

**AGENT-BASED MODELING OF NANOPARTICLES AT  
GAS-LIQUID INTERFACE WITH EMPHASIS ON  
ENVIRONMENTAL SYSTEMS**

**ÇEVRESEL SİSTEMLER VURGUSU İLE GAZ-SIVI  
ARAYÜZÜNDEKİ NANOPARTİKÜLLERİN  
AJAN TABANLI MODELLEMESİ**

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*In memory of*

My mother,

**Şerife TÜRKER**

(1937-2020)

My aunt,

**Meliha KEŞKEKÇİ**

(1932-2020)

## **ABSTRACT**

# **AGENT-BASED MODELING OF NANOPARTICLES AT GAS-LIQUID INTERFACE WITH EMPHASIS ON ENVIRONMENTAL SYSTEMS**

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The main objective of this thesis is to investigate the effects of nanoparticles on surface tension in the presence of SDS at gas-liquid interface. This thesis also aims to model the behavior of same-charged and uncharged nanoparticles as well as SDS molecules with agent-based modeling approaches to simulate their effects on surface tension.

To investigate the surface tension and its dependency on the nanoparticles and SDS, various pendant drop surface tension experiments conducted for different types of nanoparticles, SDS concentrations, and solvents at Hacettepe University Advanced Technologies Application and Research Center. The experimental results revealed that both nanoparticles and SDS have the ability to decrease the surface tension of solvents.

These experimental results used as reference for the agent-based models to computationally mimic the behavior of surface tension for selected SDS concentrations varying between  $0.1 \times \text{CMC}$  to  $10 \times \text{CMC}$ . At the model development stage, agent schema developed at first and it has been used to create the agent-based models to picture the

behavior of surface tension at gas-liquid interface with the aid of Waterfall Software Development Methodology. All agents defined as sets of attributes consisting real life counterparts of nanoparticles, SDS, and interface. Agent-based models designed to simulate the agents to reside in 12 different solvents with density values varying between 0.49 g/ml to 1.45 g/ml. Agent-based models designed to allocate the micelle formation under certain conditions.

Throughout the thesis, agent-based models implemented in NetLogo to run on both Linux and Windows based systems. Models have been subjected to validation, verification, sensitivity, and load tests prior to their deployment. Each test executed twice for  $5 \times 10^3$ ,  $7.5 \times 10^3$ ,  $10 \times 10^3$ ,  $12.5 \times 10^3$ ,  $15 \times 10^3$ ,  $50 \times 10^3$ , and  $75 \times 10^3$  same-charged and uncharged nanoparticles as well as SDS molecules. Load tests exposed that the computer system used in this thesis is capable of implementing models with less than  $200 \times 10^3$  agents.

The analysis of experimental results from HUATARC and agent-based models showed that agent-based models are capable of predicting the steady state of the surface tension. The relation between as average # nanoparticles at the interface and measured surface tension values are non-linear and this condition cannot be defined by normal distribution. Spearman and Kendall correlation analysis applied and their coefficients for the mentioned variables have been calculated as -0.999 and -0.995, respectively. Time correlation analysis for surface tension experiments and agent-based models has been done for the selected models. The results showed that each tick corresponds to 2.49 ms.

In addition to above studies, this thesis intended to analyze and identify the effects of nanoparticles and SDS to surface tension by developing a simple, practical, and low cost measurement technique. The experimental results of the technique intended to be used in the implementation of artificial neural network (ANN) models for simulating the behavior of surface tension under certain conditions. Since, the total number of data from the experiments found to be insufficient for ANN models, this part of the study put on hold.

**Keywords:** Nanoparticles, interface, agent-based modeling, artificial neural networks

## ÖZET

# ÇEVRESEL SİSTEMLER VURGUSU İLE GAZ-SIVI ARAYÜZÜNDEKİ NANOPARTİKÜLLERİN AJAN TABANLI MODELLEMESİ

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Bu tezin temel amacı, gaz-sıvı arayüzünde SDS'nin olduğu durumlarda nanopartiküllerin yüzey gerilimi üzerindeki etkilerini araştırmaktır. Bu tez aynı zamanda, aynı yüklü ve yüksüz nanopartiküllerin davranışını ve SDS moleküllerinin yüzey gerilimi üzerindeki etkilerini ajan tabanlı modelleme yaklaşımıyla tanımlamayı amaçlamaktadır.

Yüzey gerilimini ve nanopartiküllere ve SDS'ye bağımlılığını araştırmak için Hacettepe Üniversitesi İleri Teknolojiler Uygulama ve Araştırma Merkezi'nde (HÜNİTEK) farklı nanopartikül türleri, SDS konsantrasyonları ve akışkanlar için yüzey gerilimi deneyleri yapılmıştır. Deneysel sonuçlar, hem nanopartiküllerin hem de SDS'nin çözücülerin yüzey gerilimini azaltma yeteneğine sahip olduğunu göstermiştir. Elde edilen sonuçlar  $0,1 \times \text{CMC}$  ile  $10 \times \text{CMC}$  arasında değişen SDS konsantrasyonları arasında yüzey geriliminin davranışını tanımlamak için geliştirilen ajan tabanlı modellerin referansları olarak kullanılmıştır. Model geliştirme aşamasında ilk olarak ajan şeması geliştirilmiş ve bu şema Şelale Yazılım Geliştirme Metodolojisi yardımıyla gaz-sıvı arayüzündeki yüzey

geriliminin davranışını tanımlayan ajan tabanlı modellerin oluşturulmasında kullanılmıştır. Tüm ajanlar, nanopartiküllerin, SDS'nin ve arayüzün gerçek hayattaki benzerlerini içeren özellik kümeleri olarak tanımlanmıştır. Ajan bazlı modeller 0,49 g/ml ile 1,45 g/ml arasında değişen yoğunluk değerlerine sahip 12 farklı akışkanı simüle etmek ve misel oluşumunu göstermek için tasarlanmıştır.

Tez çalışmasında geliştirilen tüm ajan tabanlı modeller hem Linux hem de Windows tabanlı sistemlerde çalışacak şekilde tasarlanmıştır. Modeller dağıtımlarından önce doğrulama, duyarlılık ve yük testlerine tabi tutulmuştur. Testler iki kere tekrarlanarak  $5 \times 10^3$ ,  $7,5 \times 10^3$ ,  $10 \times 10^3$ ,  $12,5 \times 10^3$ ,  $15 \times 10^3$ ,  $50 \times 10^3$  ve  $75 \times 10^3$  adet aynı yüklü ve yüksüz nanopartiküller ile SDS molekülleri için çalıştırılmıştır. Yük testleri, bu tezde kullanılan bilgisayar sisteminin  $200 \times 10^3$  adet ajandan daha az modeller için çalıştırabildiğini ortaya koymuştur.

HÜNİTEK'te yapılan deneylere ait sonuçlar ile ajan tabanlı modellerden elde edilen verilerin analizleri, ajan tabanlı modellerin yüzey geriliminin denge durumunu tahmin etme konusunda başarılı olduğunu göstermiştir. Arayüzde bulunan ortalama nanopartikül sayısı ile ölçülen yüzey gerilim değerleri arasındaki ilişkinin doğrusal olmaması nedeniyle Spearman and Kendall korelasyon analizi yapılmış ve korelasyon katsayıları -0,999 ve -0,995 olarak hesaplanmıştır. Netlogo ajan tabanlı modellerde kullanılan zaman birimi "tick" ile günlük hayatta kullanılan zaman birimleri ile ilişkilendirilmesi için yapılan hesaplamalarda 1 tick'in 2,49 ms olduğu bulunmuştur.

Belirtilen çalışmalara ek olarak, bu tez çalışması kapsamında yüzey gerilimi ölçümü için basit, pratik ve düşük maliyetli bir ölçüm tekniği geliştirilmesi amaçlanmıştır. Bu teknik kullanılarak elde edilen sonuçlar ile deney düzeneğinin yapay sinir ağları (YSA) modelleri tasarlanmıştır. Ancak, yüzey gerilimi ölçümlerinden elde edilen verilerin yeterli sayıda olmaması nedeniyle YSA modelleri çalıştırılmamıştır.

**Anahtar Kelimeler:** Nanopartikül, arayüz, ajan tabanlı modelleme, yapay sinir ağları

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## LIST OF SYMBOLS AND ABBREVIATIONS

### Symbols

$A_{SDS}$	Function for SDS molecule
$A_i$	Function for interface
$A_{np}$	Function for nanoparticle
$A_w$	Function for world
$C_m$	Mean curvature of meniscus
$\vec{E}$	Electric field vector
$F_C$	Coulomb force of nanoparticle
$F_{vDW}$	van der Waals force of nanoparticle
$P_C$	Relative pressure for capillarity
$P_r$	Prandtl number
$R_a$	Rayleigh number
$T_t$	Total number of ticks
$V_{SDS}$	Velocity of the SDS molecule
$V_{np}$	Velocity of nanoparticle
$c_{SDS_1}$	Color of hydrophobic component
$c_{SDS_2}$	Color of hydrophilic component
$c_i$	Color of the interface
$c_{np}$	Color of nanoparticle
$c_w$	Color of the world
$d_{SDS_1}$	Diameter of hydrophobic component
$d_{SDS_2}$	Diameter of hydrophilic component
$d_{np}$	Diameter of nanoparticle
$k_C$	Coulomb's constant
$m_1$	Mass of hydrophobic component
$m_2$	Masses of hydrophilic component
$m_{np}$	Mass of nanoparticle
$np_{sc}$	Same charged nanoparticle

$np_{uc}$	Uncharged nanoparticle
$q_{SDS_1}$	Electrostatic charge of hydrophobic component
$q_{SDS_2}$	Electrostatic charge of hydrophilic component
$q_{np}$	Electrostatic charge of nanoparticle
$r_m$	Mean radius of curvature
$x_{SDS_1}$	$x$ coordinate of hydrophobic component of SDS molecule
$x_{SDS_2}$	$x$ coordinate of hydrophilic component of SDS molecule
$x_i$	$x$ coordinate of the interface
$x_{np}$	$x$ coordinate of the nanoparticle
$x_w$	$x$ coordinate of the world
$y_{SDS_1}$	$y$ coordinates of hydrophobic component of SDS molecule
$y_{SDS_2}$	$y$ coordinates of hydrophilic component of SDS molecule
$y_i$	$y$ coordinate of the interface
$y_{np}$	$y$ coordinate of the nanoparticle
$y_w$	$y$ coordinate of the world
$\alpha_{SDS_1}$	Critical contact distance of hydrophobic component
$\alpha_{SDS_2}$	Critical contact distance of hydrophilic component
$\alpha_{np}$	Critical contact distance of nanoparticle
$\beta_{SDS_1}$	Repelling distance of hydrophobic component
$\beta_{SDS_2}$	Repelling distance of hydrophilic component
$\beta_{np}$	Repelling distance of nanoparticle
$\epsilon_0$	Permittivity of free space
$\theta_h$	Boolean switch for horizontal of the world
$\theta_v$	Boolean switch for vertical wraps of the world
$\rho_E$	Electric charge density
$\Delta P$	Pressure gradient
$\alpha$	Inclination angle
$C$	Surfactant concentration
$P$	Phase space
$R$	Universal gas constant
$T$	Absolute temperature
$V$	Volume of the closed surface



$l$	Length of the link between hydrophobic and hydrophilic components
$p$	Patch size of the world
$q$	Electrical charge
$s$	Distinctive state
$\varepsilon$	Switch for screen updates of the world
$\eta$	Thickness of the interface
$\lambda$	Wavelength
$\mu$	Location of origin in Cartesian coordinates of the world
$\sigma$	Surface tension
$\varphi$	Dispersion
$\omega$	Frame rate of the world
$\vartheta$	Font size of the world

## Abbreviations

ABM	Agent-Based Modeling
AFM	Atomic Force Microscope
AIAA	American Institute of Aeronautics and Astronautics
ANN	Artificial Neural Network
ASP	Active Server Page
ASTM	American Society for Testing and Materials
AVI	Audio Video Interleave
BOD	Biological Oxygen Demand
CAGR	Compound Annual Growth Rate
CalTech	California Institute of Technology
CLR	Common Language Runtime
CMC	Critical Micelle Concentration
CNF	Carbon Nanofiber
CNT	Carbon Nanotube
COD	Chemical Oxygen Demand
CTAB	Cationic Hexadecyltrimethylammonium Bromide
DEB	Dynamic Energy Budget
DI	Distilled Water

DLVO	Derjaguin, Landau, Verwey, and Overbeek
DMS	Dimethylsulphide
DNA	Deoxyribonucleic Acid
DRAM	Dynamic Random Access Memory
DTAB	Lauryltrimethylammonium Bromide
E. Coli	Escherichia coli
eFAST	Extended Fourier Amplitude Sensitivity Test
ENP	Engineered Natural Nanoparticle
EOR	Enhanced Oil Recovery
EPA	Environmental Protection Agency
EPO	European Patent Office
EU	European Commission
FAST	Fourier Amplitude Sensitivity Test
FLAME	Flexible Larger-scale Agent-based Modelling Environment
FOD	Function Oriented Design
FTP	File Transfer Protocol
GALATEA	Glider with Autonomous, Logic-based Agents, Temporal Reasoning and Abductions
GPL	General Public License
GSO	Global Sensitivity Analysis
GUI	Graphical User Interface
HDD	Hard Disk Drive
HIV	Human Immunodeficiency Virus
HUATARC	Hacettepe University Advanced Technologies Application and Research Center
HVAC	Heating, Ventilating, Air Conditioning
IC	Information Criterion
IDE	Integrated Development Environment
IEM	Integrated Environmental Modelling
IIS	Internet Information Server
IR	Infrared
ISO	International Organization for Standardization
IT	Information Technology
JADE	Java Agent Development Framework

JRE	Java Runtime Environment
JVM	Java Virtual Machine
LED	Light Emitting Diode
LISP	List Programming Language
LM	Levenberg-Marquardt Algorithm
LNG	Liquefied Natural Gas
MAML	Multi-Agent Modelling Language
MAPE	Mean Absolute Percent Error
MAS	Manual Arm Strength
MASON	Multi-Agent Simulator of Neighbors or Networks
MD	Molecular Dynamics
MII	<a href="#">Mutual Information Index</a>
MIT	Massachusetts Institute of Technology
MLP	Multilayer Perceptron
MLR	Multiple Linear Regression
MPR	Multivariate Parametric Regression
MRAM	Magnetoresistive Random Access Memory
MRI	Magnetic Resonance Imaging
MTPRNG	Mersenne Twister Pseudorandom Number Generator
MWCNT	Multi-Wall Carbon Nanotube
NAR	Nonlinear Autoregressive
NIC	Network Information Criterion
NIRF	Near-infrared Fluorescence
NIST	National Institute of Standards and Technology
NMR	Nuclear Magnetic Resonance
NNP	Natural Nanoparticle
OAT	One at a Time
OBEUS	Object Based Environment for Urban Simulations
OFAT	One Factor at a Time
OOP	Object Oriented Design
PDMAS	Parallel and Distributed Multi-Agent Model
PNG	Portable Network Graphics
RAM	Random Access Memory
RBSA	Regression Based Sensitivity Analysis

RGB	Red Green Blue
RSM	Response Surface Method
RMSE	Root Mean Squares Error
SAR	Sodium Adsorption Ratio
SBR	Sequencing Batch Reactor
SDS	Sodium Dodecyl Sulphate
SMTP	Simple Mail Transfer Protocol
SQL	Structured Query Language
SRS	Software Requirements Specifications
STM	Scanning Tunneling Microscope
SWCNT	Single-Wall Carbon Nanotube
SWNT	Single-Walled Nanotube
TEM	Transmission Electron Microscope
TRNG	True Random Number Generator
USA	United States of America
UTF-8	Unicode Transformation Format-8
UV	Ultraviolet
UVA	Ultraviolet A
UVB	Ultraviolet B
VBA	Visual Basic for Applications
WSDM	Waterfall Software Development Methodology
XOR	Exclusive Or

## FOREWORD

The ideas and concepts behind nanoscience and nanotechnology started with a talk entitled “There’s Plenty of Room at the Bottom” by Feynman at American Physical Society meeting held at California Institute of Technology (CalTech) on December 29, 1959 long before the term “nanotechnology” used by Taniguchi in 1974 [1, 2]. In his speech, Feynman described a process, which could be able to manipulate and control individual atoms as well as molecules. He proposed shrinking computing devices toward their physical limits, where “wires should be 10 or 100 atoms in diameter”. Also, Feynman mentioned that focused electron beams could write nanoscale features on a surface called “e-beam lithography” [3].

According to Feynman, a top-down perspective can achieve reaching to nanoscale. Regarding his judgements about miniaturization, building smaller and smaller machines, and ultimately using these to build machines in the smallest imaginable scale can be accomplished by “maneuvering things atom by atom”.

Feynman noted that many of the most fundamental questions in biology could be solved if we only had the ability to see the molecules directly. Today, new inventions such as the scanning tunneling microscope (STM), atomic force microscope (AFM) and the transmission electron microscope (TEM) achieved resolution at the scale where individual atoms can be actually seen and manipulated [4-6].

Feynman argued that Encyclopedia Britannica could be written on to a pin’s area if the manuscript were reduced by a factor of  $25 \times 10^3$ . He offered a prize to the first person capable of printing one page of any book at this scale [1]. Newman first accomplished this in 1986 with reprinting of the first page of Dickens’ “A Tale of Two Cities” [7].



# 1. INTRODUCTION

Nanomaterials have at least one dimension less than 100 nm, nano-objects have two dimensions less than 100 nm and nanoparticles have all three dimensions less than 100 nm in accordance with International Organization for Standardization's (ISO) Technical Specifications<sup>1</sup> [8, 9]. In addition, European Commission (EU) published a study involving the definition of nanomaterials the proposed size limits for nanoparticles should be between 1 to 100 nm [10]. It must be noted that a nanometer approximately equals to the total width of 10 hydrogen (H) atoms. Also, a red blood cell is ~3500 nm in radius and the size of some viruses are known to be 60 to 100 nm [11]. The schematic comparison of nanoparticles with selected entities can be seen in Figure 1.1 [12].

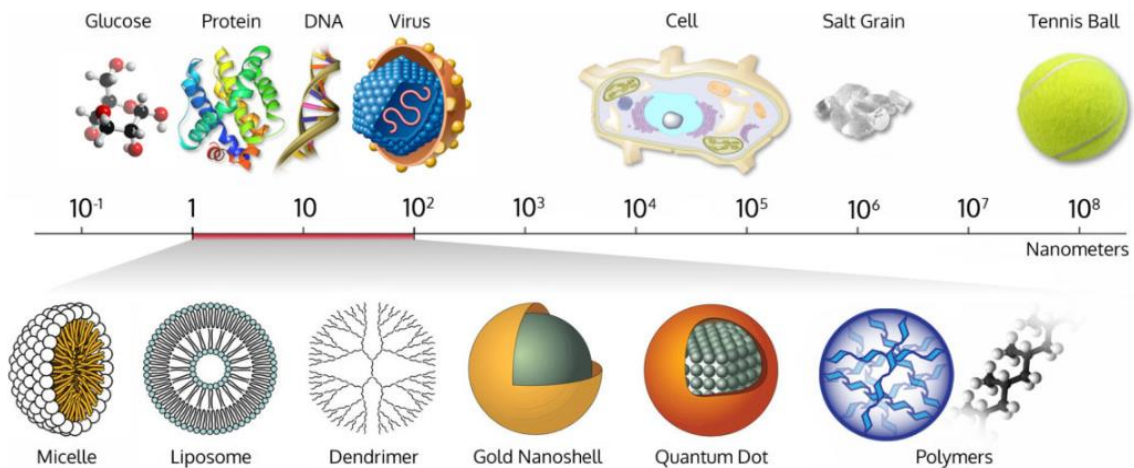


Figure 1.1 Nanoparticle size comparison scale [12]

Nanoparticle categorization can be defined by their origins as natural (NNP) and engineered nanoparticles (ENP). NNPs reached the environment before nanotechnology developed and they have been formed through geological, chemical, and biological processes. The most important sources of NNPs in the environment are the combustion of fuels, aerosols from atmosphere, activity of volcanoes, and erosion. ENPs include metals, metal oxides, alloys, carbon based materials like fullerenes, nanotubes, silicates, and quantum dots as well as polymer composites [13]. They have been used in distinctive

<sup>1</sup> ISO/TS 27687:2008 and its replacement ISO/TS 80004-2:2015

areas such as electronics, biomedicine, pharmaceuticals, cosmetics, and material sciences. For instance,  $\text{TiO}_2$  nanoparticles accepted as good semiconductors due to their significant band gaps between their shells as 3.2, 3.02, and 2.96 eV [14]. Among the other ENPs, CdS, CdSe, and cadmium telluride (CdTe) quantum dots used as semiconductors and attracted a special interest for applications in molecular biology, medicine, and information technology (IT).

In addition to NNPs and ENPs, particular microorganisms induce the formation of nanoparticles. Biogenic nanoparticles directly formed by specific organisms for their metabolic requirements. For instance, magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles intracellularly produced by bacteria for its mobility. Nanoparticles also formed as an indirect result of microbial activity when a microorganism induces redox transformation of a metal [15].

In general, nanotechnology represents all processes that include design, production, and application of materials in the atomic, molecular, and macromolecular scales to produce new nano-sized materials. Nanoparticles create a link between bulk materials and molecular structures. When ordinary materials like carbon and silicon reduced to nanoscale they display extraordinary and unpredictable properties such as high strength, chemical reactivity, electrical conductivity, and other characteristics that the same material does not possess at its micro or macro scales [16]. For instance, nanoparticles have a very large surface area to volume ratio, which reduces the melting temperature of nanoparticles. As the dimensions of a matter decrease towards to the atomic scale its melting temperature decreases and this phenomenon called “melting temperature depression” [17]. In other words, melting temperature is directly proportional to dimensions of the matter. This condition can be observed predominantly in nanowires, nanotubes, and nanoparticles that all melt at lower temperatures than macro scale of the same material.

### **1.1. Nanoparticles in the Environment**

In the last decades, nanoparticles are gaining popularity in agriculture, manufacturing, electronics, pharmaceuticals, cosmetics, consumer products, and environmental pollution control such as wastewater, and air pollution treatment processes [18-30].



For instance, Vance et al. studied on the distribution and quantity of consumer products containing nanoparticles [31]. The results showed that there are 1814 consumer products on the market supplied by 622 establishments as of October 2013. Ag found to be the mostly used nanoparticle in overall consumer products accompanied by titanium nanoparticles. The merchandises contained Ag reaches to 24% of all products in the market. The combinations of the nanoparticles used in consumer products analyzed so that titanium nanoparticles along with Ag and ZnO nanoparticles discovered to be the most used mixtures as in Table 1.1.

Table 1.1 The matrix for the types and numbers of nanoparticles used together in consumer products [31]

	Gold	Carbon	Copper	Ceramics	Iron	Calcium	Magnesium	Silicon	Zinc oxide	Titanium	Silver
Gold	7	1		1				1		1	3
Carbon	1	10	1		2					2	3
Copper		1	10		1	1	1	2	1		1
Ceramics	1			11				1		2	7
Iron		2	1		11	1	1			2	1
Calcium			1		1	13	8	1			
Magnesium			1		1	8	13	1			
Silicon	1		2	1		1	1	14	1	2	4
Zinc oxide			1					1	14	10	2
Titanium	1	2		1	2			2	10	30	10
Silver	3	3	1	7	1			4	2	10	35

The extensive utilization of nanoparticles in selected sectors examined briefly as follows,

- Food Sector:** Nanotechnology utilization in food sector is reaching to a greater extent with the new technical progresses. Nanotechnology related to many areas in food sector, such as food security, as well as delivery systems, and prolonged residence time in the gastrointestinal tract, efficient absorption through cells, bioavailability, and pathogen detection. Furthermore, bio-nanocomposites used in packaging protects the food such as Ag nanoparticles are being used as antibacterial agents to identify the food degradation [32]. Nanotechnology also prolongs the shelf life of food, as well

as reduces the requirement of plastic packaging materials usage that avoids the environmental pollution so that TiO<sub>2</sub> nanoparticles generally used for antimicrobial plastic packaging [33, 34].

- **Cosmetic Sector:** Cosmetic and personal care producers prefer nanoscale versions of bulk ingredients to offer better UVB<sup>2</sup> and UVA<sup>3</sup> protection, improved dermatological penetration, enduring effects, enhanced color, and better finish quality in their products. In general, nanoparticles of TiO<sub>2</sub>, ZnO, iron oxides, boron nitride (BN), and bismuth oxychloride (BiClHO) used in cosmetics [35, 36]. For instance, toothpastes and some sunscreens contains from 1% to >10% Ti nanoparticles by weight. Additionally, a good number of shampoos, deodorants, and shaving creams contain <0.01 µg/mg Ti [37].
- **Health Sector:** The wide range of medical implementations of Ag nanoparticles range from dental resin composites, coatings of medical equipment as catheters, infusion systems, and sterilization of medical devices [38]. Ag nanoparticles are the most widely used antimicrobials with low human toxicity. In addition, its unique optical scattering properties allow Ag nanoparticles to be used in biosensing and imaging applications. Ag nanoparticles in the range of 1 to 10 nm in diameter have been shown to interact with the human immunodeficiency virus (HIV-1) and constrain its ability to attach the host cells [39]. Shahverdi et al. showed that Ag nanoparticles increased antibacterial activities of antibiotics when used on *Staphylococcus aureus* and *Escherichia coli* (E. Coli) [40].
- **Information Technology (IT) Sector:** Magnetic storage components manufactured using nanotechnology denser than the existing hard disk drives (HDD) on the market. The bottom-up design of nanostructures yields to an unconventional form of magnetism called “antiferromagnetism” [41]. This new technology uses less surface area than the conventional HDDs, and needs  $\sim 1 \times 10^6$  atoms to store a single bit of information. The capability of designing the storage medium on the atomic level leads to manufacture smaller, faster, and more energy efficient IT peripherals [42]. On the

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<sup>2</sup>  $\lambda_{UVB} = (290-320)$  nm

<sup>3</sup>  $\lambda_{UVA} = (320-440)$  nm

other hand, there is a limiting factor that ferroelectric materials that smaller than 10 nm can switch their magnetization directions at room temperature. In the light of this information, ferromagnetic materials has been considered impractical for data storage in electronic devices under critical size [43]. Magnetoresistive random access memories (MRAMs) manufactured with nanometer-scale magnetic tunnel junctions lets computers to start instantaneously, also they have has the benefits of non-volatility, low energy consumption, fast switching speed, and robustness over dynamic random access memories (DRAMs) [44].

- **Wastewater Treatment Sector:** Wastewater treatment with nanoparticles is gaining more popularity in the recent years. For instance,  $\text{TiO}_2$  nanoparticles can be utilized for the treatment of wastewater as well as polluted groundwater. Li et al. worked on the potential impacts of  $\text{TiO}_2$  nanoparticles on nitrogen (N) removal from activated sludge using sequencing batch reactor (SBR) [45]. In their study, it has been found that the addition of 2 to 50 mg/l  $\text{TiO}_2$  nanoparticles did not adversely affect N removal from activated sludge but when 100 to 200 mg/l of  $\text{TiO}_2$  nanoparticles used, total N removal efficiency increased up to 36.5%. Furthermore, the addition of 100 to 200 mg/l  $\text{TiO}_2$  nanoparticles into activated sludge drastically reduced the microbial diversity. In addition to  $\text{TiO}_2$  nanoparticles, iron oxide (II, III) ( $\text{Fe}_3\text{O}_4$ ) nanoparticles have gained attention because of their size, high surface area to volume ratio, and magnetic properties. Adsorption process combined with magnetic separation methods used extensively in water treatment [46]. Iram et al. studied on the removal of contaminants from water with the aid of magnetic  $\text{Fe}_3\text{O}_4$  nanospheres [47]. They experimented nanosphere adsorbents for the removal of natural red dye contaminants. The monolayer adsorption capacity of magnetic  $\text{Fe}_3\text{O}_4$  nanospheres for natural red dye in the concentration range calculated as 105 mg/g from the Langmuir isotherm model at 25 °C. They concluded that adsorption processes are spontaneous and endothermic as well as  $\text{Fe}_3\text{O}_4$  nanospheres can be useful for the separation process in wastewater treatment. Girginova et al. used silica coated  $\text{Fe}_3\text{O}_4$  nanoparticles to remove mercury (II) cation ( $\text{Hg}^{+2}$ ) from wastewater [48]. The experiments reported that tested nanoparticles showed 74% efficiency for  $\text{Hg}^{+2}$  uptake. Magnetic nanoparticles yielded vast potential for the removal of heavy metal ions from polluted

water with magnetic separation. Peng et al. performed experiments for assessing the removal efficiency of adsorbents for cupric ion ( $\text{Cu}^{+2}$ ) and found that chitosan coated magnetic nanoparticles yielded highly favorable utilization results so that the adsorption efficiency reached over 90% [49].

- **Forest Products Sector:** Nanotechnology initiated new possibilities to manufacture wood-based products that have UV, moisture, fungal, pest, and fire resistance. Additionally, nanotechnology introduced alternative ways in the production of raw materials as well as creates innovative products for paper products and new generations of functional nanoscale materials. Wood and paper-based products with nanosensors developed to estimate and detect the humidity, temperature, pressure, and wood decay by fungi.

The potential benefits of nanotechnology generally well described and analyzed but the toxicological effects and impacts of nanoparticles did not receive significant attention. The rapid introduction nanoparticles into our daily lives need deep understanding of their negative impacts on humans and environment. Advances in nanotechnology caused more ENPs discharge to the environment than ever. For instance, Keller et al. studied on the types and quantities of ENPs released from the personal care products [50]. As a result, they estimated that 870 to  $1 \times 10^3$  mt of  $\text{TiO}_2$  and  $1.8 \times 10^3$  to  $2.1 \times 10^3$  mt of ZnO ENPs released annually in the USA. The environmental fate and toxicity of ENPs depends on numerous factors, including their size and size distribution, solubility, mass concentration, shape, surface area, and electrostatic charge. Furthermore, ENPs can react with chemicals in the environment and act as catalysts for the chemical reactions or inhibit the occurrence of chemical reactions. Another and the foremost important danger of ENPs is their undesirable side effects to humans. Nanoparticles can enter the human body via oral ingestion, inhalation, dermal penetration, injection, and propagate to internal organs. The small size of nanoparticles increases their potential to cross through cell membranes.

It must be noted that not all nanoparticles are benign so that some of them have the capability to create confrontational biological effects at cellular, subcellular, and molecular levels. Nanoparticles are in the range of cellular components like ribosomes<sup>4</sup>

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<sup>4</sup> The size of the ribosomes within cells changes depending on the cell type and on factors such as whether the cell is resting or replicating. The ribosome of E. coli is  $\sim 100 \text{ \AA}$  in radius.

and able to interact with proteins and nucleic acids. These interactions can affect the vital processes such as enzyme functions, gene translations, and transcriptions. Other possible harmful effects enhanced by the ability of nanoparticles to penetrate cell membrane, and accumulate in mitochondria. Above all, the large surface area of nanoparticles increases their role as carriers for other contaminants, thereby providing them instant, and long-range transportation medium. [51, 52]. For instance, Adams et al. researched the toxicity of TiO<sub>2</sub>, ZnO, and silicon dioxide (SiO<sub>2</sub>) ENP-water suspensions for *Bacillus subtilis* and *E. coli* [53]. They concluded that all ENPs were detrimental to varying levels by the antibacterial activity. Increment of ENP concentrations indicated a steady increase in toxicity on *E. coli* and *Bacillus subtilis*. The experiments showed 72% and 99% growth reduction in cells that exposed to ENPs, respectively. Another ENP that can be harmful to humans is Ag nanoparticles. Besides their benefits, studies on the health risks of Ag nanoparticles showed that they could initiate reproductive failure, developmental malformations, and morphological deformities. Gonzalez et al. indicated that 14% of all Ag nanoparticles used in consumer products released into the air while they are being manufactured and deposited in different regions of the respiratory system [54]. In their study, Zou et al. mentioned that Ag exposure to rats exhibited a mitochondrial dysfunction leading to permanent or temporary hearing loss based on the dose [55]. Ag nanoparticles with 4 µg/ml concentration caused hearing loss with partial recovery at seven days, whereas 20 µg/ml caused irreversible hearing loss. Even though, Maneewattanapinyo et al. stated that the oral administration of at a limited dose of 5 mg/kg Ag nanoparticles caused neither mortality nor acute toxic signs throughout the observation period [56]. In vitro results reported that Ag nanoparticles produced toxicity including lung, liver, brain, vascular system, and reproductive organs. Milic et al. worked on the treatment of kidney cells with Ag nanoparticles [57]. The results showed that toxic effects observed in higher doses with the accumulation inside of the kidneys and might be the reason for toxicity, in vivo. Pulmonary toxicology studies on animals showed that being exposed to nanoparticles produced enhanced levels of lung inflammation, fibrosis, and tumors [11]. Elder et al. indicated that the rats which subjected to manganese (II) oxide (MnO) nanoparticles for 12 days resulted increment in olfactory bulb concentrations by 3.5 times [58].

In addition, nanoparticles can be toxic and hazardous to marine life. Blinova et al. investigated the acute toxicity of CuO and ZnO nanoparticles for crustaceans *Daphnia magna* and *Thamnocephalus platyurus*, and protozoan *Tetrahymena thermophile* [59]. Results showed that water has the ability to mitigate the toxic effects of CuO nanoparticles but not ZnO nanoparticles on the selected crustaceans and protozoan. Miller et al. tested the effects of TiO<sub>2</sub> and ZnO nanoparticles on the population growth rates of phytoplankton [60]. Although, TiO<sub>2</sub> nanoparticles presented no measurable effects on the growth rates of any species, ZnO nanoparticles showed inhibitory effects. Toxicity of ZnO nanoparticles on phytoplankton population likely due to dissolution, release, and uptake of free Zn ions, but specific nanoparticulate effects may be difficult to unravel from effects. Also, in this study, a modeling approach based on Dynamic Energy Budget (DEB) framework managed to estimate the lethal effects of nanoparticles on phytoplankton populations [61]. Smith et al. showed that the aqueous exposure of SWCNTs in 1 to 3 nm in diameter to rainbow trout and observed the respiratory distress triggered by the mechanical blockage of the gills, also verified by gill pathologies [62]. Another study on the rainbow trout's exposure to nanoparticles created by Federici et al. [63]. Exposure to TiO<sub>2</sub> nanoparticles caused some gill pathologies of trout. They concluded that the respiratory distress caused sub-lethal toxicity that involves oxidative stress, organ pathologies, and the induction of anti-oxidant defenses. In addition to mentioned health hazards, several studies that state the potential applications and toxicity effects of selected nanoparticles summarized in Table 1.2.

The production of nanoparticles can be energy intensive. In a study conducted by Isaacs et al. revealed that the life cycle of single-walled nanotubes (SWNTs) is highly energy demanding so that it needed  $1.44 \times 10^{12}$  to  $2,80 \times 10^{12}$  MJ/kg energy [64]. The life cycle energy requirements of CNTs are 13 to 50 times that of aluminum (Al) on an equal mass basis. A comparison can be made of the damage and indicators evaluated in the process life cycle assessment of carbon nanofibers (CNF). There are several reasons for this difference is the high-temperature vapor-phase procedure required for CNF synthesis has low efficiency and it requires significant amount of energy usage [65].

Table 1.2 Potential applications and toxicity effects of selected nanoparticles

<b>Nanoparticle</b>	<b>Potential Applications</b>	<b>Potential Toxicity Effects</b>	<b>References</b>
Gold	Cancer and gene therapy, fuel cells, detection of biomarkers in the diagnosis	Liver damage, activation of hepatic macrophages, genotoxicity and cell toxicity	[66-71]
Platinum	Diagnosis, electronics, medicine, electrocatalysts and catalytic converters, magnetic nanopowders, polymer membranes, cancer therapy	Liver and kidney damage, drop in heart rate, abnormal cardiac morphology, circulatory defects, malformation in the eyes	[72-75]
Copper	Ink jet printers, high strength metals and alloys, capacitors, anti-microbial, and anti-fungal agent	Alterations in the histopathology of the pulmonary tissues, liver and kidney damage, increment in the cellular level of various types of proteins	[76-82]
Iron	Biomedical applications, contaminated land and groundwater remediation, arsenic removal, magnetic data storage and magnetic resonance imaging (MRI)	Cytotoxicity in cells, deoxyribonucleic acid (DNA) damage, genotoxicity, developmental toxicity, neurotoxicity, kidney damage	[71, 83-87]
Silver	Biosensors, drug delivery, diagnosis, medical imaging, antibacterial applications	Kidney damage, inflammation, mineralization, toxicity on internal organs	[88-92]
Titanium dioxide and zinc oxide	Dermatological drug delivery, food additive, paints, food packaging, paper industry for improving the opacity of paper	Inflammation, liver damage, cell and DNA damage, metabolic change, phototoxicity upon UV irradiation	[93-98]

As indicated in previous Sections, nanomaterials used in every aspect of our daily lives. As the global demand for nanomaterials increases, the market revenue of nanomaterials increases consistently. There are numerous reports investigating and projecting the economic size of nanomaterials trade. For instance, Zion Market Research calculated the revenue of the global nanomaterials market as USD  $7.3 \times 10^9$  in 2016 and expected to increase by 130.14% to USD  $16.8 \times 10^9$  in 2022 [99]. Inkwood Research projected the global nanomaterials market grow from USD  $4.7 \times 10^9$  in 2017 to USD  $13 \times 10^9$  in 2024 with an increment of 176.68% [100]. Global market for nanotechnology products expected to reach USD  $3 \times 10^9$  by 2020 [101]. In another study, it has been forecasted that global nanomaterials market will increase by 175.61% from USD  $4.1 \times 10^9$  to USD  $11.3 \times 10^9$  between 2015 and 2020 [102].

## 1.2. Surfactants and Their Presence in the Environment

The word “surfactant” derived by Antara Products in the 1950s for the phrase “surface active agent”. This expression covers the manufactured goods having surface activity such as detergents, and foaming agents [103]. Surfactants are amphiphilic molecules and they represent double affinity on behalf of their polarization duality. All surfactants have the common properties such as consisting of both polar and non-polar groups. They can construct self-assembled aggregates in liquids as a part of their chemical structure. A structural characteristic of the most surfactants is the presence of at least one (non-polar) hydrophobic region and at least one (polar) hydrophilic region. This enables that a surfactant molecule resides both polar (hydrophilic, lipophobic, or oleophobic) head groups and non-polar (hydrophobic, lipophilic, or oleophilic) tail groups as in Figure 1.2. In general, hydrophilic and hydrophobic parts of a surfactant called as “head” and “tail”, respectively. The hydrophobic part of surfactant has an affinity for fats and oils. On the other hand, hydrophilic part of the surfactant has an affinity for water [104].

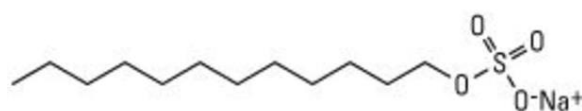


Figure 1.2 Surfactant molecule [105]



Regarding on the types of hydrophilic components, surfactants can be categorized as anionic, cationic, and nonionic. Anionic surfactants can disassociate in water as negatively and positively charged ions. The hydrophilic head is anion and they are the most common. They are inexpensive surfactants so that they have been used generally in detergents and personal care products. Cationic surfactants dissociate in water as negatively and positively charged ions where hydrophilic head is cation. The positive charge of the head group, cationic surfactants strongly adsorbed by negatively charged surfaces. [106].

Surfactants consumed for various applications on behalf of their significant effects on surfaces and interfaces. To name a few, textiles, leather, paints, paper and cellulose products, plant protection and pest control, food, packaging, plastics and composite materials, pharmaceuticals, and medicine. Industrial and technological areas that also use surfactants are display and printing technologies, microcircuit and storage media manufacturing as well as in metal-processing, petrochemical, and agrochemical industries [107].

Surfactants can self-organize in solutions to form different structures with distinctive morphologies. Beyond a critical concentration, which is known as “critical micelle concentration” (CMC), surfactant molecules instinctively gather to construct superior aggregates called “micelles”.

Micelles can survive in nature from  $\sim 10^{-5}$  s to more than three months. This self-assembly phenomena called as “micellization”. The history of micellization research goes back to McBain in the early 20<sup>th</sup> century [108]. The initial studies on micelles substantially focused on experimental methods for classifying the size and shape of the aggregates until late 1940s when the first theory on micellization published by Debye in 1949 [109]. Self-assembly represented as spontaneous association of organized structures into defined three-dimensional geometry to form structured separate components under boundary conditions. A well-organized systematic structure emerges naturally from disorder through a process that involves pre-existing components as in Figure 1.3 [110]. Self-assembly processes are reversible and controlled by design of the components, environment, and the major forces in the medium [111, 112].

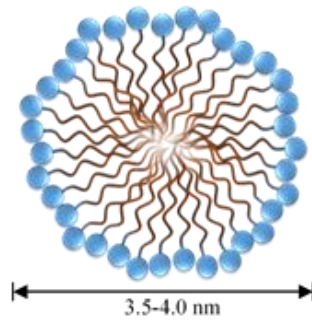


Figure 1.3 Schematic representation of a self-assembled structure [110]

Due to extensive use of surfactants, global demand accomplished as  $15.93 \times 10^6$  tons that has the main share of home care treatment in 2014. It has been expected to reach  $24.19 \times 10^6$  tons by 2022, with growing at a compound annual growth rate (CAGR) of 5.4% from 2015 to 2022. Moreover, the category of surfactants used in personal care products projected to have the maximum growth of 6.3% from 2015 to 2022 [113]. The global surfactant market expected to reach USD  $44.9 \times 10^9$  by 2022 from USD  $36 \times 10^9$  in 2017. The annual revenue of personal care products category expected to increase from USD  $4.5 \times 10^9$  in 2017 to USD  $5.8 \times 10^9$  in 2022 at a CAGR of 5.1% [114].

### 1.3. Importance and Benefits of Surface Tension

Surface tension is a phenomenon that effects our everyday life in many ways. The understanding of surface tension is great interest for every sector. Medical application, food, painting, pharmacological goods, packaging and almost all sectors related with surface tension [115]. The importance of surface tension in selected industries as follows,

- **Detergents:** The high surface tension of water makes it a moderately inadequate cleaning medium, alone. Although, any increment in the water temperature results in decreasing the surface tension of water, it is not sufficient to clean goods. In this situation, addition of detergent required. In the process of developing detergent formulations, surface tension values of water routinely measured.
- **Food products:** Most of the food products in our daily diet are emulsions such as mayonnaise, milk, margarine, and ice cream. Regarding its nature, an emulsion formed by the dispersion of two immiscible liquids with one to other with relatively small droplets such as oil and water. Even though oil-water emulsions can be prepared by homogenizing both liquids together, emulsion will not be stable so that

it will separate rapidly. To avoid this phenomenon, emulsifiers can be used. Thus, in preparation of emulsifiers, surface tension plays an important role.

- **Paints:** One of the fundamental requirements for paints is that it can create a consistent, defect-free coating on the applied medium. Surface imperfections originating from quality of the paint like levelling and peeling, generally related to surface tension. To decrease the surface tension of the paint, necessary amount of surfactants must be added. As a result, surface tension can be related to better wetting of the substrate. Paints with reasonably low surface tension values are advantageous. It must be mentioned that excessively low surface tension can cause levelling issues on the surface.
- **Pharmaceutical products:** Surface tension plays an important role in numerous pharmaceutical practices from coating of tablets to solubility and stability of drugs. In order to enrich the outer shell, camouflage the taste and odor, and regulate the level of drug release coatings for tablets stereotypically used. In general, polymers selected as coating materials and surface tension of the polymer coatings influence on the efficiency of the drug. During this process, surface-active molecules supplemented to polymer coating solutions in order to decrease surface tension. For this reason, knowledge on the CMC of surfactants is crucial in pharmaceutical industry. In addition, surface tension effects on the solubility of the drugs. For instance, liposomes are comprised of both phospholipids and cholesterol. The surface tension of liposomes has great importance on the optimum drug delivery and timely release in the body.

#### **1.4. Modeling Ecological Behavior of Nanoparticles and Surfactants**

The roots of word “model” goes back to Latin “modellus” which means “a small measure, standard” and defined as “human way of coping with the reality”. Anthropologists believe that the ability to construct conceptual models from scratch is one of the most significant competencies of homosapiens over all other living beings [116].

In modern days, modeling comprehended to simulate or describe the behavior of a real system to understand its mechanism. Environmental Protection Agency (EPA) defines modeling as “formal representation of the behavior of system processes, often in mathematical or statistical terms” [117, 118]. In another point of view, Wallace

considered models as analogies that assist the interpretation of a selected phenomenon that cannot be understood with experience [119].

Models are abridged versions of real world with the lack of its complication apart from the selected properties considered as critical to the interpretation of the system in the digital world or *in silico*<sup>5</sup>. The increasing computing power makes it possible to model complex phenomena that could not be done previously. For instance, the number of transistors per microprocessor has increased from  $2.3 \cdot 10^3$  to  $1.92 \cdot 10^{10}$  between 1971 and 2017 [120]. The advances in memory technology and prices<sup>6</sup> enabled to deal with the enormous number of parameters that resemble systems so that this capacity has encouraged modeling very complex systems such weather. As early as 1972, Meadows et al. developed a model called “World3” that portrayed 12 different scenarios of world development and their environmental consequences for 200 years from 1900 to 2100 [121]. Randall et al. created “General Circulation Models” concept to model the entire earth’s surface, atmosphere, and oceans to foretell global events such as global warming, rain, and snowfall [122].

Modeling can provide risk-free and cost effective environment to analyze the system in question, presents numerous visualization options, as well as lets the coordination of parameters to gain insight into dynamics of the system. Furthermore, constructing models assist to detect and classify the relationships among components of the system. It must be mentioned that a fair amount of skepticism raised by some researchers such as Box<sup>7</sup> who stated in more than a few studies “models are wrong, but some are useful” [123-125]. Besides, developments in hardware and software technology enabled researchers to create more complicated models, as mentioned earlier. Any unrestrained increments in the complexity of models, lead to a point where the model becomes incomprehensible. At a critical instant, the model will no longer function as a description of the phenomena with

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<sup>5</sup> “*In silico*” is a Latin word that means “in silicon” and it is used for to mention that the study performed on computer or via computer simulation.

<sup>6</sup> The price of computer memory dropped from USD  $411 \cdot 10^6$ /MB to USD  $6.8 \cdot 10^{-3}$ /MB between 1957 and 2018 [138].

<sup>7</sup> Box is the co-creator of Box-Jenkins method which first published in “Time Series Analysis: Forecasting and Control” [126]. Box-Jenkins method used for forecasting data from the specified time series. The widely used autoregressive integrated moving average (ARIMA) models are the types of Box-Jenkins methods.

selected properties therefore it will be a replication of the real system which is out of the modeling context.

The one of the most important aim in modeling studies must be to exhibit and define system with a straightforward and uncomplicated set of properties and rules of interaction. Models sometimes designed so complex that they become incomprehensible to the phenomena. For instance, Banini concluded that the tweaking of the models beyond a critical point is counterproductive which led to a paradox known by his name [126]. He stated, “As a model of a complex system becomes more complete, it becomes less understandable”. This proposition can be further extended with Korzybski’s “the map is not the territory” statement. If the scale of a map increases up to 1:1, it will be beyond useful for any practical usage [127].

There are numerous techniques and approaches stated in literature to predict the surface tension by modeling. For instance, agent-based modeling (ABM), artificial neural networks (ANN), arrangement of state equations with Butler equation, Barker-Henderson perturbation theory, Butler equation, closely-related density functional theory, corresponding state theory, density gradient theory, Fowler-Kirkwood-Buff approximation, molecular dynamics, parachor methods, Pazuki-Nikookar equation of state, and radial distribution function used for surface tension estimations [128-140].

This thesis took the advantage of using and comparing different modeling approaches and assessing the benefits of each for the surface tension models. Before starting to modelling studies, ABM and ANN techniques compared in detail.

In the light of the previous conclusions, surface tension values of 12 different solvents modeled with the addition of various amounts of MWCNTs, and graphene as well as SDS. In the following Section, ABM and its techniques will be discussed.

#### **1.4.1. Agent-based Modeling**

ABM focuses on modeling complex and dynamical systems comprised of autonomous and interacting entities. ABM has become a widely used modeling approach for understanding complex and nonlinear systems. ABM’s background lies back to von Neumann machine which is a theoretical machine competent of reproducibility that led to the cellular automata principle [141, 142].

ABM has been proven itself as an effective approach to analyze, reconstruct, and predict systems with various entities. ABM used in diverse research areas in natural, social, and applied sciences for the reason of its complexity, randomness, heterogeneity, and flexibility [143]. Epstein and Axtell modeled communal lifespan named “Sugarscape” [144]. In their study, they designed an ecosystem in a computerrarium and studied social interactions among its virtual habitants as in Figure 1.4.

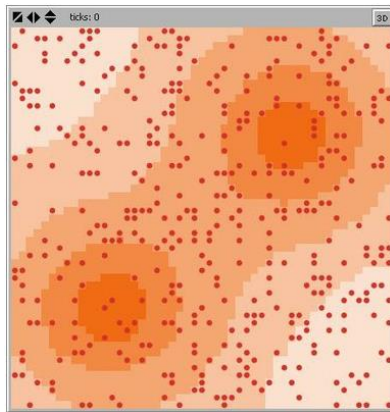


Figure 1.4 Sugarscape agent-based model created by NetLogo

Stummer et al. used ABM to overcome the limitations of traditional approaches used in diffusion of repetitive product purchases in competitive markets [145]. Their model addressed the heterogeneity of consumer behavior and market diffusion of products, in addition to marketing strategies. They improved a bottom-up multi-agent design approach to model self-directed elements. In addition to above studies, there has been a significant effort to incorporate numerous interdisciplinary researches in ABM. Bithell and Brasington studied on farming with individual-based forest models and dynamical models of water distribution with ABM [146]. Another study is done by Crabtree and Kohler for analyzing the ancient socio-ecological systems for longstanding interactions between demography, human groups, environmental variables, and social contacts [147].

In the recent decades, numerous commercial and free/open source ABM development software have been progressed with particular encoding syntax, logic, and semantics such as GridABM NetLogo RePast, and Swarm, etc. [148-151]. Aforementioned software classified by depending on their targeted domains, modifiability, usability, and overall performance. The features and comparison of selected ABM development environments adapted from the literature survey of Abar et al. and represented in Table 1.3 [128].

Regarding their properties and capabilities of mentioned packages, NetLogo selected to implement all agent-based models in this thesis [149].

NetLogo which was formerly branded as StarLogo, is an open source powerful programming language with an integrated graphical interface [152] NetLogo developed at Northwestern University in 1999 and it is the successor of list processing language (LISP) that created by McCarthy in late 1950s at Massachusetts Institute of Technology (MIT) [153, 154]. NetLogo developed with the intention of simulating distributed, discrete, and non-centralized complex systems. [155]. It has been built up as a multi-agent modeling language (MAML) to optimize and handle large amount of objects, synchronously. Its built-in functions, graphing capabilities, and coding features eased the agent-based model development and implementation period.

Primary components of ABM are mobile and stationary agents, interaction, and time<sup>8</sup>. In ABM terminology, independent, autonomous, heterogeneous, state-based objects called as “agents”. Epstein and Axtell defined agents as the “people of artificial societies” including “internal states and behavioral rules” [156]. Gilbert and Troitzsch interpreted agents as self-contained programs that can handle their specific actions depending on the perceptions of the environment [157].

There are numerous definitions of “agent” in literature such as Jennings and Wooldridge stated that an agent is a computer system, which is capable of autonomous action in its environment to endure its design intents [158]. Quang et al. defined agents as basic building blocks of systems in agent-based models which can act autonomously and interact with each other [159]. Hewitt defined an agent as a concept of a self-contained, interactive, and synchronously implementing entity as an “actor” [160]. Moulin et al. described agent as the combination of definition, organization, and cooperation/coordination layers [161]. Heppenstall et al. conceived agent as a representation of a virtual decision-making element that includes self-directed objects with certain behaviors and exhibit delimited rationality and they have the ability of making verdicts on their own [162].

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<sup>8</sup> Time concept in NetLogo discussed in Section 4.1.1.

There are three different types of built-in agents in NetLogo as turtles, patches, and observer. All other agents used in agent-based models inherit their properties from these agents. Turtles are the mobile agents confined in the world and have ability to move under the given limitations. World is a user defined 2D space that composed of patches where turtles reside and observer is the entity that perceives the behavior of turtles in the world.

Agents in the models move in a constrained space where they can interact with each other concurrently within a matrix of square shaped cells called “patches”. In NetLogo, patches are stationary agents and they have coordinates. The total number of patches for an agent-based model can be set from the interface as well as from the code before run-time. An output of a NetLogo model to illustrate the patches of a world filled with random colors can be seen in Figure 1.5.

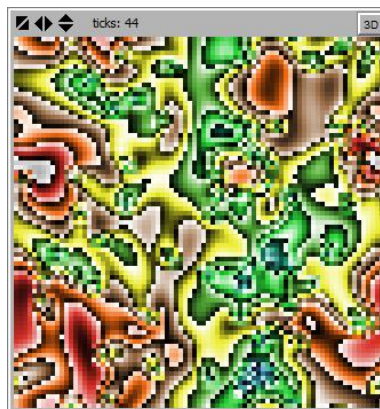


Figure 1.5 Random colored patches in NetLogo

Apart from the code, NetLogo supports the visualization of all agents in 2D and 3D in real-time. Besides, it consists more than a few specialized tools such as BehaviorSpace that enables to explore a widespread parameter space by running numerous agent-based models and logging data without any human interaction [163].



Table 1.3 Comparison of selected ABM development environments [128]

<b>Package</b>	<b>License</b>	<b>Source Code</b>	<b>IDE<sup>9</sup></b>	<b>Compiler</b>	<b>Reference</b>
AgentCell	Open source	Java	Eclipse	JRE	[164]
AgentScript	Open source	Java	CoffeeScript	JavaScript Console	[165]
FLAME <sup>10</sup>	Open source	C	GUI	GNU C, Xparser, Graphviz	[166]
FlexSim	Closed source	Microsoft Visual C++	GUI	Microsoft .NET Compiler	[167]
GALATEA <sup>11</sup>	Open source	Java	Eclipse	Java Development Kit	[168]
GridABM	Open source	Java	Eclipse	JRE	[148]
GrowLab	Open source	Java	Eclipse	JRE	[169]
Janus	Open source	Java	Eclipse, Maven	JRE	[170]
MASON <sup>12</sup>	Open source	Java .NET	Eclipse, NetBeans	JRE	[171]
NetLogo	Open source	Java	NetLogo	JRE	[172]
OBEUS <sup>13</sup>	Closed source	Microsoft .NET Framework	GUI	Microsoft .NET Compiler	[173]
Repast	Open source	Java, C#	Eclipse	JRE, Microsoft .NET Compiler	[150]
Swarm	Open source	Java, Objective C	Eclipse	JRE	[151]

<sup>9</sup> IDE is the abbreviation for Integrated Development Environment

<sup>10</sup> FLAME is the abbreviation for Flexible Larger-scale Agent-based Modeling Environment

<sup>11</sup> GALATEA is the abbreviation for Glider with Autonomous, Logic-based Agents, Temporal Reasoning, and Abductions

<sup>12</sup> MASON is the abbreviation for Multi-Agent Simulator of Neighbors or Networks

<sup>13</sup> OBEUS is the abbreviation for Object Based Environment for Urban Simulations.

NetLogo originally implemented in Java 1.1 and inherited the same pros and cons of this programming language. Java was chosen for both programming language and graphical user interface (GUI) libraries because of its cross-platform support and its high performance in Java virtual machines<sup>14</sup> (JVM) [174]. On the other hand, NetLogo's dependence on JVM constrains the maximum number of objects to  $2^{31}-1$  by means of array indices signed as 32-bit integers. NetLogo's official document states that it has 1 GB upper limit on how much total random access memory (RAM) it can use. Beyond this critical value, NetLogo becomes unresponsive due to out of memory error [175]. In addition, Java enables the agent-based models to run in multiple operating systems since the core language and GUI libraries are compatible with widely used operating systems such as Microsoft Windows, Linux, and Mac OS X [176-178].

In this thesis, following agent schema used to create models for revealing the behavior of surface tension at interfaces with the aid of Waterfall Software Development Methodology (WSDM) [179]. As it can be seen from Figure 1.6, all agents have their origins in the environment and they are considered as the counterparts of the real world entities. Agents designed in a way so that they resemble the most relevant definition of entities with the selected set of attributes in the agent-based models. Every agent can interact among each other without any restriction of its type and all interactions specified within agents defined in the agent-based models. In the model run-time, agents continuously create information on behalf of their attributes and interactions with other agents in the middle information layer. All information integrated and assessed in the top information layer to form the agent-based models.

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<sup>14</sup> Java virtual machine enables a runtime environment that allows the Java bytecode to execute.

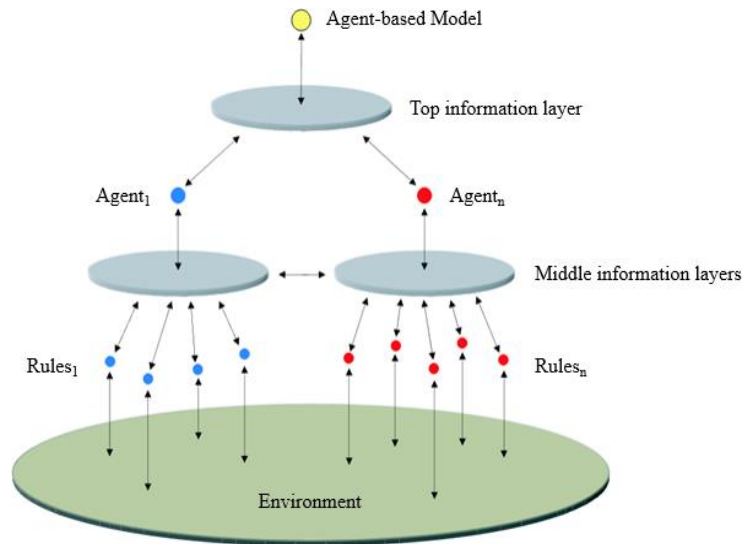


Figure 1.6 Agent-based model structure (adapted from [180])

There are numerous techniques for developing agent-based models such as PARTE and WSDM [179, 181]. Former technique name is the abbreviation of the words “properties”, “actions”, “rules”, “time”, and “environment”. The initial three elements (properties, actions, and rules) define the agents, while the latter ones (time and environment) define the context of the technique. Regarding its widespread usage and documentation, all agent-based models developed with the WSDM, which is also known as linear sequential life cycle model. Although, implementation of WSDM originates back to 1960s, Royce credited with the first formal description of it in his article dated 1970. WSDM controls the software development by sectionalizing the whole process into separate subprocesses [182]. Numerous alternatives of WSDM exist with each one citing different tags for the subprocesses. In this methodology, development categorized into hierarchically ordered six subprocesses, which can be seen in Figure 1.7. As the figure implies, WSDM outlined as a cascade of consecutive subprocesses followed with one another.

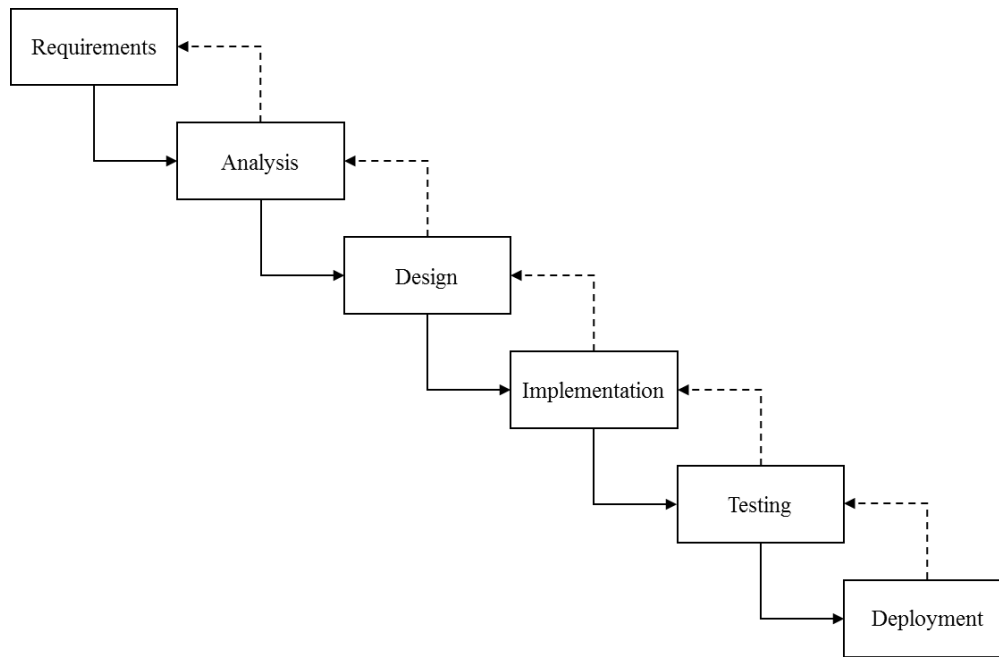


Figure 1.7 Waterfall software development methodology

Apart from the requirements stage, each stage depends on its predecessor as an input. Every single subprocess developed and completed separately throughout the WSDM. Feedbacks exist among all subprocess in order to modify the complete agent-based model development process when an unpredicted condition occurred and/or a problem detected. Furthermore, iterations such as reassessing the preceding subprocesses and considering new results from the succeeding subprocesses takes an important role in WSDM. The subprocesses utilized for agent-based modeling can be expressed as follows,

1. **Requirements:** In this subprocess, all requirements and prerequisites collected and documented for the agent-based models. This documentation is known as Software Requirements Specification (SRS) and lies in the foundation of the agent-based models. SRS defines the interaction of software and hardware, additional software and end-users under different real-world circumstances [183]. In SRS, software and hardware parameters such as availability, maintainability, and security, etc. assessed. Procedures of defining SRS expressed in ISO/IEC/IEEE 29148:2011 standard [184].
2. **Analysis:** All activities involved in converting requirements into design and implementation subprocesses are known as “analysis”. Every bit of collected requirements analyzed whether they are valid and reasonable. Additionally,

limitations of the software and hardware identified as well as scope and schedule of ABM defined.

3. **Design:** In this subprocess, software and hardware requirements planned in detail. Additionally, flowcharting, performance, security issues, and integrated development environment (IDE) selection put into practice. There are numerous software design approaches such as structured design, object oriented design (OOP), and function oriented design (FOD) [185-187]. In this thesis, bottom-up structural design used to create agent-based models. It can be briefly mentioned as a “divide and conquer” approach. It is based on the logic of breaking the main problem into little chunks and solving each chunk exclusively until the main problem solved completely.
4. **Implementation:** Agent-based model code developed using NetLogo programming language with its IDE to achieve the goals that specified in the previous three subprocesses. In this part of WSDM, code-reuse implemented where possible and version management issued. Throughout the implementation, naming conventions, control structures, functions, variables, and operators, etc. standardized.
5. **Testing:** After implementation, agent-based models subjected to tests including validation, verification, and calibration tests in order to check if they operate to the same extent as predicted. Validation, verification, and calibration are common processes that used in modeling studies.
6. **Deployment:** If all subprocesses ended without any kind of issues, agent-based models deployed and released to consumption of end-users with necessary manuals.

In this thesis, one of the most important objective of ABM is to create analogies between the real world and representative computer code. This urge instinctively raises the question of validity of the agent-based models. It must be taken into account that large agent-based models with numerous non-linear relationships is likely to behave in a highly random and disordered manner so that it should be difficult to follow the interactions yield the requested specific kind of behavior. For this reason, agent-based models with thousands of agents and parameters as in this thesis need to be defined, validated, verified, and calibrated, appropriately with a utilitarian approach.

The roots of word “valid” goes back to 17<sup>th</sup> century, which means “sufficiently supported by facts or authority, well-grounded” [188]. Validation is essential in the reliability confirmation of the models. In literature, there are numerous definitions for “model validation” such as, Midgley et al. described validation as demonstrating correct equations that have been solved by referencing an external and independent test [189]. Casti defined validation as the level that the model adequately represents the system being modeled [190]. Schlesinger et al. explained it as “substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy with the intended application of the model” [191]. Macal stated that validation as the process of determining the degree that a model characterizes the “real” world [192]. American Institute of Aeronautics and Astronautics (AIAA) defined validation as determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses [193].

The word “verify” originates from the combination of Latin words “*verus*” and “*facere*” which can be combined as “make true” [194]. Besides its etymological roots, verification can be expressed as the process of investigating the reasoning of the model is adequate [195]. In the verification process, agent-based models debugged and checked to be error-free and executing accurately. Verification step starts by taking into account of each process defined in the model and associates the outcomes with experimental data. Sargent explained verification as “ensuring that the computer program of the computerized model and its implementation are correct” [196]. Oberkampf et al. stated the relation between conceptual and computerized models with their relation to validation and verification as in Figure 1.8 [197]. In their study, validation thought to be critical entity between “reality” and “computerized model” coupled with the verification, which is considered the connection between “computerized model” and “conceptual model”.

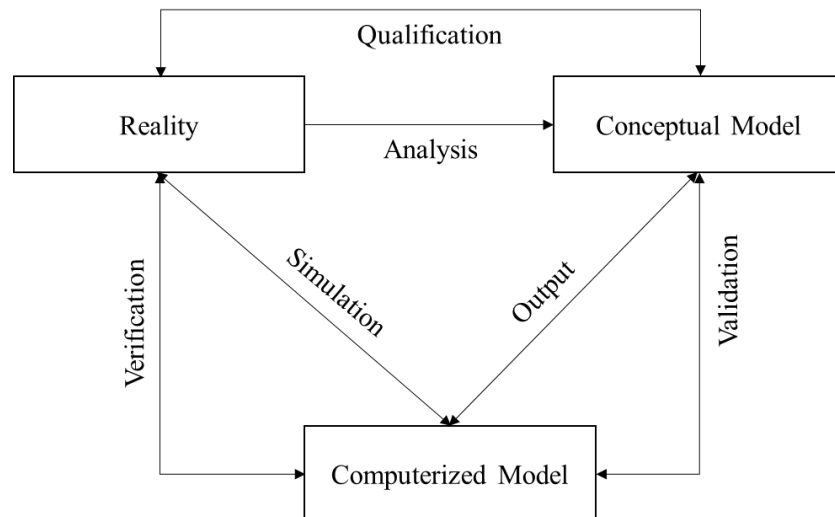


Figure 1.8 Validation and verification stages in modeling [197]

In particular to ABM, Bharathy mentioned the foremost controversy as the dilemma on validation and verification of models [198]. Non-linear behavior, abundant patterns of emergence, modeling dynamics, chaotic nature, and complexity of ABM makes the validation and verification challenging. For instance, Galan et al. indicated that agent-based models are hard to validate for their high tendency of yielding errors [199]. Lucas et al. stated the immense number of agents in the models could cause trap of tweaking variables [200]. In their study, Fagiolo et al. mentioned the high complexity of agent-based models can make the process of empirical validation a hard problem [201]. Finally, Moss stated by regarding of agents' behavior and interactions that agent-based models are difficult to validate and verify [202].

There is not a broadly accepted single method for validation and verification of agent-based models. Selected methods from literature that adopted to this thesis summarized as, Darvishi and Gholamreza grouped agent-based model validation to three stages [203], Balci outlined 15 principles validation and verification in his study [204], and a different approach to validation and verification is the three steps proposed by Naylor and Finger [205].

Besides validation and verification, calibration is also an important process in modeling. Calibration is the adjustment and modification of agent-based models to adapt the experimental data. In addition, it involves with the tweaking of agents and the interactions among them to fit their behavior to the real world objects and yield consistent results with

the particular values in the experimental results. The agent-based models simplified therefore surface tension values cannot exactly match the experimental data. For this reason, results must be calibrated to evaluate the competence of agent-based models for predicting the values in the acceptable range.

### **1.5. Thesis Outline**

The overall organization of thesis consists of six chapters, with this chapter. After presenting background and introductory information about the thesis in Chapter 1, literature review on fate of nanoparticles in air, water bodies, and soil presented in Chapter 2. In addition, surface tension and effects of nanoparticles on surface tension researched. In Chapter 3, objectives and boundaries of the thesis mentioned. Chapter 4 includes the detailed information about ABM approaches as well as experimental setups. Chapter 5 is concerned with the results gathered from the experiments held in this thesis. The results of models and experiments evaluated and discussed. Detailed analysis performed to investigate the feasibility and performance of all agent-based models and experimental setups. Recommendations for the future studies represented in Chapter 6 and as a final point, an alternative experimental setup as well as ANN modeling approach portrayed in Annex.



## 2. LITERATURE REVIEW

This chapter attempts to review the relevant literature and research related to the fate of nanoparticles, surface tension, and effects of nanoparticles on surface tension. The purpose of this literature review is to investigate the connections among the surface tension and nanoparticles. The chapter first discusses the fate of nanoparticles in air, water bodies, and soil followed by surface tension. The final section is examines the effects of nanoparticles on surface tension which has controversial results.

### 2.1. Fate of Nanoparticles in the Environment

Nanoparticles, nanospheres, nanotubes, and nanofibers and their byproducts have the capability to develop concerns for humans and the environment. Nanoparticle cycle from anthroposphere to environment resented in Figure 2.1 [206].

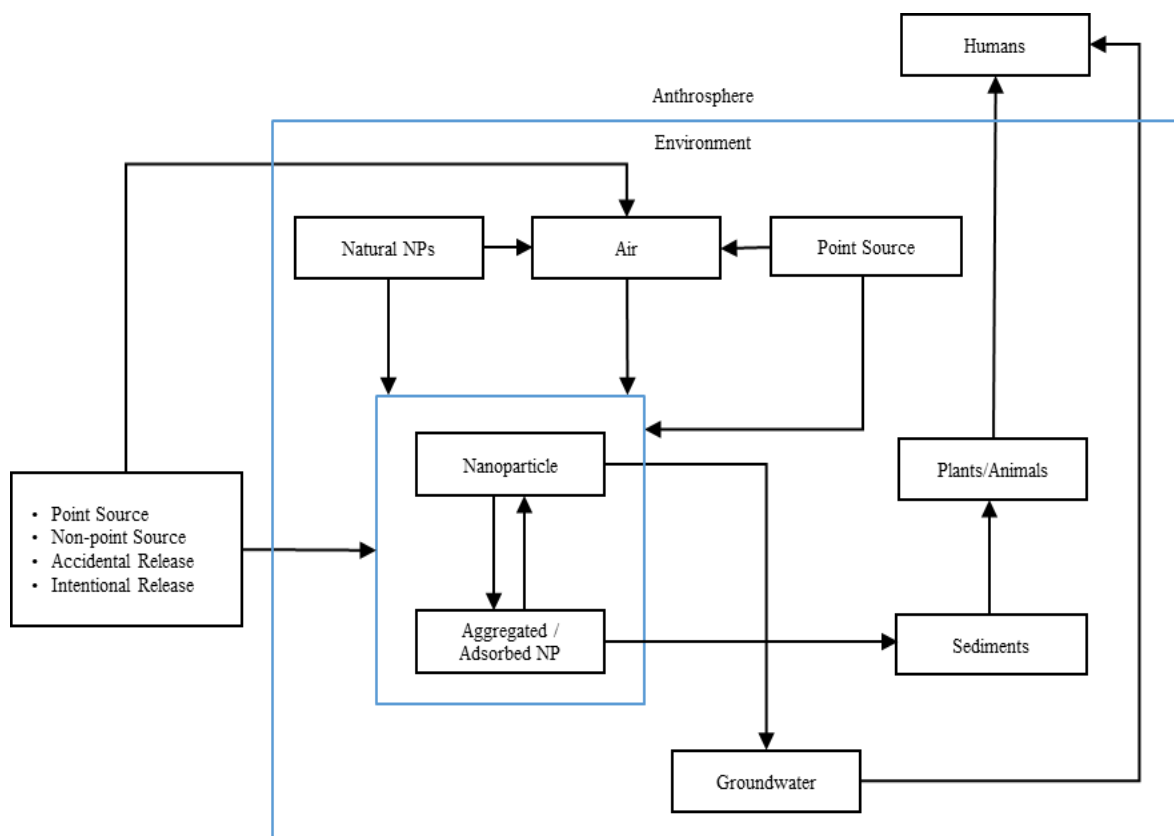


Figure 2.1 Nanoparticle cycle from anthroposphere to environment [206]

Engineered and naturally occurring nanoparticles can be transported, distributed, and transformed in the environment, and can possibly have impacts on humans as well as on environment. The behavior of nanoparticles in different medium such as air, water, and soil examined as follows,

### **2.1.1. Fate of Nanoparticles in the Air**

Nanoparticles govern the total number of particles in the atmosphere although they correspond to extremely insignificant amount of the total particle mass. Eggersdorfer et al. stated that shape of atmospheric nanoparticles varies from perfect spheres to fractals like agglomerates [207]. In addition, nanoparticles can be categorized by regarding their mean primary particle and mobility-equivalent diameters.

Natural resources of nanoparticles in the atmosphere originate from numerous sources such as volcanic eruptions, precipitation, hydrothermal ventilation, forest fires, and biological processes. Anthropogenic sources involve emissions from transportation, power plants, and manufacturing, etc. Nanoparticle cycle in the atmosphere represented in Figure 2.2. As mentioned in preceding chapter, between 2010 and 2014 production of ENPs increased by 24%. Farre et al. predicted that the amount of nanoparticles released to atmosphere due to human activity calculated as more than 36% of the entire released particulate concentrations [51].

Nanoparticles can contend with different processes in the atmosphere so that they can increase their sizes more than 100 nm in diameter to act as nuclei for cloud condensation that can critically contribute to global warming [208, 209]. Nanoparticle growth in the atmosphere appears with coagulation and condensation processes. Condensation and vaporization processes influence the changes in the physical properties of nanoparticles. Consequently, Kelvin effect reduces the condensation of semi-volatile mixtures causing substantial growth for the nanoparticles with >5 nm in diameter, [210]. There is a strong expectancy in the increment of nanoparticles in atmosphere caused by anthropogenic activity.

Nanoparticles can go through numerous manners in atmosphere so that they can reach up to >100 nm in diameter to act as nuclei for cloud condensation which can participate to global warming. Nanoparticle size increment in the atmosphere arises because of

coagulation and condensation. Condensation and vaporization guide to changes in the physical properties of nanoparticles but do not affect the total number concentration.

In Table 2.1 particular metal ENPs found in the atmosphere with their selected origins represented.

Table 2.1 Particular metal ENPs in the atmosphere associated with their selected origins

<b>Nanoparticles</b>	<b>Source</b>	<b>References</b>
Al, Fe, Mg, and Zn	Diesel	[211]
Al, Ca, Fe, Ni, and Zn	Diesel	[212]
Ca, P, Zn, and Mg	Lubricating oil	[213]
Fe, Mn, and Ce	Fuel-borne catalysts	[214, 215]
Fe, Cu, Sn, and Zn	Brakes	[216]
Fe, K, Na, Pb, and Zn	Metalworking	[217]
Ce, Fe, Na, and K	Power generation	[218]
Cd, Pb, and Zn	Incinerators	[218]

Meteorological conditions in the region can affect the nanoparticle concentrations in the atmosphere [219]. In addition, any increment in the density of nanoparticles influences the cloud concentration and reflectivity that have impacts on the precipitation and dimming. Extinction durations of nanoparticles are remarkably short but their persistent replacement from the aforementioned sources results in considerable concentrations in the atmosphere. The lifetimes of nanoparticles varies between minutes to days, depending on their properties [220].

Nanoparticles are the main predecessors of larger particles in the atmosphere. Depending on their types, sizes, physical and chemical properties, nanoparticles can effect global climate through warming or cooling effects. Nanoparticles in the atmosphere can scatter sunlight ensuing in net cooling of earth. On the other hand, opposite phenomenon occurs when nanoparticles absorbs sunlight. When nanoparticle concentration increased with the amount of greenhouse gases in the atmosphere, cooling effect of nanoparticles screened by greenhouse warming. [221]. The screening effect can be considerably immense by considering the projected power of nanoparticles as  $1.20 \text{ W/m}^2$  compared with  $2.64 \text{ W/m}^2$

for greenhouse gases (1.66 W/m<sup>2</sup> for CO<sub>2</sub>, 0.16 W/m<sup>2</sup> for nitrous oxide (N<sub>2</sub>O), 0.34 W/m<sup>2</sup> for halocarbons, and 0.48 W/m<sup>2</sup> for CH<sub>4</sub>) [222].

On the other hand, nanoparticles can initiate negative effects in cloud formations and structure. In unpolluted air, clouds comprised of moderately insignificant amount of large droplets so that formed clouds become dark and translucent. In highly polluted areas with nanoparticles, H<sub>2</sub>O can easily condense on nanoparticles by causing large number of small droplets in the form of dense, reflective, bright, and white clouds. These types of clouds are the foundations of large reductions in the total amount of solar radiation reaching to earth's surface. In addition, they can cause atmospheric heating, variations in atmospheric thermal structure, and changes in local atmospheric circulation systems that causes as monsoons.

Although, these processes occur can naturally they can be artificial too. In a study conducted by Maruyama et al. offered the planned dispersal of nanoparticles to the stratosphere for reducing the solar irradiation and global warming. In this study, it has been concluded that in order to drop 3% of global radiation  $3 \times 10^7$  tons of nanoparticles in dimension of 350-450 nm dispersed in the stratosphere. Regarding the lifespan of nanoparticles in the stratosphere, decrement in amount of radiation can be accomplished by projectiles and dispersing 10 tons of nanoparticles. This procedure planned to take place in 100 launch sites around the earth with a frequency of 19 times/day. The maximum energy and the electrical power required for the operation estimated to be in order of  $2.6 \times 10^4$  MJ and 0.8 GW, respectively [223, 224].

Nanoparticles in the atmosphere can reduce visibility depending on their type, size, and composition. This phenomenon occurs as a result of absorption and scattering of sunlight in the environment [225]. For instance, C and NO<sub>3</sub><sup>-</sup> nanoparticles can cause 5% to 40% and 60% to 95% overall reduction in visibility through light absorption, respectively [226]. Representation of nanoparticle cycle in the atmosphere can be seen in Figure 2.2.

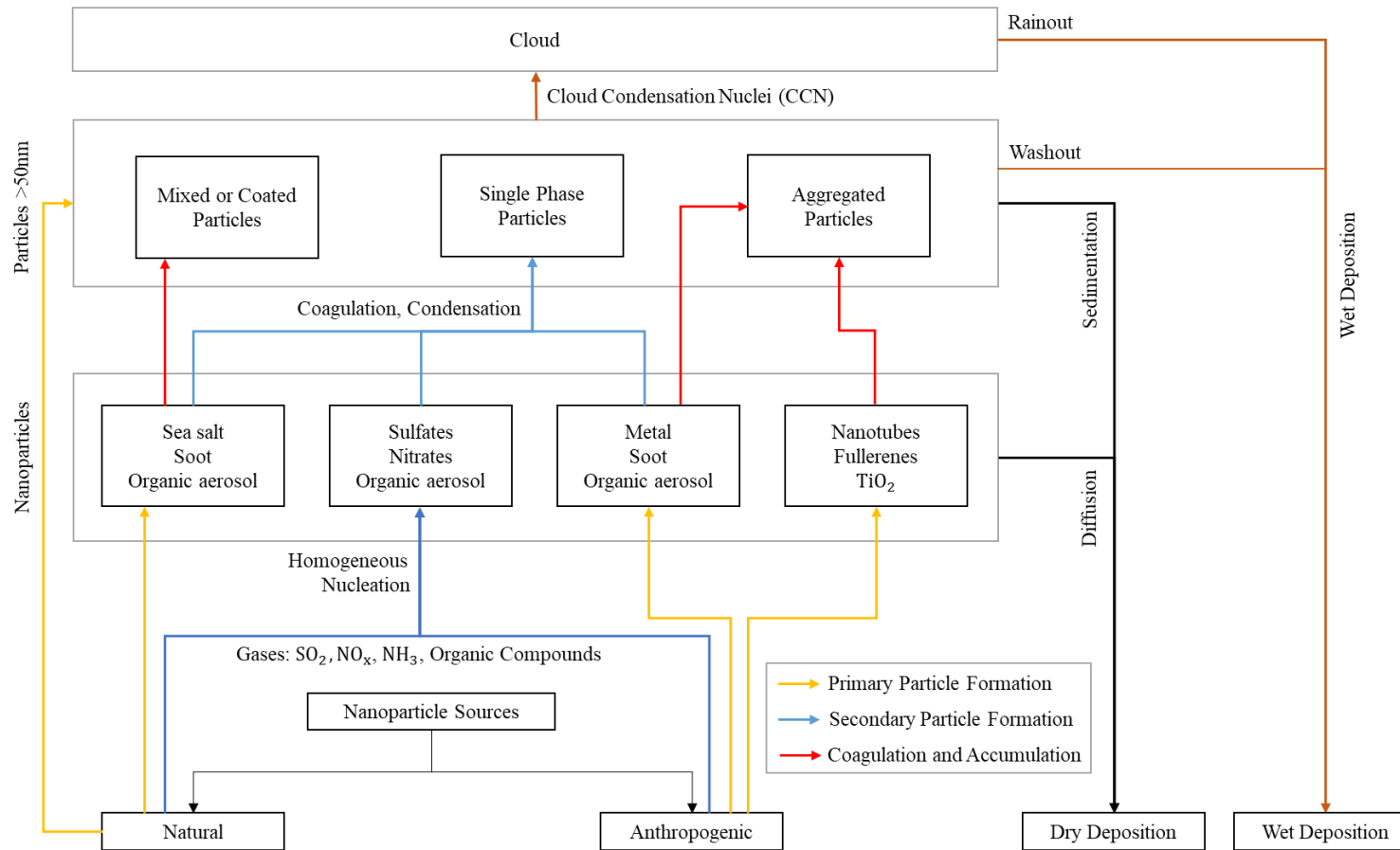


Figure 2.2 Nanoparticle cycle in the atmosphere [227]

### **2.1.2. Fate of Nanoparticles in the Water Bodies**

Nanoparticles can adhere to the aqueous medium during production, usage, and disposal of products containing nanoparticles as well as depositions from the atmosphere. They are also influenced by dispersion, diffusion, aggregation, disaggregation, sedimentation, degradation (both biotic and abiotic), accumulation, and transformation processes. Undergoing these processes can cause modification in the physical and chemical properties of nanoparticles and change their behaviors in the water bodies [228].

Dumont et al. studied to quantify the fate of ENPs in the surface waters of EU to evaluate the environmental risks that linked to the household usage of items containing ENPs as a part of project NanoFATE<sup>15</sup> [229]. In this study, Global Water Availability Assessment (GWAVA) model used in simulating concentrations of Ag and ZnO<sub>2</sub> nanoparticles over continental Europe [230]. The results yielded that less populated countries such as Iceland and Scandinavia have less of concentrations both ENPs than the more populated inhabited countries, predictably.

Because of precipitation and surface run off, marine ecosystems considered as the biggest sink for nanoparticles. In literature, it has been has shown that nanoparticle contamination of nanoparticles cause numerous effects on marine life, including fertilization immune and repertory systems, and even life expectancy. Nanoparticles can also accumulate in marine invertebrates and get involved in the food chain. Hence, eating seafood contaminated with nanoparticle can create possible health risks for humans, which mentioned in Section 1.1.

Furthermore, nanoparticles interact among each other or with bigger particles. The aggregate formation among these particles in natural systems can be comprehended by considering physical processes like Brownian diffusion [231]. Although, nanoparticles can be transported particularly extensive distances in water stream, their stability changed with water characteristics. The abundant dissolved organic matter can also affect stability of nanoparticles. In addition, nanoparticles collected from river can be stabilized by the involvement with organic colloids on mineral surfaces [15].

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<sup>15</sup> NanoFATE is an EU funded project gathering nine European countries between 2010 and 2014. During project, environmental fate and effects of ENPs studied.

Graca et al. found the occurrence density of nanoparticles in the Baltic Sea fluctuated from undetectable amounts to  $38 \times 10^3/\text{cm}^3$  [232]. In this study, nanoparticles at sea have various morphologies and sizes varying between 15 to 55 nm identified. They discovered nanoparticle distribution in the water column of Baltic Sea is seasonally dependent.

### **2.1.3. Fate of Nanoparticles in the Soil**

The fate of nanoparticles released to soil depends on their chemical and physical properties. Common natural nanoparticles in soil include inorganic matter (phyllosilicates, chlorite, iron oxide, and aluminum oxide) and organic matter (carbohydrates, proteins, and humic acid). ENPs in soil consist of fullerene ( $\text{C}_{60}$ ), CNTs, metals (Ag, Au, and Fe), metal oxides ( $\text{TiO}_2$ ,  $\text{FeO}_2$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{SiO}_2$ ) [233]. Kumar et al. mentioned that significant amount nanomaterials manufactured every year which are metal and metal oxide nanoparticles, eventually accumulate in soil [234]. After arriving in the soil, nanoparticles can critically distress the microorganisms and disrupt essential functions of soil.

In addition, common soil and plant treatment techniques in agriculture increased the rapid and bulk amount of nanoparticle development for farming and other agriculture sectors, which caused additional chances of deposition of nanoparticles in the soil. ENPs can accumulate in soil as the results of human activities including application of fertilizers or pesticides in agriculture, soil and water remediation technology or water and sewage sludge applied to the landfill, in addition nanoparticles released in the form of aerosols to the atmosphere and surface water which ends in soil. Soil is also affluent with NNPs as both in the form of primary particles as well as aggregates. Introduction of nanoparticles to soil into the soil can have significant consequences, so that they can be resilient to depreciation and result in accumulation in the soil. It has been shown that microscopic properties of soil effected by nanoparticles. The protection of soil microbial biomass and diversity is one of the major issues in the field of sustainable management of soil [235].

Nanoparticles are insignificant enough to fit into smaller gaps among soil particles or can be strongly bound with organic matters in the soil. The sorption strength and transportation rate of nanoparticles to soil dependent on its size, charge, chemistry, and application conditions. One of the main destinations of nanoparticles in soil to bound with

soil organic matter and immobilization through soil microorganisms. There is a correlation between organic carbon (C) content and nanoparticles sorption potential, which can be originated from binding of C to organic matter. In the adsorption process, the movement of nanoparticles decreases and their effects on the microbial activities decreases, considerably. Generally, microorganisms in the soil interact with nanoparticles through passive and active mechanisms caused by the changing microbial activities. Mobility of nanoparticles in soil related to numerous factors such as pH, soil type, nanoparticle size, and groundwater flow [236]. Nanoparticles found to be influencing bacteria activity and population in soil explored in various studies. The studies on FeO nanoparticles showed that nanoparticles drift from centimeters up to meters from the point of addition. For instance, Ge et al. presented that TiO<sub>2</sub> and Zn nanoparticles can cause undesirable effects on bacteria population in soil [237]. Also, Both, Ben-Moshe et al. and Kumar et al. revealed that even moderate concentrations of nanoparticles have the potential to adversely disturb overall bacterial population in soil [238, 239].

In addition to effects on soil, nanoparticles directly and/or indirectly effect the plants. Nanoparticles effect plants so that they trigger toxicity resulting in the productivity reduction of vegetation by changing their biochemical, and genetic properties. Nanoparticles can cause numerous morphological and physiological transformations in plants. The intensity of consequences varies with the size, type, reactivity characteristics, chemical and physical properties, structure, and surface coating of nanoparticles [240].

Literature has many examples on effects of nanoparticles on plant growth and development depending upon their properties, type of application as well as plant species. For instance, single-walled carbon nanotubes (SWCNTs) caused 300% higher photosynthetic yield in the chloroplasts attributable to the quick transport of electrons. In addition, silica and TiO<sub>2</sub> nanoparticles increased the photosynthetic rate through better oxygen transport or higher light absorbance. In contrast, some nanoparticles such as TiO<sub>2</sub> and Ag prevented photosynthesis because of their toxic actions. ZnO nanoparticles created a comparable oppressive influence on photosynthesis by restraining the photosynthesis controlling genes [241]. Thuesombat et al. studied on the impacts of Ag nanoparticles with varying diameters from 20 to 150 nm and concentrations from 0.1 to 1000 mg/l in the growth of jasmine rice [242]. The results showed that seed germination and growth are indirectly proportional to the diameter and concentrations of Ag



nanoparticles. The uptake ratio in the roots of jasmine rice found to be higher with the smaller Ag nanoparticles. The increment in the dimensions and concentrations of the Ag nanoparticles caused the deformation of leaf cells during seed germination. This study revealed that Ag nanoparticles exhibited phytotoxic effects on of jasmine rice seeds. Mirzajani et al. studied on the effects of Ag nanoparticles to the roots of the Asian cultivated rice (*Oryza sativa* L.) [243]. The experimental outcomes indicated that the escalated concentration of Ag nanoparticles up to 60 µg/ml, caused the nanoparticles penetrate through the cell wall and damaged the cell morphology as well structural features of the Asian cultivated rice. In a similar study, Nair and Chung studied on the effects of Ag nanoparticles to the Asian cultivated rice, as well [244]. In their study, rice seedlings exposed to 0.0, 0.2, 0.5, and 1.0 mg/l Ag nanoparticle concentrations for a week. The results showed that exposure to Ag nanoparticles caused reduction in root continuation, overall weight, and chlorophyll contents of rice. In addition, significant increment in hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) formation and decrement in sugar observed. Besides the mentioned studies, the effects of selected nanoparticles on plants mentioned in Table 2.2.

## 2.2. Surface Tension

History of surface tension has a long history, which goes back to BC 4<sup>th</sup> century. Natural philosophers have noticed the effects of surface tension since Aristotle, whom documented that small pieces of Fe and Pb can stay on surface of water. Studies on capillarity of liquids go back to Leonardo da Vinci. The theory of surface tension published independently by Young and Laplace in the beginning of 19<sup>th</sup> century [245].

Young-Laplace equation defines capillarity as functions of pressure and curvature of meniscus as follows [246],

$$\Delta P = \sigma \cdot C_m = \frac{2\sigma}{r_m} = \sigma \cdot \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \quad \text{Equation 2.1}$$

In the above equation,  $\Delta P$  is pressure gradient between gas and interface phases,  $C_m$  is mean curvature of meniscus, and  $r_m$  is the mean radius of curvature.

Additionally, all these equations, Kevin stated the relation among molar volume of liquid ( $V_L$ ), and relative pressure for capillarity ( $P_C$ ) as in Equation 2.2 [247].

$$P_c = \exp\left(\frac{2\sigma \cdot V_L}{r_m \cdot R \cdot T}\right) \quad \text{Equation 2.2}$$

Where,  $R$  defined as universal gas constant ( $=8.31 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ) and  $T$  is absolute temperature.

Borozzi and Angeli concluded that the capillary rise for six borosilicate glass tubes with different inner diameters gradually reduces by increasing the declination angle,  $\alpha$  of capillary tubes [248]. They observed that the meniscus does not fail to keep its axial symmetry with the inclination of the tube.

In literature, there are numerous studies involving capillary techniques used for surface tension measurements, such as Andbaeva and Khotienkova used the capillary rise to determine the capillary constant and surface tension of liquefied natural gas (LNG) components at high temperatures [249]. They showed that surface tension of ethane was indirectly proportional with both pressure and concentration of methane in LNG. In the experiments, they used glass capillaries with internal radii of 0.6393, 0.2297, and 0.09607 mm. Sobolev et al. studied on the measurement of the surface tension of water in capillaries with radii between 40 to 200 nm, which manufactured from high purity quartz tubes. They found that surface tension approximately constant and consistent to values stated in literature with 1% experimental error [250].

Table 2.2 Effects of selected nanoparticles on plants

Nanoparticle	Physiological changes	References
Ag	Addition of 1-10 mg/l and $1 \times 10^3$ - $3 \times 10^3$ mM Ag nanoparticles adversely affect seedling growth and chlorophyll fluorescence of <i>Triticum aestivum</i> L. and <i>Pisum sativum</i> L., respectively.	[251, 252]
	Ag nanoparticles with 10, 20, 40, and 50 ppm concentrations to <i>Triticum aestivum</i> L. caused incorrect chromosomal breakage/gaps, fragmentation, and distributed and lagging chromosomes.	[253]
	Ag nanoparticle uptake due to root versus foliar exposure for soybean and rice following compared and foliar exposure caused 17-200 times more bioaccumulation than root exposure of nanoparticles.	[254]
Al <sub>2</sub> O <sub>3</sub>	Activity of superoxide dismutase (SOD) in <i>Triticum aestivum</i> L. increased with the treatments of $10$ - $1 \times 10^3$ mg/l Al <sub>2</sub> O <sub>3</sub> nanoparticles at concentration of 200 and 500 mg/l.	[255]
Au	Exposure of 25-100 mg/l Au nanoparticles to <i>Arabidopsis thaliana</i> caused 75% reduction in root length and significant accumulation in the plant.	[256]
CuO	Height and the root length of transgenic cotton harboring the isopentenyl transferase (Ipt) gene decreased after exposure to $1 \times 10^3$ mg/l CuO nanoparticles.	[257]
S and ZnO	Treatment of $500$ - $4 \times 10^3$ ppm concentrations of S and ZnO nanoparticles increased the total lipids, proteins and chlorophyll.	[258]
TiO <sub>2</sub>	Application of 200 mg/l TiO <sub>2</sub> nanoparticles had a significant effect on chlorophyll A and B.	[259]
	Exposure of <i>Lemna minor</i> to $10$ - $2 \times 10^3$ mg/l TiO <sub>2</sub> nanoparticles increased the activities of enzymes.	[260]
ZnO	Spraying cluster beans with 10 mg/l ZnO nanoparticles yielded a substantial escalation in chlorophyll content (276.2 %), acid phosphatase (73.5%), total soluble leaf protein (27.1%), and alkaline phosphatase (48.7%).	[261]

### 2.3. Effects of Nanoparticles on Surface Tension

Surface tension of a liquid changed by the presence of surface-active agents and/or nanoparticles. Solutions containing surface active molecules such as surfactants, amphiphilics, lipids, and proteins typically cause decrement in surface tension, as a result of adsorption processes took place at interface [262].

The chronologically ordered studies from literature that cover both increment and decrement of surface tension dealing with different nanoparticles and/or liquids represented in the following paragraphs,

Bhuiyan et al. studied nanofluids with  $\text{Al}_2\text{O}_3$ ,  $\text{TiO}_2$ , and silicon dioxide ( $\text{SiO}_2$ ) nanoparticles in DI at various concentrations from 0.05 to 0.25% by volume and temperature from 303 to 323 K [263]. In their study, Du Nouy ring method used and their findings implied that the surface tension of the nanofluids directly proportional to nanoparticle volume fractions. The deviation in the concentration of nanofluids showed that surface tension is directly proportional with the nanoparticle quantity as mentioned in the studies of Godson and Tanvir [264, 265].

Esmailzadeha et al. investigated surface tension behavior at air/ $\text{H}_2\text{O}$  and oil/ $\text{H}_2\text{O}$  interfaces containing surfactants and zirconia ( $\text{ZrO}_2$ ) nanoparticles with du Nouy ring method [266]. The results showed that accumulation of anionic, cationic, and non-ionic surfactants decreased the air/ $\text{H}_2\text{O}$  surface tension.  $\text{ZrO}_2$  nanoparticles with negative electrostatic charges significantly changed the effects of SDS molecules at aforementioned interfaces.

Lu et al. calculated the surface tension, viscosity, and rheology of Au- $\text{H}_2\text{O}$  nanofluids using molecular dynamics simulation methods that provide a microscopic interpretation for the modified properties on the molecular level [267]. It is found that the addition of nanoparticles increased the surface tension of the nanofluid depending on Au- $\text{H}_2\text{O}$  interaction parameter,  $\epsilon$ . The addition of nanoparticles changed the surface tension with respect to  $\epsilon$ .

Moghadam and Azizian investigated the effects of ZnO nanoparticles to interfacial tension with cationic hexadecyltrimethylammonium bromide [268]. The results yielded

that ZnO nanoparticles solely have little to none effect on surface tension. Nanoparticles increase CTAB efficiency in decreasing surface tension due to synergistic effect.

Tanvir and Qiao examined the surface tension of ethanol ( $C_2H_6O$ ) and n-decane ( $C_{10}H_{22}$ ) with aluminum (Al), and boron (B), and  $Al_2O_3$  nanoparticles along with MWCNTs [265]. Surface tension measured using the pendant drop method. The results showed that surface tension increases with particle concentration above a critical concentration as well as particle size for all cases. However, at low particle concentrations change in surface tension was altered depending on fluid and type.

Moosavi et al. showed that surface tension of ethylene glycol ( $C_2H_6O_2$ ) base fluid increases ~7% with the addition of 3% (by volume) ZnO nanoparticles with Du Nouy tensiometer [269]. They concluded that the surface tension ratio of suspensions containing particles directly proportional to the nanoparticles.

Blute et al. measured interfacial tensions of air/ $H_2O$  with numerous types of silica nanoparticles by modifying pH and nanoparticle concentration [270]. Measurements have done by Sigma 70 du Nouy tensiometer [271]. Bindzil CC30 silica nanoparticles presented the highest surface activity, which is indirectly proportional with concentration although indirectly proportional with pH.

Godson et al. studied on surface tension of Ag- $H_2O$  nanofluids with varying particle volume concentrations and temperatures from 50 to 90°C with bubble pressure method [264]. They found that surface tension of nanofluids significantly indirectly proportional to temperature and directly proportional to particle volume concentration.

Vefaei et al. studied on the of bismuth telluride ( $Bi_2Te_3$ ) nanoparticles in aqueous solutions with thioglycolic acid ( $HSCH_2CO_2H$ ) [272]. For nanoparticles sized 10.5 and 2.5 nm in diameter using sessile drop method indicates that surface tension firstly drops inconsistently with the concentration of nanoparticles, and conclusively increased again after a critical value. The observed maximum deterioration is up to 50% in the surface tension appeared for minor sized nanoparticles. It has been observed that the surface tension of the nanofluid consist of 10.4 nm nanoparticles is larger than the one has 2.5 nm sized nanoparticles at the same concentration.

Jeong et al. showed that the surface tension of tri-sodium phosphate ( $\text{Na}_3\text{PO}_4$ ) solutions and aluminum oxide ( $\text{Al}_2\text{O}_3$ ) nanofluids decreased almost 20% for 4% (by volume) nanoparticle concentration [273]. In general, it has been determined that surface tension is inversely proportional to the concentration of  $\text{Na}_3\text{PO}_4$  solutions.

Murshed et al. worked on the surface tension of  $\text{TiO}_2$ - $\text{H}_2\text{O}$  nanofluid with a tensiometer [274]. They indicated that with the increment of  $\text{TiO}_2$  nanoparticles decreased the surface tension of the nanofluid at room temperature. They reported that this condition could be because of Brownian motion as well as adsorption of  $\text{TiO}_2$  nanoparticles at the interface [275, 276].

Dong and Johnson analyzed surface tension of  $\text{TiO}_2$  dispersions at selected pH values [277]. It has been concluded that surface tension values initially decreased drastically with an increase in the nanoparticle population and then it began to increase after a critical value.

Vignati et al. investigated the interfacial tension of an oil droplet in  $\text{H}_2\text{O}$  with silica nanoparticles and hexamethyldisilazane [278]. It has been found that there is no variation in surface tension values as the nanoparticle concentration and/or hydrophobicity of the surface transformed.

Okubo studied on the  $\text{H}_2\text{O}$ /air surface tension with several types of mono dispersed polystyrene and silica colloidal nanoparticles (6-460 nm in diameter) using Wilhelmy method [279]. It has been investigated that interfacial tension decreased considerably as soon as self-assembly of the polystyrene particles, completed with the creation of crystalline structures at interface. For the silica particles at the interface, independent

The sources and effects of nanoparticles in the environment have made significant progress in recent decades. On the other hand, approaches that are more systematic needed for uncovering the role of nanoparticles [280, 281]. In the light of previous studies, this thesis aims to model the nanoparticle behavior at the interfaces to understand the mechanisms underlying the relevant advances.

In summary, there are conflicting results in literature for surface tension with the accumulation of nanoparticles. The results express that surface tension of nanofluids increases directly proportional to nanoparticle concentration. On the contrary, there are opposing studies representing that the surface tension drops with the escalation of nanoparticle concentration.

### **3. OBJECTIVES OF THE THESIS**

This chapter intends to evaluate objectives and boundaries of the thesis. In this thesis, it has been aimed to assess the effects of selected nanoparticles and SDS to surface tension.

#### **3.1. Objective of the Thesis**

The most important purpose of the thesis is to investigate and analyze the impact of nanoparticles at the liquid/gas interfaces of the environmental systems. This thesis will examine the way in which the surface tension can be modelled.

This thesis implemented so that it has both experimental and modeling approaches to fulfill each other. In the course of this thesis, a simple, practical, and low cost technique employed to determine the surface tension and the effects of SDS, graphene, and multiwall carbon nanotubes (MWCNTs) to the various solvents. In addition, surface tension experiments held for 12 different solvents with varying nanoparticle and SDS concentrations at Hacettepe University Advanced Technologies Application and Research Center (HUATARC). This thesis also intends to demonstrate the behavior of the above-mentioned entities and non-linear dynamical systems using ABM techniques on behalf of the selected programming languages and software packages.

#### **3.2. Boundaries and Limitations of the Thesis**

Experimental and modeling limitations can affect the overall validity and reliability of the thesis therefore; they must be mentioned, in detail. The boundaries of this thesis include, but are not restricted as follows,

- The total number of variables used to define the agents in the agent-based models restricted to achieve optimum performance from the computers. Load tests ran to find ideal number of variables for the models' best execution performance as well as to detect the critical overload of models. Agents representing nanoparticles, SDS molecules, world, and interface defined as functions that consist of 12, 21, 11, and four variables, respectively.
- The dimensions of the world in agent-based models used to accommodate agents in the models limited to attain most favorable results. In order to get ideal dimensions,



initial tests ran for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds with different number of agents.

- NetLogo's built-in Mersenne twister pseudorandom number generator (MTPRNG) algorithm strictly dependent on software version, so that same seed value generates diverse set of random numbers for different versions of the same software [282].
- Regarding the memory limitations of NetLogo and MATLAB in agent-based modeling development process and data analysis; it can be argued that alternative software packages can be used or developed from scratch<sup>16</sup> [149, 283].
- The interactions among the agents and world simplified to avoid computational performance problems<sup>17</sup>. More accurate modeling can be done by taking into more number of forces such as magnetic and viscous drag forces.
- In the agent-based modeling approach, the forces other than electrostatic and mechanical forces neglected due to their magnitude and availability. Electrostatic interactions among nanoparticles and as well as nanoparticles and SDS molecules due to their charges are taken into consideration in all agent-based models. However, their interactions with the world and the other agents neglected. These behaviors interpreted through the Gauss' Law and can be briefly expressed in differential and integral forms as in following equations [284]. In the latter equation, first integral is the surface integral over the closed boundary and the second integral is volume integral over the 3D space.

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho_E}{\epsilon_0} = 4\pi \cdot k_C \cdot \rho_E \quad \text{Equation 3.1}$$

$$\oint_{\delta V} \vec{E} \cdot d\vec{A} = 4\pi \iiint_V \rho_E dV = 4\pi \cdot k_C \cdot \rho_E \quad \text{Equation 3.2}$$

In the above equations,  $\vec{E}$  is electric field vector,  $\rho_E$  is electric charge density,  $\epsilon_0$  is permittivity of free space ( $=8.85 \times 10^{-12} \text{ C}^2/\text{N} \cdot \text{m}^2$ ),  $q$  is total electrical charge,  $k_C$  is Coulomb's constant ( $=8.99 \times 10^9 \text{ N} \cdot \text{m}^2/\text{C}^2$ ), and  $V$  is volume of the closed surface.

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<sup>16</sup> Technical limitations of NetLogo and MATLAB can be seen in Section 1.4.

<sup>17</sup> Software and hardware configurations of computers used in this thesis represented in Appendix 19.

Throughout the thesis, magnetic properties of the all agents neglected. Representation of electrostatic repulsion of the same-charged nanoparticles applied to agent-based models in accordance with Coulomb's Law, which can be seen in Figure 3.1. In all models, it has been assumed that when two same-charged nanoparticles positioned in the neighboring patches, they repel each other one patch. This assumption is also valid for the interactions of nanoparticles with the hydrophobic and hydrophilic components of the SDS molecules, which have the corresponding electrostatic charges.

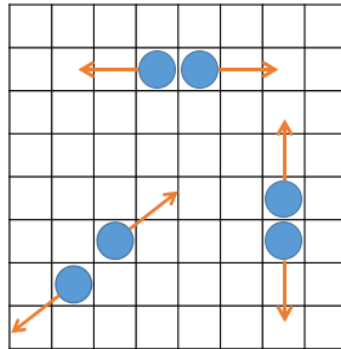


Figure 3.1 Representation of electrostatic repulsion forces on the same-charged nanoparticles in NetLogo agent-based models

- In the thesis, contacts among the container and nanoparticles as well as SDS molecules modelled the considering conservation of momentum to ease the computational load on hardware and software in all NetLogo agent-based models.
- The collision of nanoparticles with each other and with SDS molecules applied into agent-based models in accordance with Newton's Third Law of Motion [285]. When two or more nanoparticles positioned in the neighboring patches collide, they repel each other one patch further in the opposite directions. However, this condition cannot be satisfied when at least one of the nanoparticles is incapable of moving due its position in the world. These restrictions may originate from the position of nanoparticles that located at the border of the world or residing at the interface for the specific time when the collision occurs. In the collision of a nanoparticle and a wall, nanoparticle bounces back one patch in the opposite direction of its initial path as in Figure 3.2.

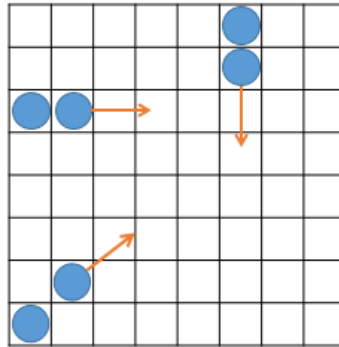


Figure 3.2 Representation of Newton's Third Law on the nanoparticles that are at the boundary conditions of world in NetLogo agent-based models

- All agent-based models ran for 12 different incompressible viscous solutions to determine the effects of density and viscosity on the nanoparticles and SDS molecules as well as surface tension. The density values for the mentioned solutions vary from  $494 \text{ kg/m}^3$  to  $1465 \text{ kg/m}^3$  for propane and chloroform, respectively. In addition, viscosity changes from  $11 \times 10^{-5} \text{ N}\cdot\text{s/m}^2$  to  $53 \times 10^{-5} \text{ N}\cdot\text{s/m}^2$  for the aforementioned solutions. The effect of density and viscosity reflected to the all agent-based models as coefficients with respect to DI.
- The measurement techniques in the experiments mentioned in Annex mainly rely on the manual procedures, which mean that results can accommodate human error.

## **4. MATERIALS AND METHODS**

In this chapter, approaches used in the creating, gathering, and analyzing of experimental results and agent-based models discussed to fulfill the objectives of the thesis. This chapter also examines the suitability and applicability of ABM techniques for surface tension modeling. Modeling techniques that comprehended through the thesis and their detailed explanations presented in the following subsections.

### **4.1. Agent-Based Modeling Approaches**

This thesis consists of modeling the accumulation of nanoparticles interface and experimental evaluation of this phenomenon. One of the projected outcomes of this thesis is to model the effects of nanoparticles and SDS molecules to the surface tension as well as their influences to the interfaces. This phenomenon can be modeled with numerous modeling techniques that use varying degrees of computational resources associated with the amount of detail provided by the model design. Throughout the thesis, non-linear, discrete, and dynamic surface tension models developed to simulate the effects of nanoparticles and SDS molecules at air-liquid interfaces at room temperature and pressure. For the modeling of surface tension in the light of experimental results, ABM techniques used. In all modeling techniques, nanoparticles, SDS molecules, solvents, and containers treated as independent objects with specific sets of attributes, which interact with each other under the given rules. All models designed to utilize the computational resources at its optimum performance and cause minimal idle time.

As defined in Section 1.4, agent-based models implemented in accordance with WSDM in NetLogo [149, 179]. The main concepts and procedures of WSDM applied to ABM as follows,

#### **4.1.1. Requirements of Agent-Based Models**

In order to avoid errors in reasoning, detailed investigations held through preparing the requirements of the agent-based models. The requirement analysis solely based on the abridged version of SRS manuscript specified in IEEE Standard 830-1998 [183, 286].

The agent-based models required to have the following core attributes so that users can,

- Define the container dimensions in 2D Cartesian coordinate system,
- Add virtually infinite number of charged/uncharged nanoparticles and SDS molecules<sup>18</sup>,
- Define the masses and velocities of nanoparticles and SDS molecules,
- Define independent random movement paths for nanoparticles and SDS molecules,
- Define different type of solvents<sup>19</sup>,
- Define different electrostatic charges for nanoparticles and SDS molecules. Also, specify Coulomb and VDW forces among them, using parameters,
- Define the critical contact distances among nanoparticles and SDS molecules independently, Prerequisite Analysis for Agents and Constraints for Agent-Based Models
- Track, plot, and log the exact positions of nanoparticles and SDS molecules (hydrophobic and hydrophilic components, separately) concurrently at any given time,
- Track, plot, and log the total number of hydrophilic components of SDS molecules at the interface in real-time,
- Track, plot, and log the number of nanoparticles and SDS molecules in the world with respect to quadrants by means of their quantity and percentages in real-time,
- Track, plot, and log the mean and median values of x and y coordinates of all nanoparticles and SDS molecules in real-time,
- Track, plot, and log the total number of occupied patches and their percentages in real-time,
- Track, plot, and log the total distance travelled by nanoparticles and SDS molecules in real-time,

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<sup>18</sup> The limiting factor for the maximum number of charged/uncharged nanoparticles and SDS molecules in the agent-based models is the software and hardware configurations of the computers. In the light of this statement, load tests had been executed for agent-based models in Section 5.1.3.

<sup>19</sup> In all agent-based models, solvent distribution designed to be continuous and homogenous throughout the world.

- Track, plot, and log the total number of collisions among nanoparticles and distribution of two, three, four, and five-body collisions with respect to quadrants by means of quantity and percentages in real-time,
- Track, plot, and log the changes in the model within the time interval of  $1 \times 10^{-3}$  s depending on computer software and hardware configuration,
- Set time and date to start the agent-based models,
- Run the agent-based models for any desired time interval,
- Access log files via FTP and send them as e-mail attachments using Gmail SMTP server, on demand.

In order to achieve necessary randomness for defining the initial conditions of agent-based models, NetLogo's built-in MTPRNG algorithm used to generate random numbers [287]. This algorithm extensively used in programming languages and software packages such as Apache, MATLAB, PHP, Python, R, Scilab, and SPSS [283, 288]. Although, the most commonly used version of this algorithm based on the Mersenne prime<sup>20</sup>. NetLogo runs with predefined seed values between  $-2^{31}-1$  to  $2^{31}-1$  [149, 287]. In this thesis, maximum positive prime number in the given interval<sup>21</sup> selected as a seed value to regenerate agent-based model results. In view of the fact that, MTPRNG algorithm dependent on NetLogo version, for overcoming the version dependency, true random number generators (TRNG) and universal constants' decimal digits (for instance, pi and Euler's number (also known as Napier's constant)) can be used as the sources for random numbers. Frequency distribution of  $10^9$  decimal digits of pi and Euler-Mascheroni's constant calculated in Appendix 1 [287].

In NetLogo, time elapses in continuous discrete intervals known as "ticks". They are the unit of erratic time measurement of NetLogo that do not have a consistent engagement with the regular time units used in daily life. Since, ticks do not map directly real-time, they are useful for making comparisons between models for maintaining the count of how many times the model updates from one state to another<sup>22</sup>. It must be mentioned that ticks

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<sup>20</sup> As of Dec 7, 2016, the largest Mersenne prime found as  $2^{77232917}-1$ . The new prime has 23,249,425 digits, which corresponds to  $\sim 1.09 \times 10^6$  more digits than the previous prime.

<sup>21</sup> Maximum positive prime number calculated as 2,147,483,647.

<sup>22</sup> In order to test reliance and consistence of agent-based models in fixed time intervals, same model ran for 100 times up to  $50 \times 10^3$  ticks.

are dependent on the dimensions of the world and total number of agents in the model as well as computational resources. All agents in the models make possible changes in their positions on behalf of the rules implied to them for every tick depending on the state of the system with respect to preceding tick. This phenomenon can be interpreted, as there is little to no data dependency in the process of phase state update for each agent for any tick. The last position of agents depends on no more than the last state of the model. In addition, ticks are reliant on visual updates of the models. In this thesis, in order to avoid performance problems of the agent-based models, all visual updates restricted.

#### 4.1.2. Types of Agents Used in Agent-Based Models

All objects treated as agents in the concept of ABM depending on their physical and chemical properties. Every agent acts according to a set of specified rules, which can be deterministic or stochastic. There are four different types of agents used to define nanoparticles, SDS molecules, world, and gas-liquid interface in all agent-based models. Each agent has its different properties which defined by selected number of static and dynamic variables throughout the models. Types of agents and their corresponding physical entities represented in Table 4.1. In addition, the allocation of static and dynamic variables for each agent can be seen in Table 4.2.

Table 4.1 Agents used in the agent-based models and their corresponding physical entities

Agent No.	Physical Entity	Agent Name	# Variables
1	Nanoparticle	Nanoparticle	12
2	SDS molecule	SDS	21
3	Container	World	11
4	Gas-Liquid Interface	Interface	4

Details of the agents used in the agent-based models are given below,

1. **Agent-1:** Nanoparticles regarded as circle shaped agents where all their masses and electrostatic charges distributed homogeneously. Depending on the model requirements, diverse number of attributes assigned to represent particular nanoparticles. Throughout the thesis, a nanoparticle defined as a function ( $A_{np}$ ), which is indicated in Equation 4.1.

$$A_{np} = f(x_{np}, y_{np}, m_{np}, V_{np}, q_{np}, d_{np}, c_{np}, \alpha, \beta, F_C, F_v, t) \quad \text{Equation 4.1}$$

In the above function  $x_{np}$  and  $y_{np}$  are the  $x$  and  $y$  coordinates of the nanoparticle,  $m_{np}$  is mass,  $V_{np}$  is velocity,  $q_{np}$  is electrostatic charge,  $d_{np}$  is diameter,  $c_{np}$  is color,  $\alpha$  is critical contact distance,  $\beta$  is repelling distance,  $F_C$  is Coulomb force,  $F_v$  is VDW force, and  $t$  is time. The schematic representation of a nanoparticle in NetLogo agent-based models can be seen Figure 4.1.



Figure 4.1 Agent-1: Nanoparticle representation in NetLogo agent-based models



Table 4.2 Allocation of static and dynamic variables for agents

<b>Agent Name</b>	<b>Variable</b>	<b>Variable Type</b>
Nanoparticle	$x$ coordinate of the nanoparticle	Dynamic
	$y$ coordinate of nanoparticle	Dynamic
	Mass	Static
	Velocity	Static
	Electrostatic charge	Static
	Diameter	Static
	Color	Static
	Critical contact distance	Static
	Repelling distance	Static
	Coulomb force	Static
	VDW force	Static
	Time	Dynamic
	SDS molecule	$x$ coordinate of the hydrophobic component
$y$ coordinate of the hydrophobic component		Dynamic
$x$ coordinate of the hydrophilic component		Dynamic
$y$ coordinate of the hydrophilic component		Dynamic
Mass of hydrophobic component		Static
Mass of hydrophilic component		Static
Velocity of SDS molecule		Static
Electrostatic charge of hydrophobic component		Static
Electrostatic charges of hydrophilic component		Static
Diameter of hydrophobic component		Static
Diameter of hydrophilic component		Static
Length of the link (straight line) between hydrophobic and hydrophilic components		Static
Color of hydrophobic component		Static
Color of hydrophilic component		Static
Critical contact distance for hydrophobic component		Static
Critical contact distance for hydrophilic component		Static
Repelling distance for hydrophobic component		Static
Repelling distance for hydrophilic component		Static
Coulomb force		Static
VDW force		Static
Time	Dynamic	

*Continued on next page,*

Agent Name	Variable	Variable Type
World	Dimension of world in $x$ coordinates	Static
	Dimension of world in $y$ coordinates	Static
	Patch size	Static
	Font size	Static
	Frame rate	Static
	Location of origin in Cartesian coordinates	Static
	Background color of the world	Static
	Boolean switch for horizontal wrap	Static
	Boolean switch for vertical wrap	Static
	Time	Dynamic
Gas-Liquid Interface	$x$ coordinate of the interface	Static
	$y$ coordinate of the interface	Static
	Color	Static
	Thickness of the interface	Static

2. **Agent-2:** SDS molecules treated as linked combinations of hydrophilic and hydrophobic components as in Figure 4.2. All linked to each other with a straight line. SDS agent defined with attributes such as electrostatic charges, component diameters, and colors. All attributes designed to be modified programmatically within NetLogo. The attributes used to define a SDS molecule can be seen as a function in Equation 4.2.

$$\begin{aligned}
& A_{SDS} \\
= & f(x_{SDS_1}, y_{SDS_1}, x_{SDS_2}, y_{SDS_2}, m_{SDS_1}, m_{SDS_2}, V, q_{SDS_1}, q_{SDS_2}, \\
& d_{SDS_1}, d_{SDS_2}, l, c_{SDS_1}, c_{SDS_2}, \alpha_{SDS_1}, \alpha_{SDS_2}, \beta_{SDS_1}, \beta_{SDS_2}, F_C, F_v, t)
\end{aligned}
\tag{Equation 4.2}$$

In the above function,  $x_{SDS_1}$  and  $y_{SDS_1}$  are the  $x$  and  $y$  coordinates of hydrophobic component,  $x_{SDS_2}$  and  $y_{SDS_2}$  are the  $x$  and  $y$  coordinates of hydrophilic component,  $m_1$  and  $m_2$  are the masses of hydrophobic and hydrophilic components,  $V$  is the velocity of the SDS molecule,  $q_{SDS_1}$  and  $q_{SDS_2}$  electrostatic charges of hydrophobic and hydrophilic components,  $d_{SDS_1}$  and  $d_{SDS_2}$  diameters of both components,  $l$  is the length of the link (straight line) between hydrophobic and hydrophilic components,  $c_{SDS_1}$  and  $c_{SDS_2}$  are the color of the components,  $\alpha_{SDS_1}$  and  $\alpha_{SDS_2}$  is the critical contact distance,  $\beta_{SDS_1}$  and  $\beta_{SDS_2}$  are repelling distances of both components,  $F_C$  is Coulomb

force,  $F_v$  is VDW force, and  $t$  is time. The SDS molecule used in NetLogo agent-based models represented in Figure 4.2.



Figure 4.2 Agent-2: SDS molecule representation in NetLogo agent-based models

3. **Agent-3:** World described as collection of patches where all agents occur and interact with each other in agent-based models. The dimensions of 2D world and the patches can be changed by either GUI or script. Patch size accepted as uniform across the world and designed to correspond to  $2 \text{ px}^{23}$ . The screen update rate of world depends on computer resources and for all agent-based models; it is set to 30 fps with 60 Hz refresh for the best performance. In this thesis, Cartesian coordinate system used to track the location data of nanoparticles and SDS molecules for all agent-based models. The center of the 2D Cartesian coordinate system positioned as in Figure 4.3. The location data consists of  $x$  and  $y$  coordinates of the particular agent with respect to the center of the world.

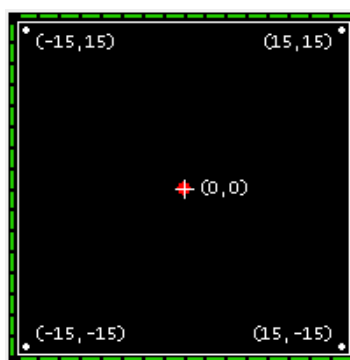


Figure 4.3 Agent-3: World representation in NetLogo agent-based models with 2D Cartesian coordinate system located

<sup>23</sup> “px” is the abbreviation of “pixel element” and it defines the basic programmable color on a computer screen or in a computer image. Each pixel has a unique location defined by  $x$  and  $y$  coordinates within the world.

In case of SDS molecules, the location data of hydrophobic and hydrophilic components recorded individually and interconnected to each other. For every single update of the world, the location data of entire dynamic agents logged into unicode transformation format-8 (UTF-8) encoded text file in real time [289]. The attributes used to define a world in the agent-based models can be seen in Equation 4.3.

$$A_w = f(x_w, y_w, p, \vartheta, \omega, \mu, \varepsilon, \theta_h, \theta_v, c, t) \quad \text{Equation 4.3}$$

In the above equation,  $x_w$  and  $y_w$  are the dimensions of the world,  $p$  is patch size,  $\vartheta$  is the font size,  $\omega$  is the frame rate,  $\mu$  is the location of origin in Cartesian coordinates,  $\varepsilon$  is the switch for screen updates,  $c$  is color, and  $t$  is time.  $\theta_h$  and  $\theta_v$  are the Boolean switches for horizontal and vertical wraps, respectively.

The monitor resolutions of the computers, which the agent-based models ran set to (1920 x 1080) px resolution with 24-bit color depth. In this configuration, every  $\text{cm}^2$  designed to reside 3612 px ( $=9715 \text{ px/in}^2$ ) on a monitor with 16:9 display aspect ratio. The (250 x 250) patch world area, which is used in main models, consists of  $250 \times 10^3$  px that constitutes the 12.05% of the viewable monitor area.

The droplet of Attension optical tensiometer and its modelled region with ABM represented in Figure 4.4 [8]. The shape of the droplet assumed to be a perfect sphere and its curvature so big when compared to size of the world. For this reason, the upper border of the world considered as linear, yielding a square shaped world.

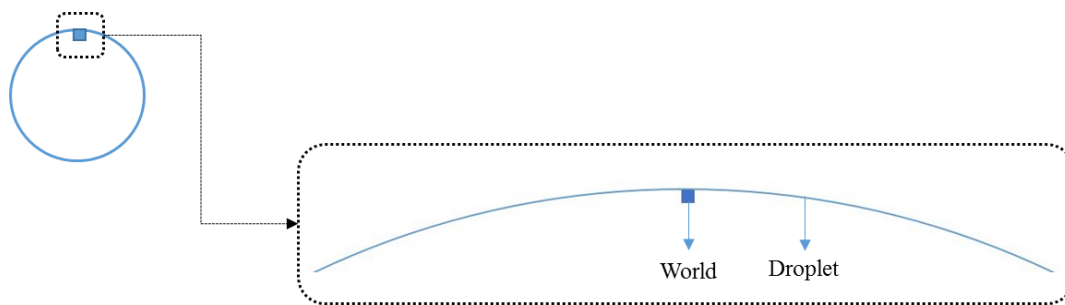


Figure 4.4 Position of agent-3 with respect to droplet created by Attension optical tensiometer [8]

In NetLogo agent-based models, world dimensions set to (250 x 250) patch to maximize the performance. Throughout the analysis of the models, it is accepted that every patch can only store one nanoparticle at a given time.

3. **Agent-4:** Interface described as the boundary where solvents and air interact. In all agent-based models, interface defined to be at the top surface of the world anywhere with its value of  $y$  coordinates equals to the  $y_{max}$  of the world. Regarding the necessities of the models, more than one interface can be defined to simulate several solvents, at once. All attributes used to specify the interface are given in Equation 4.4,

$$A_i = f(x, y, c, \eta) \quad \text{Equation 4.4}$$

In the above function  $x$  and  $y$  are the coordinates of the interface,  $c$  is color,  $\eta$  is the thickness of the interface. The horizontal interface in a rectangular form colored in yellow, which is consisting of (80 x 20) patches with the presence of other agents shown in Figure 4.5.

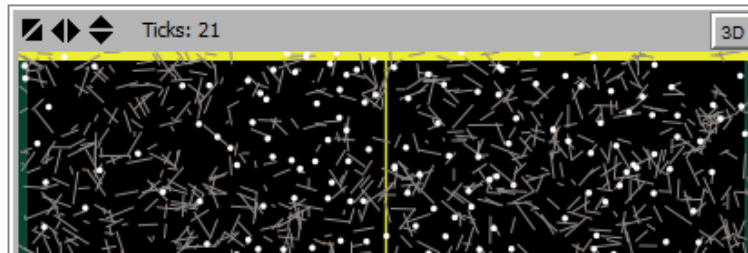


Figure 4.5 Agent-4: Interface representation in NetLogo agent-based models

#### 4.1.3. Design of Agent-Based Models

Software design is the practice of defining procedures, functions, objects, boundary conditions, and interactions among objects to assure the fulfillment of requirements [290]. In the thesis, during the design process of agent-based models two types of breeds developed nanoparticles and SDS molecules. In order to implement the best practice in agent-based model design, various algorithms created and tested to deal with the behavior of agents that simulate the surface tension. The implemented models designed to retain the requirements stated in Section 4.1.1 as well as in accordance with the functions  $A_{np}$ ,  $A_{SDS}$ ,  $A_w$ , and  $A_i$ .

#### 4.1.4. Implementation of Agent-Based Models

ABM is computationally competent for big systems and extended periods when compared to other modeling techniques by means of development cycle. Additionally, the discrete nature of the ABM makes it an ideal candidate for parallel<sup>24</sup> and distributed computing efficiency [291].

In this thesis, two particular approaches used for the ABM implementation. The first one is to code all modeling steps from scratch. For this purpose, initially Microsoft Visual Basic .NET programming language which is the part of component-based Microsoft Visual Studio Ultimate 2013 IDE suite selected [292, 293]. Nevertheless, concerning its performance, Microsoft Visual C# programming language working with .NET Framework 4.5.51641 preferred for implementation of all agent-based models [294, 295].

Microsoft Visual C# is an object oriented programming language like Microsoft Visual Basic .NET, which released in 2002 as a simplified version of C++. .NET Framework is a programming platform for implementing and running distributed applications by Microsoft. This context comprehends a class library and reusable types to perform shared tasks such as file operations and database management. .NET Framework also includes an IDE for executing applications using the .NET library named Common Language Runtime (CLR), which is responsible for running software and runtime services [296]. Initial conditions of the agent-based models and compulsory randomness generated with Knuth's modified subtractive random number generator algorithm [297].

Even though the implemented model works as designed, there are some significant issues raised skepticism for the core algorithm such as the tracking movement of nanoparticles, SDS molecules, and micelle formations in real-time. The developed code on behalf of the agent-based model puts temporary locks to selected nanoparticles, SDS molecules and micelles, sequentially. These locks avoid real-time comparison, in the view of the fact that any locked object can neither move nor interact any other entity in the system. In addition, these locked objects cannot contribute to the overall system dynamics. The

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<sup>24</sup> Parallel computing is to breakdown a selected job into smaller pieces and executing these pieces concurrently on dedicated CPUs or on batch of computers that connected together.

interface of the agent-based model developed for SDS molecules in Microsoft Visual C# IDE can be seen in Figure 4.6.

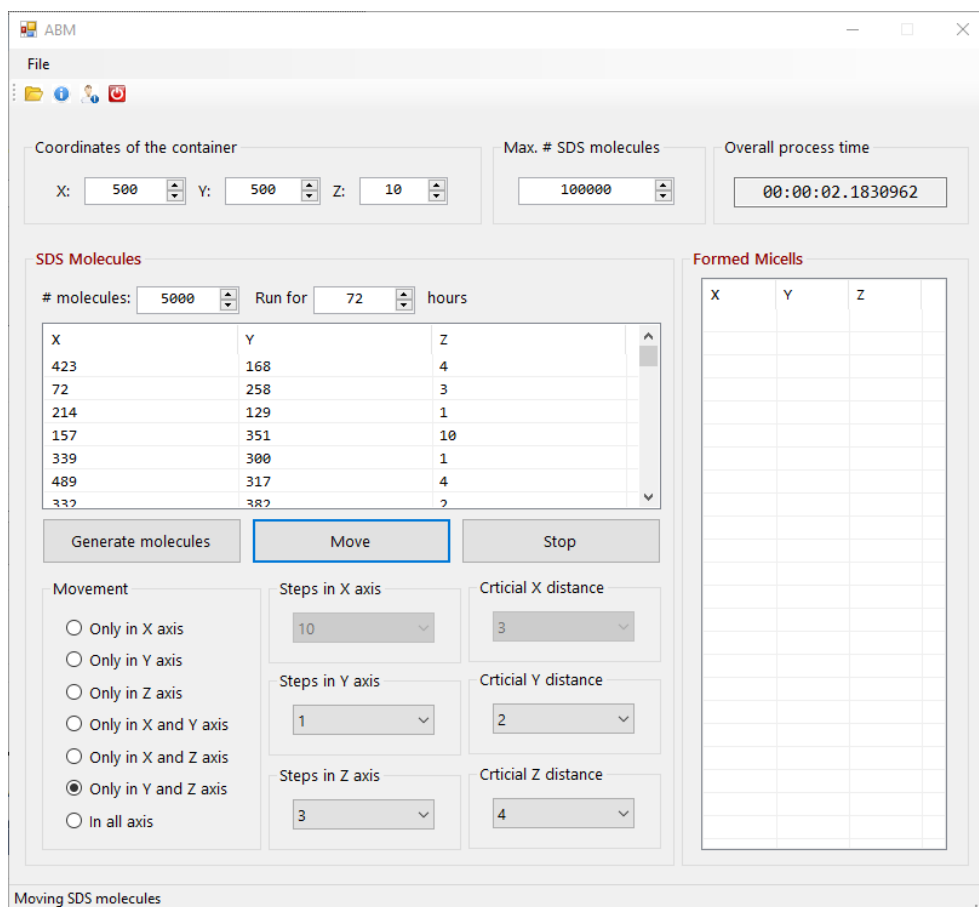


Figure 4.6 Interface of agent-based models developed with Microsoft Visual C#

With reference to the previously mentioned tryouts resulted without any significant accomplishments, NetLogo selected to analyze and model the effects of nanoparticles and SDS molecules to surface tension as a replacement for Microsoft Visual C# [149].

After implementing and testing agent-based models for nanoparticles and SDS molecules individually, both gathered to create an integrated model that resemble their effects on the surface tension. In this agent-based model, 41 variables can be tracked and controlled in real-time. The algorithm of the agent-based model designed so that users can,

- Define the dimensions of world in 2D,
- Add virtually infinite number of nanoparticles and SDS molecules,
- Add virtually infinite number interfaces vertically and horizontally,

- Define the independent random movement paths for each nanoparticle and SDS molecule in selected dimensions,
- Define the electrostatic charges of nanoparticles and SDS molecules,
- Define the masses of nanoparticles and SDS molecules,
- Detect the exact position of all nanoparticles and SDS molecules concurrently at any given time,
- Track the instantaneous and total number of SDS molecules at the interface,
- Track distributions of nanoparticles and SDS molecules in the world with respect to quadrants by means of their quantity and percentages,
- Track total distance travelled by all nanoparticles and SDS molecules,
- Track total number of occupied patches and their percentages,
- Track mean and median values of x and y coordinates of all nanoparticles and SDS molecules,
- Define virtually infinite type and number of solvents,
- Track total number of collisions among nanoparticles and distribution of collisions with respect to quadrants by means of quantity and percentages,
- Run the model for any desired time interval,
- Set time and date to start agent-based model,
- Send the logged results as mail attachments via Gmail Simple Mail Transfer Protocol (SMTP) server and access them through file transfer protocol (FTP), on demand,
- Log model outcomes into UTF-8 encoded text files and store them in the HDDs [289].

The basic flowchart of agent-based models used thesis represented in Figure 4.7.



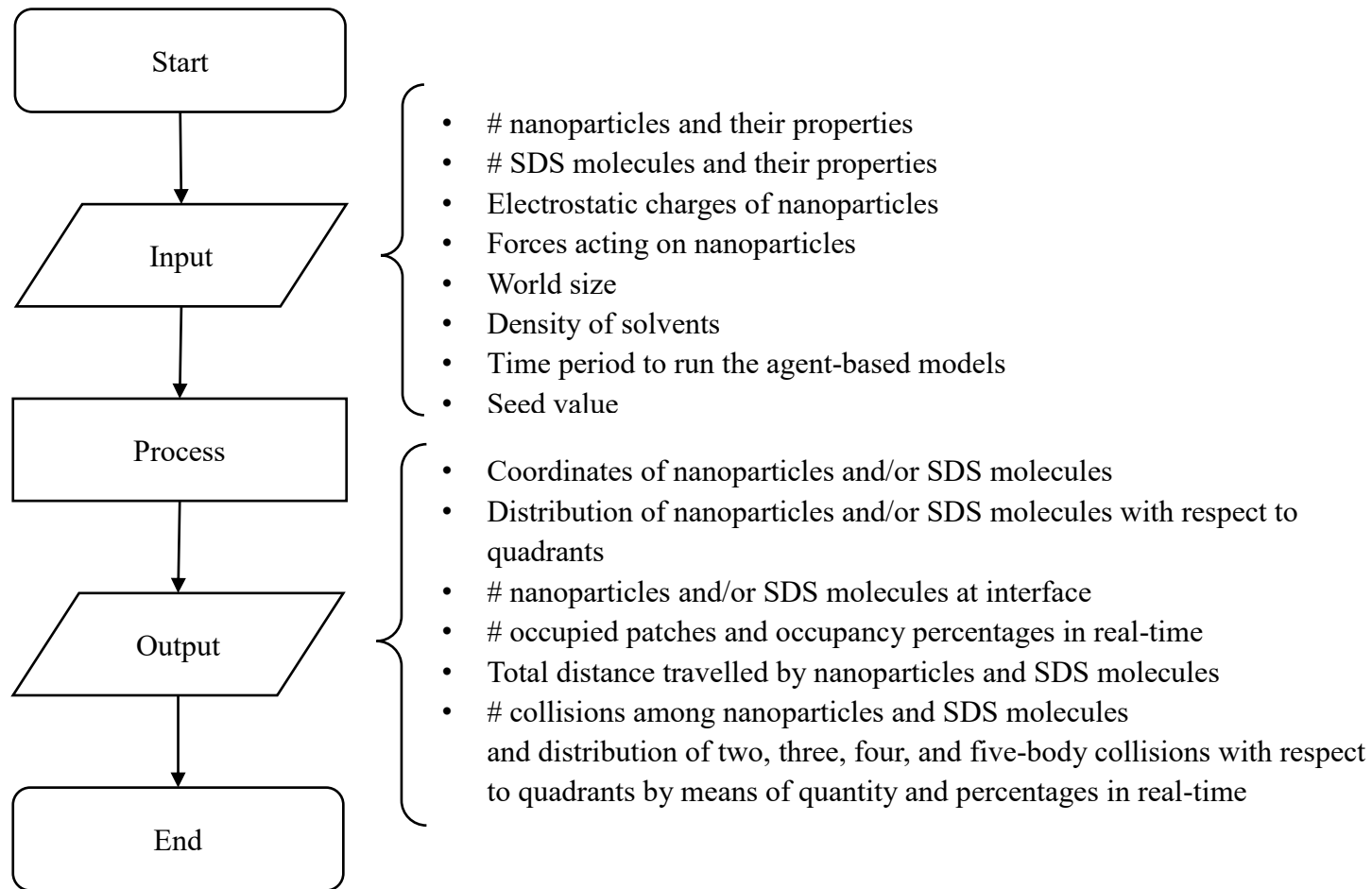


Figure 4.7 Basic flowchart for NetLogo agent-based models with selected input and outputs

The screenshots of NetLogo agent-based models represented from Figure 4.8 through Figure 4.10.

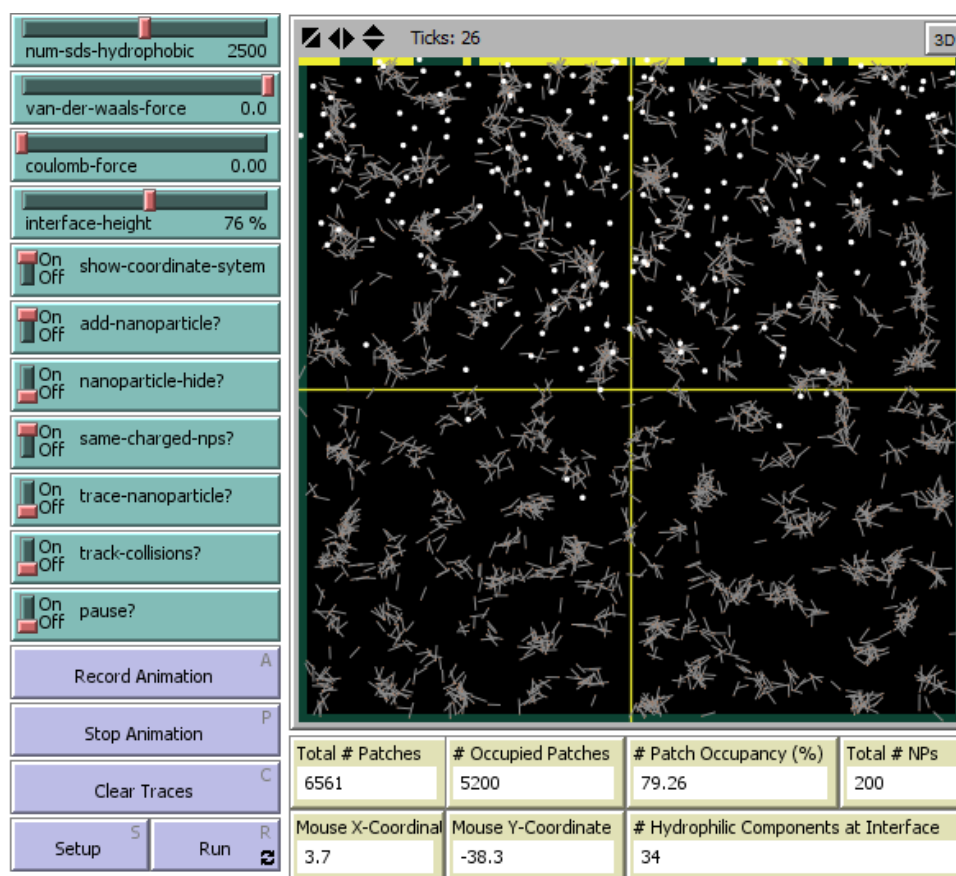


Figure 4.8 Interface of agent-based models developed with NetLogo (a)

#### 4.1.5. Testing, Validating, and Verifying the Agent-Based Models

All agents individually tested for their behaviors and randomness in numerous agent-based models under different scenarios. In order to ensure reliability of the models, nanoparticles and SDS molecules in various environmental conditions investigated. The same-charged and uncharged 10, 100, and  $1 \times 10^3$  nanoparticles individually tested for the interactions with each other as well as with the interface for different sized worlds such as (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch for 24 and 48-hours. In addition, SDS molecules tested for the same conditions mentioned above, as well. All tests repeated for two times on dedicated computers and their results analyzed to examine the behaviors of nanoparticles in addition to consistency of randomness of the agent-based models.

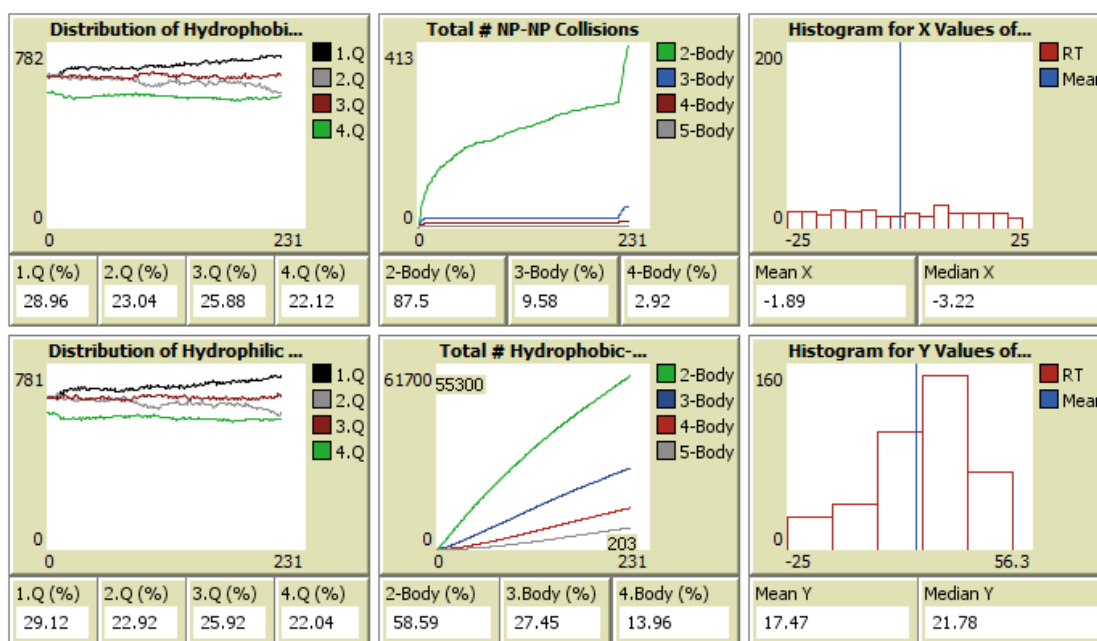


Figure 4.9 Interface of agent-based models developed with NetLogo (b)

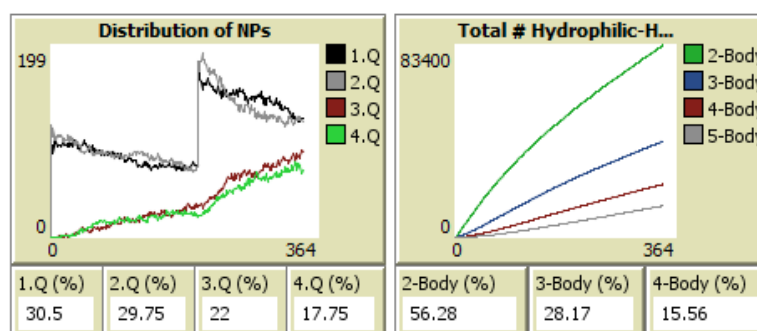


Figure 4.10 Interface of agent-based models developed with NetLogo (c)

In each run, 26 parameters that are given in the following seven categories selected to define the behavior and randomness of all agents in the models. The parameters logged into UTF-8 encoded text file in real time as follows [289],

- Ticks,
- Current time and date information (time-stamp),
- Distribution of nanoparticles/SDS molecules in the world with respect to quadrants by means of their quantity and percentages,
- Mean and median values of  $x$  and  $y$  coordinates of nanoparticles/SDS molecules,
- Total distance travelled by nanoparticles/SDS molecules in the world,

- Total number of collisions between nanoparticles/SDS molecules and distribution of collisions with respect to quadrants by means of quantity and percentages,
- Total number of occupied patches and their percentages.

All tests for uncharged and same-charged nanoparticles with DI took 2,592 hours of CPU time (=108 days) to complete. Tests generated log files with  $17.62 \times 10^6$  and  $12.90 \times 10^6$  lines of data for uncharged and same-charged nanoparticles, respectively. In the course of testing, total number of  $793.41 \times 10^6$  parameters logged for both types of nanoparticles. The initial test results for nanoparticles represented in Appendix 3 and Appendix 4.

The tests for SDS molecules with DI took 1,296 hours of CPU time (=54 days) to finish and generated log files including  $16.94 \times 10^6$  lines<sup>25</sup>. Throughout the testing total number of  $440.38 \times 10^6$  parameters logged in real-time. The initial test results for SDS molecules submitted in Appendix 5. In another set of tests, all agent-based models experimented for 12 different solvents for 72-hours to investigate the behavioral effects of density on nanoparticles and SDS molecules influenced by the surface tension. Density values of the selected solvents at 25°C vary from 494.00 kg/m<sup>3</sup> for propane to 1,465.00 kg/m<sup>3</sup> for chloroform. The density values of all solvents represented in Appendix 2 [298].

Each test for every solvent ran twice for  $5 \times 10^3$ ,  $7.5 \times 10^3$ ,  $10 \times 10^3$ ,  $12.5 \times 10^3$ ,  $15 \times 10^3$ ,  $50 \times 10^3$ , and  $75 \times 10^3$  same-charged and uncharged nanoparticles as well as SDS molecules, independently. All tests took 36,288 hours of CPU time (=1,512 days) to finish and created  $55.70 \times 10^6$  lines of log file. During all tests, total number of  $1.45 \times 10^9$  variables recorded in real-time to HDDs.

Besides, agent-based models for nanoparticles and SDS molecules also subjected to load testing in order to establish stability and threshold state of computers. The main objective of this test to ensure the model does not crash in conditions of inadequate hardware and/or software resources and determines the critical breaking point for total number of agents. As mentioned in Section 1.4, NetLogo implemented in Java and inherits its all limitations [149]. For this reason,  $100 \times 10^6$  and  $200 \times 10^6$  same-charged and uncharged nanoparticles

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<sup>25</sup> In all tests, following DOS and Linux commands used to count the total number of lines in a log folder,  
 DOS: (for %a in (Log\*.txt) DO @(findstr /R /N "" %a & echo:)) | find /c ":"  
 Linux: wc -l /var/log/Log-\*.txt

in addition to SDS molecules tested with screen updates off, one a time. Tests created  $12.50 \times 10^6$  and  $41.55 \times 10^3$  lines of log files for all nanoparticles and SDS molecules, respectively. During tests, it has been detected that performance of agent-based models dropped drastically due to number of agents in the world. The recorded variables in the log files decreased by 99.86% as the number of SDS molecules increased from  $5 \times 10^3$  to  $200 \times 10^3$ .

All tests created extensively big log files that have more than ten thousands of lines therefore it has been unattainable to open these files for a plain text editor. For this reason, open source Glogg log analyzer software used to examine the results [299]. Hardware and software configurations of computers used in agent-based models are given in Appendix 19.

#### **4.1.6. Deployment of Agent-Based Models to Selected Operating Systems**

Deployment consists all of the activities that enable agent-based models to be accessible to the end-user. It includes all procedures required for a model to run and operate in a specific environment such as Microsoft Windows 10 Enterprise version 1803 (64 bit) or Ubuntu 16.04.2 LTS (64 bit) [176, 300]. Deployment process consists of manually or automatically installation, configuration, and optimization of the agent-based models. Up to this final subprocess, all agent-based models must pass every single test and verified to demonstrate the real environmental conditions.

All agent-based models deployed to aforementioned Windows and Linux operating systems, independently [177]. Ubuntu 16.04.2 LTS (64 bit) distro selected for its stability, scalability, maintainability for an alternative open source computer operating system [300]. In order to run the agent-based models, NetLogo 5.3.1 (64 bit) IDE manually installed on each computer and agent-based models deployed to relevant folders on the computers [172]. For Linux, Xftp 5 FTP and Xshell 5 terminal emulator used to deploy agent-based models. [301, 302]. Prior to the deployment of the models, HDDs of all computers checked to ensure that there is enough free space to keep log files.

All agent-based models ran concurrently on six computers that have the similar hardware and software configuration, which represented in Appendix 19. The logged data matched with ticks to analyze the dependency of NetLogo agent-based models to computer

resources [149]. Hardware and software utilization monitored in computers with Microsoft Windows 10 Enterprise version 1803 (64 bit) using HWInfo diagnostic freeware and the same monitoring has been done by open source software Glances on Ubuntu 16.04.2 LTS (64 bit) operating systems [176, 300, 303, 304].

During the utilization of NetLogo agent-based models more than 20 parameters in five categories logged in real-time to each computer's local HDD. Selected critical parameters that monitored in both operating systems are page file usage (%), physical memory load (%), and total CPU usage.

A faulty deployment can cause a configuration error across the agent-based models, which leads to malfunction. As a result, valuable time and effort will be misused in identifying and addressing difficulties arising from the flawed agent-based models. In the course of a crashed deployment, old agent-based models backed-up to roll back to a known-working version. In addition to models, operating systems and log files backed-up periodically by Macrium Reflect Free to Seagate Flexagent Goflex and Seagate Extension Portable external storage units to make sure that the computers will be online within the shortest possible time without any data loss, in case of computer failure due to hardware malfunction, software virus, etc. [305-307]. The incremental backing-up of computers scheduled daily and there is no requirement to start the processes manually, in terms of human interaction.

All software used in this thesis is freeware and/or open source except Microsoft products, SPSS, and MATLAB [283, 288]. In order to avoid cross-platform operating system issues and assure a homogeneous topology, Microsoft Windows 10 Enterprise version 1803 (64 bit) operating system preferred on all computers with the exception of running NetLogo agent-based models on Ubuntu 16.04.2 LTS (64 bit) operating system [176, 300].

#### **4.1.7. Sensitivity Analysis of Agent-Based-Models**

Agent-based models express non-linear interactions and emergent behaviors, which limit the information flow between input and output values of the models as in typical sensitivity analysis techniques. To overcome this inadequacy, Broekea et al. evaluated the performance of three sensitivity analysis techniques as follows [308],

1. **One-factor-at-a-time (OFAT) sensitivity analysis** built on picking a fixed variable configuration (also known as nominal set) and a changing variable with respect to time. The effects of the changing variable to the output of the agent-based model with nominal set investigated. This analysis shows that the response of the model can be either linear or non-linear, effects of the fixed variable to model, and whether it caused any breaking points. Besides, another sensitivity analysis technique based on OFAT is one-at-a-time (OAT) technique, which approximates the sensitivity values as derivatives of the models outputs depending on inputs. OAT investigates the response of minor variations of changing variable to values on the agent-based model outcomes [309].
2. **Global sensitivity analysis (GSO)** studies on the relations and interactions of the variables by sampling the agent-based model outcomes over an extensive range of input variables. Input variables selected from the variable space and consequent outputs analyzed. The sensitivity of an agent-based model to a selected input variable expressed as the fraction of overall variance to deviation in selected agent-based model variable [310].
3. **Regression based sensitivity analysis (RBSA)** relates the variation of the agent-based models outputs to the input variables by fitting regression function. This technique has the advantage of summarizing complex relationships of agent-based models between inputs and outputs into descriptive relations that can be examined with  $R^2$  analysis.

In addition to Broekea et al, there are numerous approaches for sensitivity analysis, as well. For instance, Massada and Carmel analyzed the sensitivity of a stochastic individual-based model that implemented to predict the changes in mosquitofish population [311]. In their study, they proposed a new sensitivity index method to determine the parameters was calculated using the mean of the output distribution through ranking model parameters corresponding to their effects on the output. The results showed that the new method and widely used standard method yielded different values for the parameters used in the model. They concluded that the proposed new index had better performance in the forecasting of parameters on model output since it accounted for the variance of the output distribution.

Campolongo et al. proposed a modified version of the Elementary Effects (EE) method, which used as an effective screening sensitivity measure to identify the significant factors in models [312, 313]. EE method based on computing for each input a number of incremental ratios (elementary effects) that are averaged to evaluate the total importance of the input. They tested their version with a multi-phase chemical model for the dimethylsulphide (DMS) oxidation and found that method performed better and yielded estimations that are more accurate.

Ascough et al. studied on the integrated natural resource models and compared Fourier Amplitude Sensitivity Test (FAST), Response Surface Method (RSM), Mutual Information Index (MII), and Sobol's sensitivity analysis methods [314]. It has been found that FAST and Sobol's methods were capable of measuring the parameter effects and all interactions related to that particular parameter. In addition, they suggested that sensitivity analysis must be employed prior and during model development as well as deployment of the model.

Blower and Dowlatabadi studied on the sensitivity analysis of HIV transmission models [314]. In the analysis, PRCC used to indicate the uncertainty in the estimation of the input parameter to the prediction of output parameter. PRCCs indicated the degree of monotonicity among input and output parameters. It has been concluded that positive values of PRCC implied that the cases would increase, and vice versa.

Thiele et al. examined a NetLogo agent-based model with R using RNetLogo package. [315]. They recommended the following sensitivity analysis techniques applied to the selected model in the given order,

1. Morris's elementary effects screening
2. Sobol's method
3. Partial rank correlation coefficients (PRCC) method
4. Extended Fourier amplitude sensitivity test (eFAST)

The comparison of sensitivity analysis methods with respect to regarding information and efficiency versus cost represented in Figure 4.11. In the plots, cost stands for the computational expenses (i.e., number of simulations, hardware and software utilization etc.) as well as the time needed to modification of the analysis methods. Information and



efficiency of the sensitivity analysis consist of features about the category of output data set and the ways to accomplish the meaningful results.

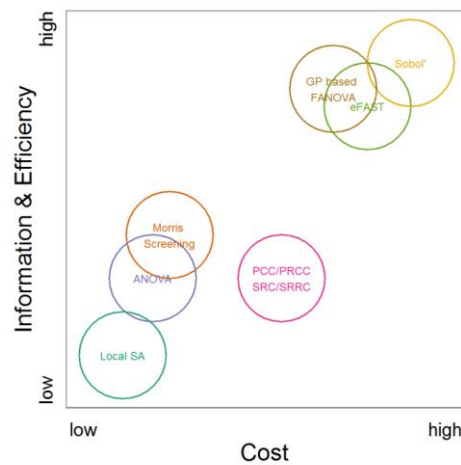


Figure 4.11 Categorization of sensitivity analysis methods [315]

They been indicated that executing the same agent-based model with the similar parameters and configuration with different random seeds for numerous times.

Inconsistent with the aforementioned approach by Thiele et al., the sensitivity analysis of the NetLogo agent-based models, regarding the previously mentioned time-consuming and tedious sensitivity analysis techniques following approach has been utilized. Firstly, 100 different random data sets generated with MTPRNG algorithm and used as inputs of the same model to examine the influences of nanoparticles and SDS molecules to the surface tension of DI [282]. Each model ran separately in a (80 x 80) patch world for  $50 \times 10^3$  number of ticks<sup>26</sup> and for each tick, 103 parameters logged in real time into UTF-8 encoded text file for future analysis.

All log files, which are in fact text files that contain  $272.72 \times 10^6$  parameters, manually imported into MATLAB and arranged as a  $(50 \times 10^3 \times 103 \times 100)$  3D matrix. In the course making analysis and running tests, computers ran “out of memory” by reaching the MATLAB’s 3 GB RAM limit<sup>27</sup> and to overcome this issue original matrix rearranged to

<sup>26</sup> Approximately, 48 hours required to reach  $50 \times 10^3$  number of ticks for each agent-based model.

<sup>27</sup> MATLAB generates an “out of memory” error when it demands a segment of memory from offered by the operating system larger than available at a specific time.

create three ( $16.67 \times 10^3 \times 103 \times 100$ ) 3D matrices [283, 316]. All statistical analysis evaluated on these matrices and every 1000<sup>th</sup> tick programmatically selected to plot with the intention of visualizing the behavior of the model. Due to the computational performance problems this technique abandoned and the succeeding solution used for the analysis. All log files trimmed down to 50 lines which represents the every 1000<sup>th</sup> tick with Notepad++ freeware text editor using regular expressions method [317, 318]. Afterwards, all log files imported into separate Microsoft Excel worksheets with a code implemented in Visual Basic for Applications (VBA) and statistically analyzed [319].

Sensitivity analysis of variables for the agents defining gas-liquid interface, world, nanoparticles, and SDS molecules for all agent-based models represented in Table 4.3 and Table 4.4, respectively.

As mentioned before, this thesis intended to explore and analyze the impact of nanoparticles and SDS molecules at liquid/gas interfaces. The pendant drop surface tension measurement experiments conducted at HUATARC experiments with Attension optical tensiometer from Biolin Scientific, Frölunda, Sweden [8, 320].

In this thesis, two main categories of experiments implemented at HUATARC [320]. Each experiment repeated for three times, individually. The experiments are as follows,

1. **Surface tension measurement experiments without graphene and MWCNTs:** DI, DI with different concentrations of SDS at, above and, below CMC, and hexane,
2. **Surface tension measurement experiments with graphene and MWCNTs:** DI, DI with different concentrations of SDS at, above, and below CMC, hexane with 2 mg graphene, and 2 mg MWCNTs<sup>28</sup>.

The inventory and results of the experiments held at HUATARC represented in Appendix 12 and Section 5.2.

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<sup>28</sup> Graphene and MWCNTs obtained from Prof.Dr. Semra İDE, H.U. Physics Engineering Department SWAXS (SAXS/WAXS) Lab.

Table 4.3 Sensitivity analysis of variables for the agents defining gas-liquid interface, world, and nanoparticle

<b>Agent Name</b>	<b>Variable</b>	<b>Impacts on Models</b>	<b>Impacts on Real Life</b>	<b>Impacts on Computation</b>
Gas-Liquid Interface	$x$ coordinate	Yes	Yes	Yes
	$y$ coordinate	Yes	Yes	Yes
	Thickness	No	No	Yes
	Color	No	No	Yes
World	$x$ coordinate	Yes	Yes	Yes
	$y$ coordinate	Yes	Yes	Yes
	Patch size	Yes	No	Yes
	Font size	Yes	No	No
	Frame size	Yes	No	Yes
	Origin of Cartesian coordinates	Yes	No	No
	Switch for screen updates	Yes	No	Yes
	Switch for horizontal wrap	Yes	No	Yes
	Color	No	No	Yes
	Time	Yes	Yes	Yes
	Nanoparticle	$x$ coordinate	Yes	Yes
$y$ coordinate		Yes	Yes	Yes
Mass		Yes	Yes	No
Velocity		No	Yes	No
Electrostatic charge		Yes	Yes	Yes
Diameter		Yes	Yes	Yes
Color		No	No	Yes
Critical contact distance		Yes	Yes	Yes
Repelling distance		Yes	Yes	Yes
Coulomb force		Yes	Yes	Yes
VDW force		Yes	Yes	Yes
Time	Yes	Yes	Yes	

Table 4.4 Sensitivity analysis of variables for the agent defining SDS molecule

Agent Name	Variable	Impact on Models	Impact on Real Life	Impact on Computation
SDS molecule	$x$ coordinate of the hydrophobic component	Yes	Yes	Yes
	$y$ coordinate of the hydrophobic component	Yes	Yes	Yes
	$x$ coordinate of the hydrophilic component	Yes	Yes	Yes
	$y$ coordinate of the hydrophilic component	Yes	Yes	Yes
	Mass of hydrophobic component	Yes	Yes	No
	Mass of hydrophilic component	Yes	Yes	No
	Velocity of SDS molecule	No	Yes	No
	Electrostatic charge of hydrophobic component	Yes	Yes	Yes
	Electrostatic charge of hydrophilic component	Yes	Yes	Yes
	Diameter of hydrophobic component	Yes	Yes	Yes
	Diameter of hydrophilic component	Yes	Yes	Yes
	Length of the link between hydrophobic and hydrophilic components	Yes	Yes	Yes
	Color of hydrophobic component	No	No	Yes
	Color of hydrophilic component	No	No	Yes
	Critical contact distance for hydrophobic component	Yes	Yes	Yes
	Critical contact distance for hydrophilic component	Yes	Yes	Yes

*Continued on the next page,*

<b>Agent Name</b>	<b>Variable</b>	<b>Impact on Models</b>	<b>Impact on Real Life</b>	<b>Impact on Computation</b>
SDS molecule	Repelling distance for hydrophobic component	Yes	Yes	Yes
	Repelling distance for hydrophilic component	Yes	Yes	Yes
	Coulomb force	Yes	Yes	Yes
	VDW force	Yes	Yes	Yes
	Time	Yes	Yes	Yes

## 5. RESULTS AND DISCUSSIONS

This thesis aimed to explore and analyze the impact of nanoparticles and SDS molecules to surface tension on liquid/gas interfaces. In addition, it has intended to create a new perspective in surface tension modeling with ABM techniques.

Following sections includes analysis, presentation, and interpretation of the agent-based models. Also, results from all experiments revealed in previous Sections presented and examined, in detail. In the first section the outcomes of the agent-based models developed for surface tension elaborated and in the latter section pendant drop experiments held at HUATARC presented and its results discussed [320].

### 5.1. Results for NetLogo Agent-Based Models

As mentioned in Chapter 3, this thesis set out with the aim of assessing the importance of agent-based modelling in the prediction of surface tension at environmental interfaces. With this objective, the results of agent-based modeling methodologies will be discussed in the succeeding sections. In the beginning this thesis, all agent-based models subjected to initial testing procedures and interaction tests under different circumstances. The performance of agent-based models on behalf of ticks documented for uncharged and same-charged nanoparticles as well as SDS molecules for 24 and 48-hour periods for two times, independently. In order to test the behaviors of all nanoparticles and SDS molecules two, three, and four-body collisions monitored and logged for  $9 \times 10^4$ ,  $25 \times 10^4$ , and  $49 \times 10^4$  patch worlds. All initial tests carried out for different number of nanoparticles and SDS molecules in numerous worlds. Additionally, randomness, frequency of collisions, and behavioral effects of density on nanoparticles and SDS molecules investigated, in detail. The density values of the particular solvents used in the agent-based models diverge from  $494.00 \text{ kg/m}^3$  to  $1465.00 \text{ kg/m}^3$  for propane to chloroform at  $25^\circ\text{C}$ , respectively. The density values of all solvents used in agent-based models can be seen in Appendix 2 [298]. The detailed results including the average and total number of ticks, frequency of collisions, and distributions of agents with respect to quadrants represented in Appendix 3, 4, and 5.

The average update interval for the position of nanoparticles and SDS molecules predominantly depends on their electrostatic charge, world area, and the total nanoparticle count. When the electrostatic charges are taken into consideration, agent-based models subjected to process and evaluate more interactions among the mentioned agents, which create an extra load on the computational resources. Because of this situation, agent-based models slow down depending on the number of nanoparticles and SDS molecules. At a critical point based on the total number of agents, models can stop responding. In this thesis, critical agent population, types of interactions and other parameters selected after compulsory load tests. The details and results of load tests of agent-based models presented in Section 5.1.3 and their data in Appendix 9 and 10, respectively.

### **5.1.1. Initial Tests for NetLogo Agent-Based Models**

An agent-based model consisting of 10 nanoparticles, the overall tick difference among uncharged and same-charged nanoparticles calculated as 44.40%, 39.68%, and 36.53% for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds for 24-hours. When the nanoparticle population in the agent-based models increased tenfold, overall ticks decreased by 94.31%, 24.25%, and 69.73%, respectively. Another tenfold increment, which tops the number of nanoparticles to  $1 \times 10^3$ , transforms the gap between uncharged and same charges nanoparticle ticks by 65.35%, 43.93%, and 40.39% for the respective worlds. In another set of initial tests, the same set of agent-based models ran for 48-hours, individually. The results of models yielded consistent outcomes with the agent-based models that ran for 24-hours. All calculations exhibited regular disparity between two periods. The agent-based model consisting total number of 10 nanoparticles yielded a tick difference among uncharged and same-charged nanoparticles as 30.38%, 17.65%, and 24.91% for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds in 48-hours, respectively. The same pattern continues and the variations in ticks calculated as 48.53%, 19.52%, and 41.40% for 100 nanoparticles for the previously mentioned worlds. Finally, agent-based models with  $1 \times 10^3$  same-charged nanoparticles created 39.52%, 29.90%, and 28.76% less ticks than the uncharged nanoparticles for the same world.

The examination of tick values indicated an important connection between electrostatic forces and functioning of agent-based models. The introduction of new controls,

limitations, and rules such as critical contact distance, repelling distance, and charge values on behalf of the electrostatic forces reduces the performance of the agent-based models, drastically.

Any increment in the nanoparticle population has a downgrading effect on the performance of the agent-based models by independent of their electrostatic charge and world size. For instance, increasing the nanoparticle population in the agent-based models tenfold causes 7.48% and 27.09% reduction in ticks for uncharged and same-charged nanoparticles operated in (150 x 150) patch world. The decrement in ticks continued indirectly proportional to the nanoparticle population so that a hundredfold increment triggered an additional tick loss of 8.62% and 18.00% for the same and uncharged nanoparticles, respectively.

The effect of world dimensions on ticks observed extensively in the agent-based models implemented in (250 x 250) patch and (350 x 350) patch worlds. As the dimensions of the world get bigger, the total number of patches that should be simultaneously tracked by the computer also increases. Any upgrade from (150 x 150) to (250 x 250) patch world adds up 177.78% more patches to be tracked, besides in a (350 x 350) patch world total number of patches increases 444.44% with reaching up to  $490 \times 10^6$  patches. For instance, an agent-model based consists of  $1 \times 10^3$  same-charged nanoparticle creates 7.25 ticks/s for a (150 x 150) patch world and 1.45 ticks/s for a (250 x 250) patch world. In a scenario, all agent-based models executed for of 24 and 48-hours to investigate the time effects on ticks, individually. In the longer period, agent-based models particularly generated reduced amount of ticks for same-charged and uncharged nanoparticles.

In the collision tests for 10, 100, and  $1 \times 10^3$  uncharged and same-charged nanoparticles, two-body collisions are predominantly more than three and four-body collisions for the both 24 and 48-hour processing time. In place of 10 uncharged nanoparticles in  $9 \times 10^4$ ,  $25 \times 10^4$ , and  $49 \times 10^4$  patch worlds average number of two-body collisions calculated as 470, 245, and 226 in 24-hours. If the agent-based model duration doubles, the total number of two-body collisions increases by 78.81%, 33.06%, and 22.22%, respectively. In case of three and four-body collisions, collision frequency of uncharged nanoparticles decreases sharply. For instance, in a (150 x 150) patch world three-body collisions is five, and four-body collisions is one for 24-hours. It has been observed that doubling the agent-



based model processing time to 48-hours increases the total number of collisions more than twofold. The total number of three-body collisions in the agent-based models remained constant for a (150 x 150) patch world, increased by 28.57% for a (250 x 250) patch world, and decreased by ~100.00% for a (350 x 350) patch world.

The total number of collisions reduces significantly with respect to the any increment in the dimensions of the world. For instance, increasing the world dimension from  $90 \times 10^3$  to  $490 \times 10^3$  patches, total number of collisions reduced by 71.43%, 43.51%, and 77.83% for 10, 100, and  $1 \times 10^3$  uncharged nanoparticles for a 24-hour processing time, respectively. When the time span increased twofold, the total number of all collisions does not double but only raise 79.43%, 53.43, and 65.56% with respect to agent-based models that ran for 24-hours. At any number of uncharged nanoparticles and worlds, the majority of collisions are two-body. The average number of collisions shows that 97.67%, 95.99%, and 95.13% of all collisions in  $9 \times 10^4$ ,  $25 \times 10^4$ , and  $49 \times 10^4$  patch worlds are two-body collisions. In addition, agent-based models for SDS molecules show the same behavior with the nanoparticles in stepping up from 24 to 48-hours. For 10 SDS molecules, total number of ticks decreased by 3.67%, 20.96%, and 35.02% with respect to ticks calculated 24-hour agent-based models that ran in for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds. The same comparison yields 14.25%, 12.06%, and 19.16% reduction for 100 SDS molecules and 16.02%, 25.09%, and 6.15% for  $1 \times 10^3$  SDS molecules, conclusively. The minimum and maximum reductions in ticks for 24 and 48-hours observed between 1.30 to 1.22 ticks/s (-6.15%) for  $1 \times 10^3$  SDS molecules and 2.17 to 1.41 ticks/s (-35.02%) for 10 SDS molecules in (350 x 350) patch worlds, respectively. Just about, 2.12%, 3.22%, and 3.93% of collisions are three-body along with 0.23%, 0.80%, and 0.95% of collisions are four-body for 24-hours, consecutively. The minimum and maximum number of collisions for uncharged nanoparticles varies correspondingly from 135 to  $4.01 \times 10^6$  collisions for 10 nanoparticles in (350 x 350) patch worlds and  $1 \times 10^3$  nanoparticles in (150 x 150) patch worlds for 24-hours. The increment from 24 to 48-hours in agent-based model execution time yields merely small changes in uncharged nanoparticle collision distributions. The average variation between two time spans is less than 1%. The total number of collisions per unit time is an important indicator of agent-based models' performance and sustainability.

The performance of agent-based models highly dependent on the world dimensions and total number of objects as well as computer configurations. For an agent-based model covering 10 uncharged nanoparticles, the collision speed calculated as  $5.43 \times 10^{-3}$ ,  $2.83 \times 10^{-3}$ , and  $1.56 \times 10^{-3}$  collisions/s for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds for 24-hour processing time. The adjustment of the world dimension from  $90 \times 10^3$  to  $250 \times 10^3$  patches decreases the collision speed by 47.88% for uncharged nanoparticles. If the dimension of world extends to  $490 \times 10^3$  patches, collision speed drops by 71.27% compared to  $90 \times 10^3$  patch world, in 48-hour time span. It has been observed that every one of agent-based models behave in consistent with the 24-hour models so that collision speed decreases with the world area. The details of uncharged nanoparticle collisions including test results of agent-based models represented in Appendix 6.

In case of same-charged nanoparticles, overall collisions have tendency to decrease sharply due to electrostatic repelling forces. Although, theoretically total number of all collisions must be equal to zero, results of the particular models does not support this hypothesis. Generally, agent-based models consist of relatively small sized world with large number of nanoparticles that yield the redundant collisions due to minimal movable area in the world. For instance, in a (150 x 150) patch world with 100 and  $1 \times 10^3$  same-charged nanoparticles, the total number of occurred collisions is  $188.43 \times 10^3$  and  $90.97 \times 10^3$  for 24-hours, respectively. These values are considerably less than the collision of the uncharged nanoparticles by 24.25% and 69.78%. When the agent-based model run time multiplied by two, total number of collisions decreased by 34.38% and 62.41%, respectively. Increasing the world dimension for the agent-based models with same-charged nanoparticles decreases the collision probability, as in uncharged nanoparticles.

At any number of same-charged nanoparticles and worlds, the majority of collisions are two-body. The calculations showed that 99.85%, 0.14%, and 0.01% of entire collisions in all same-charged initial tests are two, three, and four-body collisions, respectively. The number of two-body collisions for 10 same-charged nanoparticles is zero in a (350 x 350) patch world, which is less than the uncharged nanoparticle collisions. In the same initial test setup, uncharged nanoparticles subjected to maximum number of  $0.14 \times 10^3$  two-body collisions for 24-hours and in the case doubling the process time, overall collisions increased by 21.43% to  $0.17 \times 10^3$ . The tenfold increment in the number of same-charged nanoparticles for the same time span, yielded  $0.02 \times 10^3$  two-body collisions and created

$11.39 \times 10^3$  more collisions for the uncharged nanoparticles. Finally, for the  $1 \times 10^3$  same-charged nanoparticles two-body collisions reached to  $1.78 \times 10^3$ , which is much less compared to uncharged nanoparticles collisions, again. The same behavior is also consistent with the initial tests processed for the different sized worlds. Approximately, all of the collisions in the same-charged initial tests observed are two-body. Apart from the initial tests of 10 same-charged nanoparticle agent-based models, only 100 and  $1 \times 10^3$  nanoparticle initial tests subjected to three-body and four-body collisions with an overall count of  $1.17 \times 10^3$  and  $40 \times 10^3$ , respectively. In other words, for every four-body collision in all same-charged nanoparticle initial tests,  $20.90 \times 10^3$  two-body and  $29.25 \times 10^3$  three-body collisions took place in the agent-based models, synchronously.

Increasing the processing time from 24 to 48-hours in initial tests showed insignificant variations in the uncharged nanoparticle collision distributions. The average variation between initial tests for two different time spans is less than 2%. For an initial test that consists of 10 uncharged nanoparticles, the two, three, and four-body collision speeds computed as zero for  $9 \times 10^4$ ,  $25 \times 10^4$ , and  $49 \times 10^4$  patch worlds for 24 and 48-hours. Correspondingly, the same collision values computed for 100 and  $1 \times 10^3$  nanoparticles. The increasing the number of  $90 \times 10^3$  patches by 277.78%, increases the collision speed of 100 same-charged nanoparticles to  $1.15 \times 10^{-6}$  collisions/s for both 24 and 48-hours. When the world extends to  $490 \times 10^3$  patches, the collision speed of 100 same-charged nanoparticles reaches to  $7.72 \times 10^{-7}$  and  $1.15 \times 10^{-6}$  collisions/s. For the  $1 \times 10^3$  same-charged nanoparticles, the number of collisions and their corresponding speeds increase with the nanoparticle population in all worlds. As in the (150 x 150) patch world the maximum collision speeds of same-charged nanoparticles calculated as 1.02 collisions/s for 24-hours and 2.15 collisions/s for 48-hours. The details of the same-charged nanoparticle collisions including both test results and average values represented in Appendix 7.

The initial tests for SDS molecules repeated for 10, 100, and  $1 \times 10^3$  agents for 24 and 48-hours, in accordance with the initial nanoparticle tests. In all tests, SDS molecules designed to be uniform and in agreement with the definitions mentioned in Section 4.1.2. The initial test with 10 SDS molecules, average number of ticks generated is  $777.28 \times 10^3$ ,  $305.18 \times 10^3$ , and  $149.33 \times 10^3$  for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds in 24-hours. When the processing time doubled, the total number of collisions increased by 204.50% and 57.78%, and 62.97% respectively. In the case of 100

SDS molecules, total number ticks observed as 778.13, 272.34, and 177.27 for 24-hours, respectively. For the 48-hour period, the total number of collisions increased by 65.10%, 75.61%, and 62.16% for the previously mentioned worlds. Finally,  $1 \times 10^3$  SDS molecules yielded the minimum number of ticks when compared to the previously completed tests. For instance,  $319.43 \times 10^3$ ,  $251.36 \times 10^3$ , and  $120.51 \times 10^3$  ticks generated for (150 x 150) patch, (250 x 250) patch, and (350 x 350) patch worlds for 24-hours. In addition, 48-hour load test results are also consistent with the other tests therefore all tests created significantly more ticks than the preceding time span with an average value of 128.28 ticks for each run. Any increment in the world dimension directly causes decrement in the collision probability of SDS molecules, as in same-charged and uncharged nanoparticles.

In distribution tests for SDS molecules, positions of hydrophobic and hydrophilic components with respect to quadrants in Cartesian coordinate system in agent-based models tracked and logged for the periods of 24 and 48-hours. In the tests, location data of every SDS molecule analyzed with respect to four quadrants, in real time. The distribution of hydrophobic and hydrophilic components of 10 SDS molecules in a (150 x 150) patch world showed that both components grouped in the fourth quadrant for 24-hour tests, predominantly. When the time span doubled, the accumulation of components shifted to the first quadrant where 36.36% of all SDS molecules resided. In a (250 x 250) patch world, the population of both components in the first quadrant drastically increased. The calculations presented a decrement 45.45% for hydrophobic and 41.67% for hydrophilic components for 24-hours. In the 48-hour tests, all first three quadrants have the same component distribution as 27.27%. Once the world dimension increased to (350 x 350) patches, the maximum number of hydrophobic and hydrophilic components happened to gather in the first and fourth quadrants with the same percentage as 30.00%. As soon as the initial test processing time doubled, hydrophobic components moved evenly to the last three quadrants and hydrophilic components showed 36.36% residence in the third quadrant.

In the case of 100 SDS molecules, the average distribution of hydrophobic and hydrophilic components in a (150 x 150) patch world indicated that 28.71% of both SDS components grouped in the fourth quadrant. When the testing time increased twofold, majority of all components shifted to the first quadrant with same percentage. In a (250 x

250) patch world, the ratio of hydrophobic and hydrophilic components increased by 29.70% in the third quadrant for 24-hours. For the 48-hour tests, both components shifted together to the first quadrant for creating the 28.80% of overall SDS molecule population. In the (350 x 350) patch world for the 24-hour tests, results showed that 27.72% of all hydrophobic and hydrophilic components happened to be in the fourth quadrant. As soon as the test processing time doubled, both SDS components moved to the third quadrant so that hydrophobic and hydrophilic components presented 32.35% and 32.67% residence, respectively.

For the  $1 \times 10^3$  SDS molecules in a (150 x 150) patch world, the maximum number of both components observed in the first quadrant with the same percentage as 37.56% for 24-hour tests. In addition, the 48-hour tests yielded those hydrophobic and hydrophilic components of SDS molecules grouped by 38.70% and 35.66% in the first quadrant, respectively. The tests ran in the (250 x 250) patch world that 27.40% of all hydrophobic and 26.97% of all hydrophilic components observed in the third quadrant for 24-hour tests. For the doubled test time, the maximum occurrence in quadrants reallocate to second and fourth quadrants with the hydrophobic (27.70%) and hydrophilic (28.67%) components, respectively. Finally, in the (350 x 350) patch world both components of SDS molecule predominantly occurred to be in the fourth quadrant for both tests.

All tests including two types of nanoparticles and SDS molecules in three different worlds took 1944 hours of CPU time (=81 days) to complete and generated  $52.86 \times 10^6$  lines of log files. Throughout all tests, total number of  $10.57 \times 10^6$  agent location data recorded.

### **5.1.2. Validation Tests for NetLogo Agent-Based Models**

The validation testing for agent-based models developed in NetLogo employed to determine the consistency and reliability of the models to the assumptions stated in Section 4.1. To begin with, agent-based model updates in the name of ticks, tested for their solvent density dependency. The model design proposes that any change in solvent density do not drastically affect overall updates to the model processing time and interfere with the randomness of the model. The same agent-based models ran twice for  $5 \times 10^3$ ,  $7.5 \times 10^3$ ,  $10 \times 10^3$ ,  $12.5 \times 10^3$ ,  $15 \times 10^3$ , and  $50 \times 10^3$  uncharged and same-charged nanoparticles as well as SDS molecules for 12 different solvents in a (250 x 250) patch world, separately. Each validation test took 72-hours to complete and overall  $36.29 \times 10^3$

hours of CPU time (=1512 days) needed to complete all validation tests. Throughout the tests, total number of  $1.45 \times 10^9$  variables recorded in  $55.70 \times 10^6$  lines of log files, in real time.

The average number of system updates based on ticks showed that chloroform and heptane generated the maximum and minimum number of ticks for  $5 \times 10^3$  uncharged nanoparticles. The difference between ticks calculated as  $40.47 \times 10^3$  for a period of 72-hours. When the uncharged nanoparticle population increased by 50%, the gap between maximum and minimum number of ticks decreased by 51.82% to  $19.50 \times 10^6$  ticks. Apart from the  $5 \times 10^3$  uncharged nanoparticles, the maximum and minimum number of ticks observed for propane as  $292.96 \times 10^3$  and xylene as  $273.46 \times 10^3$ , respectively. At the initial tests executed for  $12.5 \times 10^3$  uncharged nanoparticles the peak tick values detected for creosote as  $94.47 \times 10^3$  and  $197.52 \times 10^3$ . The average number of minimum updates calculated as  $53.09 \times 10^3$  for  $10 \times 10^3$ , uncharged nanoparticles, respectively. Toluene created the minimum tick value calculated as  $124.72 \times 10^3$  for  $12.5 \times 10^3$  uncharged nanoparticles. Increasing the uncharged nanoparticle population to  $15 \times 10^3$  resulted as xylene to have the minimum number of ticks as  $124.33 \times 10^3$ . In the last test,  $50 \times 10^3$  uncharged nanoparticles used to validate agent-based models. The calculations showed that the maximum and minimum number of ticks observed for water as  $105.29 \times 10^3$  and pentane as  $64.08 \times 10^3$ , respectively.

The variation of total number of ticks for  $5 \times 10^3$ ,  $12.5 \times 10^3$ , and  $50 \times 10^3$  uncharged nanoparticles analyzed in 12 different solvents placed in a (250 x 250) patch world for 72-hours. The results showed that number ticks in all validation tests with the exception of creosote are indirectly proportional to the total number of uncharged nanoparticles. In the validation tests for  $5 \times 10^3$  uncharged nanoparticles placed in creosote showed that the number of ticks observed are 13.50% more than  $12.5 \times 10^3$  uncharged nanoparticles.

Besides, relative tick updates among the validation tests with selected number of uncharged nanoparticles investigated and compared with each other. For this thesis, the changes between two pairs of nanoparticles are taken into consideration. In the first pair, the variation of ticks among  $5 \times 10^3$  and  $12.5 \times 10^3$  uncharged nanoparticles tested. The calculations showed a consistent decline in total number of ticks in all solvents except creosote. The average reduction computed as 26.02% for all solvents. Within all

validation tests, xylene showed the maximum reduction where total number of ticks dropped 41.55% from  $215.30 \times 10^3$  to  $125.85 \times 10^3$  ticks. In the second pair of tests, the same pattern also observed for the ticks among  $12.5 \times 10^3$  and  $50 \times 10^3$  uncharged nanoparticles. In this case, creosote also showed harmonious behavior with other solvents and the total number of ticks decreased entirely. The average reduction in ticks calculated as 40.57% for all solvents. The maximum decline in ticks performed by pentane as 67.16% with a decrement from  $195.11 \times 10^3$  to  $64.08 \times 10^3$ .

In case of same-charged nanoparticles, the number of system updates based on ticks showed that creosote and heptane generated the maximum and minimum average number of ticks for  $5 \times 10^3$  same-charged nanoparticles. The difference between ticks calculated as  $30.48 \times 10^3$  for a period of 72-hours. When the same-charged nanoparticle population increased by 50%, the gap between maximum and minimum number of ticks decreased by 1.94% to  $5.75 \times 10^6$  ticks. Apart from the  $5 \times 10^3$  same-charged nanoparticles, the maximum and minimum number of ticks observed for hexane as  $144.80 \times 10^3$  and pentane as  $118.13 \times 10^3$ , respectively. In the tests executed for and  $12.5 \times 10^3$  same-charged nanoparticles the peak tick values detected for xylene as  $94.39 \times 10^3$  and for creosote as  $83.81 \times 10^3$ . Expanding the same-charged nanoparticle population to  $15 \times 10^3$  resulted as water to have the minimum number of ticks as  $56.85 \times 10^3$ . In the concluding test,  $50 \times 10^3$  same-charged nanoparticles used to validate agent-based models. The calculations indicated that the maximum and minimum number of ticks observed for water as  $105.29 \times 10^3$  and pentane as  $54.58 \times 10^3$ , respectively.

The deviation of total number of ticks for  $5 \times 10^3$ ,  $12.5 \times 10^3$ , and  $50 \times 10^3$  same-charged nanoparticles analyzed in 12 different solvents placed in a (250 x 250) patch world for 72-hours. In all tests, the average number of total ticks decreased when the same-charged nanoparticle population increased to  $7.50 \times 10^3$ . The relative changes in the number of ticks vary from 17.01% to 41.33% with an average value of 24.31% for the same-charged nanoparticles. The most significant change detected in creosote which presented 41.33% decrement from  $142.86 \times 10^3$  to  $83.81 \times 10^3$  ticks. Besides, the results indicated that total number ticks for in five of 12 solvents used in  $12.5 \times 10^3$  same-charged nanoparticles generated less ticks than  $50 \times 10^3$  same-charged nanoparticles. These solvents found to be benzene, chloroform, creosote, toluene, and water. The mentioned solvents have the five of the six topmost density values in all solvents. Water has the maximum variation such

when the total number of system updates escalated from  $89.51 \times 10^3$  to  $105.29 \times 10^3$ . In other solvents, tick increments fluctuated from 1.84% to 17.98% for creosote and chloroform.

The variation in total number of ticks for  $5 \times 10^3$ ,  $12.5 \times 10^3$ , and  $50 \times 10^3$  SDS molecules investigated in 12 different solvents placed in a (250 x 250) patch world for 72-hours. In all agent-based models, the average number of total ticks decreased when the number of SDS molecules increased. For  $7.5 \times 10^3$  SDS molecules, the maximum and minimum number of ticks recorded as  $111.05 \times 10^3$  and  $47.30 \times 10^3$  for toluene and pentane, respectively. When the total number of SDS molecules increased by  $5 \times 10^3$  to  $12.5 \times 10^3$ , different solvents exposed the boundary conditions for ticks. In this case, creosote generated 41.65% and pentane generated 50.04% less ticks than the previous tests with  $7.5 \times 10^3$  SDS molecules. Finally, for the  $50 \times 10^3$  SDS molecules the maximum and minimum number of ticks decreases further and drops to  $5.42 \times 10^3$  and  $1.62 \times 10^3$  ticks for DI and hexane, respectively. The results showed that tick generation inversely proportional to the overall SDS molecules as in uncharged and same-charged nanoparticles.

In all agent-based modeling validation tests, the most significant tick variation detected in benzene for the alterations of SDS molecules. Benzene presented 66.47% decrement from  $93.28 \times 10^3$  to  $31.28 \times 10^3$  ticks with the addition of  $5 \times 10^3$  SDS molecules. When the population of SDS molecules quadrupled to  $50 \times 10^3$ , number of ticks decreased by 95.97% to  $1.62 \times 10^3$ . As a result, density of the solvents does not directly affect the agent-based model updates in the name of ticks. This property originates from the model design and the outcomes from this approach can be seen in the total number of ticks and collisions.

### **5.1.3. Load Tests for NetLogo Agent-Based Models**

The load testing for NetLogo agent-based models implemented to determine the models' performance and response under the peak loads for  $100 \times 10^3$  and  $200 \times 10^3$  charged and uncharged nanoparticles in 12 different solvents. The results of the load test models pinpoint the maximum operational capacity and threshold values of the variables for models, as well as bottlenecks and limitations depending on the total number of agents, interactions, and dimensions of the world. In load tests, every model executed twice for a period of 72-hours on dedicated computers, independently. It took 3456 hours of CPU



time (=144 days) to complete and created  $191.98 \times 10^6$  lines of log files. The world area for all models fixed to (250 x 250) patches and the entire screen updates restricted. The performance of the agent-based models traced and logged by HWInfo and Glances for Microsoft Windows 10 Enterprise version 1803 (64 bit) and Ubuntu 16.04.2 LTS (64 bit) operating systems, respectively [176, 300, 303, 304].

NetLogo agent-based models with  $100 \times 10^3$  uncharged nanoparticles updated themselves in the range of 37.73 ticks/min to 56.85 ticks/min for ammonia and pentane, respectively. When uncharged nanoparticle population doubled in the models, the average speed gap between minimum and maximum number of ticks increased by 211.02%. The twofold increment in the number of nanoparticles decreased their average speed by -10.19% from 191.98 ticks/min to 172.42 ticks/min. The most significant change in speed in all solvents calculated -36.24% for hexane. In this case, the slowest and the fastest nanoparticles observed in creosote and water with model speeds of 35.38 ticks/min and 110.78 ticks/min, respectively.

In the following group of load tests, same-charged nanoparticles used under the equivalent settings that applied to uncharged nanoparticles. The agent-based models with  $100 \times 10^3$  same-charged nanoparticles updated themselves with a speed in the range of 106.31 ticks/min to 226.07 ticks/min for propane and chloroform, respectively. When same-charged nanoparticle population doubled in agent-based models, the average speed gap between minimum and maximum values of ticks increased by 222.21%. The slowest and the fastest nanoparticles observed in pentane and chloroform as 91.46 ticks/min and 177.78 ticks/min, respectively. When the number of nanoparticles doubled, the average speed declined by -34.90% from 113.14 ticks/min to 73.65 ticks/min. The most noteworthy change in speed for all solvents calculated for toluene by 37.84% decrement.

In the first and second tests for the  $100 \times 10^3$  uncharged nanoparticles it has been observed that pentane and propane have the maximum cumulative population at the interface as  $98.86 \times 10^6$  and  $98.88 \times 10^6$ , respectively. The average number of maximum uncharged nanoparticles at the interface found to be  $98.54 \times 10^6$  for propane. On the other hand, chloroform yielded the minimum uncharged nanoparticle population for both tests and the average nanoparticle count at the interface calculated as  $96.35 \times 10^6$ . The variation between maximum and minimum uncharged nanoparticles determined to be 2.27%. For

the equivalent number of same-charged nanoparticles, the cumulative maximum number of nanoparticles at the interface observed as  $99.69 \times 10^6$  for heptane and  $99.01 \times 10^6$  for hexane. The maximum average number of same nanoparticles at the interface calculated as  $99.38 \times 10^6$  for heptane. When it comes to the minimum nanoparticle counts, both propane and seawater exhibited the lowest values such as  $99.18 \times 10^6$ . The average minimum value of the same-charged nanoparticles presented to be  $98.27 \times 10^6$ . The difference between maximum and minimum same-charged nanoparticles determined to be 1.11% for 12 different solvents.

When the overall nanoparticle population increased twofold, the maximum number of uncharged nanoparticles accumulated at the interface of pentane and propane as  $198.79 \times 10^6$  and  $191.64 \times 10^6$  for both tests, respectively. The average maximum number of uncharged nanoparticles at the interface calculated as  $194.82 \times 10^6$  for propane. This behavior is consistent with the results of the  $100 \times 10^3$  uncharged nanoparticle tests, which indicated the same solvents for the maximum nanoparticles at the interface. Regarding the cumulative uncharged nanoparticle population, xylene and seawater have the minimum values as  $191.41 \times 10^3$  and  $191.64 \times 10^3$  for both tests. The variation between maximum and minimum number of nanoparticles at interface nanoparticles for all solvents calculated as 1.01% which is approximately half of the value calculated for  $100 \times 10^3$  uncharged nanoparticles.

For the equivalent number of same-charged nanoparticles, the maximum cumulative number of nanoparticles at the interface observed  $99.69 \times 10^6$  for heptane and  $99.01 \times 10^6$  for hexane. The number of maximum average number of same nanoparticles at the interface found to be  $99.38 \times 10^6$  for heptane. When it comes to the minimum nanoparticle counts, both propane and seawater exhibited the lowest values such as  $99.18 \times 10^6$ . The average minimum value of the same-charged nanoparticles presented to be  $98.27 \times 10^6$ . The distinction between the maximum and minimum same-charged nanoparticles at the interface determined to be 1.11% for 12 different solvents, used in all agent-based models.

The load tests of uncharged and same nanoparticles showed that same-charged nanoparticles have more tendency to accumulate on the interface in all solvents. Regarding all test results from 12 different solvents, calculations revealed that for every 100 same-charged nanoparticles, there is 99.16 uncharged nanoparticles at the interface

after 72-hours. The maximum number of cumulative nanoparticle count observed for  $200 \times 10^3$  same-charged nanoparticles in pentane. For pentane, 46 same-charged nanoparticles reached to the interface for every minute. In addition, the probability of a patch to be subjected to a same-charged nanoparticle at the interface is 9.20% per minute.

The load tests for  $100 \times 10^3$  uncharged and same-charged nanoparticles in 12 different types of solvents showed that two-body collisions are significantly more than three and four-body collisions. In the first and second load tests, 77.17% and 77.30% of all collisions occurred as two-body collisions, respectively. This percentage drops down to 16.13% and 16.03% for three-body collisions, and finally to 6.70% and 6.67% for four-body collisions. Even though, propane has the maximum two-body collision percentage (78.91%) among all solvents, the minimum number of two-body collisions observed as  $23.24 \times 10^3$  for the same solvent. The similar relationship also valid for chloroform where it has the minimum two-body collision percentage (74.92%) and the maximum number of two-body collisions as  $57.86 \times 10^3$ . From the previously mentioned findings, both agent-based models are consistent with each other and yielded approximately the same results<sup>29</sup>.

The distribution of collisions with respect to quadrants in the world revealed that the majority of the collisions occurred in the first and second quadrants for all solvents. In the first and second load tests, 89.77% ( $33.43 \times 10^6$  collisions) and 89.17% ( $33.65 \times 10^6$  collisions) of all two-body uncharged nanoparticle collisions detected in the first two quadrants. The same behavior of the load tests also valid for three-body collisions so that 59.60% ( $7.78 \times 10^6$ ) and 60.17% ( $7.81 \times 10^6$  collisions) of collisions occurred in the first and second quadrants, respectively. The same pattern continues for the four-body collisions by settling most of the collisions to first and second quadrants without leaving any collisions left to other quadrants. The calculations showed that in the first load test 100.00% ( $3.25 \times 10^6$ ) and in the second load test, 100.00% ( $3.26 \times 10^6$ ) of four-body collisions took place in the mentioned quadrants.

The average collision frequencies depending on quadrants show that uncharged nanoparticles subject to 9.27 two-body collisions/s, 1.96 three-body collisions/s, and 0.81 four-body collisions/s for all load tests. On the solvent basis, chloroform has the highest

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<sup>29</sup> The difference in the number of collisions for two-body collisions is 0.17%, three-body collisions is 0.62%, and four-body collisions is 0.45% in all agent-based models.

collision frequency in all quadrants reaching to its peak value as 109.24 two-body collisions. All load tests for  $100 \times 10^3$  uncharged nanoparticles took 840 hours of CPU time to complete and created overall  $1.16 \times 10^9$  collisions, which indicates 383.60 collision/s.

When the number of uncharged nanoparticles doubled to  $200 \times 10^3$ , the two-body collisions also increases and its ratio in overall collisions turn out to be considerably greater than three and four-body collisions. In the first and second load tests, 78.14% and 72.12% of all collisions occurred as two-body collisions. This percentage drops down to 15.51% and 17.57% for three-body collisions, and finally to 6.35% and 10.31% for four-body collisions. The average number of two, three, and four-body collisions for uncharged nanoparticles  $1.28 \times 10^9$ ,  $275.55 \times 10^6$ , and  $9 \times 10^6$ , respectively. The distribution of collisions with respect to quadrants in the world revealed that the majority of the collisions occurred in the first and second quadrants for all solvents. In the first and second load tests, 89.77% ( $33.43 \times 10^6$  collisions) and 89.17% ( $33.65 \times 10^6$  collisions) of all two-body uncharged nanoparticle collisions detected in the first two quadrants. The same behavior of the load tests also valid for three-body collisions so that  $7.78 \times 10^6$  (59.60%) and  $7.81 \times 10^6$  collisions (60.17%) of collisions occurred in the first and second quadrants, respectively. This outline continues for the four-body collisions by settling most of the collisions to first and second quadrants without leaving neglectible number of collisions left to other quadrants. The calculations showed that in the first load test 99.99% ( $132.64 \times 10^6$ ) and in the second load test, 100.00% ( $133.59 \times 10^3$ ) of all four-body collisions took place in the previously mentioned quadrants.

The average collision frequency calculations show that  $200 \times 10^3$  uncharged nanoparticles subjected to  $98.93 \times 10^9$  two-body collisions/s,  $2.13 \times 10^3$  three-body collisions/s, and  $1.03 \times 10^3$  four-body collisions/s for all load tests. Depending on the solvents, chloroform has the highest collision frequency in all quadrants with reaching to its peak value as  $92.47 \times 10^6$  for two-body collisions. All load tests for  $200 \times 10^3$  uncharged nanoparticles took 840 hours of CPU time to complete and created overall  $3.38 \times 10^9$  collisions, which indicates  $13.04 \times 10^3$  collision/s. When compared to the load tests with  $100 \times 10^3$  uncharged nanoparticles, the collisions increased by 291.28%. The details of the uncharged nanoparticle collisions including test results and analysis represented in Appendix 9.

The overall comparison of update frequency measures for same-charged nanoparticles in 12 different solvents showed that the density dependency of the load tests is insignificant. Furthermore, update frequency is indirectly proportional to the uncharged and same-charged nanoparticle population. Nanoparticles (in more general manner, agents) play crucial a role for the model performance and stability. When the nanoparticle population increased, computer resources used more aggressively therefore model updates become less frequent. The real-time system utilization logged by HWInfo and Glances showed that doubling number of uncharged nanoparticles raised the CPU and memory usages as well as average HDD access by 15.23%, 23.59%, and 6.87%, respectively<sup>30</sup> [303, 304]. For the same-charged nanoparticles, system information data yielded that twofold increment in the nanoparticle population also sharply elevated the CPU and memory consumption and average HDD access so that CPU and memory consumption rates frequently topped to 100.00%. Due to the overload of the system, load tests frequently became unresponsive and the stability of the operating systems turned out to be questionable.

In addition, previously mentioned nanoparticle tests replicated for the  $100 \times 10^3$  SDS molecules. The results presented that two-body collisions in 12 different solvents are considerably more than three and four-body collisions. In the first and second load tests, 46.23% and 46.38% of all collisions occurred as two-body collisions, respectively. This percentage drops down to 30.60% for three-body collisions for both tests and finally to 30.55% and 31.49% for four-body collisions. On the average, more than half of the two-body SDS molecule collisions (50.95%) observed for toluene. When it comes to the average number of three and four-body collisions, creosote and hexane have the maximum values as 31.21% and 27.78%. The minimum number two-body collisions observed for seawater and three and four-body collisions observed for propane. The percentages calculated as 43.99%, 29.40%, and 19.65%, respectively. The difference between maximum and minimum number of two-body collisions calculated as  $6.40 \times 10^6$ . The distinction found to be  $3.82 \times 10^6$  and  $2.72 \times 10^6$  for the three and four-body collisions, respectively where 66.67% and 58.33% of all solvents exposed to less collisions. The distribution of SDS collisions with respect to quadrants revealed that all collisions

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<sup>30</sup> The changes calculated with respect to the idle condition of the computer.

distributed almost evenly in all solvents as it can be seen in Figure 5.1 so that it can be concluded that distribution of the collisions reached to steady state.

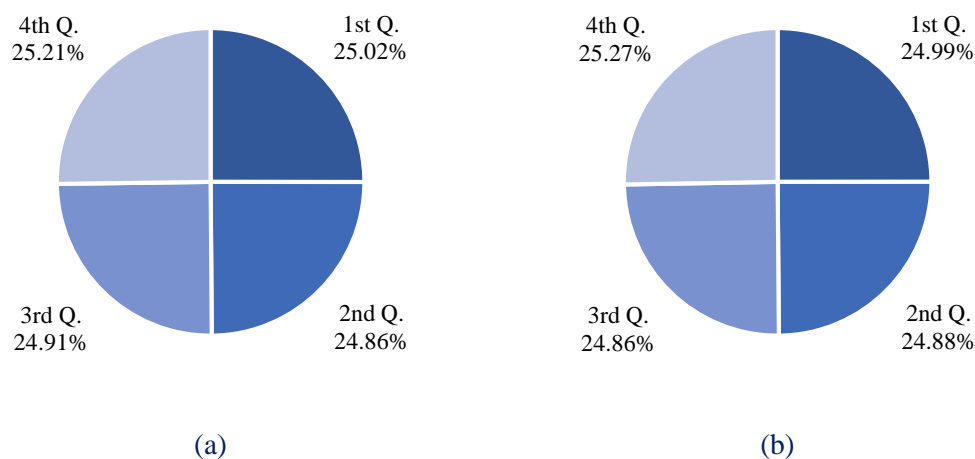


Figure 5.1 The distribution of two, three, and four-body average collisions for SDS molecules with respect to quadrants

The frequency of average collisions depending on quadrants show that SDS molecules subjected to 255.56 two-body collisions/s, 167.32 three-body collisions/s, and 124.42 four-body collisions/s in all agent-based model load tests. The comparison of frequency values of nanoparticles and SDS molecules indicate a considerable difference. This phenomenon originates from the design of nanoparticles and SDS molecules. On the solvent basis, toluene and xylene have the highest collision frequencies in all quadrants with reaching to its peak values as  $18.24 \times 10^6$  and  $18.86 \times 10^6$  collisions/s for the first and second tests, respectively. The minimum collision frequencies calculated for chloroform as  $6.53 \times 10^6$  for benzene and  $5.09 \times 10^6$  for hexane. It has been determined that there is 279.99% difference between maximum and minimum average frequency values, for all agent-based model tests.

#### 5.1.4. Accumulation of Nanoparticles and SDS Molecules at Liquid/Gas Interface in NetLogo Agent-Based Models

The number of nanoparticles at the interface has a great importance on the behavior of the surface tension as discussed in Chapter 1. The studies from the literature include both increment and decrement of surface tension due to particular environmental conditions.

By the reason of this indication, in all agent-based models, the cumulative number of uncharged and same-charged nanoparticles as well as SDS molecules at the interfaces of 12 different solvents logged in real-time for 72-hours. The agent-based models with same configuration operated twice for  $5 \times 10^3$ ,  $7.5 \times 10^3$ ,  $10 \times 10^3$ ,  $12.5 \times 10^3$ ,  $15 \times 10^3$ , and  $50 \times 10^3$  agents. All models ran in a (250 x 250) patch world in order to normalize the effects of the confined area for each agent. It has been observed that the cumulative number of nanoparticles at the interface either same-charged or uncharged related to the overall nanoparticle population. Additionally, same condition observed for the agent-based models with SDS molecules. For instance, the cumulative number of hydrophobic components of SDS molecules at the interface of ammonia increased by 21.27% when the total number of SDS molecules in the agent-based model doubled. Subsequently, the total SDS molecule count increased to  $10 \times 10^3$  and as a result collective hydrophobic component population at the interface escalated by 32.66%. For the agent-based models with  $12.5 \times 10^3$  and  $50 \times 10^3$  SDS molecules, overall accumulation at the interface increased by 66.12% and 560.43%, respectively as in Figure 5.2.

In addition, the cumulative number of nanoparticles at the interface depends on the electrostatical charges. The uncharged nanoparticles found to have more presence at the interface than the same-charged nanoparticles for all agent-based models. For instance, the cumulative number of  $5 \times 10^3$  uncharged nanoparticles at the interface of ammonia is 41.73% more than the same-charged nanoparticles. The same behavior also observed for different number of nanoparticles resided in ammonia that facilitates 25.36%, 6.03%, 0.49%, and 5.01% difference between the same-charged and uncharged nanoparticles, respectively.

The discrepancy of uncharged and same-charged nanoparticles accumulated at the interface of 12 solvents is indirectly proportional to the total number of nanoparticles in the agent-based models. When the overall nanoparticle population increased from  $5 \times 10^3$  to  $50 \times 10^3$ , the average difference between uncharged and same-charged nanoparticle population at the interface decreased from 42.20% to 17.22%. The cumulative number of same-charged, uncharged nanoparticles and SDS molecules at the interface of 12 different solvents in a (250 x 250) patch world presented in the following tables.

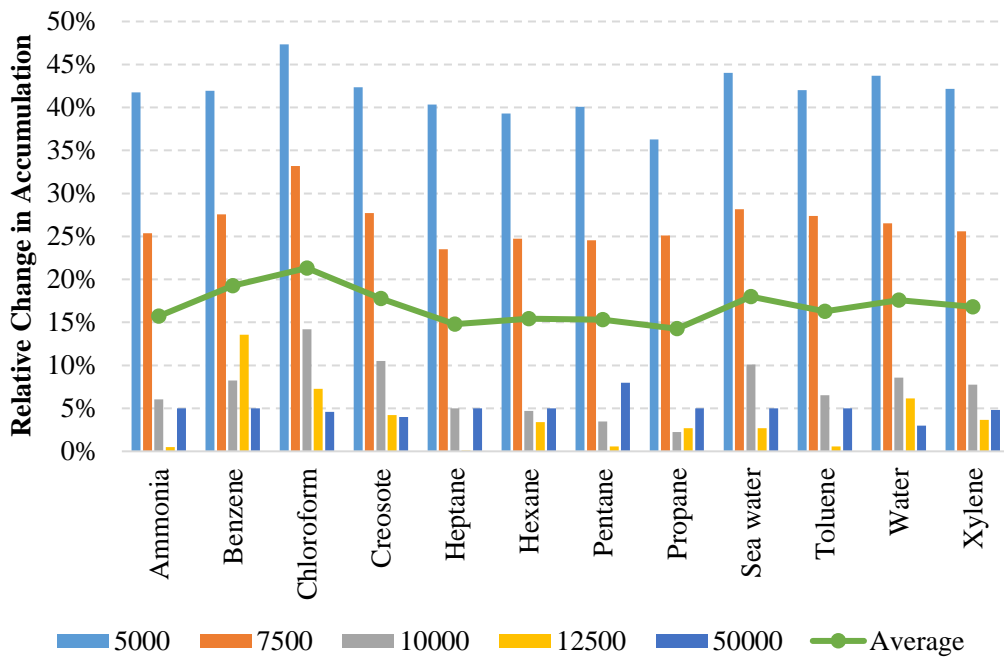


Figure 5.2 The relative change in the cumulative number of uncharged and same-charged nanoparticles at the interface of 12 different solvents

## 5.2. Results of Surface Tension Experiments at HUATARC

The pendant drop surface tension measurement experiments conducted at HUATARC with Attension optical tensiometer from Biolin Scientific, Frölunda, Sweden [8, 320]. Ahead of the experiments, Attension optical tensiometer calibrated for pendant drop method with DI, which is prepared at Hacettepe University Environmental Engineering Department Research Laboratory. The details of DI preparation method represented in Section 8.1.1.2. Throughout the calibration process, total number of 65 measurements recorded within 2.49 s and the average value of surface tension calculated as 72.20 dynes/cm for DI.



Table 5.1 The cumulative number of uncharged nanoparticles at the interface of 12 different solvents in a (250 x 250) patch world ( $10^6$ )

Solvent	# Uncharged Nanoparticles				
	$5 \times 10^3$	$7.5 \times 10^3$	$10 \times 10^3$	$12.5 \times 10^3$	$50 \times 10^3$
Ammonia	7.38	8.95	9.79	12.26	48.74
Benzene	7.39	8.96	9.83	13.87	48.85
Chloroform	7.33	8.89	9.78	12.25	48.09
Creosote	7.32	8.88	9.80	12.28	48.41
Heptane	7.41	8.98	9.79	12.27	48.98
Hexane	7.43	9.01	9.81	12.29	48.94
Pentane	7.36	8.92	9.82	12.35	48.92
Propane	7.39	8.96	9.85	12.34	49.01
Sea water	7.38	8.95	9.79	12.25	48.47
Toluene	7.38	8.95	9.79	12.26	48.85
Water	7.37	8.94	9.79	12.37	48.69
Xylene	7.35	8.91	9.78	12.26	48.60
<b>Average</b>	<b>7.37</b>	<b>8.94</b>	<b>9.80</b>	<b>12.42</b>	<b>48.71</b>

Table 5.2 The cumulative number of same-charged nanoparticles at the interface of 12 different solvents in a (250 x 250) patch world ( $10^6$ )

Solvent	# Same-charged Nanoparticles				
	$5 \times 10^3$	$7.5 \times 10^3$	$10 \times 10^3$	$12.5 \times 10^3$	$50 \times 10^3$
Ammonia	4.30	6.68	9.20	12.20	46.30
Benzene	4.29	6.49	9.02	11.99	46.41
Chloroform	3.86	5.94	8.39	11.36	45.88
Creosote	4.22	6.42	8.77	11.76	46.47
Heptane	4.42	6.87	9.30	12.26	46.53
Hexane	4.51	6.78	9.35	11.87	46.49
Pentane	4.41	6.73	9.48	12.28	45.01
Propane	4.71	6.71	9.63	12.01	46.56
Sea water	4.13	6.43	8.80	11.92	46.05
Toluene	4.28	6.50	9.15	12.19	46.41
Water	4.15	6.57	8.95	11.61	47.23
Xylene	4.25	6.63	9.02	11.81	46.26
<b>Average</b>	<b>4.29</b>	<b>6.56</b>	<b>9.09</b>	<b>11.94</b>	<b>46.30</b>

Table 5.3 The cumulative number of hydrophobic components of SDS molecules at the interface of 12 different solvents in a (250 x 250) patch world ( $10^6$ )

Solvent	# Hydrophobic Components of SDS Molecules				
	$5 \times 10^3$	$7.5 \times 10^3$	$10 \times 10^3$	$12.5 \times 10^3$	$50 \times 10^3$
Ammonia	24.73	180.61	221.99	325.74	529.18
Benzene	20.40	245.14	280.33	496.74	740.52
Chloroform	30.98	184.38	224.49	275.96	460.44
Creosote	45.58	185.80	233.56	438.19	452.02
Heptane	30.85	232.66	255.49	323.15	508.49
Hexane	34.68	230.41	218.27	318.77	565.50
Pentane	36.45	233.48	294.75	325.00	612.94
Propane	43.81	501.25	501.96	837.74	984.24
Sea water	35.53	216.87	195.76	299.01	577.09
Toluene	34.85	232.34	242.12	360.61	612.92
Water	38.89	190.34	202.59	383.39	435.90
Xylene	41.10	207.98	232.74	312.54	401.69
<b>Average</b>	<b>34.82</b>	<b>236.77</b>	<b>258.67</b>	<b>391.40</b>	<b>573.41</b>

In this thesis, two main categories of experiments implemented at HUATARC [320]. Each experiment repeated for three times, individually. The experiments are as follows,

1. **Surface tension measurement experiments without graphene and MWCNTs:** DI, DI with different concentrations of SDS at, above and, below CMC, and hexane,
2. **Surface tension measurement experiments with graphene and MWCNTs:** DI, DI with different concentrations of SDS at, above, and below CMC, hexane with 2 mg graphene, and 2 mg MWCNTs<sup>31</sup>.

The image of DI pendant drop created by Attension optical tensiometer and the variation of surface tension with respect to time and volume during the calibration process represented in Figure 5.3 and Figure 5.4 [8].

<sup>31</sup> Graphene and MWCNTs obtained from Prof.Dr. Semra İDE, H.U. Physics Engineering Department SWAXS (SAXS/WAXS) Lab.

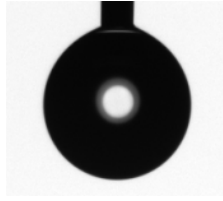


Figure 5.3 The pendant drop of DI by Attension optical tensiometer [8]

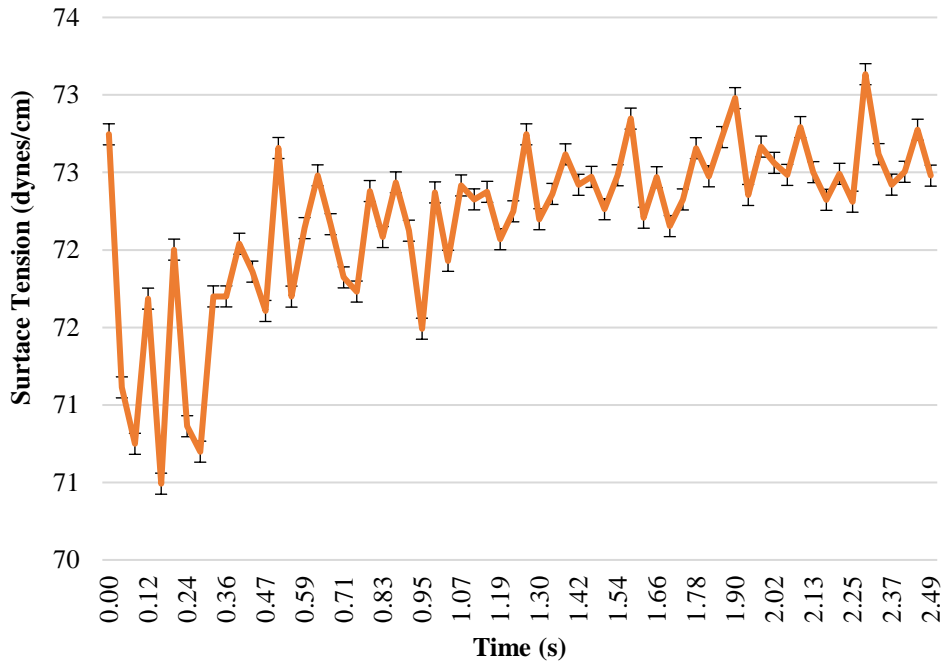


Figure 5.4 Variation DI surface tension values with respect to time in pendant drop surface tension calibration with Attension optical tensiometer at HUATARC [8, 320]<sup>32</sup>

<sup>32</sup> Throughout the thesis, standard error bars added to all plots. Standard error (*SE*) values for the respective data sets calculated by the following formula,

$$SE = \frac{S}{\sqrt{n}} = \sqrt{\frac{\sum_{s=1}^m \sum_{j=1}^n y_{is}^2}{n_y \cdot (n_y - 1)}}$$

where *S* and *n* are standard deviation and total number of measurements, respectively. In the second mathematical expression, *s* is series number, *i* is point number in series, *m* is specified number of series for point *y* in chart, *n* is number of points in each series, *y<sub>is</sub>* value of series *s*, point *i*, and *n<sub>y</sub>* is the data value of series *s* and point *i*.

The matching of time in the surface tension experiments to agent-based models is one of the critical points of this thesis. In the light of this determination, time dependency of surface tension for all solvents and their responses to graphene and MWCNTs derived from experimental data gathered from HUATARC [320].

In the following subsections, average time gaps among surface tension measurements and overall durations for surface tension experiments with Attension optical tensiometer analyzed [8]. The univariate quadratic polynomials derived to determine the time dependency of surface tension values from the statistically analyzed experimental data.

The computations showed that the average surface tension experiment duration decreased with the addition of various constituents to DI. MWCNTs and graphene exhibited impacts on the average time gaps between measurements and overall duration of DI surface tension experiments. As it can be seen from Table 5.4, addition of 2 mg MWCNTs and 2 mg graphene reduced the experiment duration by 6.91%. Both of the constituents initiated 0.03% and 0.02% decrements in the average time gaps between measurements, respectively. Furthermore, addition of SDS results an 80.11% decrement in time gaps with respect to DI experiments. The adding up of graphene and MWCNTs to DI + SDS solutions demonstrates the similar effects on time gaps. In both cases, average time gaps between measurements calculated as 13.17 ms, which is 52.69 ms less than the measurements of DI experiments. It can be concluded that one of the main factors on time gap decrements and surface tension values originates from the introduction of SDS to DI. In addition, SDS has a significant dominance on influencing the entire time dependent factors other than graphene and MWCNTs, in all experiments.

Table 5.4 The average time gaps among surface tension measurements and overall durations for pendant drop surface tension experiments with Attension optical tensiometer at HUATARC [8, 320]

<b>Experiments</b>	<b>Avg. Time Gaps Between Measurements (ms)</b>	<b>Avg. Experiment Duration (s)</b>
DI	65.86	10.01
Hexane	70.00	4.48
DI + graphene	65.84	9.94
DI + MWCNT	65.85	9.94
DI + SDS + graphene	13.17	1.99
DI + SDS + MWCNT	13.17	1.99

The time dependency of surface tension values for DI, hexane, and their solutions with 2 mg graphene and 2 mg MWCNTs presented as functions in Table 5.5. The univariate quadratic functions of surface tension exhibit the same behavior and they are consistent with each other. All functions have the same pattern in form of  $\sigma(t) = a \cdot t^n$  where  $\forall \{(a > 0) \wedge (n > 0) \wedge [(a \wedge n) \in \mathbb{R}]\}$ .

Table 5.5 The time dependency of surface tension values for DI, hexane, and their solutions with 2 mg graphene and 2 mg MWCNTs measured with Attension optical tensiometer at HUATARC [8, 320]

<b>Solution</b>	<b>Function</b>
DI	$\sigma(t) = 70.14 t^{1.6 \times 10^{-3}}$
Hexane	$\sigma(t) = 28.02 t^{1.4 \times 10^{-3}}$
DI + graphene	$\sigma(t) = 70.53 t^{-3.0 \times 10^{-6}}$
DI + MWCNTs	$\sigma(t) = 69.79 t^{8.0 \times 10^{-4}}$
Hexane + graphene	$\sigma(t) = 27.71 t^{5.8 \times 10^{-3}}$
Hexane + MWCNTs	$\sigma(t) = 27.85 t^{2.7 \times 10^{-3}}$

The time dependency of DI + SDS, DI + SDS + graphene, and DI + SDS + MWCNT solutions exhibit mostly identical behaviors depending on the SDS concentrations for the surface tension. At CMC, all surface tension values drop to their minimum values as expected. The difference between the measured and literature values of surface tension

reduced by 1.96% to 70.77 dynes/cm. On the other hand, surface tension measurement results for hexane generated more divergence from the values mentioned in the literature. The average surface tension value of hexane with measured Attension optical tensiometer determined as 28.86 dynes/cm, which is approximately 10 dynes/cm more than the value stated by the same resource.

The average values of the last 15 surface tension measurements with Attension optical tensiometer for DI and hexane with graphene, MWCNTs<sup>33</sup> at various SDS concentrations presented from Table 5.6 through Table 5.8 [8]. The average surface tension value of DI from three experiments measured by the Attension optical tensiometer found to be 70.59 dynes/cm, which is 1.96% less than the value mentioned in literature [8, 321]. The last 15 measurements, average surface tension value of DI calculated as 0.18% more. The difference between the measured and literature values of surface tension reduced by 1.96% to 70.77 dynes/cm. On the other hand, surface tension measurement results for hexane generated more divergence from the values mentioned in the literature. The average surface tension value of hexane with measured Attension optical tensiometer determined as 28.86 dynes/cm, which is approximately 10 dynes/cm more than the value stated by the same source, in accordance with the previous paragraph [8, 321]. For every DI + SDS and DI + SDS + graphene experiment, the minimum value of surface tension determined at the values less than CMC. Apart from both experiments, DI + SDS + MWCNT measurements revealed that the minimum value of surface tension determined at SDS concentration of 21.44 mM. The calculations showed that the difference between two values is 0.24 dynes/cm, which corresponds to 1.56% divergence from the CMC.

The most significant purpose of evaluating the mentioned number of measurements is to compute the steady state values of surface tension. In this state, the effects of all solvents and constituents to the surface tension are minimalized as well as concentration and time dependency of surface tension can be neglected. The inspection of calculated values shows that there are no outliers in the surface tension values and they are consistent with each other.

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<sup>33</sup> In all experiments, 2 mg of graphene and 2 mg of MWCNTs used, separately.

Table 5.6 The time dependency of surface tension values for DI + SDS solutions with varying SDS concentrations measured with Attension optical tensiometer at HUATARC [8, 320]

SDS Concentration (mM)	Function
0.82	$\sigma(t) = -2 \times 10^6 t^2 - 4.8 \times 10^{-3} t - 41.307$
3.00	$\sigma(t) = -3 \times 10^{-7} t^2 - 3.1 \times 10^{-4} t + 21.693$
6.00	$\sigma(t) = -6 \times 10^{-7} t^2 - 1 \times 10^{-3} t + 24.024$
8.20	$\sigma(t) = 1 \times 10^5 t^2 - 3.5 \times 10^{-3} t + 21.878$
44.30	$\sigma(t) = -4 \times 10^{-6} t^2 - 1.1 \times 10^{-3} t + 26.673$
59.00	$\sigma(t) = -4 \times 10^{-6} t^2 - 4.3 \times 10^{-3} t + 26.399$
82.00	$\sigma(t) = -8 \times 10^{-6} t^2 - 2.4 \times 10^{-3} t + 22.915$

Table 5.7 The time dependency of surface tension values for DI + SDS + 2 mg MWCNT solutions with varying SDS concentrations measured with Attension optical tensiometer at HUATARC [8, 320]

SDS Concentration (mM)	Function
0.82	$\sigma(t) = -3 \times 10^{-7} t^2 - 3 \times 10^{-4} t - 21.917$
3.00	$\sigma(t) = -3 \times 10^{-7} t^2 - 3 \times 10^{-4} t - 21.917$
6.00	$\sigma(t) = -1 \times 10^{-6} t^2 - 9 \times 10^{-4} t + 24.721$
8.20	$\sigma(t) = 3 \times 10^{-6} t^2 - 1.5 \times 10^{-3} t + 21.844$
44.30	$\sigma(t) = -2 \times 10^{-7} t^2 - 1.2 \times 10^{-3} t + 26.768$
59.00	$\sigma(t) = 4 \times 10^{-6} t^2 - 9 \times 10^{-4} t + 23.799$
82.00	$\sigma(t) = -7 \times 10^{-6} t^2 - 1.0 \times 10^{-3} t + 25.903$

Table 5.8 The time dependency of surface tension values for DI + SDS + 2 mg graphene solutions with varying SDS concentrations measured with Attension optical tensiometer at HUATARC [8, 320]

SDS Concentration (mM)	Function
0.82	$\sigma(t) = 4 \times 10^{-5} t^2 - 3.3 \times 10^{-3} t - 50.111$
3.00	$\sigma(t) = 2 \times 10^{-7} t^2 - 4 \times 10^{-4} t + 21.888$
6.00	$\sigma(t) = 5 \times 10^{-6} t^2 - 4.4 \times 10^{-3} t + 25.236$
8.20	$\sigma(t) = 5 \times 10^{-6} t^2 - 3.2 \times 10^{-3} t + 21.833$
44.30	$\sigma(t) = 7 \times 10^{-6} t^2 - 2.2 \times 10^{-3} t + 27.402$
59.00	$\sigma(t) = 1 \times 10^{-5} t^2 - 8 \times 10^{-6} t + 24.597$
82.00	$\sigma(t) = -8 \times 10^{-6} t^2 - 1.4 \times 10^{-3} t + 25.942$

Within the scope of last 15 measurements, the average surface tension value calculated as 27.98 dynes/cm which is again more than the values in the literature [322]. For every DI + SDS and DI + SDS + graphene experiment, minimum values of surface tension determined at the values less than CMC. Apart from both experiments, DI + SDS + MWCNT measurements revealed that the minimum value of surface tension determined at SDS concentration of 21.44 mM. The difference between two values calculated to be 0.24 dynes/cm, which corresponds to 1.56% divergence from CMC value.

The following plots from Figure 5.5 through Figure 5.7 are drawn with the average values of pendant drop surface tension experiments and exhibit the dependence of surface tension to the SDS concentration, as mentioned before. In this thesis, all surface tension measurements accomplished in the SDS concentration range of  $0.1 \times \text{CMC}$  to  $10 \times \text{CMC}$ . The average time intervals among all measurements is  $\sim 10$  ms in accordance with Berry et al. [323]. For all experiments, surface tension sharply decreases with the upsurge of SDS concentration up to point *C*, as it can be seen in Figure 5.5. Between points *C* and *E*, there is an escalation in the surface tension. At point *D*, an unpredicted increment observed for the surface tension for all experiments, such as 10.25%, 12.64%, and 12.97% for DI + SDS, DI + SDS + MWCNT, and DI + SDS + graphene, respectively. At point *E*, where SDS reaches its CMC, surface tension decreases to its minimum. Beyond this point, surface tension fluctuates up to point *H*. Between points *E* and *F* surface tension increases for all solutions but in contradiction to surface tension of DI + SDS + graphene



so that all other surface tension values increases between points *F* and *G*. The increment of surface tension continues between points *E* and *G*, with the exception of DI + SDS + graphene. Briefly, surface tension of DI + SDS + graphene behaved distinctively with DI + SDS and DI + SDS + MWCNT among points *G* through *H*. The surface tension difference between points *E* and *H* is 5.07% for DI + SDS, 19.83% for DI + SDS + graphene, and 18.75% for DI + SDS + MWCNT. The surface tension values for DI and hexane with graphene, MWCNTs, and varying SDS concentrations measured with Attension optical tensiometer at HUATARC.

The sharp decrement at point *C* observed in the experiments also mentioned in a white paper published by Biolin Scientific, which is the manufacturer of the Attension optical tensiometer used for all pendant drop surface tension experiments at HUATARC [8, 324]. Both, Miles and Shedlovsky and aforementioned white paper came to conclusion that this phenomenon is the result of the impurities residing in the solution [325]. According to ISO 4311:1979 standard, the minima in the plot must be detected at CMC [326].

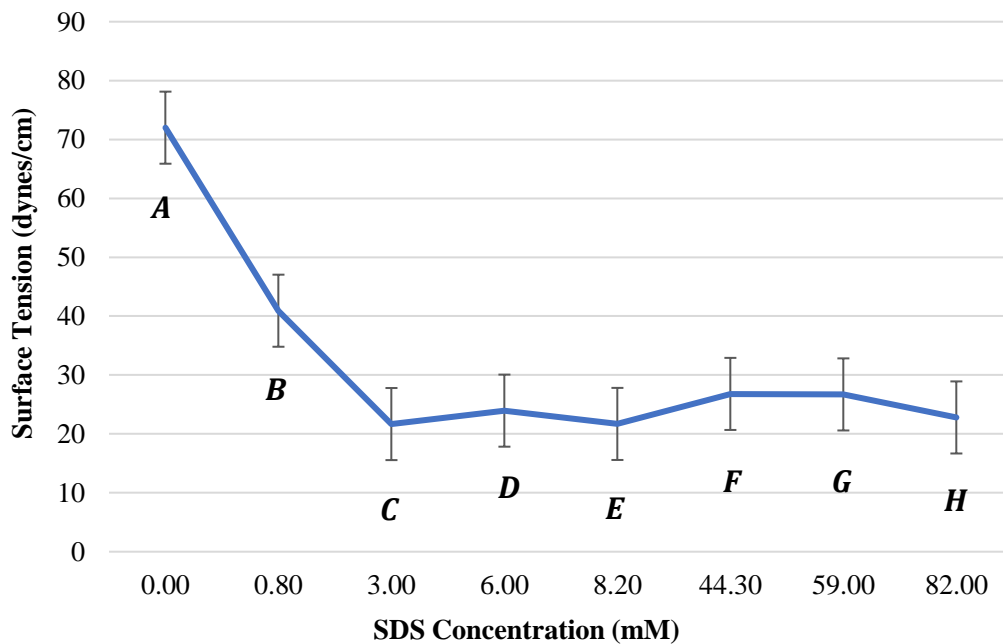


Figure 5.5 Average values of HUATARC pendant drop surface tension experiment results for DI + SDS in different SDS concentrations [320]

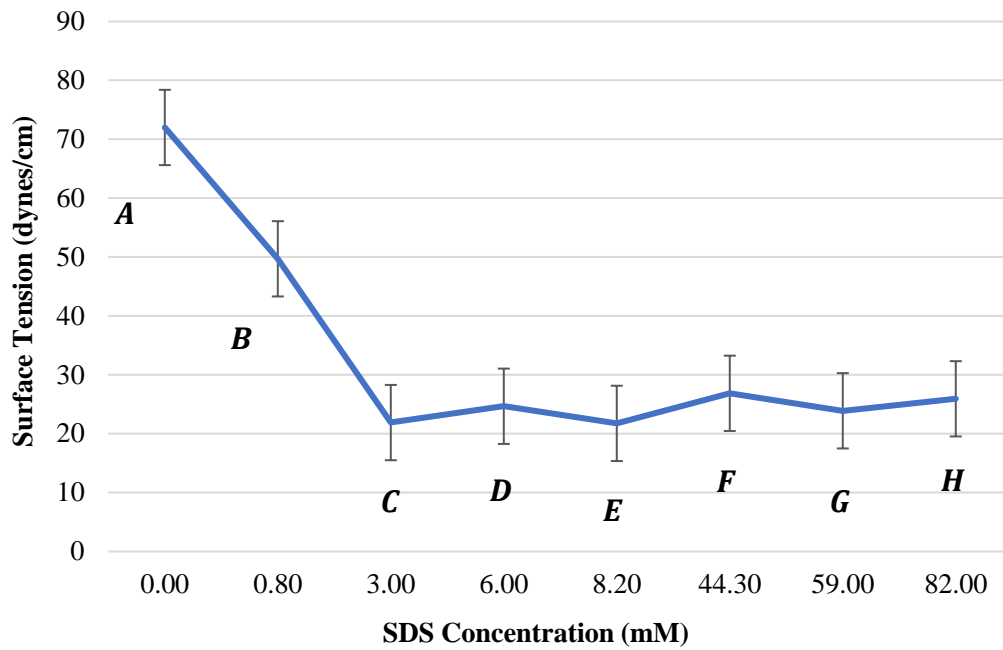


Figure 5.6 Average values of pendant drop surface tension experiment results for DI + SDS with 2 mg MWCNT in different SDS concentrations [320]

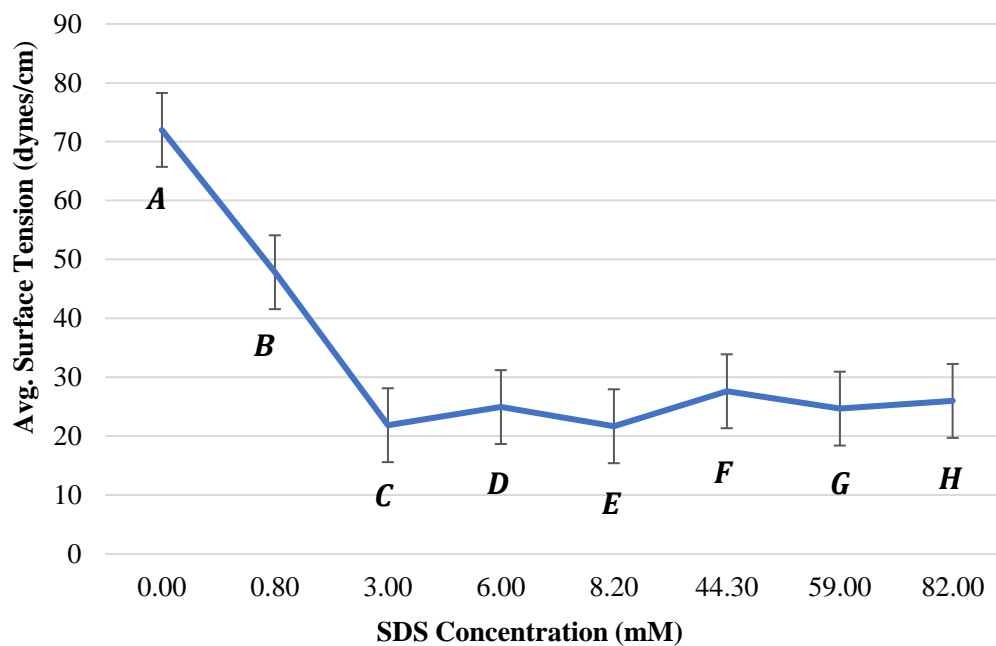


Figure 5.7 Average values of pendant drop surface tension experiment results for DI + SDS with 2 mg graphene in different SDS concentrations [320]

Other selected studies supporting this deduction as follows, Sutton and Harden investigated the effects of residual impurities on surface tension of nitroglycerine ( $C_3H_5N_3O_9$ ) with two different experimental techniques [327]. The results presented that bubble pressure and capillary techniques dependent on the amount of impurities in the system. The effect of residual impurities is noticeably higher with the capillary technique than with the bubble-pressure technique. Surface tension values varied 2.44% and 34.21% for bubble pressure and capillary techniques with different impurity levels, respectively. Ponce-Torres and Vega measured the influences of uncleanness on the surface tension for DI and DI + SDS (at CMC) with setups under different atmospheric conditions such as uncontrolled ambient air as well as controlled environments of saturated air and argon (Ar)<sup>34</sup> [321, 328]. Experimental results showed that ambient contamination created an evident reduction on the surface tension of DI and DI + SDS and in all other controlled environments surface tension experiments yielded results that are more accurate.

Berry et al. found that cetyl trimethylammonium bromide (CTAB) surface tension values measured with pendant drop technique at the concentration of 10 mM is considerably lower than the values given in literature which can be possibly caused by the residual impurities such as alcohol remaining from the surfactant synthesis [323]. El-Hefian and Yahaya investigated the influences of impurities on DI + SDS solutions with SDS concentrations in the range of 1 to 15 mM. In presence of the impurities, surface tension values of solutions reached their minimum values at 3.90 mM, which is 52.44% below CMC in the literature as shown in Figure 5.8 [329].

When experimental results of Attension optical tensiometer compared with the aforementioned study, it can be concluded that the behavior of surface tension with respect to various SDS concentrations approximately similar to the results of the experiments in this thesis Attension optical tensiometer at HUATARC [8, 320].

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<sup>34</sup> Density of air is  $1.18 \times 10^{-3}$  g/cm<sup>3</sup> (with 50% relative humidity, 0.04% CO<sub>2</sub> at 100 kPa and 20°C) and density of argon is  $1.63 \times 10^{-3}$  g/cm<sup>3</sup> (at 100 kPa and 20°C).

Table 5.9 The surface tension values for DI and hexane with graphene, MWCNTs and varying SDS concentrations measured with Attension optical tensiometer at HUATARC [8, 320]

Solution	SDS Concentration (mM)	Surface Tension (dynes/cm)					
		1 <sup>st</sup> Exp.	2 <sup>nd</sup> Exp.	3 <sup>rd</sup> Exp.	Min.	Max.	Avg.
DI	0.00	70.30	70.64	70.82	69.47	72.00	70.59
DI + graphene	0.00	70.81	70.17	70.60	69.08	71.90	70.53
DI + MWCNT	0.00	69.92	70.05	70.08	68.00	72.47	70.01
Hexane	0.00	28.39	27.82	28.19	27.61	28.46	28.13
Hexane + graphene	0.00	28.37	28.06	28.68	26.97	28.82	28.37
Hexane + MWCNT	0.00	27.91	28.30	28.03	27.76	28.46	28.08
DI + SDS	0.82	41.29	40.92	40.55	39.92	42.28	40.92
	3.00	21.78	21.40	21.84	21.38	21.87	21.67
	6.00	23.66	24.09	24.10	23.58	24.07	23.90
	8.20	21.66	21.68	21.75	21.52	22.40	21.69
	44.30	26.50	26.74	27.12	26.36	27.22	26.79
	59.00	27.06	26.86	26.18	25.78	27.30	26.70
	82.00	22.68	22.69	23.01	22.38	23.08	22.79
DI + SDS + graphene	0.82	48.27	47.76	47.48	45.27	50.96	47.84
	3.00	22.61	21.42	21.55	21.40	22.71	21.86
	6.00	25.85	24.88	24.08	23.95	26.44	24.94
	8.20	21.72	21.67	21.66	21.51	21.97	21.68
	44.30	27.67	28.24	26.96	26.75	28.50	27.62
	59.00	24.53	25.23	24.26	24.06	25.33	24.67
	82.00	25.85	25.96	26.15	25.78	26.23	25.98
DI + SDS + MWCNT	0.82	48.20	50.87	49.71	46.60	51.71	49.69
	3.00	21.46	22.43	21.78	21.43	22.52	21.89
	6.00	24.27	24.41	25.30	24.18	25.36	24.66
	8.20	21.78	21.70	21.77	21.63	22.86	21.75
	44.30	27.23	26.65	26.69	26.54	27.33	26.86
	59.00	24.41	23.77	23.49	23.45	25.76	23.89
	82.00	25.69	26.06	26.02	25.64	26.10	25.93

The difference between SDS concentrations observed for the minimum surface tension values in both studies computed as 0.4 mM. Lin et al. and Tofani et al. also described a minimum as a function of SDS concentration due to the influence of impurities as result of the unsealed ambient [330, 331]. In addition to the effects of impurities on the measurement of the surface tension, extra concerns occur on droplet fluctuation induced by peripheral vibrations and air streams during experiments. Both unwanted effects can be prevented with an anti-vibration tables and sealed experimental setups, respectively.

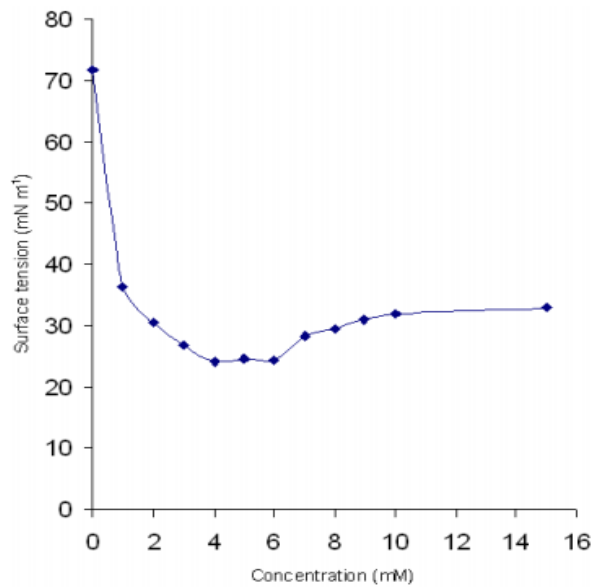


Figure 5.8 Influence of impurities on the surface tension of DI + SDS solution [329]

HUATARC pendant drop surface tension experiment results showed that DI + SDS, DI + SDS with 2 mg MWCNT, and DI + SDS with 2 mg graphene solutions reached their steady state standpoints after 0.72 s, 0.96 s, and 1.03 s, respectively [320]. These results can be interpreted as DI + SDS solutions accomplished their steady state in the first 36.00% of the experimentation time. From the calculations, it has been found that addition of graphene to DI + SDS solution increases the proportion more than the addition of MWCNTs. DI + SDS solutions with graphene reached their steady state at 51.76% of the experimentation time compared to 48.24% for MWCNTs.

It must be mentioned that Harikrishnan et al. studied the influences of five kinds of metal oxide nanoparticles<sup>35</sup> in addition to three kinds of surfactants<sup>36</sup> to the surface tension of DI, ethylene glycol (C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>), and glycerol (C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) with pendant drop technique [332]. The experiments divided into three types with each resembling the different combinations of base fluids, surfactants, and nanoparticles as in Table 5.10.

Table 5.10 Types of experiments in the study of Harikrishnan et al. [332]

Surface Tension Measurements	Type			
	A	B	C	D
Base fluid	+	+	+	+
Surfactant		+		+
Nanoparticle			+	+

In “Type B” experiments, the effects of surfactants on the surface tension inspected. All surfactants exhibited consistent behaviors on the solvents that can summarized with the function  $\sigma(C) = m + n \cdot C^{-2}$ . In this function,  $\sigma$  is surface tension,  $C$  is surfactant concentration in accordance with  $\forall \{(m > 0) \wedge (n > 0)\} \in \mathbb{R}$ . There is a constant decrement in the surface tension up to CMC and the minimum values for the surface tension observed at CMC for all surfactants. Beyond CMC, surface tension values remain constant up to the maximum concentration value ( $=2 \cdot \text{CMC}$ ) covered by the study. It has been examined the consequences of surfactants cannot be tied to their anionic and cationic nature such as DTAB found to be most effective surfactant followed by SDS and finally with CTAB. In “Type C” experiments, the effects of nanoparticles on the surface tension examined. All nanoparticles showed the consistent behavior on DI that can summarized with a monotonic sigmoid function<sup>37</sup> which is confined in the first quadrant. The behavior

<sup>35</sup> Nanoparticles of copper (II) oxide (CuO) in (30 and 80) nm, aluminum oxide (Al<sub>2</sub>O<sub>3</sub>) in 20 nm, bismuth(III) oxide (Bi<sub>2</sub>O<sub>3</sub>) in 20 nm, zinc oxide (ZnO) in 80 nm, and magnesium oxide (MgO) in ~100 nm diameter used.

<sup>36</sup> SDS selected as anionic surfactant, CTAB and lauryltrimethylammonium bromide (DTAB, CH<sub>3</sub>(CH<sub>2</sub>)<sub>11</sub>N(CH<sub>3</sub>)<sub>3</sub>Br) selected as cationic surfactants.

<sup>37</sup> In this thesis, sigmoid function used as a non-linear activation function for ANN models.

of the surface tension with respect to surfactant concentrations can be expressed with the Gudermann function as in Equation 5.1 and Equation 5.2 [333].

$$f(x) = gd(x) = \int_0^x \operatorname{sech}(t) dt = \int_0^x \frac{1}{\cosh(t)} dt \quad \text{Equation 5.1}$$

$$f(x) = \int_0^{\sinh(x)} \frac{1}{1+u^2} du = \arctan(\sinh(x)) \quad \text{Equation 5.2}$$

where,

$$u = \sinh(t) = \frac{e^t - e^{-t}}{2} \quad \text{Equation 5.3}$$

$$du = \cosh(t) dt \quad \text{Equation 5.4}$$

$$1 + u^2 = 1 + \sinh^2(t) = \cosh^2(t) \quad \text{Equation 5.5}$$

The accumulation of nanoparticles in DI increased the value of surface tension. Among all nanoparticles, bismuth(III) oxide ( $\text{Bi}_2\text{O}_3$ ) expressed the maximum enhancement of surface tension followed by zinc oxide ( $\text{ZnO}$ ), zinc oxide ( $\text{CuO}$ ), and  $\text{Al}_2\text{O}_3$  nanoparticles. The surface tension of DI increased by 0.3% to 0.5% more with  $\text{CuO}$  nanoparticles 80 nm in diameter than the same kind of identical nanoparticles 30 nm in diameter. The accumulation of  $\text{Bi}_2\text{O}_3$  and  $\text{CuO}$  nanoparticles in glycerol created a hysteresis on the surface tension values.  $\text{CuO}$  concentrations up to 0.4% (by weight) cause decrement on the surface tension and beyond that point, surface tension increases up to its maximum value as  $\sim 65.80$  dynes/cm at 2.5% (by weight). In a similar manner,  $\text{Bi}_2\text{O}_3$  nanoparticles effect the surface tension of glycerol with a decrement up to 0.3% (by weight) followed by an increment to 2.5% (by weight). Finally, another decrement occurs ahead of mentioned  $\text{BiO}_2$  nanoparticle concentration.

The both nanoparticles caused fluctuating changes in the surface tension value which stayed well below the surface tension of pure ethylene glycol. The experiments showed the minimum surface tension value for ethylene glycol is 43.9 dynes/cm and 43.5 dynes/cm for  $\text{CuO}$  nanoparticles addition. For both nanoparticles used in glycerol and ethylene glycol experiments, the behavior of surface tension cannot be related to compliant functions as a result of inconsistent behavior. In “Type D” experiments,

influences of nanoparticles and surfactants to the surface tension of  $C_2H_6O_2$  and  $C_3H_8O_3$  examined, consecutively. The results showed that all three surfactant and nanoparticle solutions caused decrease in surface tension. As in “Type B” experiments the behavior of surface tension can be expressed with the function  $\sigma(C) = m + n \cdot C^{-2}$  where  $\sigma$  is surface tension,  $C$  is surfactant concentration in accordance with  $\forall \{(m > 0) \wedge (n > 0)\} \in \mathbb{R}$ . Any raise in CMC coefficient ( $n$ ) from 0.25 to 1 yielded significant reductions in the surface tension values. Harikrishnan et al. concluded that addition of nanoparticles adjusted the CMC so that surface tension turned out to be indirectly proportional to the overall nanoparticle population and this phenomena explained by referring to adsorption kinetics [332].

Although, several experimental similarities can be observed between aforementioned study and this thesis, the concentration ranges of surfactants are significantly different. The concentration ranges in the experiments of this thesis and Harikrishnan et al. vary from 0.0 to  $10.0 \times CMC$  and 0.0 to  $2.0 \times CMC$ , respectively. In brief, this thesis covers fivefold more concentration range than Harikrishnan et al. [332]. In addition to differences in CMC range, this thesis recommends a new surface tension measurement technique as well as several modeling techniques.

In resemblance to ABM, molecular dynamics (MD) is a technique of solving the equations of motion within the interacting objects of a system [334]. MD is a solely deterministic technique based on the computationally solving Newton’s Laws. Regarding the lack of adequate data about micellization span in ABM, the time specifics used in MD taken into consideration. Selected studies with MD time span information as Bruce et al. investigated the micelle properties that composed of 60 SDS molecules for 5 ns and found that a stable distribution of counter ions and an equilibrated, non-spherical, micelle shape formed in 1 ns of simulation [335]. Sammalkorpi et al. examined the micellization of SDS molecules that are randomly dispersed and filled with 7,902 water molecules to create the process. The model ran for 200 ns with a time step of 2 fs [336]. Lebecque et al. firstly run for a 500 ps simulation with SDS, sodium octylsulfate (SOS,  $CH_3(CH_2)_7OSO_3Na$ ), and tetradecyl phosphocholine (TPC,  $C_{36}H_{76}NO_6P$ ) with a 2 fs time step for a 10 ns overall time period [337]. The area for the models arranged as  $\sim (7.5 \times 7.5 \times 7.5)$  nm. Chun et al. and Mackerell investigated micelle formation consisting of 60 SDS molecules



in H<sub>2</sub>O for a 20 ns period with 120 ps time steps using MD simulation method, respectively [338, 339].

In order to correlate ABM and MD time span with each other, an agent-based model implemented similar to Bruce et al. [335]. The agent-based model ran for 24-hours in a (80 x 80) patch world that created  $4.77 \times 10^6$  ticks and several micelle formations observed.

The steady state values of surface tension and time required to reach this state for DI + SDS, DI + SDS with 2 mg MWCNT, and DI + SDS with 2 mg graphene solutions determined in the light of Table 5.5 through Table 5.8, respectively. Surface tension values of each point obtained from the plots for three different values of time ( $t$ ) at various SDS concentrations. As it can be seen from Table 5.11, surface tension values of DI + SDS solution inversely proportional to SDS concentration for all values of time. Apart from points  $F$  and  $G$ , surface tension values decreased with time as estimated. At point  $F$ , surface tension increased by 0.56% between  $t = 1$  s and  $t = 2$  s. In the same time interval, increment in the surface tension calculated as 0.67% for point  $G$ . The main source of these preventable deviations from the expected behavior is the impurities in the solution and vibrations of the experimental setup, as mentioned earlier. Relative changes among point  $H$  and selected points that resemble the results of HUATARC pendant drop surface tension experiment results for DI + SDS at different SDS concentrations compared. [320]. The minimum variation between the selected points considered to satisfy the most proper conditions for steady state conditions. From the results presented in aforementioned table, minimum variation for the surface tension of DI + SDS at different SDS concentrations observed between the points  $D$  and  $H$  as 4.71%.

Table 5.11 Average values of HUATARC pendant drop surface tension experiment results for DI + SDS at different SDS concentrations and time [320]

<b>Points</b>	<b><math>C</math> (mM)</b>	<b><math>\sigma(C)</math> at <math>t = 0</math> (dynes/cm)</b>	<b><math>\sigma(C)</math> at <math>t = 1s</math> (dynes/cm)</b>	<b><math>\sigma(C)</math> at <math>t = 2s</math> (dynes/cm)</b>	<b>Avg. <math>\sigma(C)</math> (dynes/cm)</b>
<i>A</i>	0.00	72.00	72.00	72.00	72.00
<i>B</i>	0.82	41.20	40.93	40.88	41.00
<i>C</i>	3.00	21.64	21.67	21.65	21.65
<i>D</i>	6.00	23.86	23.95	23.89	23.90
<i>E</i>	8.20	21.69	21.68	21.57	21.65
<i>F</i>	44.30	26.79	26.78	26.93	26.83
<i>G</i>	59.00	26.70	26.73	26.98	26.80
<i>H</i>	82.00	22.79	22.79	22.74	22.77

Table 5.12 Relative changes between selected points of HUATARC pendant drop surface tension experiment results for DI + SDS at different SDS concentrations and time [320]

<b>Between Points</b>	<b><math>\sigma(C)</math> at <math>t = 0</math> (dynes/cm)</b>	<b><math>\sigma(C)</math> at <math>t = 1s</math> (dynes/cm)</b>	<b><math>\sigma(C)</math> at <math>t = 2s</math> (dynes/cm)</b>	<b>Avg. <math>\sigma(C)</math> (dynes/cm)</b>
<i>C</i> and <i>H</i>	5.31%	5.17%	5.03%	5.17%
<i>D</i> and <i>H</i>	4.48%	4.84%	4.81%	4.71%
<i>E</i> and <i>H</i>	5.07%	5.12%	5.42%	5.20%
<i>F</i> and <i>H</i>	14.93%	14.90%	15.56%	15.13%
<i>G</i> and <i>H</i>	14.64%	14.74%	15.72%	15.04%

The same logic used for (DI + SDS and 2 mg MWCNT) and (DI + SDS and 2 mg graphene) solutions to determine the steady state conditions. The results showed that steady state occurred between *F* and *H* for both solutions with variation of 0.59% and 4.41%, respectively. The results of all calculations represented from Table 5.13 through Table 5.16.

Table 5.13 Average surface tension values of HUATARC pendant drop experiment results for DI + SDS and 2 mg MWCNT at different SDS concentrations and time (dynes/cm) [320]

<b>Points</b>	<b>C (mM)</b>	<b><math>\sigma(C)</math> at <math>t = 0</math></b>	<b><math>\sigma(C)</math> at <math>t = 1s</math></b>	<b><math>\sigma(C)</math> at <math>t = 2s</math></b>	<b>Avg. <math>\sigma(C)</math></b>
<i>A</i>	0.00	72.00	72.00	72.00	72.00
<i>B</i>	0.82	50.70	47.73	45.86	48.10
<i>C</i>	3.00	21.84	21.85	21.82	21.84
<i>D</i>	6.00	24.60	24.90	24.68	24.73
<i>E</i>	8.20	21.75	21.68	21.53	21.65
<i>F</i>	44.30	26.86	27.60	22.89	25.78
<i>G</i>	59.00	28.90	24.65	24.81	26.12
<i>H</i>	82.00	25.83	26.01	25.97	25.94

Table 5.14 Relative changes between selected points of HUATARC pendant drop surface tension experiment results for DI + SDS and 2 mg MWCNT at different SDS concentrations and time [320]

<b>Between Points</b>	<b><math>\sigma(C)</math> at <math>t = 0</math></b>	<b><math>\sigma(C)</math> at <math>t = 1s</math></b>	<b><math>\sigma(C)</math> at <math>t = 2s</math></b>	<b>Avg. <math>\sigma(C)</math></b>
<i>C and H</i>	18.27%	19.04%	19.02%	18.78%
<i>D and H</i>	5.00%	4.46%	5.23%	4.89%
<i>E and H</i>	18.76%	19.97%	20.62%	19.78%
<i>F and H</i>	3.83%	5.76%	13.46%	0.59%
<i>G and H</i>	10.62%	5.52%	4.68%	0.70%

Table 5.15 Average values of HUATARC pendant drop surface tension experiment results for DI + SDS and 2 mg graphene at different SDS concentrations and time (dynes/cm) [320]

<b>Points</b>	<b><math>C</math> (mM)</b>	<b><math>\sigma(C)</math> at <math>t = 0</math></b>	<b><math>\sigma(C)</math> at <math>t = 1s</math></b>	<b><math>\sigma(C)</math> at <math>t = 2s</math></b>	<b>Avg. <math>\sigma(C)</math></b>
<i>A</i>	0.00	72.00	72.00	72.00	72.00
<i>B</i>	0.82	50.20	49.69	49.81	49.90
<i>C</i>	3.00	21.82	21.89	21.85	21.85
<i>D</i>	6.00	24.65	24.66	24.60	24.64
<i>E</i>	8.20	21.68	21.75	21.68	21.70
<i>F</i>	44.30	27.62	26.85	26.94	27.14
<i>G</i>	59.00	24.67	23.89	24.00	24.19
<i>H</i>	82.00	25.98	25.94	25.90	25.94

Table 5.16 Relative changes between selected points of HUATARC pendant drop surface tension experiment results for DI + SDS and 2 mg graphene at different SDS concentrations and time (dynes/cm) [320]

<b>Between Points</b>	<b><math>\sigma(C)</math> at <math>t = 0</math></b>	<b><math>\sigma(C)</math> at <math>t = 1s</math></b>	<b><math>\sigma(C)</math> at <math>t = 2s</math></b>	<b>Avg. <math>\sigma(C)</math></b>
<i>C</i> and <i>H</i>	19.07%	18.50%	18.54%	18.70%
<i>D</i> and <i>H</i>	5.40%	5.19%	5.28%	5.29%
<i>E</i> and <i>H</i>	19.83%	19.26%	19.46%	19.52%
<i>F</i> and <i>H</i>	5.94%	3.39%	3.86%	4.41%
<i>G</i> and <i>H</i>	5.31%	8.58%	7.92%	7.25%

As stated in Section 4.1, NetLogo uses “ticks” for distinct update steps for defining time [149]. Since, ticks do not map directly to real-time so that they are merely useful for making comparisons among the agent-based models for maintaining the count of how many times the model updates itself from one state to another succeeding state. The ticks generated per unit time for models are not standard therefore; the properties of agents and interactions among them effect the overall updates numbers and frequency. For instance, the total number of ticks in ABM initial tests for 10, 100, and  $1 \times 10^3$  uncharged

nanoparticles in the (150 x 150) patch world generated average number of  $1.34 \times 10^6$ ,  $1.23 \times 10^6$ , and  $1.11 \times 10^6$  ticks, respectively for 48 hours.

The change in the ticks showed that any increment in the nanoparticle count causes a decline in the number of ticks. In addition, the “world” which is itself a stationary agent has a significant impact on the tick generation. When the world size increases, total number of patches that will be tracked by the agent-based model expands drastically. The difference between (150 x 150) and (350 x 350) patch worlds is  $400 \times 10^3$  patches which causes slowdown in the updates of agent-based models. The same agent-based model used for ABM initial tests with 10, 100, and  $1 \times 10^3$  uncharged nanoparticles ran for the (350 x 350) patch world and the average number of ticks generated found to be  $244.08 \times 10^3$ ,  $215.73 \times 10^3$ , and  $214.18 \times 10^3$ , respectively. The relative changes in ticks due to world area resizing calculated as -81.79% for 10, -82.46% for 100, and -80.53% for  $1 \times 10^3$  uncharged nanoparticles. Apart from the number of agents and size of the world, properties of the agents effect the tick generation. For instance, modifying the previously mentioned agent-based model with same-charged nanoparticles reduces overall the number of ticks significantly. The average number of ticks generated for the 10 nanoparticles decreased by -27.27% and -24.91% for (150 x 150) and (350 x 350) patch worlds, respectively when the charges of the nanoparticles switched from uncharged to same-charged. The same behavior also observed in the agent-models with 100 and  $1 \times 10^3$  nanoparticles so that the number of ticks for the agent-based models with 100 nanoparticles decreased by  $287.92 \times 10^3$  (-23.43%) for (150 x 150) and  $41.22 \times 10^3$  (-19.11%) for (350 x 350) patch worlds, respectively. Another tenfold increment in the nanoparticle population in the agent-based models caused the maximum decrement in the tick count so that the average gap between the uncharged and same-charged nanoparticles calculated as  $295.70 \times 10^3$  and  $45.24 \times 10^3$  for (150 x 150) and (350 x 350) patch worlds, respectively. The overall comparison of ticks generated by the same agent-based models for both types of worlds consists of 10, 100, and  $1 \times 10^3$  uncharged and same-charged nanoparticles can be seen in Figure 5.9.

The variation of ticks with respect to world size presented an uniform behavior with a constant decrement so that it can be summarized with the first order polynomial function  $T(n_p) = -m \cdot x(n_p) + c$ . In this function,  $T$  is total number of ticks,  $x(n_p)$  is overall

number of patches in the confined 2D space, finally  $c$  is constant in accordance with  $\forall \{(m < 0) \wedge (c > 0)\} \in \mathbb{R}$ .

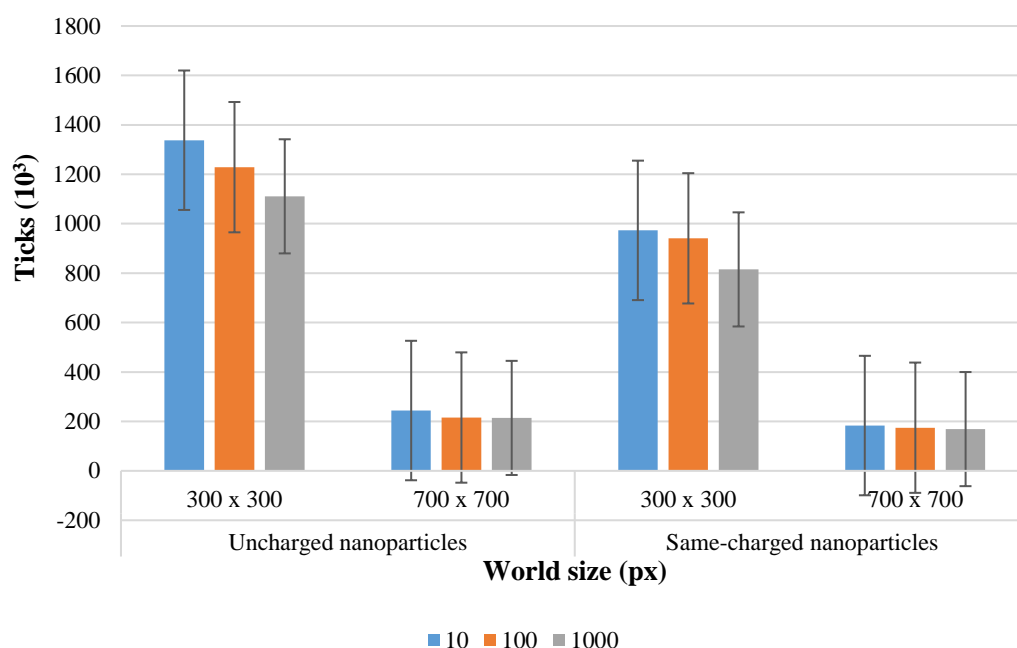


Figure 5.9 Comparison of ticks generated by the same NetLogo agent-based models for uncharged and same-charged nanoparticles in different sized worlds

Furthermore, the total number of ticks in the same agent-based models do not necessarily equal to each other. This reasoning originates itself from the fundamentals of agent-based models mentioned in Section 4.1.5.

In the following paragraphs, time to reach to the interface of the selected NetLogo agent-based models for the various types and numbers of nanoparticles discussed. In the selected model,  $5 \times 10^3$ ,  $15 \times 10^3$ ,  $50 \times 10^3$ ,  $100 \times 10^3$ , and  $200 \times 10^3$  same-charged and uncharged nanoparticles tested in 12 different solvents for 72 hours, individually. It has been observed that required time to contact to the interface is significantly more for the same-charged nanoparticles compared to uncharged nanoparticles without resembling any dependence to solvents as in Table 5.17. The time difference between both types of nanoparticles varies from 61.96% to 98.95% depending on the nanoparticle population of the agent-based models.

It must be mentioned that with the increment of number of nanoparticles in the models, time gap between the different types of nanoparticles increased. For instance, average

time gap to reach the interface between uncharged and same-charged  $5 \times 10^3$  nanoparticles calculated to be 161 s. When the nanoparticle count in the models extended to  $15 \times 10^3$ , average time difference increased by 16.77% to 188 s with respect to  $5 \times 10^3$  nanoparticles. For the  $50 \times 10^3$  nanoparticles, time difference increased to 709 s that corresponds to 601.98% upsurge. Increasing the nanoparticle population by twenty and fortyfold with respect to  $5 \times 10^3$  nanoparticles increases the time gap between uncharged and same-charged nanoparticles drastically. The average gap reaches to  $1.95 \times 10^3$  s and  $21.81 \times 10^3$  s that correspond to 88.25% and 95.45% difference for same-charged and uncharged nanoparticles, respectively. In the same models, number of ticks also recorded in the log files in real time, which can be seen in Table 5.18. The analysis of ticks showed apart from the results mentioned above, the required ticks to reach to the interface are almost similar to same-charged nanoparticles and uncharged nanoparticles. For 12 solvents, average numbers of ticks necessitated to reach to the interface for same-charged and uncharged nanoparticles computed are 36 and 32, respectively. It has been observed that, total ticks are indirectly proportional to the overall nanoparticle population. For instance, the average number of ticks declined from 36 to 27 by 25% when the number of same-charged nanoparticles increased from  $5 \times 10^3$  to  $200 \times 10^3$ . For the uncharged nanoparticles under the same conditions, the average number of ticks decreased to 25 from 32 by 21.88%. The maximum and minimum number of ticks observed for propane as 129 and chloroform as 43, respectively. In addition, average number of ticks in the agent-based models presented little to no dependence on the solvent type in accordance with the previous time computations in seconds.

Finally, the aforementioned computations used to determine the relation of ticks to time concept used in real-life. Every model starts to run with random initial conditions, so that results of the models do not necessarily consistent with each other as mentioned in Section 1.4.1. As the number of nanoparticles and the rules increase in models, seconds to ticks ratio increases, either. The rate of increment in the corresponding seconds to ticks is observed to be higher in same-charged nanoparticles rather than uncharged nanoparticles. For  $5 \times 10^3$  same-charged and uncharged nanoparticles, each tick corresponds to 4.37 s and 1.97 s, respectively. When the nanoparticle count in the agent-based models increased to  $15 \times 10^3$ , tick corresponds to 8.22 s for same-charged and 1.57 s for uncharged nanoparticles, on the average. For  $50 \times 10^3$  nanoparticles, average number of seconds

corresponding to both types of nanoparticles increased by 763.16% and 68.53% with respect to  $5 \times 10^3$  nanoparticles. Increasing the nanoparticle population by twentyfold increases the number of ticks to seconds ratio for both of the same-charged and uncharged nanoparticles, significantly. The average number of seconds corresponding to a single tick reaches to 90.78 and 3.36 that correspond to 1977.35% and 80.71% increment for  $100 \times 10^3$  same-charged and uncharged nanoparticles, respectively. When the number of nanoparticles in the agent-based models upsurges to  $200 \times 10^3$  which is in the operating limits of hardware used in this thesis, one tick equals to 939.84 s (~16 min) for same-charged nanoparticles and 9.38 s (~0.20 min) for uncharged nanoparticles. In Table 5.19, the calculations for each tick's equivalent to the corresponding number of seconds for the selected number of same-charged and uncharged nanoparticles represented. Time reach to the interface of NetLogo agent-based models for the selected number uncharged and same-charged nanoparticles with respect to 12 solvents represented in Figure 5.10 and Figure 5.11, respectively.

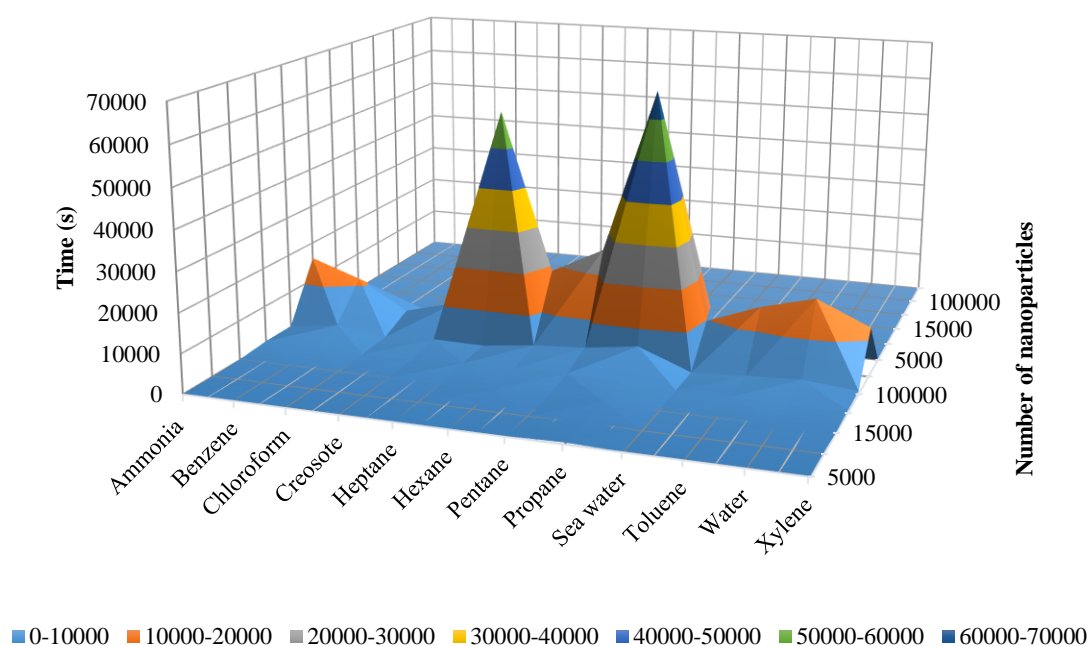


Figure 5.10 Time required to reach to the interface of NetLogo agent-based models for the selected number uncharged nanoparticles (s)



Table 5.17 Time to reach to the interface of an agent-based model for the selected number of same-charged and uncharged nanoparticles (s)

Solvent	5×10 <sup>3</sup> nanoparticles		15×10 <sup>3</sup> nanoparticles		50×10 <sup>3</sup> nanoparticles		100×10 <sup>3</sup> nanoparticles		200×10 <sup>3</sup> nanoparticles	
	<i>np<sub>sc</sub></i> <sup>38</sup>	<i>np<sub>uc</sub></i> <sup>39</sup>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>
Ammonia	120	77	130	44	765	93	797	116	15.84×10 <sup>3</sup>	215
Benzene	106	85	107	30	695	93	2.54×10 <sup>3</sup>	65	11.42×10 <sup>3</sup>	286
Chloroform	87	60	57	61	260	129	738	130	3.96×10 <sup>3</sup>	362
Creosote	101	56	148	56	441	84	1.64×10 <sup>3</sup>	75	7.40×10 <sup>3</sup>	230
Heptane	211	87	165	32	1.06×10 <sup>3</sup>	82	1.47×10 <sup>3</sup>	86	59.17×10 <sup>3</sup>	246
Hexane	177	26	476	52	1.25×10 <sup>3</sup>	72	3.04×10 <sup>3</sup>	60	18.82×10 <sup>3</sup>	97
Pentane	212	37	296	39	1.54×10 <sup>3</sup>	74	3.95×10 <sup>3</sup>	63	25.55×10 <sup>3</sup>	240
Propane	493	51	833	38	1.10×10 <sup>3</sup>	56	5.83×10 <sup>3</sup>	90	66.87×10 <sup>3</sup>	216
Sea water	113	90	85	59	551	105	686	124	9.83×10 <sup>3</sup>	310
Toluene	118	85	102	37	749	91	1.42×10 <sup>3</sup>	72	14.86×10 <sup>3</sup>	289
Water	102	49	196	49	534	101	2.08×10 <sup>3</sup>	108	18.34×10 <sup>3</sup>	46
Xylene	114	41	196	43	628	88	808	119	12.45×10 <sup>3</sup>	284
<b>Average</b>	163	62	233	45	798	89	2.08×10 <sup>3</sup>	92	22.04×10 <sup>3</sup>	235

<sup>38</sup> SC is the abbreviation of “same-charged”

<sup>39</sup> UC is the abbreviation of “uncharged”

Table 5.18 Time to reach to the interface of an agent-based model for the selected number of same-charged and uncharged nanoparticles (ticks)

Solvent	$5 \times 10^3$ nanoparticles		$15 \times 10^3$ nanoparticles		$50 \times 10^3$ nanoparticles		$100 \times 10^3$ nanoparticles		$200 \times 10^3$ nanoparticles	
	$np_{sc}$	$np_{uc}$	$np_{sc}$	$np_{uc}$	$np_{sc}$	$np_{uc}$	$np_{sc}$	$np_{uc}$	$np_{sc}$	$np_{uc}$
Ammonia	30	31	19	28	18	26	16	25	17	25
Benzene	29	32	19	29	16	27	16	26	16	26
Chloroform	22	43	15	39	13	37	13	35	14	34
Creosote	24	36	17	33	15	30	15	30	13	29
Heptane	45	28	26	25	23	23	22	23	21	22
Hexane	41	27	30	25	26	23	24	22	25	21
Pentane	49	26	33	24	27	22	27	22	27	21
Propane	84	23	84	21	108	19	113	19	129	18
Sea water	25	36	16	32	16	30	15	29	14	28
Toluene	28	32	19	29	17	27	16	26	15	25
Water	26	34	17	31	15	30	15	29	15	28
Xylene	24	32	19	30	15	27	16	26	15	26
<b>Average</b>	<b>36</b>	<b>32</b>	<b>26</b>	<b>29</b>	<b>26</b>	<b>27</b>	<b>26</b>	<b>26</b>	<b>27</b>	<b>25</b>

Table 5.19 Each tick equals to the following number of seconds for the selected number of same-charged and uncharged nanoparticles

Solvent	<b>5×10<sup>3</sup> nanoparticles</b>		<b>15×10<sup>3</sup> nanoparticles</b>		<b>50×10<sup>3</sup> nanoparticles</b>		<b>100×10<sup>3</sup> nanoparticles</b>		<b>200×10<sup>3</sup> nanoparticles</b>	
	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>	<i>np<sub>sc</sub></i>	<i>np<sub>uc</sub></i>
Ammonia	4.00	2.48	6.84	1.57	42.50	3.58	49.81	4.64	931.65	8.60
Benzene	3.66	2.66	5.63	1.03	43.44	3.44	158.88	2.50	713.81	11.00
Chloroform	3.95	1.40	3.80	1.56	20.00	3.49	56.77	3.71	282.64	10.65
Creosote	4.21	1.56	8.71	1.70	29.40	2.80	109.40	2.50	569.46	7.93
Heptane	4.69	3.11	6.35	1.28	46.09	3.57	66.82	3.74	2.82×10 <sup>3</sup>	11.18
Hexane	4.32	0.96	15.87	2.08	47.92	3.13	126.50	2.73	752.72	4.62
Pentane	4.33	1.42	8.97	1.63	57.15	3.36	146.41	2.86	946.22	11.43
Propane	5.87	2.22	9.92	1.81	10.19	2.95	51.60	4.74	518.38	12.00
Sea water	4.52	2.50	5.31	1.84	34.44	3.50	45.73	4.28	702.36	11.07
Toluene	4.21	2.66	5.37	1.28	44.06	3.37	88.56	2.77	990.40	11.56
Water	3.92	1.44	11.53	1.58	35.60	3.37	138.40	3.72	1.23×10 <sup>3</sup>	1.64
Xylene	4.75	1.28	10.32	1.43	41.87	3.26	50.50	4.58	829.93	10.92
<b>Average</b>	<b>4.37</b>	<b>1.97</b>	<b>8.22</b>	<b>1.57</b>	<b>37.72</b>	<b>3.32</b>	<b>90.78</b>	<b>3.56</b>	<b>939.84</b>	<b>9.38</b>

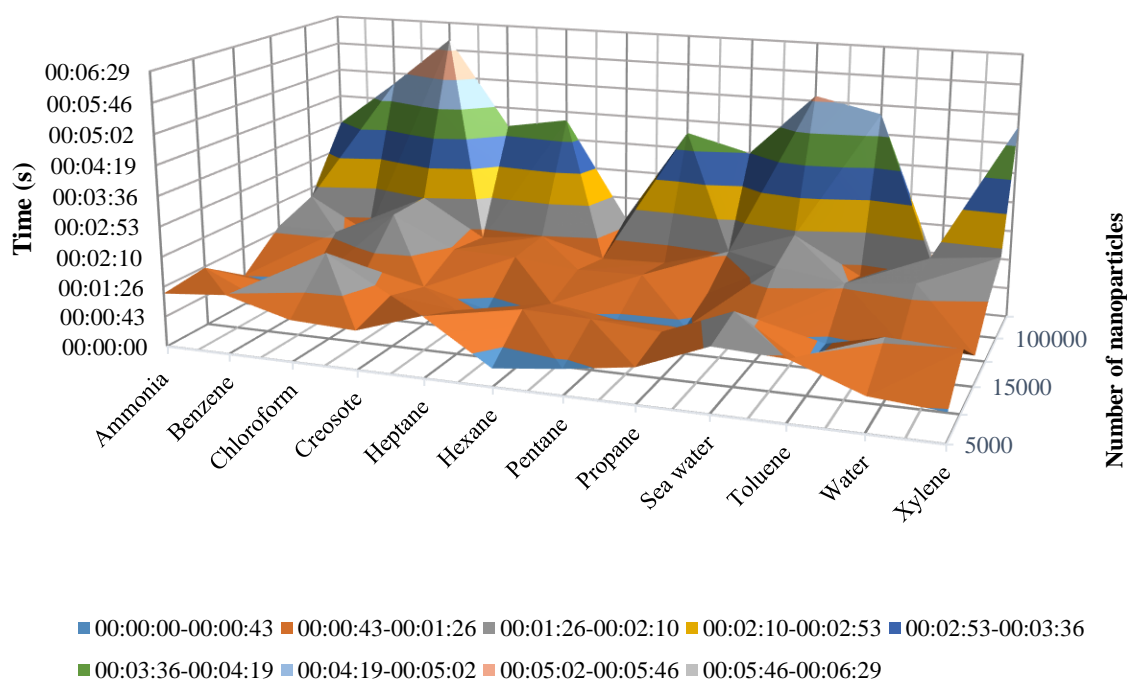


Figure 5.11 Time reach to the interface of NetLogo agent-based models for the selected number same-charged nanoparticles (s)

In another attempt to relate ticks to the time in seconds, a particular agent-based model tested consecutively for five times until the model updated itself to  $1.15 \times 10^3$  times<sup>40</sup>. Agent-based model designed to consist of  $1.45 \times 10^3$  uncharged nanoparticles, which reside in DI. During the model run-time, ticks, time in seconds and number of uncharged nanoparticles at the interface logged into a text file in real-time. After reaching the determined upper limit of ticks, descriptive statistics of nanoparticles at the interface and time data for the five tests analyzed and their results represented in Appendix 20.1 and Appendix 20.2, respectively. Due to randomness in the agent-based models, initial conditions of every model are unique. For this reason, the number of uncharged nanoparticles at the interface at fundamental stage varies from 41 to 61 with an average value of 54 among five models.

It can be concluded that as the time reaches to  $<10 \times 10^3$  ticks, any change in the number of nanoparticles at the interface significantly decreases. This phenomena can be seen in

<sup>40</sup> All agent-based models executed consecutively on the same computer in order to provide consistency. Hardware and software configurations of the computer represented in Appendix 19.1 and 19.2, respectively.

the Figure 5.12, as the number of nanoparticles starts to reach steady state at  $3.0 \times 10^3$  ticks (= 524 s). Beyond this point, the average variation in the number of nanoparticles at the interface is 2.81%. It can be concluded that time (both in ticks and in seconds) and variation in the number of nanoparticles at the interface is inversely proportional. This phenomenon can be described best by a limit function as in Equation 5.9.

$$\lim_{t \rightarrow \infty} \frac{\partial N_{np}(t)}{\partial t} \rightarrow 0 \quad \text{Equation 5.6}$$

Where  $N_{np}$  is the number of uncharged nanoparticles at the interface and  $t$  is time.

In addition to above calculations, data gathered from the five agent-based models used to correlate ticks to time in seconds. It has been determined that the relation between two variables exhibit corresponding behaviors that can be summarized in the form of univariate quadratic polynomial as  $f(x) = a_1x^n + b_1x + c_1$  where  $\forall \{(a_1 \wedge b_1 \wedge c_1) > 0\} \wedge [(a_1 \wedge b_1 \wedge c_1 \wedge n) \in \mathbb{R}]$ . This behavior represented visually in Figure 5.13 and it has been established that it can be denoted by a function such as  $f(x) = 1.67x^2 + 67.88x + 66.06$  where  $R^2$  calculated as 0.99. From this plot, it can be concluded that corresponding ticks per unit time in seconds are not constant and increases directly proportional with model run-time. For instance, at the 500<sup>th</sup> update of the agent-based model, one tick matched to 0.14 s and at the 5000<sup>th</sup> tick, it increased by 21.42% to match 0.17 s. Finally, at the 10000<sup>th</sup> tick one tick equaled to 0.21 s by 46.54% growth with respect to 500<sup>th</sup> update. This condition can be interpreted by increment of nanoparticle-nanoparticle, nanoparticle-interface, and nanoparticle-world interactions with model execution time. These phenomena also detected in other models and the increment in corresponding ticks per unit time found to be consistent with all initial, validation, verification, and load tests mentioned throughout Section 5.1.1, 5.1.2, and 5.1.3, respectively.

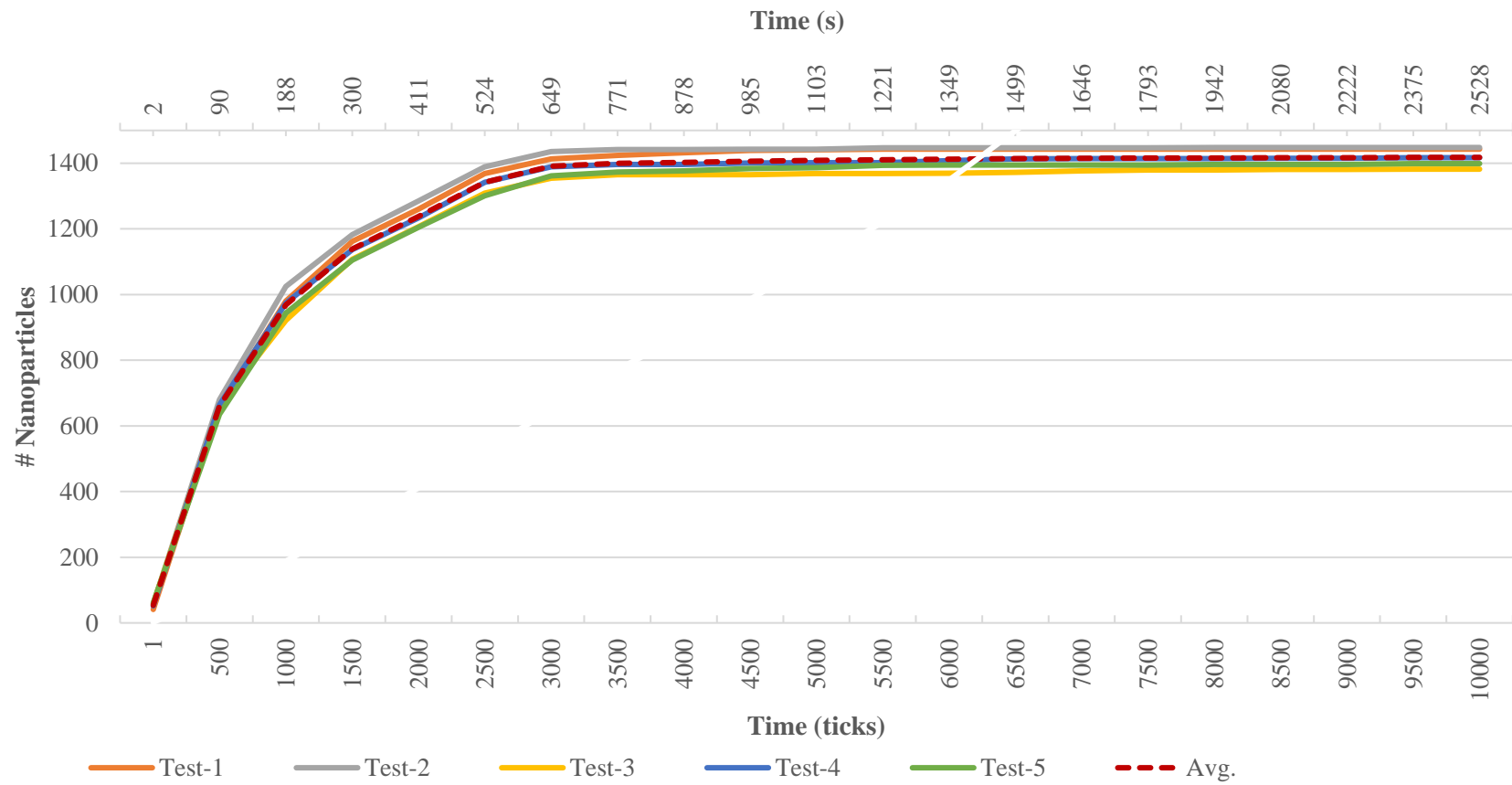


Figure 5.12 Dependency of number of nanoparticles at the interface of an agent-based model to ticks and time in seconds

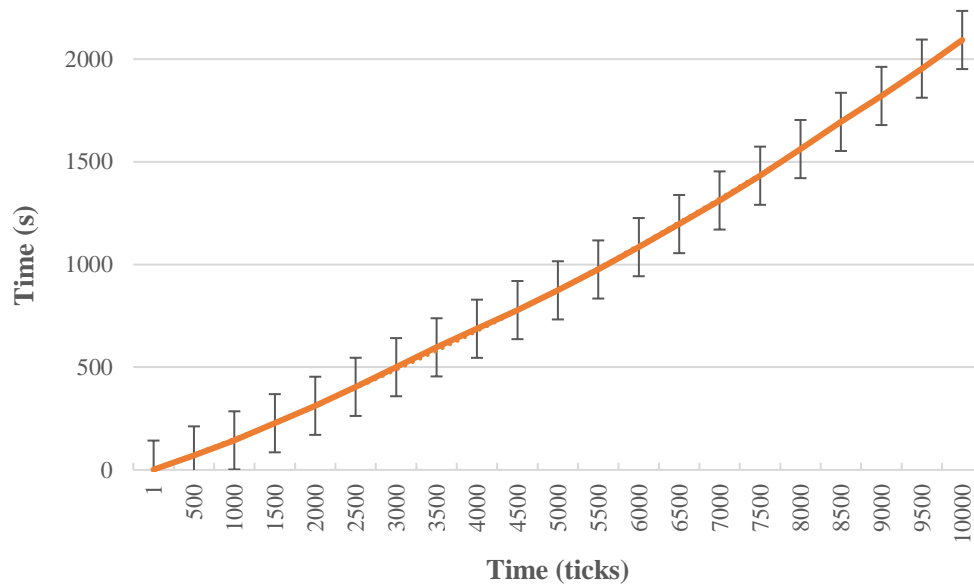


Figure 5.13 Relation between ticks and time in seconds

For understanding the relation between surface tension values gathered from the experiments at HUATARC and number of uncharged nanoparticles at the interface of the selected agent-based model, following plot has been charted [320]. It has been observed that by the increment of uncharged nanoparticle population with respect to time, surface tension decreases, as expected.

In order to understand the relation between the variables non-parametric correlation analysis techniques used. Non-parametric analysis mainly preferred in situations when data do not fit any probability distribution. Kolmogorov-Smirnov and Shapiro-Wilks tests showed that instantaneous nanoparticle population at the interface did not provide the conditions to satisfy normal distribution [340]. Both tests yielded p-values as 0.00, which are lower than the critical value, 0.05. In addition, quantile to quantile<sup>41</sup> (Q-Q) plot used to double check if instantaneous nanoparticle population at the interface consistent with normal distribution.

<sup>41</sup> Quantile defined as the part of a data set distributed into equal-sized adjoining subsets. There are several commonly used quantiles named as quartiles, deciles, and percentiles, which divides the data set into four, 10, and 100 equivalent parts, respectively.

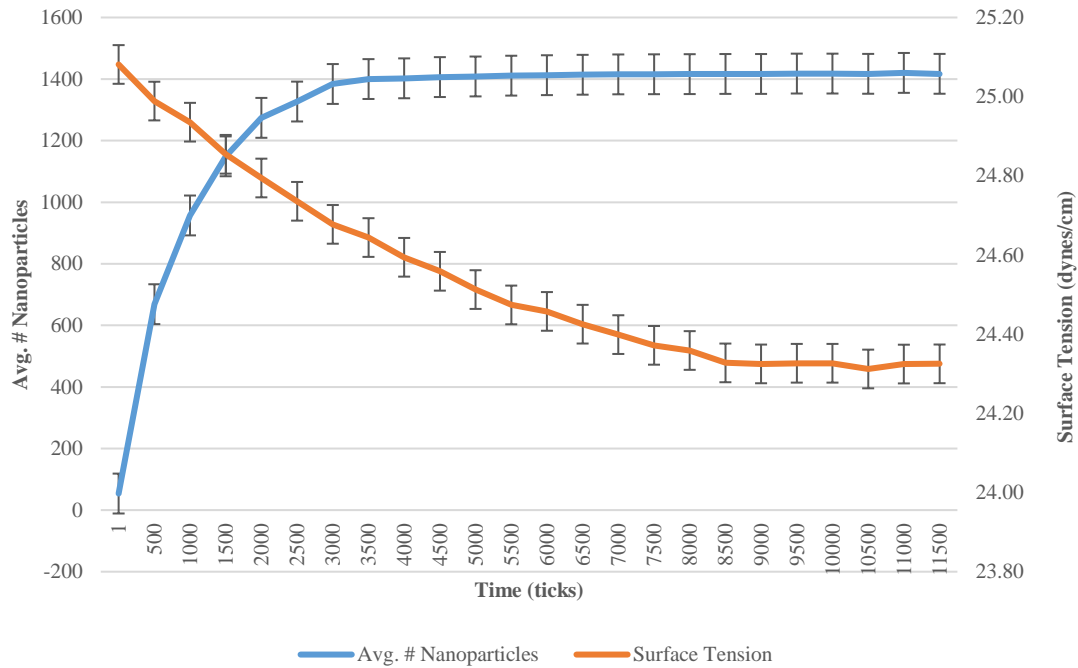


Figure 5.14 Relation between ticks and time in seconds for the elected agent-based model

Theoretically, normal distribution for respective data sets yields the same behavior so that the points on the Q-Q plot would perfectly locate around a line with an inclination of  $45^\circ$ . On the contrary, distribution of data points is far from to show uniform position as in Figure 5.15. Results represent remarkable nonlinear tendency by implying the nanoparticle population did not distributed normally at the interface.

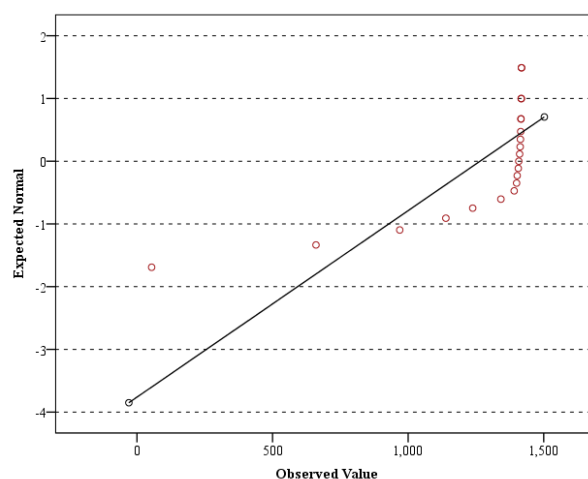


Figure 5.15 Q-Q plot for instantaneous nanoparticle population at the interface



Since, the relation found be nonlinear and cannot be defined by normal distribution, Spearman ( $r_s$ ) and Kendall ( $r_k$ ) correlation coefficients calculated to investigate the monotonic relationship<sup>42</sup> between the variables. Spearman ( $r_s$ ) and Kendall ( $r_k$ ) correlation coefficients calculated by Equation 5.7 and Equation 5.8, respectively [341].

$$r_s = \frac{\sum R_{np}(n_o) \cdot \sum R_{st}(n_o) - n_o \cdot \left(\frac{n_o + 1}{2}\right)^2}{\sqrt{\sum R_{np}(n_o)^2 - n_o \cdot \left(\frac{n_o + 1}{2}\right)^2} \cdot \sqrt{\sum R_{st}(n_o)^2 - n_o \cdot \left(\frac{n_o + 1}{2}\right)^2}} \quad \text{Equation 5.7}$$

$$r_k = \frac{n_c - n_d}{\frac{1}{2} \cdot n_o \cdot (n_o - 1)} \quad \text{Equation 5.8}$$

Where  $R_{np}(n_o)$  and  $R_{st}(n_o)$  are the ranks of the individual observations of the average number of nanoparticles at the interface of an agent-based model and experimental surface tension values, respectively.  $n_o$  is the total number of observations, and  $n_c$  and  $n_d$  are the number of concordant and discordant pairs<sup>43</sup>.

Spearman and Kendall correlation coefficients calculated for average number of nanoparticles at the interface versus surface tension values gathered from the experiments at HUATARC as -0.999 and -0.995 and represented in Table 5.20. Correlation coefficients in the ranges of (0.9 to 1.0) and -(0.9 to 1.0) can be interpreted as the aforementioned parameters are significantly correlated. Negative values of correlation coefficients refer to relationship between the two variables so that for each increment in one variable corresponds to decrement of a fraction in the other variable. This condition

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<sup>42</sup> A monotonic function is one that either never increases or decreases as its independent variable increases. Briefly, a function can said to be monotonic whether its first derivative with respect to independent variable does not its change sign.

<sup>43</sup> Concordant and discordant data pairs can be defined as the condition of selecting distinct couples through a set of two variables. For instance let  $\alpha, \alpha_2, \alpha_3, \dots, \alpha_n$  be the sample data set for variable  $A$  and let  $\beta_1, \beta_2, \beta_3, \dots, \beta_n$  be the sample data set for variable  $B$ . There will be  $P(n, 2)$  probable states to select distinct pairs such as  $(\alpha_i, \beta_j)$  and  $(\alpha_j, \beta_i)$ . For the consignment of variables, each data pair defined as concordant and disconcordant under the following conditions,

- Concordant, if  $[(\alpha_i > \alpha_j) \wedge (\beta_i > \beta_j)] \vee [(\alpha_i < \alpha_j) \wedge (\beta_i < \beta_j)]$
- Disconcordant, if  $[(\alpha_i > \alpha_j) \wedge (\beta_i < \beta_j)] \vee [(\alpha_i < \alpha_j) \wedge (\beta_i > \beta_j)]$
- Neither, if  $[(\alpha_i = \alpha_j) \vee (\beta_i = \beta_j)]$

Depending on the number of concordant and discordant pairs for a given data set,  $\tau$  can be calculated as follows,

$$\tau = \frac{n_c - n_D}{P(n, 2)}$$

Where,  $n_c$  and  $n_D$  are total number of concordant and discordant data pairs.

can be perfectly seen in Figure 5.14 so that any increment in the average number of nanoparticles at the interface responded by a decrement in the experimentally obtained surface tension values until the steady state condition achieves.

Table 5.20 Spearman and Kendall correlation coefficients of experimental surface tension values and average number of nanoparticles at the interface of an agent-based model in real time

	Correlation Coefficients	Variables	
		Avg. # NPs	Surface Tension
Spearman	Avg. # nanoparticles	1.000	-0.999
	Surface Tension	-0.999	1.000
Kendall	Avg. # nanoparticles	1.000	-0.995
	Surface Tension	-0.995	1.000

Regarding the results of Spearman and Kendall correlation coefficients, it can be concluded that the average number of nanoparticles at the interface and surface tension values experimentally obtained from HUATARC related. Finally, these results lead to the conclusion that agent-based models have capability of showing the changes in surface tension in real world.

In all agent-based models throughout the thesis, agents acted autonomously under the particular instructions and initial conditions of the models set randomly with NetLogo's built-in Mersenne twister pseudorandom number generator (MTPRNG) [282]. Although, the behaviors of agents defined by the rules of classical physics, they cannot be interpreted purely with deterministic methods. As the dynamic agents behave autonomously in a stochastic manner, the behaviors of the agent-based models are irreversible with respect to time. Even though, the models designed purely in deterministic point of view, there are some exceptions of time reversibility. For instance, Norton's Dome is a paradigm of a Newtonian system that defies the condition at a single position, which points irreversibility [342]. The simple outline of Norton's Dome states that the force on a homogeneous ball located on the top of a dome as in Equation 5.9. The first derivative of  $F(x)$  which cannot be defined in at  $x = 0$  as a result of division by zero error which triggers

the irreversibility of the movement in 3D Cartesian coordinate system which mentioned in Equation 5.12.

$$|\vec{F}(x)| = \sqrt{x} \quad \text{Equation 5.9}$$

$$\frac{|\vec{F}(x)|}{\partial x} = \frac{1}{2\sqrt{x}} \quad \text{Equation 5.10}$$

The basic representation of Norton's Dome can be seen in Figure 5.16 [342].

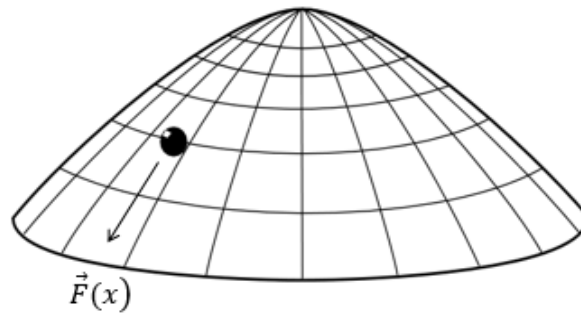


Figure 5.16 Norton's Dome [342]

Each agent-based model represents a dynamical system that starts with a different set of initial conditions and runs randomly under the defined rules for a given interval of time. Dynamical systems based on the combination of a phase space (also known as state space) and changing aspects of the system with a restricted degrees of freedom. The number of independent directions in which a system can have the ability to move defined as the number of degrees of freedom [343]. All agents apart from the stationary ones in the agent-based models designed with four degrees of freedom, which are the total of two degrees of freedom for translational and rotational motions in 2D Cartesian coordinate system. It can be regarded as a model defining the temporal progression (also known as evolution) of a system therefore  $R_s: P \times t \rightarrow P$  where  $s \in P$ . In this argument,  $P$  is phase space,  $t$  is set of time,  $s$  is any distinctive state, and  $R_s$  is progression. In this case, progression provides a prediction of the succeeding state of the system that depends on the current phase space which can be governed by on the deterministic or stochastic nature of the system. In dynamical systems, orbit or trajectory of a phase space defined as the chronologically ordered collection of phases in accordance with the progression rule [344]. An individual phase can be expressed with phase variables ( $P_v(t)$ ) that their

initial conditions represent the minimum crucial information to compute the output of the system ( $f_o(t)$ ) as mentioned in Equation 5.11.

$$P_v(t) = \begin{bmatrix} P_{v_1}(t) \\ P_{v_2}(t) \\ P_{v_3}(t) \\ \dots \\ P_{v_n}(t) \end{bmatrix} \in \mathbb{R} \text{ and is consistent with } f_o(t) \rightarrow \begin{cases} f_i(t), & t \geq t_0 \\ P_v(t), & t = t_0 \end{cases} \quad \text{Equation 5.11}$$

Phase space consists of position and momentum information that describes the system, in particular [345]. The position of every agent in the agent-based models defined by the values of  $x$  and  $y$  components in Cartesian coordinate system so that at any tick an agent will have an specific set of component pairs with respect to its position. The state of motion for dynamic agents defined by their momentum and this is also known as “quantity of motion”. Momentum of a dynamic agent ( $\vec{P}_a$ ) can be formulated as  $m \cdot \vec{V}_a$  where  $m$  is mass, and  $\vec{V}_a$  is velocity. For this reason, every dynamic agent<sup>44</sup> experiences a distinctive phase space at any given time. In agent-based models, an agent designed for a nanoparticle in 2D space defined by its position ( $\vec{r}_n(t)$ ) and momentum ( $\vec{P}_n(t)$ ) vectors as in Equation 5.12 and Equation 5.13.

$$\vec{r}_n(t) = r_n(x_n \hat{i}, y_n \hat{j}) \quad \text{Equation 5.12}$$

$$\vec{P}_n(t) = P_n(P_{x_n} \hat{i}, P_{y_n} \hat{j}) = P_n(m_n \cdot V_{x_n} \hat{i}, m_n \cdot V_{y_n} \hat{j}) \quad \text{Equation 5.13}$$

In the above equations,  $\hat{i}$  and  $\hat{j}$  are unit vectors of  $x$  and  $y$  coordinates, respectively. Both vectors  $\vec{r}_n(t)$  and  $\vec{P}_n(t)$  are functions of time as a result of the agent-based models’ dynamic behavior so that a nanoparticle can be described with four time dependent vectors as follows,

$$\vec{A}_n(t) = f(\vec{r}_n(t), \vec{P}_n(t)) \quad \text{Equation 5.14}$$

In the case of other agents with more complex geometries like SDS molecules, phase space becomes more complicated. As mentioned earlier, SDS molecules in the agent-

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<sup>44</sup> The term “dynamic agent” stands for the all agents whose momentum is different from zero at least in one dimension.

based models designed as linked combinations of hydrophilic and hydrophobic components represented in Figure 4.11. Each component shaped as perfect circles relative to their geometrical forms and connected through a line. The position ( $\vec{r}_{SDS}(t)$ ) and momentum vectors ( $\vec{P}_{SDS}(t)$ ) on behalf of time dependent phase space defined in Equation 5.15 through Equation 5.17. The substitution of these equations into Equation 5.18 yields the final form of the phase space characterization of a SDS molecule in 2D.

$$\vec{r}_{SDS}(t) = r_{SDS}(x_{SDS(C_1)}\hat{i}, y_{SDS(C_1)}\hat{j}, x_{SDS(C_2)}\hat{i}, y_{SDS(C_2)}\hat{j}) \quad \text{Equation 5.15}$$

$$\vec{P}_{SDS}(t) = P_{SDS}(P_{x_{SDS(C_1)}}\hat{i}, P_{y_{SDS(C_1)}}\hat{j}, P_{x_{SDS(C_2)}}\hat{i}, P_{y_{SDS(C_2)}}\hat{j}) \quad \text{Equation 5.16}$$

$$\vec{P}_{SDS}(t) = P_{SDS}(m_{SDS(C_1)} \cdot V_{x_{SDS(C_1)}}\hat{i}, m_{SDS(C_1)} \cdot V_{y_{SDS(C_1)}}\hat{j}, m_{SDS(C_2)} \cdot V_{x_{SDS(C_2)}}\hat{i}, m_{SDS(C_2)} \cdot V_{y_{SDS(C_2)}}\hat{j}) \quad \text{Equation 5.17}$$

$$\vec{A}_{SDS}(t) = f(\vec{r}_{SDS}(t), \vec{P}_{SDS}(t)) \quad \text{Equation 5.18}$$

$$\vec{A}_{SDS}(t) = f\left(r_{SDS}(x_{SDS(C_1)}\hat{i}, y_{SDS(C_1)}\hat{j}, x_{SDS(C_2)}\hat{i}, y_{SDS(C_2)}\hat{j}), P_{SDS}(m_{SDS(C_1)} \cdot V_{x_{SDS(C_1)}}\hat{i}, m_{SDS(C_1)} \cdot V_{y_{SDS(C_1)}}\hat{j}, m_{SDS(C_2)} \cdot V_{x_{SDS(C_2)}}\hat{i}, m_{SDS(C_2)} \cdot V_{y_{SDS(C_2)}}\hat{j})\right) \quad \text{Equation 5.19}$$

Where,  $C_1$  and  $C_2$  denotes the hydrophobic and hydrophilic components of the SDS molecule, respectively. For any dynamic agent in 2D space, the divergence of phase space equals to non-zero<sup>45</sup>.

$$\nabla \cdot \vec{A}_{SDS} = \left[\frac{\delta}{\delta x}\hat{i} + \frac{\delta}{\delta y}\hat{j}\right] \cdot [\vec{A}_{SDS}(x, t)\hat{i} + \vec{A}_{SDS}(y, t)\hat{j}] \quad \text{Equation 5.20}$$

$$\nabla \cdot \vec{A}_{SDS}(t) = \frac{\partial}{\partial x} A_{SDS}(x, t) + \frac{\partial}{\partial y} A_{SDS}(y, t) \quad \text{Equation 5.21}$$

$$\nabla \cdot \vec{A}_{SDS} = \frac{\delta}{\delta t} \left[ f\left(r_{SDS}(x_{SDS(C_1)}\hat{i}, x_{SDS(C_2)}\hat{i}), P_{SDS}(m_{SDS(C_1)} \cdot V_{x_{SDS(C_1)}}\hat{i}, m_{SDS(C_2)} \cdot V_{x_{SDS(C_2)}}\hat{i})\right) \right] \quad \text{Equation 5.22}$$

$$+ \frac{\delta}{\delta t} \left[ f\left(r_{SDS}(y_{SDS(C_1)}\hat{j}, y_{SDS(C_2)}\hat{j}), P_{SDS}(m_{SDS(C_1)} \cdot V_{y_{SDS(C_1)}}\hat{j}, m_{SDS(C_2)} \cdot V_{y_{SDS(C_2)}}\hat{j})\right) \right]$$

$$\nabla \cdot \vec{A}_{SDS} \neq 0 \quad \text{Equation 5.23}$$

<sup>45</sup> It must be mentioned that  $\vec{A}_{SDS} = \vec{A}_{SDS}(t)$ .

The discussion of dynamical systems leads to chaos theory, which portrays the behavior of complex systems. The roots of chaos theory go back to 19<sup>th</sup> century when Poincare [346] showed that Newton's theory of gravity<sup>46</sup> could be used to interpret two celestial bodies' orbit under bilateral attraction and within the inclusion of a third body caused unsolvable differential equations in 1887 [347]. The leading leap in chaos theory achieved by Lorenz in early 1960s. In his prominent study, he stated that the computer simulation of a set of first order differential equations yielded complicated behaviors which influenced extremely by the initial conditions [348].

$$\frac{\partial x}{\partial t} = P_r(y - x) \quad \text{Equation 5.24}$$

$$\frac{\partial y}{\partial t} = x(R_a - z) - y \quad \text{Equation 5.25}$$

$$\frac{\partial z}{\partial t} = xy - \beta z \quad \text{Equation 5.26}$$

In the above equations,  $x$ ,  $y$ , and  $z$  define the state of the system in 3D space,  $t$  is time,  $P_r$  is Prandtl number,  $R_a$  is Rayleigh number, and  $\beta$  is the system parameter which are entirely positive real numbers. Lorenz used 10, 2.67, and 28 for  $\sigma$ ,  $\rho$ , and  $\beta$  to demonstrate the chaotic behavior of the stated system, respectively.

In this thesis, every one of the agent-based models including initial, validation, verification, load, and main models ran twice and the average number of ticks generated by both models accepted as the absolute ticks for the models. As an example, total number of ticks and real- time correlated for an ABM initial test for 10 uncharged nanoparticles in the three different types of worlds for 24 and 48-hours. From the aforementioned comprehensions, every test has generated different number of ticks for the same nanoparticle count, world area, and time. For instance, 10 uncharged nanoparticles in a (150 x 150) patch world generated  $732.35 \times 10^3$  and  $630.48 \times 10^3$  ticks for 24-hours coupled

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<sup>46</sup> Newton's theory of gravity states that every single object attracts all other objects in the universe. The gravitational force can be represented as follows,

$$F_g(r) = G \frac{m_1 \cdot m_2}{r^2}$$

with  $1,502.58 \times 10^3$  and  $1,173.06$  ticks for 48-hours. The correlation of ticks to real-time calculated with the average values of ticks compiled from the both agent-based models, which are calculated as  $681.41 \times 10^3$  and  $1.34 \times 10^6$ . The average tick values correlated to real-time with therefore agent-based models generated  $28.39$  ticks/h ( $=7.83 \times 10^{-3}$  ticks/s) and  $27.87$  ticks/h ( $=7.67 \times 10^{-3}$  ticks/s) for 24 and 48 hours, respectively.

## 6. RECOMMENDATIONS FOR FUTURE WORK

The evaluation that has been undertaken for this thesis has drawn attention on to several issues, which further research considered necessary. Besides, regarding the boundaries of this thesis discussed in Section 3.2, following recommendations can be made to address new research areas for the future studies,

1. Further research needed to create more comprehensive and complex agent-based models to simulate the effects of nanoparticles and SDS molecules on surface tension. In these studies, agents can be determined with taking more variables into account<sup>47</sup>, which mentioned in Section 4.1.
2. All models in this thesis implemented in agent-based techniques are stand-alone and do not use any shared components with any other models. As it can be explored from literature, numerous technologies<sup>48</sup> developed to allocate routines, classes, and components simultaneously in numerous models. In future studies, reusing and distributing components of models will ease the model development processes and required time interval [349].
3. This thesis has investigated the implications of variations the in surface tension for selected nanoparticles and SDS molecules. The types of nanoparticles can be increased to compare the effects of nanoparticles to the surface tension and create a more comprehensive research.
4. More advanced cameras whose technical properties superior than 30 fps can be used to generate supplementary images for the experiments, which can solve the lack of data problem. Also, any upgrade in the Attension optical tensiometer's camera<sup>49</sup> will create more accurate results in experiments [8].
5. In this thesis, 12 different types of Newtonian fluids used in agent-based models as stated in Appendix 2. A further study with focus on the effects of nanoparticles and SDS molecules to the surface tension of non-Newtonian fluids is therefore suggested.

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<sup>47</sup> In this thesis, agents for a nanoparticle and a SDS molecule defined with 12 and 21 variables, respectively.

<sup>48</sup> For instance, Microsoft COM, Microsoft .NET, CORBA, and Java NetBeans.

<sup>49</sup> Max. resolution and measuring speed of Attension optical tensiometer's camera is (1280 x 1080) px and 2068 fps, respectively.



6. As previously mentioned in Section 3.2, interactions among the world and nanoparticles as well as SDS molecules modelled only the in view of conservation of momentum<sup>50</sup> to ease the computational load on hardware and software in all NetLogo agent-based models, throughout the thesis. Succeeding studies can include other interactions with the aid of more sophisticated computing systems to model the behavior of nanoparticles at solid/liquid interfaces as well as their interactions with the container with aid of EDL, VDW, and steric forces (ST).

In literature, there are numerous studies to define the interactions between nanoparticles and a planar surface. For instance, Petosa et al. described this phenomena using electric EDL, VDW, and ST as in Equation 6.1 to Equation 6.4 [350]. In their study, nanoparticles treated as ideal spherical objects as in this thesis<sup>51</sup>.

$$V_{EDL} = 64 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_r \cdot a_p \cdot \sqrt{\frac{k_B \cdot T}{z \cdot e}} \cdot \Gamma_1 \cdot \Gamma_2 \cdot e^{-\kappa \cdot h} \quad \text{Equation 6.1}$$

$$V_{VDW} = \frac{A_{123} \cdot a_p}{64 \cdot h \cdot \left(1 + \frac{14 \cdot h}{\lambda}\right)} \quad \text{Equation 6.2}$$

$$F_{ST} = 2 \cdot \pi \cdot a_p \cdot \left(\frac{k_B \cdot T}{s^3}\right) \cdot \left\{ \left(\frac{8 \cdot l}{7}\right) \cdot \left[\left(\frac{2 \cdot l}{h}\right)^{\frac{5}{4}} - 1\right] + \left(\frac{8 \cdot l}{7}\right) \cdot \left[\left(\frac{h}{2 \cdot l}\right)^{\frac{7}{4}} - 1\right] \right\} \quad \text{Equation 6.3}$$

$$V_{VDW} = - \int_{\infty}^h F_{ST} dh \quad \text{Equation 6.4}$$

7. In determining the movement of nanoparticles, aggregation and deposition phenomena must be considered. In this thesis, both processes did not taken into account in NetLogo agent-based models due to software and hardware limitations. The development of computational methodologies for modeling of nanoparticle aggregation is a problematic situation so that the aggregation processes can take place

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<sup>50</sup> In thesis, collisions among all agents accepted to be elastic.

<sup>51</sup> The details of nanoparticle design for NetLogo agent-based models represented in Section 4.1.2.

ranging from nanometer scale to the size of the world in NetLogo. In the range of <1 nm, high concentration of chemicals results nucleation and nuclei growth form nanoparticles in the dimension between (10 to 50) nm [351]. At the dimensions between (1 to 100) nm, Brownian motion causes aggregation of nanoparticles developing the local aggregates<sup>52</sup> [352]. For larger scales<sup>53</sup>, shear forces lead to aggregation and breaking of local aggregates. Finally, in the scale of world in NetLogo agent-based models, turbulence governs the aggregation process. Selected experimental studies for aggregation and deposition of nanoparticles in different solutions and at pH values represented in Table 6.1 and Table 6.2, respectively.

8. For this thesis, all experiments held under room temperature and pressure as mentioned in Section 4.1 and Section 8.1.2. Further research can be done to investigate the effects of varying temperature and pressure to surface tension and the results used to create new agent-based models.
9. Hardware that is more powerful can be used for implementing the agent-based models, which will enable to produce more data about the system as well as ease the critical performance problems.
10. Integrated environmental modeling (IEM) is a new concept for defining and managing environmental estimations. EPA defines IEM as “using cross-disciplinary science and computer capabilities to characterize environmental problems in selected levels” [353]. In the future agent-based models implemented throughout this thesis can be used as the components of IEM.
11. The development of more accurate agent-based models needs advanced computational power. The utilization of parallel computing techniques can overcome the restrictions of centralized systems for ABM. Regarding these necessities, parallel and distributed multi-agent model (PDMAS) development environments elaborated to develop and run agent-based models on topologies designed for parallel computing [354]. Recommended PDMAS platforms represented given below,
  - **MACE3J** is a Java-based multi-agent model (MAS) development platform. It can run on multiprocessors and in cluster environments to ensure wide range of scalability. MACE3J developed at University of Illinois [355].

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<sup>52</sup> d = (0.1 to 10)  $\mu\text{m}$

<sup>53</sup> d = (0.01 to 10) mm

- **Java Agent Development Framework (JADE)** consists of modified properties to ease the development and deployment of agent-based models. It can be issued to multiple computers as well as its configuration can be managed through a central GUI. Jade developed at Telecom Laboratory of Italia [356].
  - **RepastHPC** is the component of a MAS suite including other components such as RepastJ and Repast Symphony. It has been particularly intended for high performance computing. RepastHPC developed using C++ programming language at Argonne National Laboratory [357].
12. Finally, the boundaries of thesis that mentioned in Section 3.2 can create awareness and advance new research visions for the future studies. While the modesty of the agent-based models can be considered as a constraint, results emphasize that general response of the surface tension can be represented with ABM.

Table 6.1 Selected experimental studies for nanoparticle aggregation

Nanoparticle	Size, Concentration	Solution	Results	References
B	d = 25 nm C = n/a	20-1000 mM NaCl 0.2-20 mM MgCl <sub>2</sub> 0.2-10 mM CaCl <sub>2</sub>	Aggregation of B nanoparticles exhibited no differences with respect to bigger colloids. The process completed in accordance with DLVO theory [358].	[359]
C <sub>60</sub>	d = n/a C = 0.22 - 2.42 mg/l	0.25-1000 mM NaCl	Phenyl alkyl ester used in the experiments increased the colloidal stability.	[360]
C <sub>60</sub>	d ≤ 200 nm C = 80-140 mg/l	0.005-85 mM NaCl 0.005-85 mM NH <sub>4</sub> Cl 0.005-85 mM CaCl <sub>2</sub> 0.005-85 mM Na <sub>2</sub> SO <sub>4</sub> 0.005-85 mM La(NO <sub>3</sub> ) <sub>3</sub>	Aggregation of C <sub>60</sub> nanoparticles exhibited no differences with respect to bigger colloids. The process completed in accordance with Schulze-Hardy rule [361].	[362]
SWNTs	d = n/a C = 100 mg/l	57.5-570 mM NaCl + 1% SDS 8.78 mM MgSO <sub>4</sub> + 1% SDS 6.9 mM MgCl <sub>2</sub> + 1% SDS 3.8 mM ErCl <sub>3</sub> + 1% SDS	Aggregation of SWNTs vastly prevented by SDS molecules in selected solutions. Any increment in SDS concentration suppressed aggregation.	[363]
TiO <sub>2</sub>	d = 6-7 nm C = 3-10 g/l	500-2000 mM KCl	Aggregation of TiO <sub>2</sub> nanoparticles depends on pH of KCl solution. Process slows at pH values 0.1 to 2.	[364]

Table 6.2 Selected experimental studies for nanoparticle deposition

Nanoparticle	Size, Concentration	Solution	Results	References
B	d = 10-20 nm d <sub>TEM</sub> = 25 nm C = 9 mg/l	0.01-0.4 M NaCl, pH = 5.6	It has observed that the attachment efficiency has been directly increased with IS.	[365]
CuO	d <sub>ELS</sub> = 118-637 nm C = 9 mg/l	0.01 M NaCl, pH = 7	CuO aggregated has been formed in the porous medium and velocity affected the deposition rate and density. SDS enriched the elution process of nanoparticles.	[366]
C <sub>60</sub>	d = 95 nm C = 1-3 mg/l	DI 1 mM CaCl <sub>2</sub> , pH = 7	Transport and deposition processes found to be consistent with DLVO theory [358].	[367]
SWNTs	d <sub>DLS</sub> = 244 nm C = n/a	0.01mM KCl, pH = 5.6, 5.8 0.03-10 mM CaCl <sub>2</sub> , pH = 5.6, 5.8	The effect of physical restraining showed great importance in deposition of SWNTs.	[368]
TiO <sub>2</sub>	d <sub>DLS</sub> = 5 nm d <sub>FCS</sub> = 7-179 nm d <sub>AFM</sub> = 30 nm d <sub>TEM</sub> = 30 nm C = 10 mg/l	1-200 mM NaNO <sub>3</sub> , pH = 3, 5, 9 1-100 mM Ca(NO <sub>3</sub> ) <sub>2</sub> , pH = 3, 9	Strong attractive forces observed at pH values of 3 and 5. General agreement to DLVO theory [358] has been stated for deposition process.	[369]

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## **8. ANNEX: AN ALTERNATIVE APPROACH FOR MEASUREMENT OF SURFACE TENSION AND MODELING ITS RESULTS WITH ARTIFICIAL NEURAL NETWORKS**

### **8.1. An Alternative Approach for Surface Tension Measurement**

In this part of the thesis, an alternative approach to modeling of surface tension has been proposed.

#### **8.1.1. Experimental Preparations**

##### **8.1.1.1. Glassware Cleaning Procedure**

Proper cleaning, sterilization, and surface preparation of laboratory glassware are among the most crucial steps in the experiments since the residual contaminants can affect the experimental results of physicochemical studies. It has been noted that 100 cm<sup>2</sup> of water surface can be contaminated by a single fingertip contact that causes 10% error in the measured value of the surface tension [370]. In this thesis, the key criterion for glassware cleaning is safety, performance, time, ease of handling, and cost. An eleven-step glassware is applied during experimental investigations of the research as follows,

1. Inspect of glassware against cracks and scratches,
2. Rough cleaning applied to glassware using tap water at room temperature,
3. Glassware kept in an ultrasonic water bath (Bandelin Waterbath, Berlin, Germany) with commercial liquid detergent (Cif Power Naturals Spray, Unilever, İstanbul, Turkey) and tap water solution for 20 minutes at room temperature,
4. Glassware washed twice with DI at room temperature,
5. Glassware immersed into acetone (C<sub>3</sub>H<sub>3</sub>COC<sub>3</sub>H<sub>3</sub>, 100% by volume, Merck, Darmstadt, Germany) for 24-hours at room temperature,
6. Glassware washed twice with DI at room temperature,
7. Glassware immersed into acidic peroxide solution which is prepared by mixing equal portions of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>, 50% by volume, Sigma-Aldrich, MO, USA), and sulfuric acid (H<sub>2</sub>SO<sub>4</sub>, 95-98% by volume, Merck, Darmstadt, Germany) for 24-hours at room temperature,
8. Glassware washed twice with DI at room temperature,

9. Glassware immersed into hydrochloric acid (HCl, 37% by volume, Carlo-Erba, Val de Reuil, France) for 24-hours at room temperature,
10. Glassware washed twice with DI at room temperature,
11. Glassware kept in the oven at 105°C for five hours.

All cleaned glassware stored in a sealed borosilicate glass case at room temperature. In each experiment, water-based markers used for labeling the glassware.

#### **8.1.1.2. DI Preparation Procedure**

In the surface tension measurement experiments ultrapure reagent grade one DI used with the compliance of ASTM D1193-99 and ISO 3936 standards [371, 372]. DI generated with Human Power I<sup>+</sup> Scholar-UV water purifier system (Seoul, South Korea) at Hacettepe University Environmental Engineering Research Laboratory with conductivity value of 50.26  $\mu\text{S}/\text{cm}$  at 23.5°C. To promote its specifications to grade one, DI distilled using a heating bath with commercial cooking oil at 175°C. After cooling, the final batch kept in an opaque glass bottle at room temperature for long-term use. For avoiding any contamination and any change of its chemical and/or physical properties, every batch renewed weekly.

#### **8.1.2. Experimental Setups**

The experimental studies of this thesis aim to provide a simple, easy to use, and cost effective device to evaluate the surface tension of numerous solvents as well as track the impacts of nanoparticles and SDS molecules. In addition, the results of the experiments intended to create a groundwork for ABM models in such way that the behavior of surface tension encountered in the experiments will be replicated to all models. In the scope of this objective, several experimental setups and surface tension measurement approaches developed throughout the thesis.

For the primary experimental setup, which is used throughout the thesis, a specially designed V-shaped soda lime glass Pasteur pipettes with different geometries used for observing the changes in surface tension of the selected solvents at room temperature and atmospheric pressure. In all experiments, relative height of the solvent in the V-shaped Pasteur pipette measured for reference. In the experiments DI, chloroform, ethanol, methanol, water from the input and output of a wastewater treatment plant of a cement

factory, water from Eymir Lake used as solvents. Afterwards, 1 and 3 mg/ml of  $\text{Fe}_2\text{O}_3$  nanoparticles and 3 mg/ml SDS molecules added to the solvents, respectively. The relative height changes due to the mentioned procedure determined with various techniques. To observe the dependence of surface tension on inclination, all experiments repeated for  $30^\circ$  and  $60^\circ$  capillary declination angles with respect to normal. All experiments implemented at atmospheric pressure and at room temperature and each replicated for five times, independently. Throughout the experiments, every result exposed to descriptive statistical analysis with the implemented code in MATLAB Statistics and Machine Learning Toolbox as well as IBM SPSS [373, 374].

The experimental setups used for the surface tension measurements are shown in Figure 8.1 and Figure 8.2. The inventory of experiments made with V-shaped Pasteur pipettes are given in Appendix 12. In order to measure the changes in the height of the solvents deposited in V-shaped Pasteur pipettes following measurement approaches used,

- **Measurement Approach-1:** Light emitting diodes<sup>54</sup> (LED) with different intensities and infrared (IR) emitter/receiver sensor pairs ( $\lambda = 700 \text{ nm}$  to  $1 \text{ mm}$ ) used to measure the changes in the height of solvents in the V-shaped Pasteur pipettes due to adjustment in surface tension with the accumulation of nanoparticles. Regrettably, IR receivers ineffectively measured the height of the fluid much below than the needed precision due to insufficient sensitivity of the receiver module, deficient light intensity, and extensive scattering of light through V-shaped Pasteur pipette. In order to increase the light intensity, standard red ( $\lambda = \sim 650 \text{ nm}$ ,  $P = \sim 5 \text{ mW}$ ) and green ( $\lambda = \sim 523 \text{ nm}$ ,  $P = \sim 10 \text{ mW}$ ) lasers used as light sources. Using lasers helped to overcome the abundant intensity problem but failed to minimize the scattering of light through the V-shaped Pasteur pipette for measuring the variation of the light intensity that resembles the surface tension, precisely.
- **Measurement Approach-2:** Photographs of the experiments for resembling the solution levels in the pipette's big and small cones are taken with 10.2 MP Nikon D3000 DSLR camera with 18-55 mm lens for every 60 seconds [375, 376]. The

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<sup>54</sup> LEDs are particular type of diodes that have comparable electrical properties to PN semiconductor junction diodes. LEDs transfer electrical current only in one direction and block in reverse direction so that electrons from the conduction band merge with holes of the valence shell by emitting energy. Finally, photons release monochromatic light in the visible range ( $\lambda = 400$  to  $700 \text{ nm}$ ).



camera secured on a tripod to avoid and if not minimize the effects of vibrations. The distinctions between consecutive photos compared after each photo optimized with the selected image enhancement techniques using Paint .Net freeware [377]. The comparison process accomplished with the code written using MATLAB in cooperation with Image Processing and Image Acquisition Toolboxes [378, 379]. Additionally, randomly selected photos analyzed with Microsoft Visio Professional 2013 to verify and validate the results of the developed code [380].

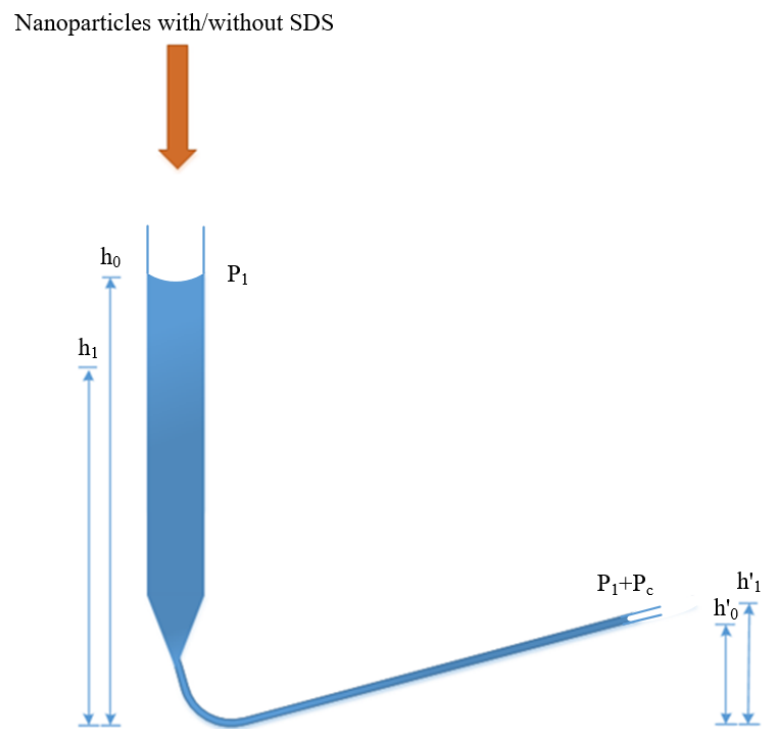
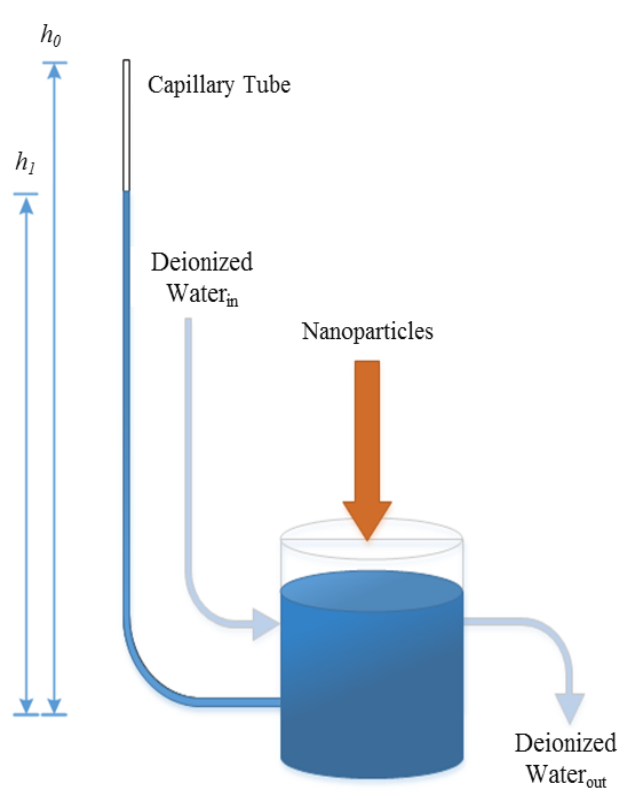
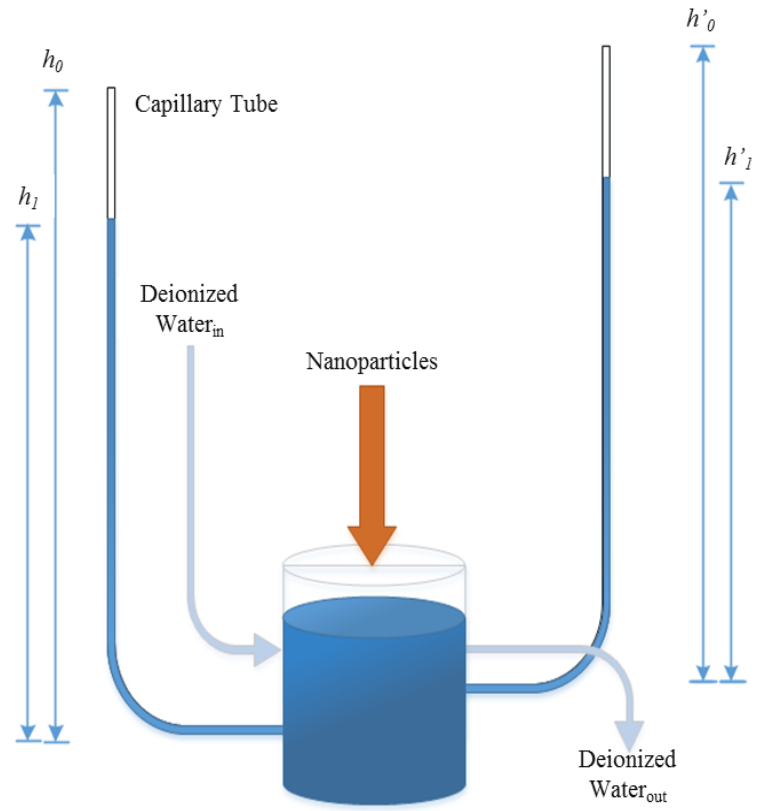


Figure 8.1 Experimental setup-1



(i)



(ii)

Figure 8.2 Experimental setup-2

In all experimental setups mentioned above, ambient temperature and humidity data logged using a DHT-21 sensor mounted on Arduino Uno for every five seconds where the equipment sited [381, 382]. The key component of sensor module is the central processing unit using 16 MHz Atmega328 based board with open source programming capability. The module encoded by Java based open-source Arduino IDE [383]. The overall setup works with 5 V/500 mA, which is supplied from the computer via USB A to B cable. Arduino Uno set to communicate sequentially with the computer via serial port through 9600 bps data transfer rate [382]. The received ambient temperature and humidity data displayed on the computer screen with its time-stamp using RS232 Port Logger Standard in real-time [384]. All data transmission processes logged into UTF-8 encoded text files for the further analysis [289].

### 8.1.3. Experimental Results for V-shaped Pasteur Pipettes

The Pasteur pipette experiments for surface tension measurements carried out at Hacettepe University Environmental Engineering Research Laboratory. The specially designed V-shaped Pasteur pipettes with two different geometries<sup>55</sup> used for measuring the changes of surface tension<sup>56</sup>.

The optical qualities of the Pasteur pipettes show great importance on the experimental results since variation in the height of solutions measured with LED and IR emitter/receiver sensor pairs as well as photo shoots and video footages as defined in Section 8.1.2. For the selection of the most appropriate pipette type, the optical properties of soda lime glass and borosilicate glass evaluated. The soda lime glass has the refractive index of 1.52 which is 5.46% less than borosilicate glass for  $\lambda = 700$  nm. Furthermore, the reflective indexes of soda lime glass and borosilicate glass are  $4.25 \cdot 10^{-2}$  and  $5.36 \cdot 10^{-2}$ , respectively<sup>57</sup> [385]. Regarding these properties, standard soda lime glass pipettes used

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<sup>55</sup> The design of all V-shaped Pasteur pipettes can be seen in Figure 8.1.

<sup>56</sup> All experiments held at room temperature.

<sup>57</sup> In addition, the dispersion formulas of soda lime and borosilicate glasses for  $\lambda = 700$  nm, as follows,

Soda lime glass: 
$$\varphi(\lambda) = -3.17 \cdot 10^{-3} \lambda^2 + 3.96 \cdot 10^{-3} \lambda^{-2} + 1.51$$

Borosilicate glass: 
$$\varphi(\lambda) = \left( \frac{-9.28 \cdot 10^{-3} \lambda^2 + 1.49 \cdot 10^{-2} \lambda^{-2} + 3.78 \cdot 10^{-4} \lambda^{-4} + 1.25 \cdot 10^{-5} \lambda^{-6} +}{7.09 \cdot 10^{-7} \lambda^{-8} + 2.54} \right)^{(1/2)}$$

instead of borosilicate glass pipettes for their refractive index, reflectance coefficient as well as extensive availability and cost, in all experiments.

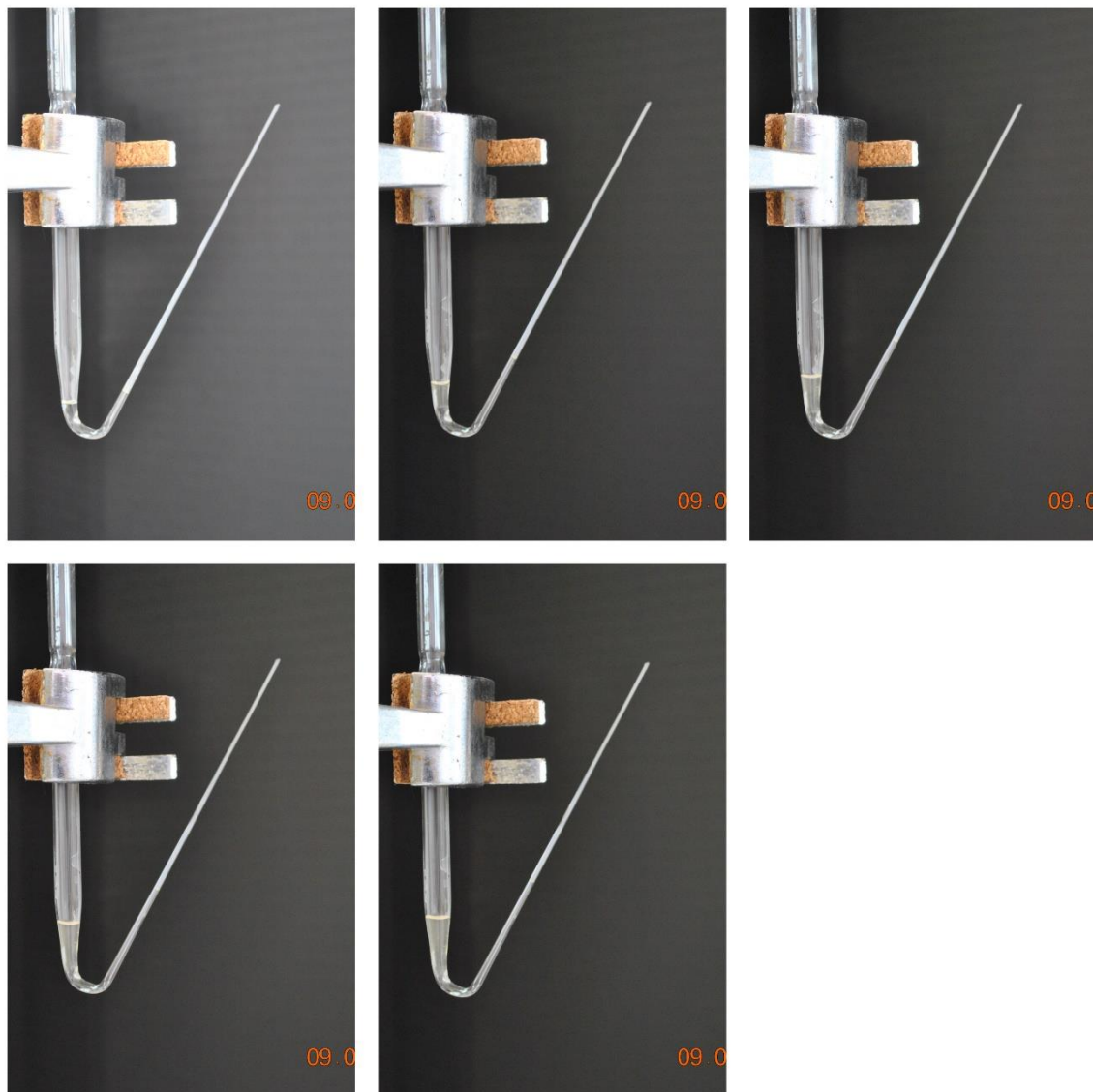


Figure 8.3 Photos of cement factory wastewater treatment input water experiments with 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles,  $\alpha = 60^\circ$

Table 8.1 Total number of ticks and real-time correlated information for an ABM initial test for 10 uncharged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours

NP Count	World Area (patches)	Time (hours)	# Ticks		Average # Ticks ( $10^3$ )	Ticks per hour	Ticks per minute
			1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )			
10	150 x 150	24	732.35	630.48	681.41	28.39	0.47
		48	1,502.58	1,173.06	1,337.82	27.87	0.46
	250 x 250	24	273.94	237.45	255.69	10.65	0.18
		48	551.97	371.62	461.79	9.62	0.16
	350 x 350	24	119.94	133.85	126.89	5.29	0.09
		48	269.72	218.43	244.08	5.09	0.08

Although, both Pasteur pipettes are identical and selected from the same batch, the principal distinction rises from the declination angles of the narrow ends of the pipettes. Each pipette bended by hand with using Bunsen burner to create 30° and 60° slopes with respect to normal. An example of a Pasteur pipette with 60° inclination presented in Figure 8.4. Before every experiment, all pipettes prepared in accordance with the glassware cleaning procedures mentioned in Section 4.1. In the experiments, various SDS concentrations and amounts of nanoparticles added to DI, methanol, input and output water of cement factory wastewater treatment plant, and water from Eymir Lake to determine their effects on the relative solution level variation in the narrow end of the V-shaped Pasteur pipettes.

The maximum number of measurements managed to record through all experiments is five. The reasons for the reduced amount of recordings are the volume of the Pasteur pipette and insufficiency of the experimental environment and equipment. Even though, five recordings are inadequate to calculate the surface tension precisely, they assist to yield the characteristic effects of SDS molecules and nanoparticles on selected solutions. Additionally, it has been observed that every set of experiment is consistent with each other.

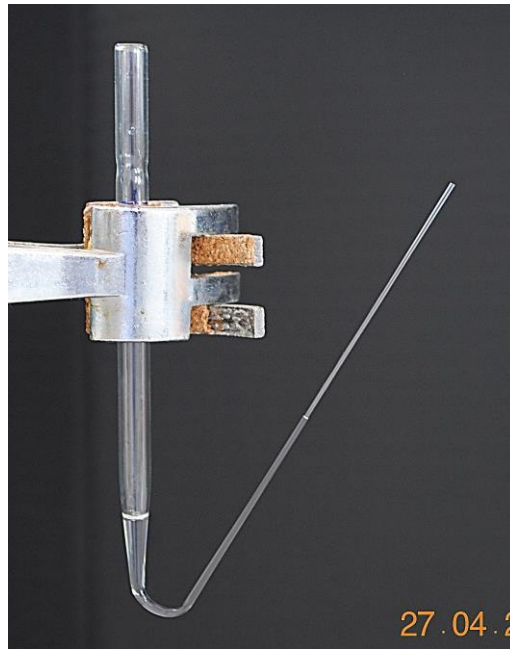


Figure 8.4 The V-shaped Pasteur pipette with 60° inclination

## 8.2. Surface Tension Modeling with Artificial Neural Networks

ANNs inspired from the human brain's problem-solving methods by simulating the behavior of biological neurons to perform calculations through digitally simulated neurons [386, 387]. The most important advantage of ANNs is that they are capable of implementing models without large amounts of data obtained from the system and the information about the underlying processes. ANNs consent the realistic modeling of a system of objects with distinctive properties such as size, mass, electrostatic charge, combined with interactions among them, as well as the environmental properties such as density and geometry<sup>58</sup>. The additional benefits of ANNs are that they represent significant amount of fault tolerance and parallelism in modeling.

The history of ANNs dates back to 1940s, which coincides the invention of the computers. In 1943, McCulloch and Pitts constructed the earliest neurological networks inspired from neurons and showed their logic and arithmetic proficiencies [388]. Hebb designed a framework for the digital representation of short and long term memories positioned in the nervous system known as "Hebbian rule" and this rule accepted as the origin of neural learning techniques [389]. In 1958, Rosenblatt designed the "perceptron" which is a two-

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<sup>58</sup> Detailed object definitions of ANN models explained in Section 8.2.

layer neural network that can learn specific categorizations with varying connection weights [306]. However, ANNs incapability of solving “exclusive or” (XOR) problems and other limitations led to the deterioration of their popularity. From the early 1980s, the interest in ANNs gained momentum once more and since then many advances made in the applications of ANN. Some of the contemporary research areas include Boltzmann machines, competitive learning models, and multilayer networks [307, 381].

There are various ANN topologies such as feedforward and feedback (recurrent) networks. Basic classification of ANNs can be seen in Figure 8.5 [390].

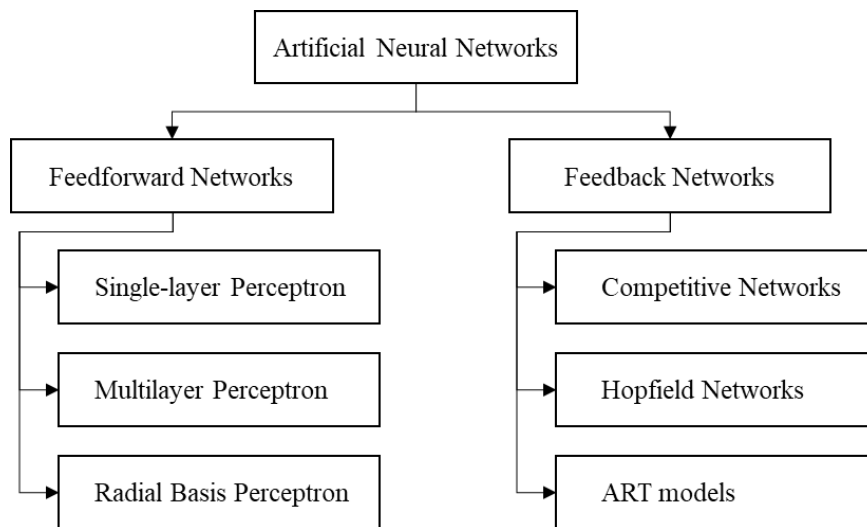


Figure 8.5 Basic classification of ANNs [390]

ANNs comprises of numerous layers of straightforward processors that transfer intelligence among layers. For instance, in a feedforward network input layer collects data and transfers it through succeeding hidden layers until a meaningful result emerges from the output layer as in Figure 8.6.

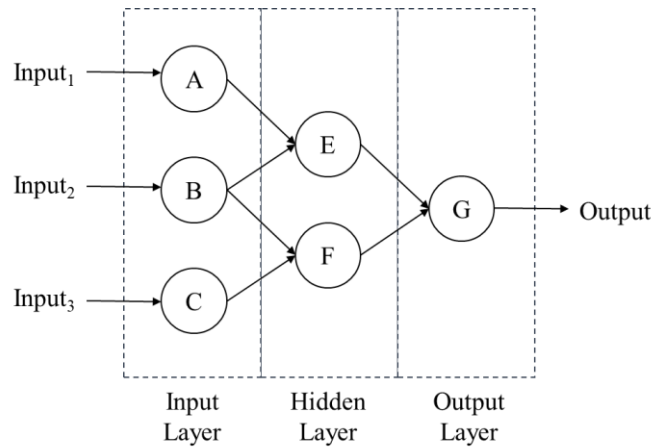


Figure 8.6 Basic feedforward ANN topology

Although, there are no *de facto* methods to calculate the optimum hidden layers count, there are studies on this subject such as Information Criterion (AIC) and its generalized version entitled as Network Information Criterion (NIC) [391, 392]. Correspondingly, Xu and Chen derived a relation to calculate the number of hidden layer nodes as in Equation 8.1 [393].

$$n = C \sqrt{\frac{N}{d \cdot \log N}} \quad \text{Equation 8.1}$$

Where,  $n$  is number of hidden nodes,  $d$  is input dimension,  $N$  is number of training pairs, and  $C$  is constant. Furthermore, if the number of hidden layers and nodes designed to be insufficient, ANNs will be unable to create a satisfactory input-output relation mapping. On the other side, if too many hidden layers are used for harvesting meaningful information, overfitting can occur. In this case, ANNs can be trained to operate thoroughly for training data but it presents poor performance for test data. It can be concluded that ANNs will not able to generalize the inputs as expected. In order to eliminate the overfitting problem, the smallest-sized ANNs must be used which can be attributed to Ockham's Razor<sup>59</sup> [394].

<sup>59</sup> Ockham is a 13<sup>th</sup> century philosopher lived in England and his well-known Ockham's Razor argument expresses that "entities should not be multiplied beyond necessity". An additional Ockham inspired quote about his idea, which is also consistent with the previous one can be stated as "plurality should not be postulated without necessity". This argument can be used as a reference to avoid unnecessary complexity in modeling, as mentioned in previous pages.



Feedforward ANNs are data based modeling approaches that can model the non-linear behaviors of a system using selected activation functions. In feedforward ANNs, data flow is strictly unidirectional and there is no information feedback. The total number of layers is not restricted and there are limitations of connections as well as type of transfer functions in ANN topology. ANNs of this type extensively used in pattern and handwriting recognition and classification [395]. Differing from feedforward ANNs, feedback ANNs have bidirectional modeling topologies. Principally, they are feedforward ANNs with back loops. In this these neural networks, signal does not transfer forward only. This circumstance exhibits a temporary dynamic state in network, which persistently changes until the equilibrium conditions occur. The basic topology of feedback ANNs can be seen in Figure 8.7 [396].

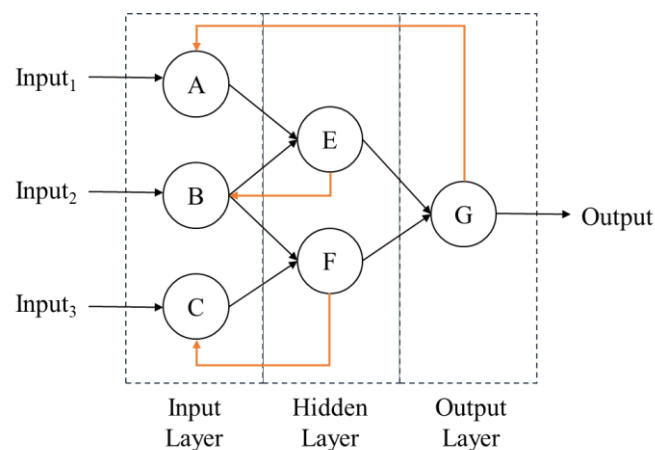


Figure 8.7 Basic feedback ANN topology

There are numerous studies involving comparison of performance and reliability of ANNs with other modeling/prediction approaches for diverse research areas. For instance, La Delfa and Potvin compared ANN and regression models in biomechanics to predict manual arm strength [397]. Data gathered from 95 participants used to evaluate the calculations and results showed that ANN predictions were more dependable than other modeling techniques. Kumar et al. matched up ANN and regression models for monthly average global solar radiation forecasts [398]. It has been found that ANN models yielded lower mean absolute percent error (MAPE) and higher R-values than regression models. Fragkaki et al. made comparisons among ANN, partial least squares,

and multiple linear regression (MLR) methods for the estimation of gas chromatographic relative retention times for trimethylsilylated (TMS) anabolic androgenic steroids [399]. ANN models returned the best root mean squares error (RMSE) values among all other methods. Tiryaki and Aydin used ANN models to calculate the compression strength of heat treated spruce, pine, chestnut, beech woods and compared with MLR method.  $R^2$  and MAPE values of ANN models calculated as 0.997% and 2.641%, respectively [400]. Results showed that ANN models yielded higher prediction rate than MLR model. Neto and Fiorelli worked on assessing the difference between ANN models and heating, ventilating, air conditioning (HVAC) design and simulation software EnergyPlus that used to forecast the energy consumption of University of São Paulo Administration Building [401, 402]. The results showed that ANN models are more suitable for energy consumption modeling. EnergyPlus forecasts yielded an error of  $\pm 13\%$  compared to ANN models' 10%. Abbasi et al. used experimental data to conjecture the best approach to determine the deformation of mouse embryos under needle injection [403]. ANN, analytical Jacobian, and nonlinear least square models returned the correlation coefficients of 0.9998, 0.9985, and 0.9964, respectively. Results showed that ANN model results superior to define embryo dimple depth by needle injection.

In addition to the above mentioned research areas ANNs broadly used in environmental sciences, as well. For instance, Birikundavyi et al. investigated the performance of ANNs for the forecasting of daily stream flows of Mistassibi River (Canada). Maier and Dandy used ANNs for the salinity estimation of River Murray (South Australia) for 14 days in advance [404, 405]. Kuo et al. and Chang et al. both studied with ANNs to forecast the effects of groundwater quality on the Blackfoot disease, which is often witnessed in southwestern Taiwan [386, 387]. Verma and Singh studied on the water quality parameters, particularly on BOD and COD via simple field parameters like temperature, and pH, etc. [406].

Adams et al. used ANN models within a framework that is inspired by land use regression for mapping real-time air pollution health risk for environmental management with mobile and stationary air pollution monitoring data recorded at Hamilton, Ontario [407].

Table 8.2 Potential applications of ANN for Natural Language Processing

Potential Applications	References
Character Recognition	[408, 409]
Language Generation and Multi-document Summarization	[410, 411]
Machine Translation	[412, 413]
Paraphrase Detection	[414, 415]
Part-of-Speech Tagging	[416, 417]
Semantic Parsing and Question Answering	[418, 419]
Speech Recognition	[420, 421]
Spell Checking/Correction	[422, 423]
Text/Document Classification and Categorization	[424, 425]

Regarding its advantages over other modeling techniques and wide spread practices, ANNs are rapidly gaining popularity to predict surface tension values, as well. Selected studies from literature in chronological order as follows,

Xu et al. studied surface tension modelling of branched alkanes using multilayer perceptron (MLP) and radial basis function (RBF) ANN models [426]. In this study, surface tension values of branched alkanes gathered from literature. The surface tension data organized so that 143 and 36 of them used for training and testing processes. The selected inputs of the both ANN models are types of alkanes, critical temperature, and ambient temperature (283.15 to 448.15 K). Results yielded that both ANN models successfully revealed expected surface tension values, though MLP ANN model found to be more accurate than others.

Lashkarbolooki and Bayat also studied on the surface tension prediction of alkanes with ANN models [427]. In their study, liquid normal alkanes, 1-alkenes, and cycloalkane modelled with Levenberg-Marquardt (LM) algorithm using linear transfer and hyperbolic tangent functions for the hidden and output layers, respectively [428]. Results showed that the developed ANN model was competent to predict and correlate the  $\sim 5.46 \times 10^3$  surface tension data of all three types of alkanes as a function of temperature. The overall surface tension data divided into two subsets to be used in training and test as 4,095 and 1,366 data points, respectively.

Soleimani et al. studied on the prediction of surface tension values of binary mixtures containing ionic liquids with an ANN model [429]. The experimental data employed for modeling consisted of 748 binary surface tension data points at atmospheric pressure were assembled from the National Institute of Standards and Technology (NIST) Standard Reference Database [430]. The ANN model based on two hidden layers that trained by using *trainbr*<sup>60</sup> training function and used for the surface tension prediction of binary mixtures containing 31 ionic liquids [431].

Gharagheizi et al. used ANN methods to forecast the surface tension of pure chemical compounds at various temperatures and atmospheric pressures [432]. In their study, more than  $4.5 \times 10^3$  surface tension data that belongs to 752 chemical compounds gathered from DIPPR. Three-layer feedforward ANN developed using MATLAB Deep Learning Toolbox (formerly Neural Network Toolbox) to predict the surface tension of 78 chemicals containing 151 functional groups that consist of organic and inorganic liquids. Results showed that adequate outcomes gained from models [388].

Pazuki et al. studied on developing a MLP back-propagation ANN model for predicting the surface tension of pure hydrocarbons [428, 433]. The model developed with using 211 experimental surface tension data from the literature and used temperature, pressure, and molecular weight as inputs. Comparison of model results with the experimental data yielded satisfactory results to use ANNs for the calculation of surface tension.

Roosta et al. predicted the pertinence of ANN models to predict the surface tension of pure organic compounds for diverse set of temperatures [129]. Models created with MATLAB Deep Learning Toolbox (formerly Neural Network Toolbox) put into operation for 82 compounds containing alkenes, alkanes, aromatics as well as sulfur, chlorine, fluorine, and nitrogen to correlate the critical pressure, temperature, and specific gravity at the normal boiling point with surface tension [388]. Results showed that ANN model with one hidden layer and 20 neurons was the most suitable model for the determination of surface tension.

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<sup>60</sup> It is an ANN training function, which renews the bias and weight coefficients in accordance with Levenberg-Marquardt optimization technique. This function minimizes the values of squared errors and weights, and determines the ideal combination to develop a generalized ANN. The overall method called Bayesian regularization.

Melo-Espinosa et al. worked on modeling the properties that establish connection between the surface tensions of 15 different vegetable oils and their fatty acid compositions regarding their importance on the quality of the fuel atomization process in diesel engines [434]. ANN and MLR models developed with experimental data available in the literature. As a result, the lowest absolute mean error values obtained with ANN models. On the contrary, the coefficient of correlation of MLR model was higher than the ANN models.

Zhang et al. studied on gas-water interfacial tension calculations for petroleum industry [435]. Three-layer network ANN model designed and trained with LM algorithm to evaluate interfacial tension of pure methane ( $\text{CH}_4$ ) and synthetic natural gas [428]. Experimental data gathered from literature that used pendant drop method or rising bubble methods. ANN models compared to multivariate parametric regression (MPR) models developed with using independent variables such as temperature, pressure, mole fractions of the gas compositions, and salt (NaCl). As a result, ANN models performed better the beyond MPR models.

Movagharnejad et al. predicted the surface tension of 61 hydrocarbons using feedforward ANN model with LM back-propagation algorithm with MATLAB Deep Learning Toolbox (formerly Neural Network Toolbox) [388, 428, 436]. In the model, temperature, critical temperature, critical pressure, boiling point temperature, and molecular weight of each hydrocarbon selected as inputs and gathered from the Landolt and Börnstein's paper [437]. Finally, the comparison of ANN model with empirical equations yielded that the accuracy of the ANN model was better than the mentioned equations.

Mulero et al. predicted the surface tension of alcohols with ANN. Selected data for 147 alcohols used for training, validating, and testing for the ANN model that consisted temperature, critical point temperature, critical density, and radius of gyration as independent input variables [438]. Finally, mean absolute percentage deviation calculated as 1.04% that yielded better results than corresponding-states principles. In another study, Mulero et al. studied on the surface tension of 76 refrigerants at the liquid-gas interface [439]. In the ANN models, reduced temperature, critical temperature, critical pressure, and acentric factor used as independent variables. Overall mean absolute percentage deviation of the models computed as 1.64%.

Nabipour and Keshavarz designed a feed-forward back-propagation neural network model to predict the surface tension of 24 pure refrigerants with several training algorithms [440]. All models used the same inputs such as temperature, critical temperature, critical pressure, and acentric factor. The outcomes of the models showed that the ANN models ability to estimate the surface tension values of refrigerants precisely with an overall MRE and R<sup>2</sup> values of as 0.0074 and 0.9996, respectively.

In the previous paragraphs, the advantages of ANNs mentioned with referencing to selected studies from literature. On the other hand, there are disadvantages of ANNs such as [441],

- ANN models are “black boxes<sup>61</sup>” that have inadequate ability to classify possible relationships among entities,
- ANN models require abundant computational resources,
- ANN models do not perform well and yield significant results on small data sets<sup>62</sup>,
- ANN models do not guarantee the correctness, precision and acceptability of the results,
- ANN models have the challenges in introduction of real world phenomenon to the problem to the network,
- Computing duration of ANN models cannot be definitely predictable,

### **8.2.1. Artificial Neural Network Modeling for Surface Tension throughout the Thesis**

MATLAB Deep Learning Toolbox (formerly Neural Network Toolbox) and its built-in Nonlinear Autoregressive (NAR) method with error backpropagation algorithm used for creating ANN models [388, 389]. NAR method deals with the implementation of models with time dependent data series, which is useful for predicting values from the past values of the data series. This method can be formulated in Equation 8.2 and Equation 8.3.

$$\theta(t) = f(\theta(t - 1), \theta(t - 2), \dots, \theta(t - n)) \quad \text{Equation 8.2}$$

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<sup>61</sup> Black box is the repetitively changing part of the ANN model, which cannot clearly be examined.

<sup>62</sup> In this thesis, insufficient number of experimental data gathered for the experiments held at Hacettepe University Environmental Engineering Research Laboratory, which led to inconsistent results to determine surface tension with ANN models.

$$\theta(t) = \int_{i=1}^{\infty} f(\theta(t-i))dt \quad \text{Equation 8.3}$$

In the ANN modeling technique following variables used as inputs,

- Initial height of the solvent in both ends of the V-shaped Pasteur pipette with respect to ground,
- Final height of the solvent in the V-shaped Pasteur pipette with respect to ground after addition of nanoparticles and SDS molecules to the selected solvent,
- Initial volume of the solvent in the V-shaped Pasteur pipette,
- Volume of the solvent infused to V-shaped Pasteur pipette at each addition of nanoparticles and SDS molecules with the selected solvent,
- Total masses of the nanoparticles added to V-shaped Pasteur pipette at every infusion,
- Declination angle of the custom made V-shaped Pasteur pipette with respect to normal,
- Ambient temperature and pressure,
- Time.

Although, the ANN models designed as mentioned in earlier, the insufficient number of data for each variable led to inconsistent results to determine surface tension. The original design of the ANN models consist of eight input variables, which gathered from different sources as, mentioned in Table 8.3.

In view of the fact that the manual measurement period of the each infusion is 60 s, for each experiment total number of data gathered for height and weight of the solution in the V-shaped Pasteur pipette did not exceed five. For instance, in cement factory wastewater treatment input water experiments with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles, total number of photos are taken is five.

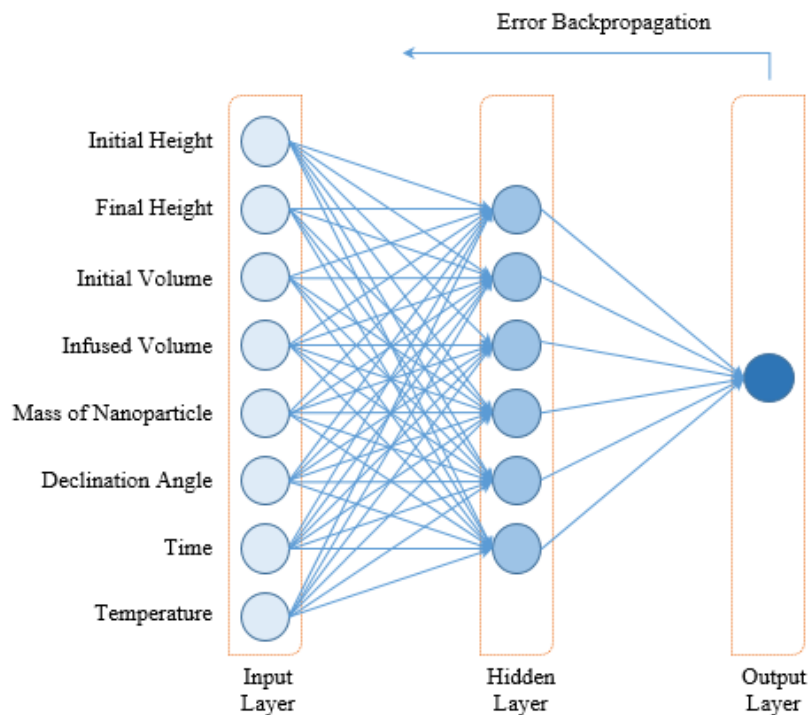


Figure 8.8 ANN topology used in surface tension modeling

Table 8.3 Input data and their sources for ANN models

Variable	Source
Initial height of solution in V-shaped Pasteur pipette	Photos taken with 10.2 MP Nikon D3000 DSLR camera with 18-55 mm Zoom-NIKKOR VR Image Stabilization Lens [375, 376]
Final height of solution in V-shaped Pasteur pipette	
Initial volume of solution in V-shaped Pasteur pipette	Measured with micropipette
Infused volume of solution in V-shaped Pasteur pipette	
Mass of nanoparticles added to V-shaped Pasteur pipette	Measured with balance
Time	Dedicated timer software installed on computer [442]
Temperature	Measurement setup designed with DHT-21 sensor mounted on Arduino Uno [382]



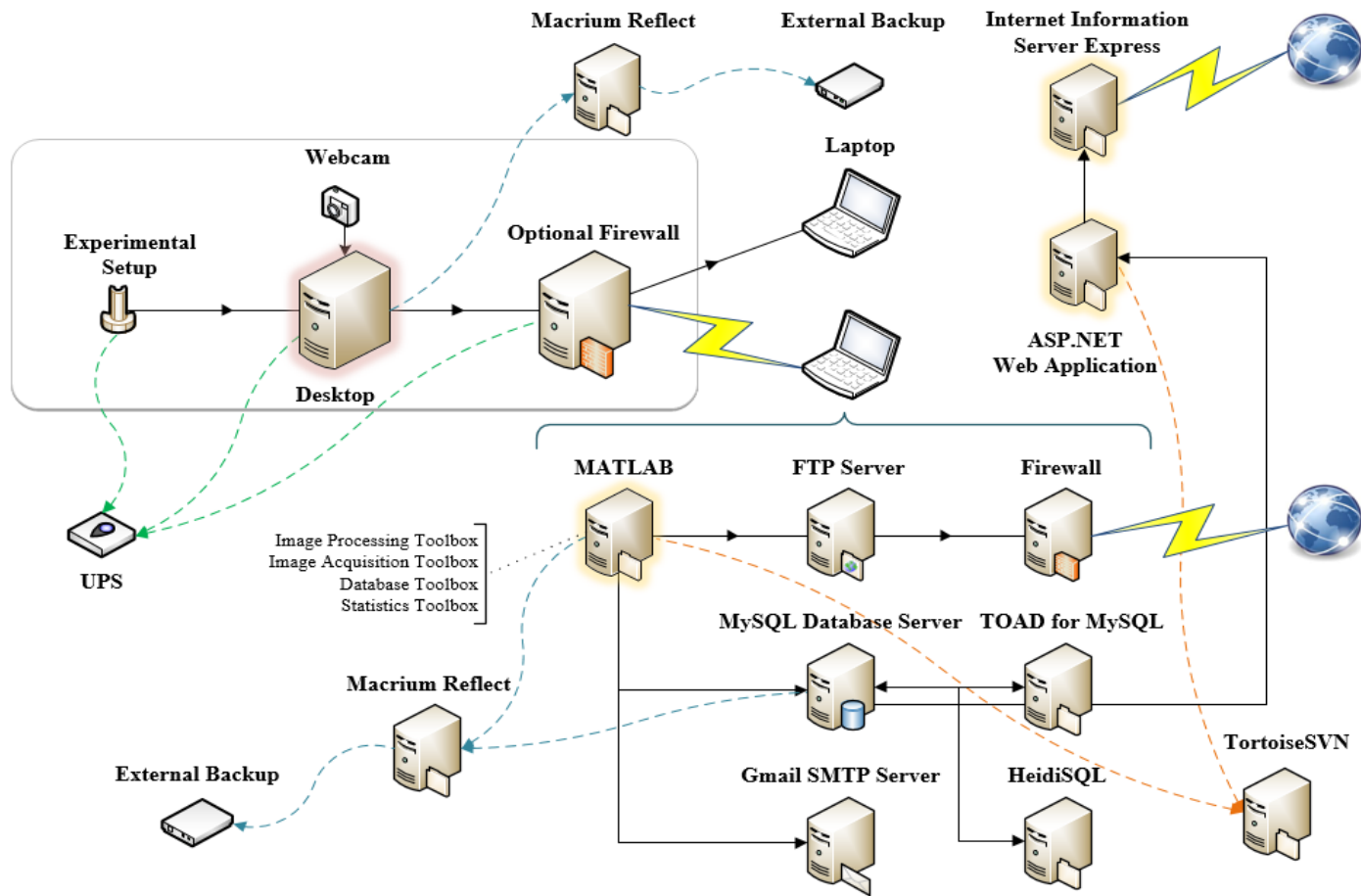


Figure 8.9 Computer topology for recommended experimental setup

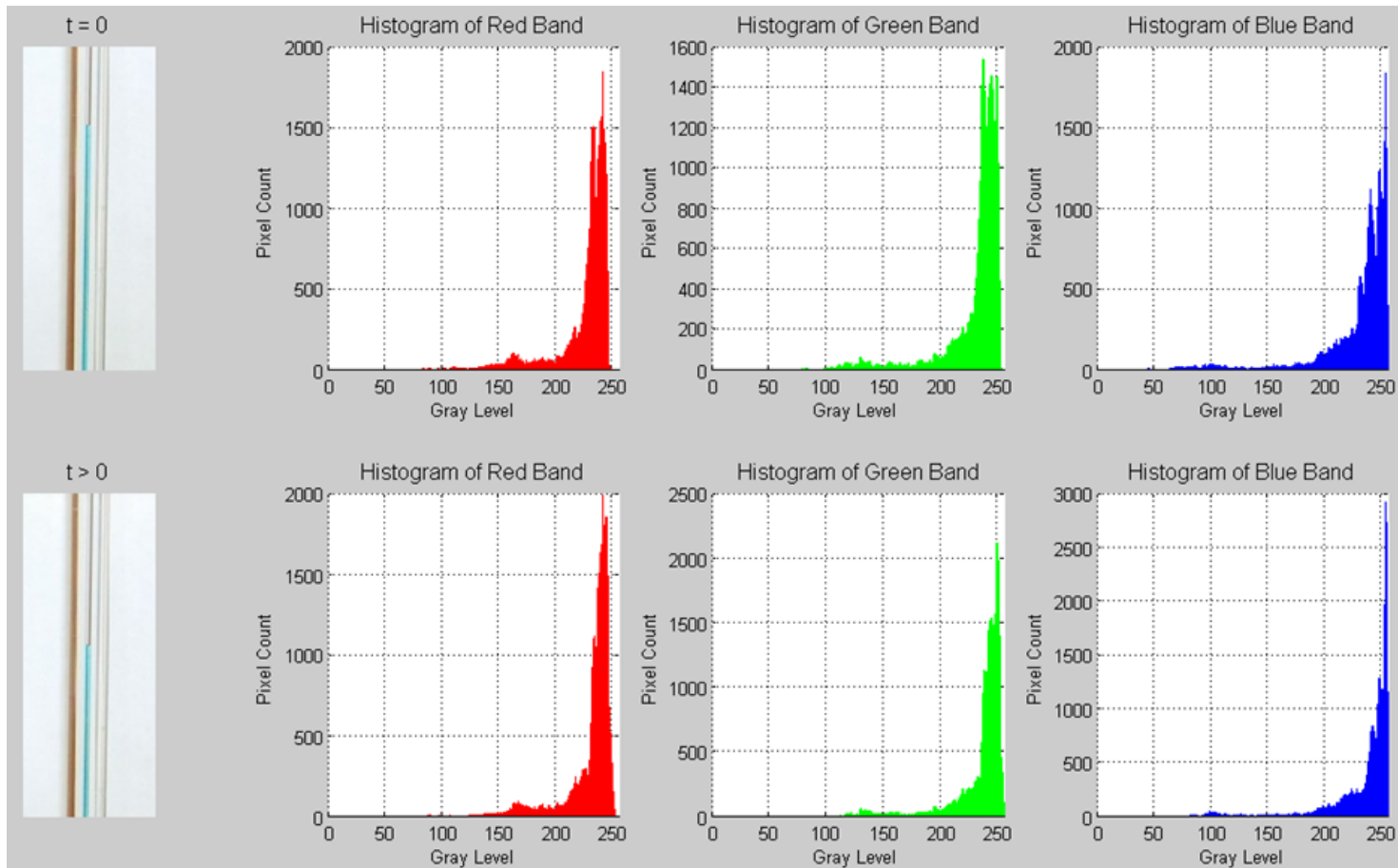


Figure 8.10 MATLAB output for recommended experimental setup-1

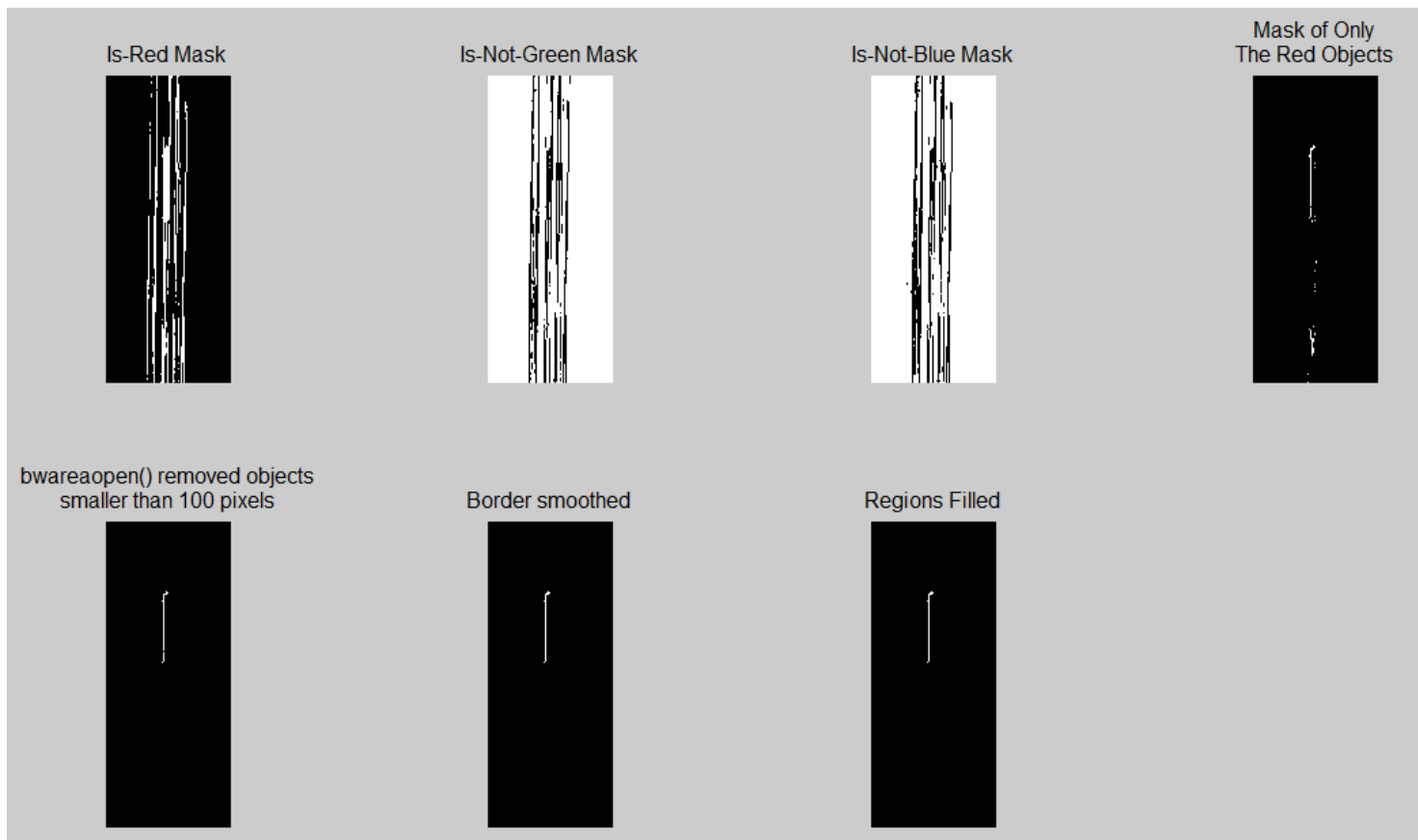


Figure 8.11 MATLAB output for the recommended experimental setup-2

## APPENDIX

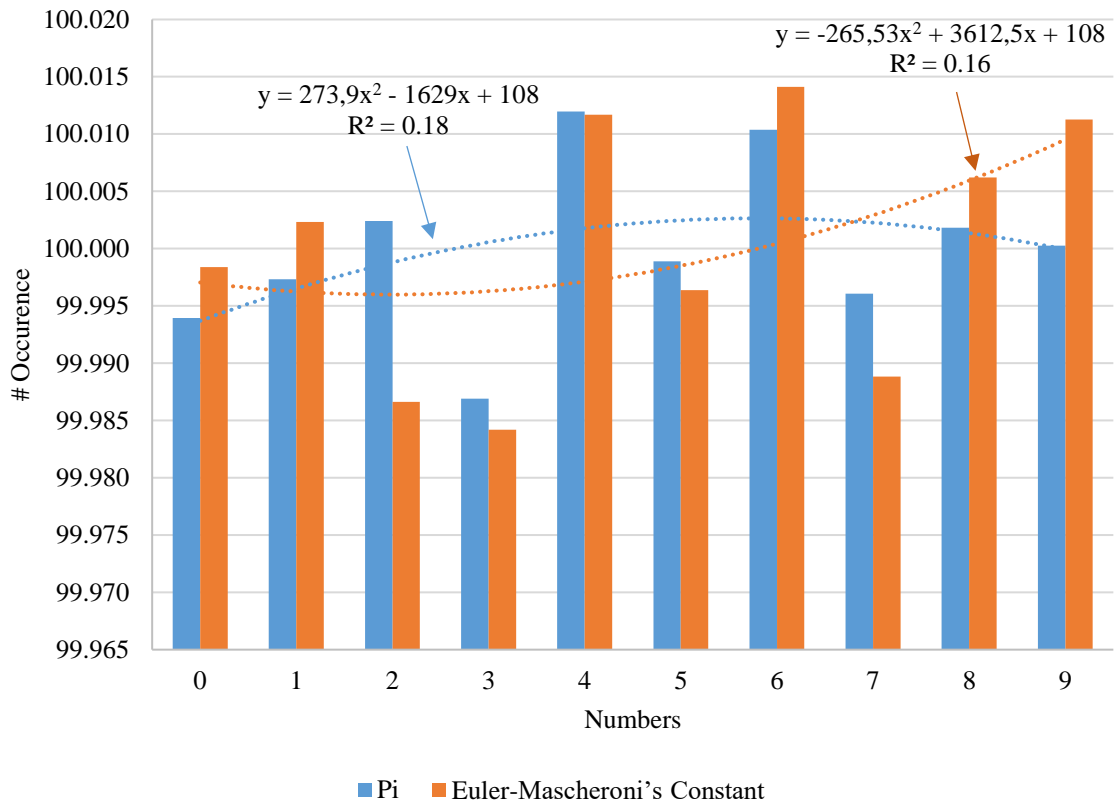
### APPENDIX 1 - Total Number of Occurrences and Frequency Distribution of $10^9$ Decimal Digits of Pi and Euler-Mascheroni's Constant

Frequency distribution of pi number's decimal digits

Number	Distribution of Decimal Digits (%)						
	$10^3$ Digits	$10^4$ Digits	$10^5$ Digits	$10^6$ Digits	$10^7$ Digits	$10^8$ Digits	$10^9$ Digits
0	9.30	9.68	10.00	10.00	9.99	10.00	10.00
1	11.60	10.26	10.14	9.98	9.99	10.00	10.00
2	10.30	10.21	9.91	10.00	10.00	10.00	10.00
3	10.20	9.74	10.03	10.02	10.00	10.00	10.00
4	9.30	10.12	9.97	10.02	10.01	10.00	10.00
5	9.70	10.46	10.03	10.04	10.00	9.99	10.00
6	9.40	10.21	10.03	9.95	9.99	10.00	10.00
7	9.50	9.70	10.03	9.98	10.00	10.00	10.00
8	10.10	9.48	9.98	10.00	10.00	10.00	10.00
9	10.60	10.14	9.90	10.01	10.00	10.00	10.00

Frequency distribution of Euler-Mascheroni constant's decimal digits

Number	Distribution of Decimal Digits (%)						
	$10^3$ Digits	$10^4$ Digits	$10^5$ Digits	$10^6$ Digits	$10^7$ Digits	$10^8$ Digits	$10^9$ Digits
0	11.10	10.04	10.07	10.02	10.00	10.00	10.00
1	9.50	10.06	9.97	10.01	10.01	10.00	10.00
2	9.70	9.67	9.82	9.98	9.99	10.00	10.00
3	10.80	9.76	9.97	10.02	10.01	10.00	10.00
4	9.00	10.14	9.87	9.98	10.01	10.01	10.00
5	9.90	9.80	10.20	10.01	10.02	10.00	10.00
6	9.00	9.88	10.10	10.02	10.00	10.00	10.00
7	11.60	10.14	9.88	9.97	9.99	10.00	10.00
8	8.10	10.33	10.11	10.01	9.99	10.00	10.00
9	11.30	10.18	10.00	9.98	10.00	10.00	10.00



Frequency distribution comparison of  $10^6$  decimal digits of pi and Euler-Mascheroni's constant

## APPENDIX 2 - Density of Solvents Used in NetLogo Models

Solvent	Chemical Formula	Density (kg/m <sup>3</sup> )	Type	Ratio
Ammonia	NH <sub>3</sub>	823.50	Hydrophilic	0.82
Benzene	C <sub>6</sub> H <sub>6</sub>	873.80	Hydrophobic	0.87
Chloroform	CHCl <sub>3</sub>	1,465.00	Hydrophobic	1.47
Creosote		1,066.83	Hydrophobic	1.07
Heptane	C <sub>7</sub> H <sub>16</sub>	679.50	Hydrophobic	0.68
Hexane	C <sub>6</sub> H <sub>14</sub>	654.80	Hydrophobic	0.65
Pentane	C <sub>5</sub> H <sub>12</sub>	625.00	Hydrophobic	0.63
Propane	C <sub>3</sub> H <sub>8</sub>	494.00	Hydrophobic	0.49
Sea water		1,025.00	Hydrophobic	1.03
Toluene	CH <sub>3</sub> -CH <sub>3</sub>	867.00	Hydrophobic	0.87
Water	H <sub>2</sub> O	1,000.00	Hydrophilic	1.00
Xylene	C <sub>8</sub> H <sub>10</sub>	860.20	Hydrophobic	0.86

### APPENDIX 3 - ABM Initial Test Results for Uncharged Nanoparticles

Total number of ticks in ABM initial tests for 10, 100, and  $1 \times 10^3$  uncharged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

NP Count	World Area (patches)	Time (hours)	# Ticks		Average ( $10^3$ )
			1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	
10	150 x 150	24	732.35	630.48	681.41
		48	1,502.58	1,173.06	1,337.82
	250 x 250	24	273.94	237.45	255.69
		48	551.97	371.62	461.79
	350 x 350	24	119.94	133.85	126.89
		48	269.72	218.43	244.08
100	150 x 150	24	731.65	615.80	673.72
		48	1,484.94	972.68	1,228.81
	250 x 250	24	225.40	242.83	234.12
		48	479.93	415.23	447.58
	350 x 350	24	193.16	115.63	154.40
		48	247.00	184.47	215.73
$1 \times 10^3$	150 x 150	24	613.39	674.13	643.76
		48	1,293.64	927.89	1,110.77
	250 x 250	24	224.48	227.31	225.90
		48	471.92	380.29	426.10
	350 x 350	24	132.81	117.48	125.14
		48	250.75	181.61	216.18

Distribution of two, three, and four-body collisions ABM initial tests with respect to quadrants for 10, 100, and  $1 \times 10^3$  uncharged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours worlds for 24 and 48-hours at 25°C

NP Count	World Area (patches)	Time (hours)	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
			2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
10	150 x 150	24	98.78	1.22	0.00	98.94	0.79	0.26	98.86	1.01	0.13
		48	99.68	0.32	0.00	99.03	0.97	0.00	99.36	0.65	0.00
	250 x 250	24	96.98	2.68	0.34	98.53	1.47	0.00	97.76	2.08	0.17
		48	97.31	2.69	0.00	94.74	4.09	1.17	96.03	3.39	0.59
	350 x 350	24	95.38	3.85	0.77	97.32	2.68	0.00	96.35	3.27	0.39
		48	98.15	1.85	0.00	95.00	4.44	0.56	96.58	3.15	0.28
100	150 x 150	24	98.78	1.22	0.00	98.33	1.35	0.32	98.56	1.29	0.16
		48	99.35	0.63	0.02	98.85	0.93	0.23	99.10	0.78	0.13
	250 x 250	24	95.10	3.79	1.11	95.92	3.37	0.72	95.51	3.58	0.92
		48	97.17	2.69	0.14	96.37	2.92	0.71	96.77	2.81	0.43
	350 x 350	24	93.98	4.73	1.29	93.82	4.82	1.35	93.90	4.78	1.32
		48	95.74	4.14	0.11	94.35	4.51	1.14	95.05	4.33	0.63
$1 \times 10^3$	150 x 150	24	97.96	1.69	0.35	98.17	1.52	0.31	98.07	1.61	0.33
		48	98.47	1.04	0.49	98.50	1.26	0.24	98.49	1.15	0.37
	250 x 250	24	94.44	4.44	1.12	94.51	4.44	1.05	94.48	4.44	1.09
		48	95.65	3.49	0.86	95.47	3.64	0.90	95.56	3.57	0.88
	350 x 350	24	92.92	5.65	1.43	92.74	5.83	1.43	92.83	5.74	1.43
		48	96.41	3.40	0.18	93.33	5.33	1.34	94.87	4.37	0.76



#### APPENDIX 4 - ABM Initial Test Results for Same-charged Nanoparticles

Total number of ticks in ABM initial tests for 10, 100, and  $1 \times 10^3$  same-charged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours

NP Count	World Area (patches)	Time (hours)	# Ticks		Average ( $10^3$ )
			1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	
10	150 x 150	24	316.67	627.11	471.89
		48	1,232.52	713.56	973.04
	250 x 250	24	123.60	242.52	183.06
		48	510.61	249.91	380.26
	350 x 350	24	61.38	124.50	92.94
		48	237.73	128.82	183.28
100	150 x 150	24	302.48	693.15	346.73
		48	1,193.82	687.95	940.89
	250 x 250	24	119.23	257.63	188.43
		48	449.98	232.10	682.08
	350 x 350	24	64.90	117.04	90.97
		48	228.05	122.82	350.87
$1 \times 10^3$	150 x 150	24	266.21	512.44	389.33
		48	1,078.08	552.05	815.07
	250 x 250	24	106.05	207.84	156.95
		48	402.98	216.10	309.51
	350 x 350	24	54.62	123.67	89.14
		48	225.83	112.04	168.94

Total number of two, three, and four-body collisions in ABM initial tests for 10, 100, and  $1 \times 10^3$  same-charged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

NP Count	World Area (patches)	Time (hours)	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
			2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )
10	150 x 150	24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	250 x 250	24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	350 x 350	24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
100	150 x 150	24	0.04	0.00	0.00	0.07	0.00	0.00	0.55	0.00	0.00
		48	0.13	0.00	0.02	0.08	0.00	0.00	0.10	0.00	0.01
	250 x 250	24	0.03	0.00	0.00	0.02	0.00	0.00	0.03	0.00	0.00
		48	0.03	0.00	0.00	0.03	0.00	0.00	0.03	0.00	0.00
	350 x 350	24	0.02	0.00	0.00	0.02	0.00	0.00	0.02	0.00	0.00
		48	0.04	0.00	0.00	0.02	0.00	0.00	0.03	0.00	0.00
$1 \times 10^3$	150 x 150	24	182.94	0.27	0.01	349.81	0.47	0.01	266.37	0.37	0.01
		48	735.91	0.95	0.01	378.28	0.47	0.01	557.10	0.71	0.01
	250 x 250	24	3.08	0.02	0.00	0.47	0.04	0.00	3.55	0.03	0.00
		48	7.74	0.03	0.01	4.84	0.03	0.01	6.29	0.03	0.01
	350 x 350	24	1.65	0.03	0.01	1.92	0.03	0.01	1.78	0.03	0.01
		48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Distribution of two, three, and four-body collisions in ABM initial tests for 10, 100, and  $1 \times 10^3$  same-charged nanoparticles in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

NP Count	World Area (patches)	Time (hours)	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
			2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
10	150 x 150	24	0.00	0.00	0.00	100.00	0.00	0.00	100.00	0.00	0.00
		48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	250 x 250	24	100.00	0.00	0.00	100.00	0.00	0.00	100.00	0.00	0.00
		48	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	350 x 350	24	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		48	100.00	0.00	0.00	0.00	0.00	0.00	100.00	0.00	0.00
100	150 x 150	24	100.00	0.00	0.00	100.00	0.00	0.00	100.00	0.00	0.00
		48	87.41	2.10	10.49	96.39	3.61	0.00	90.35	2.63	7.02
	250 x 250	24	100.00	0.00	0.00	100.00	0.00	0.00	100.00	0.00	0.00
		48	96.15	3.85	0.00	96.43	3.57	0.00	96.30	3.70	0.00
	350 x 350	24	100.00	0.00	0.00	94.74	5.26	0.00	94.74	5.26	0.00
		48	94.87	5.13	0.00	100.00	0.00	0.00	96.43	3.57	0.00
$1 \times 10^3$	150 x 150	24	99.85	0.15	0.00	99.86	0.14	0.00	99.86	0.14	0.00
		48	99.87	0.13	0.00	98.75	1.24	0.01	99.87	0.13	0.00
	250 x 250	24	99.16	0.77	0.06	92.53	7.27	0.20	99.08	0.86	0.06
		48	99.47	0.41	0.12	92.37	6.30	1.34	99.35	0.52	0.13
	350 x 350	24	97.80	1.90	0.30	98.06	1.69	0.26	97.91	1.81	0.27
		48	97.44	2.15	0.41	97.64	2.04	0.32	97.48	2.12	0.40

## APPENDIX 5 - ABM Initial Test Results for SDS Molecules

Total number of ticks in ABM initial tests for SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

SDS Molecules Count	World Area (patches)	Time (hours)	# Ticks		Average (10 <sup>3</sup> )
			1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	
10	150 x 150	24	795.39	759.17	777.28
		48	1,592.34	1,585.80	1,589.07
	250 x 250	24	283.32	327.03	305.18
		48	388.72	574.32	481.52
	350 x 350	24	146.98	151.68	149.33
		48	203.90	282.84	243.37
100	150 x 150	24	757.12	799.15	778.13
		48	1,102.11	1,467.36	1,284.73
	250 x 250	24	272.49	272.18	272.34
		48	411.82	544.69	478.26
	350 x 350	24	134.53	154.02	144.27
		48	204.68	263.22	233.95
1×10 <sup>3</sup>	150 x 150	24	295.02	343.84	319.43
		48	421.63	554.77	488.20
	250 x 250	24	212.38	218.34	251.36
		48	334.66	419.19	376.93
	350 x 350	24	118.75	122.26	120.51
		48	185.30	236.70	211.00

Distribution of two, three, and four-body collisions in ABM initial tests with respect to quadrants for 10, 100, and for  $1 \times 10^3$  SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

NP Count	World Area (patches)	Time (hours)	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
			2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
10	150 x 150	24	59.90	0.09	40.01	0.00	0.00	0.00	59.90	0.09	40.01
		48	39.19	0.01	60.80	100.00	0.00	0.00	39.26	0.01	60.73
	250 x 250	24	61.44	0.00	38.56	0.00	0.00	0.00	61.43	0.00	38.57
		48	51.20	0.00	48.80	100.00	0.00	0.00	51.30	0.00	48.70
	350 x 350	24	97.46	0.00	2.54	0.00	0.00	0.00	96.67	0.00	3.33
		48	9.26	0.00	90.74	100.00	0.00	0.00	9.35	0.00	90.65
100	150 x 150	24	47.31	0.79	51.89	98.14	0.26	1.59	47.82	0.79	51.40
		48	41.62	0.69	57.69	96.48	2.31	1.21	42.23	0.71	57.06
	250 x 250	24	49.35	0.03	50.62	98.71	0.65	0.65	49.52	0.03	50.45
		48	44.34	0.31	55.35	98.34	0.67	1.00	44.52	0.32	55.16
	350 x 350	24	42.35	0.02	57.63	100.00	0.00	0.00	42.46	0.02	57.52
		48	8.65	0.24	91.11	99.44	0.56	0.00	8.86	0.24	90.90
$1 \times 10^3$	150 x 150	24	39.40	12.46	48.15	55.94	22.97	21.09	42.86	14.66	42.48
		48	37.87	12.91	49.22	54.05	25.17	20.78	41.57	15.72	42.72
	250 x 250	24	47.00	3.94	49.06	80.67	11.43	7.90	48.79	4.33	46.88
		48	43.25	4.41	52.34	78.11	9.23	12.65	45.13	4.67	50.20
	350 x 350	24	47.93	1.58	50.48	99.19	0.44	0.36	48.81	1.56	49.63
		48	43.46	1.51	55.03	96.11	3.85	0.03	44.46	1.55	53.99

Total number of hydrophobic and hydrophilic components in the first ABM initial test with respect to quadrants for 10, 100, and for  $1 \times 10^3$  SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

SDS Molecule Count	World Area (patches)	Time (hours)	Components								
			Hydrophobic				Hydrophilic				
			1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant	1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant	
10	150 x 150	24	2	3	3	2	2	3	3	2	
		48	4	4	0	2	4	4	0	2	
	250 x 250	24	3	1	3	3	3	2	2	3	
		48	2	3	2	3	2	3	2	3	
	350 x 350	24	3	3	2	2	3	3	2	2	
		48	1	2	2	5	1	2	2	5	
	100	150 x 150	24	24	24	24	28	24	23	25	28
			48	31	27	16	26	32	27	16	25
250 x 250		24	20	33	22	25	20	33	22	25	
		48	30	23	23	24	29	24	25	22	
350 x 350		24	26	25	26	23	25	25	26	24	
		48	22	21	32	25	22	21	32	25	
$1 \times 10^3$		150 x 150	24	426	170	215	189	424	170	216	190
			48	336	128	308	228	328	138	307	227
	250 x 250	24	253	230	279	238	253	235	273	239	
		48	206	314	216	264	215	300	223	262	
	350 x 350	24	244	232	262	262	245	233	260	262	
		48	253	268	242	237	254	267	243	236	

Total number of hydrophobic and hydrophilic components in the second ABM initial tests for 10, 100, and for  $1 \times 10^3$  SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours for 24 and 48-hours at 25°C

SDS Molecule Count	World Area (patches)	Time (hours)	Components								
			Hydrophobic				Hydrophilic				
			1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant	1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant	
10	150 x 150	24	2	1	2	5	2	2	1	5	
		48	3	2	3	2	3	2	3	2	
	250 x 250	24	6	1	3	0	6	1	3	0	
		48	3	2	4	1	3	2	4	1	
	350 x 350	24	3	1	2	4	3	1	2	4	
		48	2	3	4	1	2	2	5	1	
	100	150 x 150	24	27	34	17	22	27	34	17	22
			48	26	21	28	25	26	20	30	24
250 x 250		24	18	24	38	20	18	24	37	21	
		48	26	27	27	20	26	27	27	20	
350 x 350		24	16	29	23	32	16	29	23	32	
		48	21	18	33	28	20	18	33	29	
$1 \times 10^3$		150 x 150	24	326	192	312	170	325	192	321	162
			48	438	102	106	354	385	100	107	408
	250 x 250	24	253	238	269	240	251	239	266	244	
		48	218	240	230	312	220	238	231	311	
	350 x 350	24	238	242	238	282	238	242	239	281	
		48	235	245	236	284	231	248	234	287	

Average number of hydrophobic and hydrophilic components in ABM initial tests for 10, 100, and for  $1 \times 10^3$  SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours at 25°C

SDS Molecule Count	World Area (patches)	Time (hours)	Components							
			Hydrophobic				Hydrophilic			
			1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant	1 <sup>st</sup> Quadrant	2 <sup>nd</sup> Quadrant	3 <sup>rd</sup> Quadrant	4 <sup>th</sup> Quadrant
10	150 x 150	24	2	2	3	4	2	3	2	4
		48	4	3	2	2	4	3	2	2
	250 x 250	24	5	1	3	2	5	2	3	2
		48	3	3	3	2	3	3	3	2
	350 x 350	24	3	2	2	3	3	2	2	3
		48	2	3	3	3	2	2	4	3
100	150 x 150	24	26	29	21	25	26	29	21	25
		48	29	24	22	26	29	24	23	25
	250 x 250	24	19	29	30	23	19	29	30	23
		48	28	25	25	22	28	26	26	21
	350 x 350	24	21	27	25	28	21	27	25	28
		48	22	20	33	27	21	20	33	27
$1 \times 10^3$	150 x 150	24	376	181	264	180	375	181	269	176
		48	387	115	207	291	357	119	207	318
	250 x 250	24	253	234	274	239	252	237	270	242
		48	212	277	223	288	218	269	227	287
	350 x 350	24	241	237	250	272	242	238	250	272
		48	244	257	239	261	243	258	239	262



Distribution of average number of hydrophobic and hydrophilic components in ABM initial tests for 10, 100, and for  $1 \times 10^3$  SDS molecules in the worlds with (150 x 150), (250 x 250), and (350 x 350) patches for 24 and 48-hours

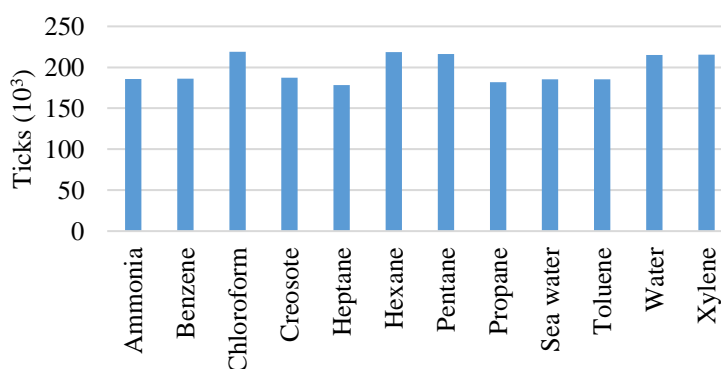
SDS Molecule Count	World Area (patches)	Time (hours)	Components							
			Hydrophobic				Hydrophilic			
			1 <sup>st</sup> Quadrant (%)	2 <sup>nd</sup> Quadrant (%)	3 <sup>rd</sup> Quadrant (%)	4 <sup>th</sup> Quadrant (%)t	1 <sup>st</sup> Quadrant (%)	2 <sup>nd</sup> Quadrant (%)	3 <sup>rd</sup> Quadrant (%)	4 <sup>th</sup> Quadrant (%)
10	150 x 150	24	18.18	18.18	27.27	36.36	18.18	27.27	18.18	36.36
		48	36.36	27.27	18.18	18.18	36.36	27.27	18.18	18.18
	250 x 250	24	45.45	9.09	27.27	18.18	41.67	16.67	25.00	16.67
		48	27.27	27.27	27.27	18.18	27.27	27.27	27.27	18.18
	350 x 350	24	30.00	20.00	20.00	30.00	30.00	20.00	20.00	30.00
		48	18.18	27.27	27.27	27.27	18.18	18.18	36.36	27.27
100	150 x 150	24	25.74	28.71	20.79	24.75	25.74	28.71	20.79	24.75
		48	28.71	23.76	21.78	25.74	28.71	23.76	22.77	24.75
	250 x 250	24	18.81	28.71	29.70	22.77	18.81	28.71	29.70	22.77
		48	28.00	25.00	25.00	22.00	27.72	25.74	25.74	20.79
	350 x 350	24	20.79	26.73	24.75	27.72	20.79	26.73	24.75	27.72
		48	21.57	19.61	32.35	26.47	20.79	19.80	32.67	26.73
$1 \times 10^3$	150 x 150	24	37.56	18.08	26.37	17.98	37.46	18.08	26.87	17.58
		48	38.70	11.50	20.70	29.10	35.66	11.89	20.68	31.77
	250 x 250	24	25.30	23.40	27.40	23.90	25.17	23.68	26.97	24.18
		48	21.20	27.70	22.30	28.80	21.78	26.87	22.68	28.67
	350 x 350	24	24.10	23.70	25.00	27.20	24.15	23.75	24.95	27.15
		48	24.38	25.67	23.88	26.07	24.25	25.75	23.85	26.15

## APPENDIX 6 - ABM Validation Test Results for Uncharged Nanoparticles

### APPENDIX 6.1 - ABM Validation Test Results for $5 \times 10^3$ Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM validation tests for  $5 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	Average (10 <sup>3</sup> )	Ratio <sup>63</sup>
Ammonia	173.17	198.24	185.71	0.86
Benzene	167.57	204.91	186.24	0.87
Chloroform	232.41	205.24	218.83	1.02
Creosote	170.15	204.45	187.30	0.87
Heptane	160.27	196.45	178.36	0.83
Hexane	232.31	204.73	218.52	1.02
Pentane	228.58	203.55	216.07	1.00
Propane	161.72	202.07	181.90	0.85
Sea water	171.94	198.59	185.27	0.86
Toluene	167.50	203.54	185.52	0.86
Water	229.70	200.57	215.14	1.00
Xylene	228.55	202.04	215.30	1.00



Comparison of average number of ticks in ABM validation tests for  $5 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>63</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	341.37	75.13	31.58	357.65	78.49	33.02	349.51	76.81	32.30
Benzene	383.78	83.62	34.80	373.27	84.74	34.93	378.52	84.18	34.86
Chloroform	630.03	139.46	57.00	596.03	134.14	55.07	613.03	136.80	56.04
Creosote	470.12	103.10	43.09	469.41	101.04	41.51	469.76	102.07	42.30
Heptane	293.35	63.90	26.44	298.43	65.62	27.48	295.89	64.76	26.96
Hexane	283.29	61.97	26.35	285.96	63.94	27.50	284.63	62.95	26.92
Pentane	290.81	62.47	25.48	281.83	62.09	25.84	286.32	62.28	25.66
Propane	234.66	50.41	21.32	217.55	49.12	21.02	226.10	49.77	21.17
Sea water	454.85	98.37	41.08	445.57	100.02	41.63	450.21	99.20	41.36
Toluene	364.19	81.65	33.90	356.61	79.05	33.54	360.40	80.35	33.72
Water	427.30	93.97	39.12	390.59	89.79	38.01	408.94	91.88	38.56
Xylene	368.89	83.80	35.79	381.07	84.74	35.62	374.98	84.27	35.70

Distribution of ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	76.19	16.77	7.05	76.23	16.73	7.04	76.21	16.75	7.04
Benzene	76.42	16.65	6.93	75.72	17.19	7.09	76.08	16.92	7.01
Chloroform	76.23	16.87	6.90	75.90	17.08	7.01	76.07	16.98	6.95
Creosote	76.28	16.73	6.99	76.71	16.51	6.78	76.49	16.62	6.89
Heptane	76.46	16.65	6.89	76.22	16.76	7.02	76.34	16.71	6.96
Hexane	76.23	16.68	7.09	75.77	16.94	7.29	76.00	16.81	7.19
Pentane	76.78	16.49	6.73	76.22	16.79	6.99	76.50	16.64	6.86
Propane	76.59	16.45	6.96	75.62	17.07	7.31	76.12	16.75	7.13
Sea water	76.53	16.55	6.91	75.88	17.03	7.09	76.21	16.79	7.00
Toluene	75.91	17.02	7.07	76.01	16.85	7.15	75.96	16.93	7.11
Water	76.25	16.77	6.98	75.35	17.32	7.33	75.82	17.03	7.15
Xylene	75.52	17.16	7.33	76.00	16.90	7.10	75.76	17.03	7.21

ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	130.66	146.32	3.42	2.90	29.34	32.63	0.00	0.00	12.72	13.63	0.00	0.00
Benzene	188.44	190.64	1.78	2.92	41.82	41.80	0.00	0.00	17.70	17.09	0.00	0.00
Chloroform	308.34	319.96	0.69	1.04	70.51	68.94	0.00	0.00	29.42	27.59	0.00	0.00
Creosote	236.95	228.83	2.07	2.26	52.08	51.02	0.00	0.00	21.67	21.42	0.00	0.00
Heptane	144.88	143.51	2.37	2.60	31.79	32.11	0.00	0.00	13.43	13.01	0.00	0.00
Hexane	130.66	146.32	3.42	2.90	29.34	32.63	0.00	0.00	12.72	13.63	0.00	0.00
Pentane	143.91	139.83	3.79	3.28	30.99	31.48	0.00	0.00	12.71	12.78	0.00	0.00
Propane	112.23	115.74	3.30	3.39	25.03	25.38	0.00	0.00	10.41	10.91	0.00	0.00
Sea water	234.03	216.39	1.95	2.49	52.24	46.14	0.00	0.00	21.69	19.39	0.00	0.00
Toluene	188.67	171.28	1.82	2.41	41.84	39.81	0.00	0.00	16.79	17.11	0.00	0.00
Water	211.90	212.60	1.45	1.35	47.62	46.35	0.00	0.00	19.79	19.33	0.00	0.00
Xylene	186.06	179.32	1.46	2.05	41.82	41.98	0.00	0.00	17.86	17.93	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	46.12	51.65	1.21	1.02	47.34	52.66	0.00	0.00	48.29	51.71	0.00	0.00
Benzene	49.10	49.67	0.46	0.76	50.01	49.99	0.00	0.00	50.88	49.12	0.00	0.00
Chloroform	48.94	50.79	0.11	0.16	50.56	49.44	0.00	0.00	51.60	48.40	0.00	0.00
Creosote	50.40	48.68	0.44	0.48	50.51	49.49	0.00	0.00	50.30	49.70	0.00	0.00
Heptane	49.39	48.92	0.81	0.89	49.75	50.25	0.00	0.00	50.81	49.19	0.00	0.00
Hexane	46.12	51.65	1.21	1.02	47.34	52.66	0.00	0.00	48.29	51.71	0.00	0.00
Pentane	49.48	48.08	1.30	1.13	49.60	50.40	0.00	0.00	49.87	50.13	0.00	0.00
Propane	47.83	49.32	1.40	1.45	49.64	50.35	0.00	0.00	48.82	51.18	0.00	0.00
Sea water	51.45	47.57	0.43	0.55	53.10	46.90	0.00	0.00	52.79	47.21	0.00	0.00
Toluene	51.81	47.03	0.50	0.66	51.24	48.76	0.00	0.00	49.52	50.48	0.00	0.00
Water	49.59	49.75	0.34	0.31	50.68	49.32	0.00	0.00	50.59	49.41	0.00	0.00
Xylene	50.44	48.61	0.40	0.55	49.90	50.10	0.00	0.00	49.91	50.09	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	178.24	176.97	1.26	1.18	38.49	40.00	0.00	0.00	15.88	17.15	0.00	0.00
Benzene	179.59	190.83	1.48	1.37	41.83	42.91	0.00	0.00	17.23	17.70	0.00	0.00
Chloroform	316.23	279.79	0.00	0.01	68.75	65.38	0.00	0.00	28.00	27.07	0.00	0.00
Creosote	230.51	238.63	0.14	0.14	50.33	50.70	0.00	0.00	20.37	21.14	0.00	0.00
Heptane	145.41	148.76	1.83	2.44	32.85	32.77	0.00	0.00	13.84	13.64	0.00	0.00
Hexane	139.99	141.52	2.26	2.19	31.75	32.19	0.00	0.00	13.50	13.99	0.00	0.00
Pentane	141.11	139.12	0.76	0.85	31.65	30.44	0.00	0.00	13.24	12.60	0.00	0.00
Propane	107.22	108.87	0.68	0.78	24.36	24.76	0.00	0.00	10.53	10.49	0.00	0.00
Sea water	218.82	225.22	0.59	0.94	49.38	50.64	0.00	0.00	20.38	21.25	0.00	0.00
Toluene	174.04	180.94	0.78	0.85	38.99	40.06	0.00	0.00	16.83	16.71	0.00	0.00
Water	194.70	195.75	0.10	0.05	43.97	45.82	0.00	0.00	18.66	19.35	0.00	0.00
Xylene	194.29	186.38	0.13	0.27	42.61	42.13	0.00	0.00	17.90	17.72	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	49.84	49.48	0.35	0.33	49.03	50.97	0.00	0.00	48.08	51.92	0.00	0.00
Benzene	48.11	51.12	0.40	0.37	49.37	50.63	0.00	0.00	49.32	50.68	0.00	0.00
Chloroform	53.06	46.94	0.00	0.00	51.26	48.74	0.00	0.00	50.84	49.16	0.00	0.00
Creosote	49.11	50.83	0.03	0.03	49.82	50.18	0.00	0.00	49.06	50.94	0.00	0.00
Heptane	48.73	49.85	0.61	0.82	50.05	49.94	0.00	0.00	50.37	49.63	0.00	0.00
Hexane	48.96	49.49	0.79	0.77	49.65	50.35	0.00	0.00	49.10	50.90	0.00	0.00
Pentane	50.07	49.36	0.27	0.30	50.97	49.03	0.00	0.00	51.24	48.76	0.00	0.00
Propane	49.28	50.05	0.31	0.36	49.60	50.40	0.00	0.00	50.10	49.90	0.00	0.00
Sea water	49.11	50.55	0.13	0.21	49.37	50.63	0.00	0.00	48.96	51.04	0.00	0.00
Toluene	48.81	50.74	0.22	0.24	49.32	50.67	0.00	0.00	50.17	49.83	0.00	0.00
Water	49.85	50.12	0.02	0.01	48.97	51.03	0.00	0.00	49.08	50.92	0.00	0.00
Xylene	50.99	48.91	0.03	0.07	50.29	49.71	0.00	0.00	50.26	49.74	0.00	0.00



Total number of collisions in ABM validation tests for  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	448.08	469.16	458.62	0.85
Benzene	502.20	492.94	497.57	0.92
Chloroform	826.49	785.24	805.87	1.49
Creosote	616.31	611.96	614.14	1.14
Heptane	383.69	391.53	387.61	0.72
Hexane	371.61	377.40	374.51	0.69
Pentane	378.76	369.76	374.26	0.69
Propane	306.39	287.69	297.04	0.55
Sea water	594.30	587.22	590.76	1.10
Toluene	479.74	469.20	474.47	0.88
Water	560.39	518.39	539.39	1.00
Xylene	488.48	501.43	494.96	0.92

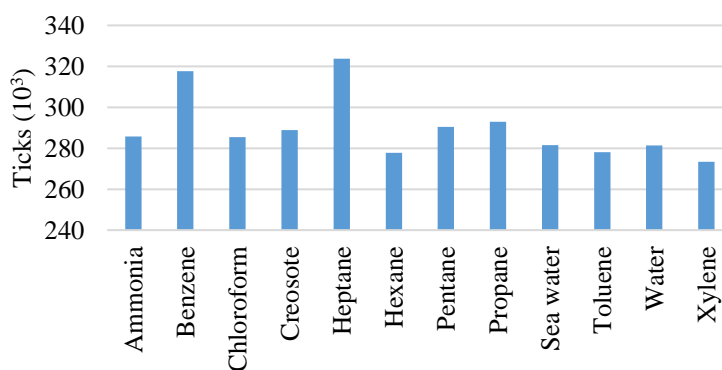
Cumulative number of uncharged nanoparticles at the interface of ABM validation test model for  $5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	7.40	7.37	7.38	1.00
Benzene	7.41	7.38	7.39	1.00
Chloroform	7.40	7.26	7.33	0.99
Creosote	7.38	7.27	7.32	0.99
Heptane	7.43	7.38	7.41	1.00
Hexane	7.43	7.43	7.43	1.01
Pentane	7.42	7.29	7.36	1.00
Propane	7.46	7.32	7.39	1.00
Sea water	7.38	7.37	7.38	1.00
Toluene	7.41	7.35	7.38	1.00
Water	7.42	7.32	7.37	1.00
Xylene	7.42	7.28	7.35	1.00

**APPENDIX 6.2 - ABM Validation Test Results for  $7.5 \times 10^3$  Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $7.5 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test</b>	<b>2<sup>nd</sup> Test</b>	<b>Average</b>	<b>Ratio<sup>64</sup></b>
Ammonia	481.93	89.62	285.78	1.02
Benzene	470.78	164.58	317.68	1.13
Chloroform	467.19	103.56	285.38	1.01
Creosote	459.35	118.50	288.93	1.03
Heptane	484.22	163.23	323.73	1.15
Hexane	474.62	80.80	277.71	0.99
Pentane	473.77	107.19	290.48	1.03
Propane	464.06	121.86	292.96	1.04
Sea water	479.37	83.62	281.50	1.00
Toluene	469.30	86.73	278.02	0.99
Water	462.93	99.91	281.42	1.00
Xylene	463.75	83.17	273.46	0.97



Comparison of average number of ticks in ABM validation tests for  $7.5 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>64</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents in the world in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	40.83	1.13	0.30	39.86	1.18	0.26	40.35	1.16	0.28
Benzene	40.32	1.15	0.29	39.31	1.20	0.30	39.82	1.18	0.29
Chloroform	32.81	0.82	0.15	30.56	0.84	0.16	31.68	0.83	0.15
Creosote	36.74	0.98	0.20	34.61	1.05	0.24	35.67	1.01	0.22
Heptane	46.87	1.33	0.30	46.80	1.38	0.37	46.84	1.35	0.34
Hexane	48.89	1.76	0.44	46.69	1.51	0.43	47.79	1.64	0.43
Pentane	50.27	1.84	0.50	48.66	1.55	0.40	49.47	1.69	0.45
Propane	61.59	1.94	0.57	61.76	2.04	0.59	61.67	1.99	0.58
Sea water	37.66	0.89	0.18	35.08	1.09	0.23	36.37	0.99	0.20
Toluene	39.39	1.21	0.28	37.61	1.19	0.26	38.50	1.20	0.27
Water	36.89	1.05	0.20	35.51	1.09	0.26	36.20	1.07	0.23
Xylene	40.17	1.16	0.27	37.62	1.21	0.29	38.90	1.19	0.28

Distribution of ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Ammonia	96.61	2.68	0.71	96.52	2.86	0.62	96.57	2.77	0.66
Benzene	96.56	2.75	0.69	96.32	2.94	0.74	96.44	2.85	0.71
Chloroform	97.13	2.44	0.43	96.84	2.65	0.51	96.99	2.54	0.47
Creosote	96.91	2.57	0.52	96.42	2.92	0.66	96.67	2.74	0.59
Heptane	96.63	2.75	0.62	96.40	2.83	0.77	96.52	2.79	0.69
Hexane	95.69	3.44	0.87	96.01	3.11	0.88	95.85	3.28	0.87
Pentane	95.56	3.49	0.95	96.14	3.06	0.79	95.84	3.28	0.88
Propane	96.09	3.03	0.88	95.91	3.17	0.92	96.00	3.10	0.90
Sea water	97.24	2.29	0.47	96.37	3.01	0.62	96.82	2.64	0.54
Toluene	96.36	2.95	0.69	96.29	3.05	0.66	96.33	3.00	0.67
Water	96.74	2.74	0.52	96.36	2.95	0.69	96.55	2.84	0.60
Xylene	96.55	2.80	0.66	96.16	3.10	0.75	96.36	2.94	0.70

ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles with respect to quadrants that in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	10.88	16.19	7.43	6.33	0.40	0.73	0.00	0.00	0.11	0.19	0.00	0.00
Benzene	13.14	13.26	6.98	6.93	0.55	0.60	0.00	0.00	0.13	0.16	0.00	0.00
Chloroform	9.26	12.98	5.56	5.00	0.28	0.55	0.00	0.00	0.05	0.10	0.00	0.00
Creosote	9.34	15.27	6.98	5.15	0.31	0.66	0.00	0.00	0.08	0.12	0.00	0.00
Heptane	18.40	11.89	7.78	8.81	0.85	0.48	0.00	0.01	0.20	0.10	0.00	0.00
Hexane	19.69	12.73	7.96	8.51	1.26	0.49	0.00	0.00	0.30	0.14	0.00	0.00
Pentane	21.02	12.40	7.24	9.61	1.31	0.51	0.00	0.01	0.37	0.13	0.00	0.00
Propane	20.48	19.25	10.57	11.28	0.99	0.92	0.01	0.02	0.30	0.27	0.00	0.00
Sea water	9.48	15.24	7.25	5.70	0.31	0.58	0.00	0.00	0.06	0.12	0.00	0.00
Toluene	14.52	12.04	6.01	6.81	0.67	0.54	0.00	0.00	0.17	0.11	0.00	0.00
Water	10.44	14.07	6.77	5.61	0.43	0.62	0.00	0.00	0.09	0.11	0.00	0.00
Xylene	10.88	15.73	7.23	6.34	0.43	0.73	0.01	0.00	0.11	0.17	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	26.64	39.66	18.21	15.50	34.86	64.61	0.35	0.18	37.58	62.08	0.00	0.34
Benzene	32.59	32.90	17.32	17.19	47.48	52.26	0.09	0.17	45.30	54.70	0.00	0.00
Chloroform	28.23	39.58	16.95	15.24	33.66	66.22	0.12	0.00	34.48	65.52	0.00	0.00
Creosote	25.43	41.57	18.99	14.01	32.10	67.38	0.21	0.31	38.07	61.93	0.00	0.00
Heptane	39.24	25.36	16.60	18.80	63.69	35.71	0.23	0.38	65.56	34.44	0.00	0.00
Hexane	40.28	26.03	16.27	17.41	71.70	28.07	0.17	0.06	67.49	32.51	0.00	0.00
Pentane	41.82	24.67	14.40	19.11	71.57	27.83	0.22	0.38	73.51	26.49	0.00	0.00
Propane	33.26	31.26	17.17	18.32	51.06	47.65	0.46	0.83	53.00	47.00	0.00	0.00
Sea water	25.16	40.45	19.26	15.13	34.39	65.16	0.45	0.00	35.36	64.64	0.00	0.00
Toluene	36.87	30.58	15.26	17.30	55.31	44.36	0.08	0.25	59.64	40.36	0.00	0.00
Water	28.29	38.14	18.35	15.22	40.63	58.89	0.19	0.29	43.94	56.06	0.00	0.00
Xylene	27.07	39.14	17.99	15.79	36.89	62.51	0.52	0.09	39.19	60.81	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	13.02	13.59	7.05	6.20	0.57	0.61	0.00	0.00	0.12	0.14	0.00	0.00
Benzene	13.82	12.39	6.25	6.86	0.62	0.57	0.00	0.00	0.18	0.13	0.00	0.00
Chloroform	8.22	13.38	4.96	4.00	0.27	0.57	0.00	0.00	0.05	0.11	0.00	0.00
Creosote	14.13	9.77	4.98	5.73	0.68	0.36	0.00	0.00	0.17	0.07	0.00	0.00
Heptane	14.23	16.07	8.43	8.07	0.65	0.72	0.00	0.01	0.16	0.21	0.00	0.00
Hexane	15.25	15.55	7.72	8.16	0.75	0.76	0.00	0.00	0.21	0.22	0.00	0.00
Pentane	19.20	13.14	7.58	8.74	1.07	0.46	0.01	0.01	0.27	0.14	0.00	0.00
Propane	16.24	23.99	11.42	10.11	0.69	1.32	0.01	0.01	0.21	0.38	0.00	0.00
Sea water	15.22	9.52	4.74	5.61	0.75	0.34	0.00	0.00	0.16	0.07	0.00	0.00
Toluene	11.64	14.23	6.20	5.55	0.52	0.67	0.00	0.00	0.10	0.16	0.00	0.00
Water	11.40	12.99	5.92	5.21	0.51	0.58	0.00	0.00	0.11	0.15	0.00	0.00
Xylene	12.27	13.62	5.90	5.83	0.54	0.67	0.00	0.00	0.14	0.15	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	32.66	34.10	17.68	15.55	48.14	51.53	0.00	0.34	46.88	53.13	0.00	0.00
Benzene	35.16	31.51	15.89	17.44	52.00	47.67	0.17	0.17	58.14	41.86	0.00	0.00
Chloroform	26.90	43.79	16.23	13.08	32.38	67.50	0.12	0.00	33.75	66.25	0.00	0.00
Creosote	40.84	28.22	14.39	16.56	65.23	34.67	0.00	0.10	69.92	30.08	0.00	0.00
Heptane	30.41	34.33	18.01	17.25	47.13	52.15	0.29	0.44	43.01	56.99	0.00	0.00
Hexane	32.67	33.31	16.54	17.48	49.60	50.00	0.13	0.26	49.06	50.94	0.00	0.00
Pentane	39.46	27.00	15.57	17.97	69.18	29.59	0.39	0.84	66.17	33.83	0.00	0.00
Propane	26.29	38.85	18.49	16.37	33.91	64.82	0.64	0.64	35.58	64.42	0.00	0.00
Sea water	43.38	27.13	13.51	15.98	68.83	31.08	0.00	0.09	69.47	30.53	0.00	0.00
Toluene	30.94	37.83	16.48	14.75	43.70	56.05	0.00	0.25	38.76	61.24	0.00	0.00
Water	32.11	36.57	16.66	14.66	46.73	53.08	0.00	0.18	43.14	56.86	0.00	0.00
Xylene	32.62	36.20	15.69	15.50	44.43	55.33	0.08	0.17	49.15	50.85	0.00	0.00



Total number of collisions in ABM validation tests for  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	42.26	41.30	41.78	1.11
Benzene	41.76	40.81	41.29	1.10
Chloroform	33.78	31.56	32.67	0.87
Creosote	37.91	35.89	36.90	0.98
Heptane	48.51	48.55	48.53	1.29
Hexane	51.09	48.63	49.86	1.33
Pentane	52.61	50.61	51.61	1.38
Propane	64.09	64.39	64.24	1.71
Sea water	38.73	36.40	37.57	1.00
Toluene	40.87	39.06	39.97	1.07
Water	38.13	36.85	37.49	1.00
Xylene	41.61	39.12	40.37	1.08

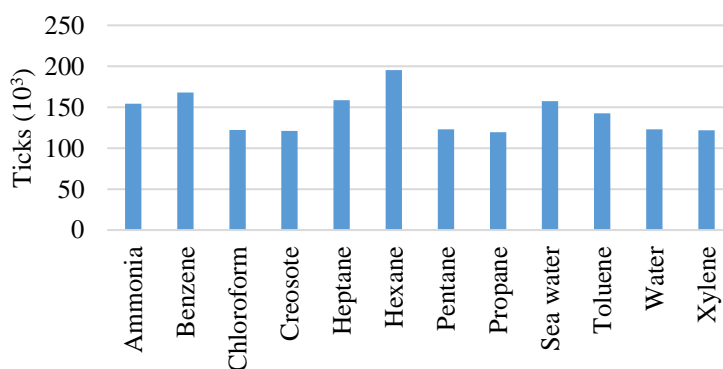
Cumulative number of uncharged nanoparticles at the interface of ABM validation tests for  $7.5 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	7.37	6.89	7.13	1.05
Benzene	7.31	6.42	6.86	1.01
Chloroform	6.87	5.89	6.38	0.94
Creosote	7.17	6.42	6.79	1.00
Heptane	7.43	7.06	7.24	1.07
Hexane	7.45	6.67	7.06	1.04
Pentane	7.46	6.87	7.16	1.06
Propane	7.49	7.17	7.33	1.08
Sea water	7.20	6.19	6.69	0.99
Toluene	7.33	6.39	6.86	1.01
Water	7.22	6.34	6.78	1.00
Xylene	7.28	6.37	6.83	1.01

**APPENDIX 6.3 - ABM Validation Test Results for  $10 \times 10^3$  Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) patch world for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $10 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (<math>10^3</math>)</b>	<b>2<sup>nd</sup> Test (<math>10^3</math>)</b>	<b>Average (<math>10^3</math>)</b>	<b>Ratio<sup>65</sup></b>
Ammonia	95.02	86.54	90.78	0.99
Benzene	92.75	195.51	144.13	1.57
Chloroform	98.44	90.31	94.38	1.03
Creosote	99.97	88.96	94.47	1.03
Heptane	98.22	86.55	92.39	1.01
Hexane	94.86	90.25	92.56	1.01
Pentane	97.41	8.76	53.09	0.58
Propane	96.52	87.15	91.84	1.00
Sea water	96.83	91.98	94.41	1.03
Toluene	98.22	87.09	92.66	1.01
Water	100.15	83.64	91.90	1.00
Xylene	97.75	88.31	93.03	1.01



Comparison of average number of ticks in ABM validation tests for  $10 \times 10^3$  uncharged nanoparticles in the (250 x 250) patch world for 72-hours at 25°C

<sup>65</sup> Ratio calculated with respect to water.

Table ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )
Ammonia	582.18	130.93	54.62	580.88	130.26	53.99	581.53	130.60	54.31
Benzene	582.61	131.40	55.04	623.49	135.56	57.21	603.05	133.48	56.13
Chloroform	962.66	213.65	88.56	984.48	224.88	95.10	973.57	219.26	91.83
Creosote	725.23	166.12	70.93	722.31	164.72	68.67	723.77	165.42	69.80
Heptane	469.28	104.41	43.83	514.27	112.77	47.40	491.78	108.59	45.62
Hexane	452.22	101.28	42.97	462.00	101.13	42.64	457.11	101.21	42.80
Pentane	462.37	99.59	41.96	464.36	103.19	43.57	463.37	101.39	42.76
Propane	367.63	80.98	34.58	365.82	81.30	34.55	366.72	81.14	34.56
Sea water	711.54	159.96	66.77	709.71	161.60	67.19	710.62	160.78	66.98
Toluene	601.06	132.32	56.15	609.98	135.47	55.46	605.52	133.90	55.81
Water	696.62	158.24	66.38	701.25	159.31	66.45	698.93	158.77	66.41
Xylene	611.52	136.19	58.04	663.47	139.94	56.98	637.50	138.07	57.51

Distribution of ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	75.83	17.05	7.11	75.92	17.02	7.06	75.88	17.04	7.09
Benzene	75.76	17.09	7.16	76.38	16.61	7.01	76.08	16.84	7.08
Chloroform	76.11	16.89	7.00	75.47	17.24	7.29	75.78	17.07	7.15
Creosote	75.37	17.26	7.37	75.58	17.24	7.19	75.47	17.25	7.28
Heptane	75.99	16.91	7.10	76.25	16.72	7.03	76.13	16.81	7.06
Hexane	75.82	16.98	7.20	76.27	16.69	7.04	76.04	16.84	7.12
Pentane	76.56	16.49	6.95	75.99	16.89	7.13	76.27	16.69	7.04
Propane	76.08	16.76	7.16	75.95	16.88	7.17	76.02	16.82	7.16
Sea water	75.84	17.05	7.12	75.62	17.22	7.16	75.73	17.13	7.14
Toluene	76.13	16.76	7.11	76.16	16.91	6.92	76.14	16.84	7.02
Water	75.62	17.18	7.21	75.65	17.19	7.17	75.63	17.18	7.19
Xylene	75.89	16.90	7.20	77.11	16.27	6.62	76.52	16.57	6.90

ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	286.09	291.03	2.19	2.88	65.40	65.52	0.00	0.00	26.91	27.71	0.00	0.00
Benzene	291.59	287.51	1.72	1.79	66.18	65.22	0.00	0.00	27.45	27.59	0.00	0.00
Chloroform	456.85	504.98	0.61	0.21	97.44	116.21	0.00	0.00	40.26	48.30	0.00	0.00
Creosote	364.36	358.70	1.12	1.05	82.51	83.61	0.00	0.00	35.25	35.69	0.00	0.00
Heptane	229.00	233.57	3.83	2.89	52.60	51.81	0.00	0.00	22.04	21.79	0.00	0.00
Hexane	223.31	222.48	3.07	3.37	50.36	50.92	0.00	0.00	21.27	21.70	0.00	0.00
Pentane	226.26	227.72	3.83	4.57	48.81	50.78	0.00	0.00	20.46	21.50	0.00	0.00
Propane	180.38	179.20	3.76	4.30	40.45	40.53	0.00	0.00	16.92	17.66	0.00	0.00
Sea water	358.71	350.08	1.56	1.18	80.03	79.92	0.00	0.00	33.37	33.39	0.00	0.00
Toluene	300.96	295.58	2.46	2.06	66.48	65.84	0.00	0.00	27.86	28.29	0.00	0.00
Water	354.69	339.26	1.27	1.40	82.53	75.71	0.00	0.00	34.09	32.30	0.00	0.00
Xylene	305.85	300.83	2.83	2.01	68.42	67.77	0.00	0.00	29.23	28.81	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	49.14	49.99	0.38	0.49	49.95	50.05	0.00	0.00	49.27	50.73	0.00	0.00
Benzene	50.05	49.35	0.30	0.31	50.37	49.63	0.00	0.00	49.86	50.14	0.00	0.00
Chloroform	47.46	52.46	0.06	0.02	45.61	54.39	0.00	0.00	45.46	54.54	0.00	0.00
Creosote	50.24	49.46	0.15	0.15	49.67	50.33	0.00	0.00	49.69	50.31	0.00	0.00
Heptane	48.80	49.77	0.82	0.62	50.38	49.62	0.00	0.00	50.28	49.72	0.00	0.00
Hexane	49.38	49.20	0.68	0.74	49.72	50.28	0.00	0.00	49.51	50.49	0.00	0.00
Pentane	48.93	49.25	0.83	0.99	49.01	50.99	0.00	0.00	48.76	51.24	0.00	0.00
Propane	49.07	48.74	1.02	1.17	49.94	50.05	0.00	0.00	48.93	51.07	0.00	0.00
Sea water	50.41	49.20	0.22	0.17	50.03	49.97	0.00	0.00	49.99	50.01	0.00	0.00
Toluene	50.07	49.18	0.41	0.34	50.24	49.76	0.00	0.00	49.62	50.38	0.00	0.00
Water	50.92	48.70	0.18	0.20	52.16	47.84	0.00	0.00	51.35	48.65	0.00	0.00
Xylene	50.01	49.19	0.46	0.33	50.24	49.76	0.00	0.00	50.36	49.64	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	301.53	274.75	1.60	2.99	66.34	63.92	0.00	0.00	27.18	26.81	0.00	0.00
Benzene	315.59	296.98	5.19	5.73	68.15	67.41	0.00	0.00	28.45	28.77	0.00	0.00
Chloroform	515.67	467.88	0.59	0.34	115.34	109.54	0.00	0.00	47.24	47.86	0.00	0.00
Creosote	364.05	356.17	0.96	1.13	82.89	81.83	0.00	0.00	34.09	34.59	0.00	0.00
Heptane	253.77	253.10	3.86	3.53	58.37	54.39	0.00	0.00	24.59	22.81	0.00	0.00
Hexane	231.72	223.29	3.52	3.47	51.65	49.48	0.01	0.00	21.67	20.96	0.00	0.00
Pentane	240.25	218.66	3.36	2.10	52.86	50.33	0.00	0.00	21.96	21.61	0.00	0.00
Propane	175.39	180.90	4.87	4.66	40.13	41.17	0.00	0.00	17.18	17.36	0.00	0.00
Sea water	355.59	351.22	1.63	1.26	81.42	80.18	0.00	0.00	33.89	33.30	0.00	0.00
Toluene	304.74	300.89	2.60	1.74	69.34	66.13	0.00	0.00	28.10	27.37	0.00	0.00
Water	345.76	352.92	1.12	1.44	79.07	80.24	0.00	0.00	32.92	33.52	0.00	0.00
Xylene	313.56	345.65	2.51	1.75	66.90	73.04	0.00	0.00	27.94	29.04	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	51.91	47.30	0.28	0.51	50.93	49.07	0.00	0.00	50.34	49.66	0.00	0.00
Benzene	50.62	47.63	0.83	0.92	50.27	49.73	0.00	0.00	49.72	50.28	0.00	0.00
Chloroform	52.38	47.53	0.06	0.03	51.29	48.71	0.00	0.00	49.68	50.32	0.00	0.00
Creosote	50.40	49.31	0.13	0.16	50.32	49.68	0.00	0.00	49.64	50.36	0.00	0.00
Heptane	49.35	49.22	0.75	0.69	51.76	48.23	0.00	0.00	51.88	48.12	0.00	0.00
Hexane	50.16	48.33	0.76	0.75	51.07	48.93	0.00	0.00	50.83	49.17	0.00	0.00
Pentane	51.74	47.09	0.72	0.45	51.23	48.77	0.00	0.00	50.40	49.60	0.00	0.00
Propane	47.94	49.45	1.33	1.27	49.36	50.64	0.00	0.00	49.74	50.26	0.00	0.00
Sea water	50.10	49.49	0.23	0.18	50.39	49.61	0.00	0.00	50.44	49.56	0.00	0.00
Toluene	49.96	49.33	0.43	0.29	51.18	48.82	0.00	0.00	50.66	49.34	0.00	0.00
Water	49.31	50.33	0.16	0.21	49.63	50.37	0.00	0.00	49.55	50.45	0.00	0.00
Xylene	47.26	52.10	0.38	0.26	47.80	52.19	0.00	0.00	49.04	50.96	0.00	0.00



Total number of collisions in ABM validation tests for  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	767.72	766.42	767.07	0.83
Benzene	769.05	809.93	789.49	0.85
Chloroform	1,264.87	1,286.69	1,275.78	1.38
Creosote	962.28	959.36	960.82	1.04
Heptane	617.52	662.51	640.01	0.69
Hexane	596.47	606.25	601.36	0.65
Pentane	603.92	605.90	604.91	0.65
Propane	483.19	481.39	482.29	0.52
Sea water	938.26	936.43	937.34	1.01
Toluene	789.53	798.45	793.99	0.86
Water	921.24	925.86	923.55	1.00
Xylene	805.76	857.71	831.73	0.90

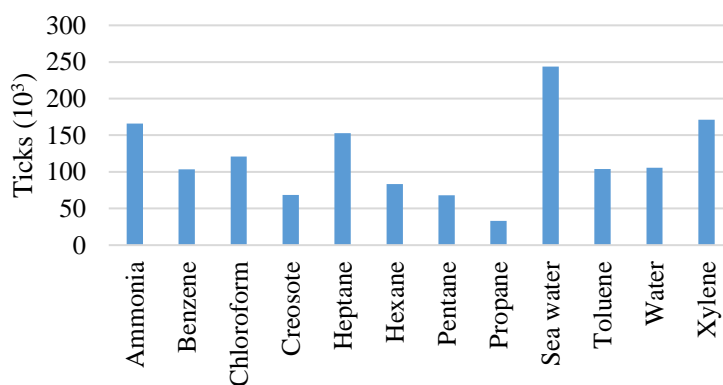
Cumulative number of uncharged nanoparticles at the interface of ABM validation tests for  $10 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	9.79	9.79	9.79	1.00
Benzene	9.80	9.85	9.83	1.00
Chloroform	9.77	9.78	9.78	1.00
Creosote	9.80	9.79	9.80	1.00
Heptane	9.82	9.76	9.79	1.00
Hexane	9.82	9.81	9.81	1.00
Pentane	9.80	9.83	9.82	1.00
Propane	9.86	9.83	9.85	1.01
Sea water	9.80	9.78	9.79	1.00
Toluene	9.80	9.78	9.79	1.00
Water	9.81	9.78	9.79	1.00
Xylene	9.79	9.77	9.78	1.00

## APPENDIX 6.4 - ABM Validation Test Results for $12.5 \times 10^3$ Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) World for 72-hours at 25°C

Total number of ticks in ABM validation tests for  $12.5 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	Average (10 <sup>3</sup> )	Ratio <sup>66</sup>
Ammonia	204.89	90.12	147.51	0.76
Benzene	158.48	99.08	128.78	0.66
Chloroform	160.38	103.21	131.80	0.68
Creosote	297.61	97.42	197.52	1.01
Heptane	155.82	97.18	126.50	0.65
Hexane	157.05	99.50	128.28	0.66
Pentane	293.25	96.96	195.11	1.00
Propane	155.64	95.52	125.58	0.64
Sea water	156.36	96.15	126.26	0.65
Toluene	156.22	93.22	124.72	0.64
Water	294.44	96.06	195.25	1.00
Xylene	154.22	97.48	125.85	0.64



Comparison of average number of ticks in ABM validation tests for  $12.5 \times 10^3$  uncharged nanoparticles in the world in a (250 x 250) patch world for 72-hours at 25°C

<sup>66</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents in the world in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )
Ammonia	851.89	186.24	78.12	888.86	190.51	79.17	870.37	188.38	78.64
Benzene	937.24	204.20	83.93	927.39	201.32	82.72	932.32	202.76	83.32
Chloroform	1,522.24	338.97	140.12	1,441.65	331.74	137.93	1,481.94	335.35	139.03
Creosote	1,211.37	256.07	105.30	1,071.43	242.25	102.31	1,141.40	249.16	103.81
Heptane	736.23	158.32	65.75	718.00	157.87	65.14	727.11	158.09	65.45
Hexane	709.23	154.69	65.15	661.23	147.88	63.94	685.23	151.28	64.55
Pentane	676.07	148.67	62.13	675.85	151.94	63.86	675.96	150.31	62.99
Propane	543.34	117.08	49.82	566.86	122.71	51.45	555.10	119.90	50.63
Sea water	1,059.45	234.78	97.64	1,027.27	233.71	97.87	1,043.36	234.25	97.75
Toluene	901.60	199.39	84.61	839.86	192.63	81.97	870.73	196.01	83.29
Water	1,047.45	225.17	93.51	1,041.23	232.10	95.95	1,044.34	228.64	94.73
Xylene	866.28	198.35	84.55	933.98	210.76	87.88	900.13	204.55	86.21

Distribution of ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	76,32	16,68	7,00	76,72	16,44	6,83	76,52	16,56	6,91
Benzene	76,49	16,66	6,85	76,55	16,62	6,83	76,52	16,64	6,84
Chloroform	76,06	16,94	7,00	75,43	17,36	7,22	75,75	17,14	7,11
Creosote	77,02	16,28	6,70	75,67	17,11	7,23	76,38	16,67	6,95
Heptane	76,67	16,49	6,85	76,30	16,78	6,92	76,49	16,63	6,88
Hexane	76,34	16,65	7,01	75,74	16,94	7,32	76,05	16,79	7,16
Pentane	76,23	16,76	7,01	75,80	17,04	7,16	76,01	16,90	7,08
Propane	76,50	16,49	7,01	76,50	16,56	6,94	76,50	16,52	6,98
Sea water	76,12	16,87	7,01	75,60	17,20	7,20	75,86	17,03	7,11
Toluene	76,05	16,82	7,14	75,36	17,29	7,35	75,71	17,04	7,24
Water	76,67	16,48	6,85	76,04	16,95	7,01	76,36	16,72	6,93
Xylene	75,38	17,26	7,36	75,77	17,10	7,13	75,58	17,18	7,24

ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	425.57	407.79	8.88	9.65	95.16	91.08	0.00	0.00	39.74	38.38	0.00	0.00
Benzene	456.90	466.21	7.56	6.57	100.45	103.74	0.01	0.00	40.98	42.95	0.00	0.00
Chloroform	777.66	740.80	1.81	1.97	173.92	165.05	0.00	0.00	71.66	68.47	0.00	0.00
Creosote	583.21	608.65	9.99	9.52	124.67	131.40	0.01	0.00	51.20	54.10	0.00	0.00
Heptane	355.47	362.53	8.81	9.42	77.80	80.51	0.01	0.00	31.73	34.02	0.00	0.00
Hexane	341.27	348.29	9.55	10.13	77.51	77.17	0.00	0.01	33.01	32.14	0.00	0.00
Pentane	322.88	334.14	8.90	10.15	71.99	76.68	0.00	0.01	30.07	32.06	0.00	0.00
Propane	268.74	255.46	9.33	9.80	59.63	57.44	0.00	0.01	25.12	24.69	0.00	0.00
Sea water	520.43	529.76	5.15	4.11	118.43	116.36	0.00	0.00	50.21	47.43	0.00	0.00
Toluene	434.42	452.87	7.61	6.70	98.78	100.60	0.00	0.00	42.20	42.41	0.00	0.00
Water	509.14	521.18	7.33	9.80	110.00	115.16	0.00	0.00	45.79	47.72	0.00	0.00
Xylene	437.95	417.40	5.17	5.75	99.01	99.34	0.00	0.00	41.86	42.69	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	49.96	47.87	1.04	1.13	51.09	48.90	0.00	0.00	50.87	49.13	0.00	0.00
Benzene	48.75	49.74	0.81	0.70	49.19	50.80	0.00	0.00	48.82	51.18	0.00	0.00
Chloroform	51.09	48.67	0.12	0.13	51.31	48.69	0.00	0.00	51.14	48.86	0.00	0.00
Creosote	48.14	50.24	0.83	0.79	48.68	51.31	0.00	0.00	48.62	51.38	0.00	0.00
Heptane	48.28	49.24	1.20	1.28	49.14	50.85	0.00	0.00	48.25	51.75	0.00	0.00
Hexane	48.12	49.11	1.35	1.43	50.11	49.89	0.00	0.01	50.67	49.33	0.00	0.00
Pentane	47.76	49.42	1.32	1.50	48.42	51.57	0.00	0.00	48.40	51.60	0.00	0.00
Propane	49.46	47.02	1.72	1.80	50.93	49.06	0.00	0.01	50.43	49.57	0.00	0.00
Sea water	49.12	50.00	0.49	0.39	50.44	49.56	0.00	0.00	51.42	48.58	0.00	0.00
Toluene	48.18	50.23	0.84	0.74	49.54	50.46	0.00	0.00	49.88	50.12	0.00	0.00
Water	48.61	49.76	0.70	0.94	48.85	51.15	0.00	0.00	48.97	51.03	0.00	0.00
Xylene	50.56	48.18	0.60	0.66	49.91	50.08	0.00	0.00	49.51	50.49	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	441.11	438.34	5.02	4.40	93.82	96.69	0.00	0.00	38.57	40.60	0.00	0.00
Benzene	462.45	456.13	3.98	4.83	99.64	101.68	0.00	0.00	40.23	42.48	0.00	0.00
Chloroform	716.15	723.91	0.58	1.02	164.60	167.14	0.00	0.00	67.54	70.39	0.00	0.00
Creosote	541.90	525.35	2.06	2.13	123.75	118.50	0.00	0.00	52.48	49.83	0.00	0.00
Heptane	358.49	346.90	7.09	5.52	80.84	77.02	0.01	0.00	33.35	31.79	0.00	0.00
Hexane	320.42	328.44	5.98	6.39	71.65	76.23	0.00	0.00	31.32	32.62	0.00	0.00
Pentane	335.99	327.45	5.32	7.09	76.31	75.62	0.00	0.00	31.80	32.06	0.00	0.00
Propane	274.26	275.17	7.64	9.80	60.90	61.80	0.01	0.01	25.57	25.88	0.00	0.00
Sea water	509.83	512.65	2.63	2.17	114.05	119.65	0.00	0.00	47.83	50.03	0.00	0.00
Toluene	415.95	417.56	2.86	3.49	98.19	94.44	0.00	0.00	41.46	40.51	0.00	0.00
Water	522.30	512.27	3.29	3.37	117.60	114.51	0.00	0.00	48.36	47.59	0.00	0.00
Xylene	467.07	458.63	3.88	4.40	107.86	102.89	0.00	0.00	45.36	42.52	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants in the world in a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	49.63	49.31	0.56	0.49	49.25	50.75	0.00	0.00	48.72	51.28	0.00	0.00
Benzene	49.87	49.18	0.43	0.52	49.49	50.51	0.00	0.00	48.64	51.36	0.00	0.00
Chloroform	49.68	50.21	0.04	0.07	49.62	50.38	0.00	0.00	48.97	51.03	0.00	0.00
Creosote	50.58	49.03	0.19	0.20	51.09	48.91	0.00	0.00	51.30	48.70	0.00	0.00
Heptane	49.93	48.32	0.99	0.77	51.21	48.79	0.00	0.00	51.20	48.80	0.00	0.00
Hexane	48.46	49.67	0.90	0.97	48.45	51.55	0.00	0.00	48.99	51.01	0.00	0.00
Pentane	49.71	48.45	0.79	1.05	50.23	49.77	0.00	0.00	49.79	50.21	0.00	0.00
Propane	48.38	48.54	1.35	1.73	49.63	50.36	0.00	0.01	49.71	50.29	0.00	0.00
Sea water	49.63	49.90	0.26	0.21	48.80	51.20	0.00	0.00	48.88	51.12	0.00	0.00
Toluene	49.53	49.72	0.34	0.42	50.97	49.02	0.00	0.00	50.58	49.42	0.00	0.00
Water	50.16	49.20	0.32	0.32	50.67	49.33	0.00	0.00	50.40	49.60	0.00	0.00
Xylene	50.01	49.10	0.42	0.47	51.18	48.82	0.00	0.00	51.62	48.38	0.00	0.00



Total number of collisions in ABM validation tests for  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	1,116	1,159	1,137	0.83
Benzene	1,225	1,211	1,218	0.89
Chloroform	2,001	1,911	1,956	1.43
Creosote	1,573	1,416	1,494	1.09
Heptane	960	941	951	0.70
Hexane	929	873	901	0.66
Pentane	887	892	889	0.65
Propane	710	741	726	0.53
Sea water	1,392	1,359	1,375	1.01
Toluene	1,186	1,114	1,150	0.84
Water	1,366	1,369	1,368	1.00
Xylene	1,149	1,233	1,191	0.87

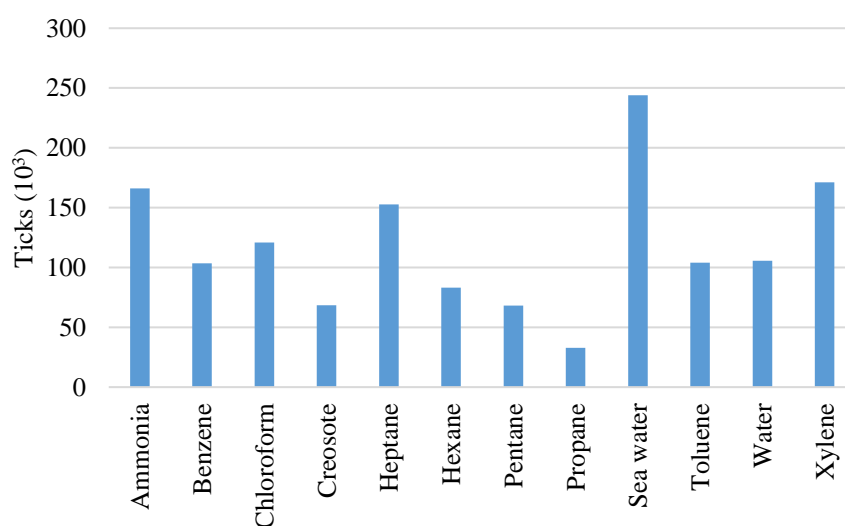
Cumulative number of uncharged nanoparticles at the interface of ABM validation tests for  $12.5 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	12.32	12.19	12.26	1.00
Benzene	12.29	12.22	12.26	1.00
Chloroform	12.26	12.24	12.25	1.00
Creosote	12.34	12.23	12.28	1.00
Heptane	12.31	12.24	12.27	1.00
Hexane	12.31	12.27	12.29	1.00
Pentane	12.44	12.27	12.35	1.01
Propane	12.40	12.29	12.34	1.01
Sea water	12.27	12.23	12.25	1.00
Toluene	12.28	12.24	12.26	1.00
Water	12.37	12.20	12.28	1.00
Xylene	12.30	12.21	12.26	1.00

**APPENDIX 6.5 - ABM Validation Test Results for  $15 \times 10^3$  Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $15 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test</b>	<b>2<sup>nd</sup> Test</b>	<b>Average</b>	<b>Ratio<sup>67</sup></b>
Ammonia	204.24	89.47	146.86	1.09
Benzene	202.37	81.87	142.12	1.05
Chloroform	206.78	116.58	161.68	1.20
Creosote	195.61	70.18	132.90	0.98
Heptane	203.62	90.71	147.17	1.09
Hexane	198.93	81.87	140.40	1.04
Pentane	206.21	105.93	156.07	1.15
Propane	207.04	68.92	137.98	1.02
Sea water	207.27	92.72	150.00	1.11
Toluene	201.65	84.81	143.23	1.06
Water	205.26	65.10	135.18	1.00
Xylene	202.64	46.02	124.33	0.92



Comparison of average number of ticks in ABM validation tests for  $15 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>67</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents in the world of a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	1139,67	255,66	108,56	1192,86	261,54	108,46	1,166.27	258.60	108.51
Benzene	1294,70	284,27	119,33	1271,57	279,97	118,20	1,283.13	282.12	118.76
Chloroform	2030,81	445,37	186,16	2017,42	453,91	192,02	2,024.11	449.64	189.09
Creosote	1536,45	342,10	143,49	1531,96	346,04	144,89	1,534.21	344.07	144.19
Heptane	1021,00	218,73	91,02	935,22	213,73	88,83	978.11	216.23	89.92
Hexane	953,42	205,24	86,23	975,31	210,65	87,00	964.36	207.94	86.62
Pentane	969,12	209,46	87,80	899,20	201,55	84,14	934.16	205.50	85.97
Propane	767,43	163,97	68,99	749,23	164,17	70,00	758.33	164.07	69.50
Sea water	1457,12	323,19	134,98	1492,85	330,48	135,83	1,474.99	326.84	135.40
Toluene	1290,32	277,29	113,69	1188,25	267,46	112,19	1,239.29	272.37	112.94
Water	1458,00	322,56	135,07	1378,51	311,32	130,74	1,418.25	316.94	132.91
Xylene	1267,93	278,25	117,31	1218,50	276,31	115,55	1,243.21	277.28	116.43

Distribution of ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	75.78	17.00	7.22	76.33	16.73	6.94	76.06	16.86	7.08
Benzene	76.24	16.74	7.03	76.15	16.77	7.08	76.19	16.75	7.05
Chloroform	76.28	16.73	6.99	75.75	17.04	7.21	76.01	16.89	7.10
Creosote	75.99	16.92	7.10	75.73	17.11	7.16	75.86	17.01	7.13
Heptane	76.72	16.44	6.84	75.56	17.27	7.18	76.16	16.84	7.00
Hexane	76.59	16.49	6.93	76.62	16.55	6.83	76.60	16.52	6.88
Pentane	76.53	16.54	6.93	75.89	17.01	7.10	76.22	16.77	7.01
Propane	76.71	16.39	6.90	76.19	16.69	7.12	76.45	16.54	7.01
Sea water	76.08	16.87	7.05	76.20	16.87	6.93	76.14	16.87	6.99
Toluene	76.75	16.49	6.76	75.79	17.06	7.16	76.28	16.77	6.95
Water	76.11	16.84	7.05	75.72	17.10	7.18	75.92	16.97	7.11
Xylene	76.22	16.73	7.05	75.67	17.16	7.18	75.95	16.94	7.11

ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	579.76	535.72	12.79	11.40	132.38	123.27	0.01	0.01	56.20	52.36	0.00	0.00
Benzene	647.18	621.06	12.55	13.91	142.87	141.39	0.00	0.00	59.14	60.18	0.00	0.00
Chloroform	1,005.00	1,015.39	5.33	5.10	226.17	219.19	0.00	0.01	94.97	91.19	0.00	0.00
Creosote	722.62	795.19	9.83	8.82	167.42	174.68	0.01	0.00	71.10	72.39	0.00	0.00
Heptane	487.80	503.71	14.94	14.55	106.27	112.44	0.01	0.01	44.21	46.81	0.00	0.00
Hexane	454.76	468.92	16.15	13.59	103.35	101.87	0.01	0.01	44.15	42.08	0.00	0.00
Pentane	458.76	478.77	14.81	16.78	102.89	106.56	0.01	0.01	43.35	44.45	0.00	0.00
Propane	364.31	367.91	16.71	18.50	81.73	82.21	0.01	0.01	34.65	34.34	0.00	0.00
Sea water	738.44	699.35	8.36	10.98	167.11	156.06	0.01	0.01	69.27	65.71	0.00	0.00
Toluene	636.35	622.65	16.30	15.03	140.42	136.85	0.01	0.01	57.78	55.91	0.00	0.00
Water	707.55	728.72	11.60	10.12	159.12	163.43	0.01	0.00	66.34	68.73	0.00	0.00
Xylene	608.57	627.84	18.11	13.41	135.78	142.45	0.01	0.01	57.37	59.94	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	50.87	47.01	1.12	1.00	51.78	48.22	0.00	0.00	51.77	48.23	0.00	0.00
Benzene	49.99	47.97	0.97	1.07	50.26	49.74	0.00	0.00	49.57	50.43	0.00	0.00
Chloroform	49.49	50.00	0.26	0.25	50.78	49.21	0.00	0.00	51.02	48.98	0.00	0.00
Creosote	47.03	51.75	0.64	0.57	48.94	51.06	0.00	0.00	49.55	50.45	0.00	0.00
Heptane	47.78	49.33	1.46	1.42	48.59	51.41	0.00	0.00	48.57	51.43	0.00	0.00
Hexane	47.70	49.18	1.69	1.43	50.36	49.64	0.01	0.00	51.20	48.80	0.00	0.00
Pentane	47.34	49.40	1.53	1.73	49.12	50.87	0.01	0.00	49.38	50.62	0.00	0.00
Propane	47.47	47.94	2.18	2.41	49.85	50.14	0.01	0.01	50.23	49.77	0.00	0.00
Sea water	50.68	48.00	0.57	0.75	51.71	48.29	0.00	0.00	51.32	48.68	0.00	0.00
Toluene	49.32	48.26	1.26	1.16	50.64	49.35	0.00	0.00	50.82	49.18	0.00	0.00
Water	48.53	49.98	0.80	0.69	49.33	50.67	0.00	0.00	49.11	50.89	0.00	0.00
Xylene	48.00	49.52	1.43	1.06	48.80	51.20	0.00	0.00	48.91	51.09	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	597.69	581.11	7.32	6.75	131.05	130.48	0.01	0.00	53.86	54.61	0.00	0.00
Benzene	628.19	633.23	4.92	5.23	139.09	140.88	0.00	0.00	58.39	59.80	0.00	0.00
Chloroform	1,030.36	982.89	2.47	1.70	236.70	217.21	0.00	0.00	99.68	92.34	0.00	0.00
Creosote	740.64	786.47	2.86	1.99	168.87	177.17	0.00	0.00	70.76	74.14	0.00	0.00
Heptane	452.56	466.78	7.21	8.67	106.34	107.37	0.01	0.01	44.27	44.56	0.00	0.00
Hexane	476.56	479.41	9.77	9.56	105.29	105.35	0.01	0.00	43.33	43.67	0.00	0.00
Pentane	440.91	436.84	10.77	10.68	102.83	98.70	0.01	0.01	42.74	41.40	0.00	0.00
Propane	362.36	366.37	9.59	10.91	81.47	82.68	0.01	0.01	34.52	35.48	0.00	0.00
Sea water	745.67	738.97	4.94	3.27	167.84	162.64	0.01	0.00	69.00	66.83	0.00	0.00
Toluene	593.71	583.58	5.44	5.52	133.49	133.97	0.00	0.01	55.44	56.76	0.00	0.00
Water	692.53	680.98	2.57	2.43	159.87	151.45	0.00	0.00	67.57	63.17	0.00	0.00
Xylene	629.94	585.16	1.63	1.76	142.92	133.39	0.00	0.00	58.80	56.75	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	50.11	48.72	0.61	0.57	50.11	49.89	0.00	0.00	49.65	50.35	0.00	0.00
Benzene	49.40	49.80	0.39	0.41	49.68	50.32	0.00	0.00	49.40	50.60	0.00	0.00
Chloroform	51.07	48.72	0.12	0.08	52.15	47.85	0.00	0.00	51.91	48.09	0.00	0.00
Creosote	48.35	51.34	0.19	0.13	48.80	51.20	0.00	0.00	48.83	51.17	0.00	0.00
Heptane	48.39	49.91	0.77	0.93	49.76	50.23	0.01	0.00	49.84	50.16	0.00	0.00
Hexane	48.86	49.15	1.00	0.98	49.98	50.01	0.00	0.00	49.80	50.20	0.00	0.00
Pentane	49.03	48.58	1.20	1.19	51.02	48.97	0.00	0.00	50.80	49.20	0.00	0.00
Propane	48.36	48.90	1.28	1.46	49.63	50.36	0.00	0.01	49.31	50.69	0.00	0.00
Sea water	49.95	49.50	0.33	0.22	50.79	49.21	0.00	0.00	50.80	49.20	0.00	0.00
Toluene	49.97	49.11	0.46	0.46	49.91	50.09	0.00	0.00	49.41	50.59	0.00	0.00
Water	50.24	49.40	0.19	0.18	51.35	48.65	0.00	0.00	51.68	48.32	0.00	0.00
Xylene	51.70	48.02	0.13	0.14	51.73	48.27	0.00	0.00	50.89	49.11	0.00	0.00



Total number of collisions in ABM validation tests for  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	14.80	14.63	14.72	7.88
Benzene	14.78	14.60	14.69	7.86
Chloroform	14.71	14.64	14.68	7.86
Creosote	14.75	14.55	14.65	7.84
Heptane	14.83	14.69	14.76	7.90
Hexane	14.84	14.63	14.74	7.89
Pentane	14.84	14.73	14.78	7.91
Propane	14.92	14.67	14.79	7.92
Sea water	14.77	14.62	14.70	7.87
Toluene	14.74	14.62	14.68	7.86
Water	14.76	14.54	14.65	7.84
Xylene	14.74	14.51	14.63	7.83

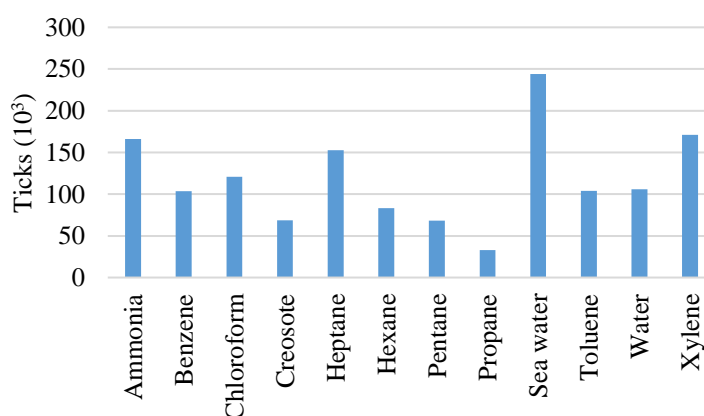
Cumulative number of uncharged nanoparticles at the interface of ABM validation tests for  $15 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	1.50	1.56	1.53	0.82
Benzene	1.70	1.67	1.68	0.90
Chloroform	2.66	2.66	2.66	1.43
Creosote	2.02	2.02	2.02	1.08
Heptane	1.33	1.24	1.28	0.69
Hexane	1.25	1.27	1.26	0.67
Pentane	1.27	1.19	1.23	0.66
Propane	1.00	0.98	0.99	0.53
Sea water	1.92	1.96	1.94	1.04
Toluene	1.68	1.57	1.63	0.87
Water	1.92	1.82	1.87	1.00
Xylene	1.66	1.61	1.64	0.88

**APPENDIX 6.6 - ABM Validation Test Results for  $50 \times 10^3$  Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $50 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio<sup>68</sup></b>
Ammonia	66.53	95.78	81.16	0.77
Benzene	68.78	138.05	103.42	0.98
Chloroform	71.35	134.66	103.01	0.98
Creosote	66.42	104.27	85.35	0.81
Heptane	64.49	90.41	77.45	0.74
Hexane	70.04	67.96	69.00	0.66
Pentane	63.48	64.68	64.08	0.61
Propane	49.87	58.22	54.05	0.51
Sea water	67.86	98.81	83.34	0.79
Toluene	66.99	131.56	99.28	0.94
Water	74.50	136.07	105.29	1.00
Xylene	67.81	98.27	83.04	0.79



Comparison of average number of ticks in ABM validation tests for  $50 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>68</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	3.35	0.40	0.11	3.33	0.40	0.11	3.34	0.40	0.11
Benzene	3.20	0.37	0.10	3.17	0.37	0.10	3.18	0.37	0.10
Chloroform	2.52	0.25	0.05	2.52	0.26	0.05	2.52	0.26	0.05
Creosote	2.80	0.31	0.07	2.78	0.30	0.07	2.79	0.30	0.07
Heptane	4.19	0.55	0.18	4.22	0.55	0.18	4.20	0.55	0.18
Hexane	4.60	0.62	0.21	4.57	0.62	0.21	4.59	0.62	0.21
Pentane	4.84	0.66	0.23	4.92	0.67	0.23	4.88	0.67	0.23
Propane	12.69	2.03	0.85	12.75	2.05	0.85	12.72	2.04	0.85
Sea water	2.87	0.32	0.08	2.83	0.31	0.08	2.85	0.31	0.08
Toluene	3.20	0.38	0.10	3.23	0.38	0.10	3.21	0.38	0.10
Water	2.94	0.33	0.08	2.89	0.32	0.08	2.92	0.33	0.08
Xylene	3.15	0.37	0.10	3.17	0.37	0.10	3.16	0.37	0.10

Distribution of ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	86.68	10.40	2.92	86.68	10.39	2.93	86.68	10.39	2.92
Benzene	87.10	10.16	2.75	87.06	10.17	2.76	87.08	10.17	2.75
Chloroform	89.09	8.99	1.92	89.05	9.02	1.93	89.07	9.00	1.93
Creosote	88.08	9.60	2.32	88.08	9.60	2.32	88.08	9.60	2.32
Heptane	85.22	11.19	3.59	85.18	11.20	3.61	85.20	11.20	3.60
Hexane	84.77	11.42	3.81	84.77	11.42	3.81	84.77	11.42	3.81
Pentane	84.45	11.60	3.95	84.46	11.58	3.96	84.46	11.59	3.95
Propane	81.49	13.07	5.45	81.48	13.08	5.44	81.48	13.07	5.45
Sea water	87.93	9.68	2.39	87.99	9.64	2.37	87.96	9.66	2.38
Toluene	87.00	10.21	2.79	87.00	10.22	2.78	87.00	10.22	2.78
Water	87.74	9.79	2.47	87.76	9.79	2.45	87.75	9.79	2.46
Xylene	87.12	10.17	2.72	87.09	10.18	2.73	87.10	10.17	2.72

ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	0.79	0.79	0.88	0.88	0.10	0.10	0.10	0.10	0.03	0.03	0.03	0.03
Benzene	0.75	0.76	0.84	0.85	0.09	0.09	0.10	0.10	0.02	0.02	0.03	0.03
Chloroform	0.59	0.59	0.67	0.68	0.06	0.06	0.06	0.07	0.01	0.01	0.01	0.01
Creosote	0.66	0.66	0.74	0.74	0.07	0.07	0.08	0.08	0.02	0.02	0.02	0.02
Heptane	1.00	1.00	1.09	1.09	0.13	0.13	0.14	0.14	0.04	0.04	0.05	0.05
Hexane	1.10	1.11	1.20	1.19	0.15	0.15	0.16	0.16	0.05	0.05	0.05	0.05
Pentane	1.17	1.17	1.25	1.25	0.16	0.16	0.17	0.17	0.06	0.06	0.06	0.06
Propane	3.12	3.12	3.22	3.22	0.50	0.50	0.51	0.51	0.21	0.21	0.21	0.22
Sea water	0.67	0.68	0.76	0.76	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02
Toluene	0.75	0.76	0.84	0.84	0.09	0.09	0.10	0.10	0.02	0.03	0.03	0.03
Water	0.69	0.69	0.78	0.78	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02
Xylene	0.75	0.74	0.83	0.84	0.09	0.09	0.09	0.09	0.02	0.02	0.02	0.03

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	23.69	23.71	26.35	26.25	24.31	24.36	25.71	25.62	24.52	24.29	25.69	25.50
Benzene	23.49	23.67	26.40	26.44	24.12	24.53	25.69	25.67	24.14	24.45	25.62	25.79
Chloroform	23.50	23.20	26.54	26.76	24.78	24.30	25.32	25.60	25.34	24.30	25.17	25.19
Creosote	23.55	23.39	26.48	26.58	24.53	24.47	25.37	25.63	24.98	24.83	24.99	25.19
Heptane	23.95	23.90	26.05	26.11	24.48	24.33	25.54	25.65	24.35	24.33	25.54	25.78
Hexane	23.93	24.16	26.01	25.90	24.11	24.61	25.79	25.49	24.06	24.43	25.86	25.65
Pentane	24.11	24.22	25.92	25.75	24.47	24.69	25.55	25.28	24.59	24.48	25.55	25.38
Propane	24.62	24.63	25.38	25.38	24.68	24.72	25.28	25.32	24.68	24.67	25.28	25.37
Sea water	23.34	23.64	26.64	26.38	24.30	24.69	25.72	25.29	24.55	24.96	25.38	25.11
Toluene	23.60	23.71	26.37	26.33	24.21	24.46	25.69	25.63	24.38	24.71	25.47	25.44
Water	23.60	23.55	26.39	26.47	24.45	24.39	25.53	25.64	24.97	24.88	24.86	25.29
Xylene	23.75	23.54	26.19	26.52	24.49	24.25	25.51	25.75	25.08	24.37	25.11	25.43

ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	0.79	0.88	0.87	0.10	0.10	0.10	0.10	0.03	0.03	0.03	0.03	0.79
Benzene	0.75	0.83	0.83	0.09	0.09	0.09	0.09	0.02	0.03	0.03	0.03	0.75
Chloroform	0.59	0.67	0.67	0.06	0.06	0.06	0.07	0.01	0.01	0.01	0.01	0.59
Creosote	0.66	0.74	0.73	0.07	0.07	0.08	0.08	0.02	0.02	0.02	0.02	0.66
Heptane	1.01	1.10	1.10	0.14	0.14	0.14	0.14	0.04	0.04	0.05	0.05	1.01
Hexane	1.10	1.18	1.19	0.15	0.15	0.16	0.16	0.05	0.05	0.05	0.05	1.10
Pentane	1.19	1.27	1.27	0.17	0.16	0.17	0.17	0.06	0.06	0.06	0.06	1.19
Propane	3.14	3.23	3.24	0.51	0.51	0.52	0.52	0.21	0.21	0.21	0.22	3.14
Sea water	0.67	0.75	0.75	0.07	0.08	0.08	0.08	0.02	0.02	0.02	0.02	0.67
Toluene	0.77	0.85	0.85	0.09	0.09	0.10	0.10	0.03	0.03	0.03	0.03	0.77
Water	0.68	0.77	0.76	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02	0.68
Xylene	0.75	0.83	0.83	0.09	0.09	0.09	0.09	0.02	0.02	0.03	0.03	0.75

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	23.82	26.44	26.15	24.24	24.48	25.81	25.48	24.11	24.72	25.72	25.46	23.82
Benzene	23.84	26.34	26.35	24.13	24.75	25.65	25.48	24.35	24.90	25.43	25.33	23.84
Chloroform	23.29	26.51	26.71	24.75	24.30	25.41	25.54	25.55	24.46	24.95	25.03	23.29
Creosote	23.61	26.57	26.37	24.36	24.73	25.64	25.26	24.44	25.23	25.42	24.91	23.61
Heptane	23.93	26.04	26.05	24.48	24.35	25.59	25.58	24.53	24.24	25.58	25.65	23.93
Hexane	24.11	25.86	25.94	24.42	24.52	25.45	25.60	24.49	24.50	25.59	25.42	24.11
Pentane	24.13	25.87	25.84	24.53	24.42	25.47	25.58	24.59	24.25	25.53	25.63	24.13
Propane	24.63	25.30	25.39	24.78	24.71	25.20	25.31	24.66	24.68	25.24	25.42	24.63
Sea water	23.59	26.56	26.42	24.16	24.75	25.66	25.42	24.34	25.16	25.51	24.99	23.59
Toluene	23.90	26.46	26.20	23.89	24.98	25.74	25.39	24.27	25.11	25.38	25.25	23.90
Water	23.59	26.58	26.33	24.30	24.66	25.52	25.53	24.40	24.83	25.51	25.25	23.59
Xylene	23.72	26.27	26.30	24.41	24.54	25.51	25.53	24.55	24.87	25.24	25.33	23.72



Total number of collisions in ABM validation tests for  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	3.86	3.84	3.84	1.16
Benzene	3.67	3.64	3.64	1.10
Chloroform	2.83	2.83	2.83	0.86
Creosote	3.18	3.16	3.15	0.96
Heptane	4.91	4.95	4.95	1.50
Hexane	5.43	5.40	5.40	1.64
Pentane	5.73	5.81	5.82	1.76
Propane	15.57	15.63	15.65	4.74
Sea water	3.26	3.22	3.22	0.98
Toluene	3.68	3.71	3.71	1.12
Water	3.35	3.30	3.30	1.00
Xylene	3.62	3.64	3.64	1.10

Cumulative number of uncharged nanoparticles at the interface of ABM validation tests for  $50 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	48.58	48.91	48.74	1.00
Benzene	48.57	49.13	48.85	1.00
Chloroform	47.76	48.41	48.09	0.99
Creosote	48.19	48.62	48.41	0.99
Heptane	48.84	49.12	48.98	1.01
Hexane	48.94	48.94	48.94	1.01
Pentane	48.92	48.92	48.92	1.00
Propane	48.93	49.09	49.01	1.01
Sea water	48.28	48.66	48.47	1.00
Toluene	48.55	49.15	48.85	1.00
Water	48.44	48.93	48.69	1.00
Xylene	48.52	48.86	48.69	1.00

## APPENDIX 7 - ABM Validation Test Results for Same-charged Nanoparticles

### APPENDIX 7.1 - ABM Validation Test Results for $5 \times 10^3$ Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM validation tests for  $5 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio<sup>69</sup></b>
Ammonia	106.48	125.88	116.18	1.02
Benzene	106.90	139.80	123.35	1.08
Chloroform	106.15	134.32	120.24	1.05
Creosote	152.97	132.74	142.86	1.25
Heptane	92.23	132.52	112.38	0.98
Hexane	103.22	138.24	120.73	1.06
Pentane	100.99	135.30	118.15	1.03
Propane	105.38	125.47	115.43	1.01
Sea water	103.28	130.24	116.76	1.02
Toluene	107.70	128.60	118.15	1.03
Water	100.44	128.28	114.36	1.00
Xylene	102.20	125.26	113.73	0.99

<sup>69</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	14.42	0.47	0.12	14.89	0.59	0.16	14.65	0.53	0.14
Benzene	14.21	0.50	0.11	14.64	0.56	0.14	14.42	0.53	0.13
Chloroform	11.57	0.42	0.11	11.31	0.30	0.05	11.44	0.36	0.08
Creosote	13.57	0.49	0.11	13.26	0.42	0.07	13.42	0.45	0.09
Heptane	17.17	0.70	0.21	16.82	0.79	0.22	17.00	0.74	0.21
Hexane	17.78	0.67	0.17	17.72	0.62	0.15	17.75	0.64	0.16
Pentane	18.37	0.70	0.18	18.19	0.75	0.24	18.28	0.73	0.21
Propane	22.75	0.88	0.31	21.82	0.94	0.35	22.29	0.91	0.33
Sea water	13.08	0.51	0.12	13.44	0.47	0.08	13.26	0.49	0.10
Toluene	13.99	0.54	0.13	14.66	0.58	0.15	14.33	0.56	0.14
Water	13.40	0.49	0.10	13.44	0.53	0.13	13.42	0.51	0.11
Xylene	13.70	0.55	0.15	14.72	0.54	0.15	14.21	0.55	0.15

Distribution of ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	96.09	3.11	0.81	95.23	3.77	1.00	95.65	3.45	0.90
Benzene	95.86	3.37	0.76	95.47	3.63	0.89	95.66	3.51	0.83
Chloroform	95.68	3.43	0.88	97.02	2.57	0.40	96.34	3.01	0.65
Creosote	95.73	3.46	0.80	96.46	3.03	0.50	96.09	3.25	0.66
Heptane	95.02	3.85	1.14	94.32	4.44	1.24	94.67	4.14	1.19
Hexane	95.54	3.58	0.89	95.82	3.36	0.83	95.68	3.47	0.86
Pentane	95.43	3.65	0.91	94.86	3.90	1.24	95.15	3.78	1.08
Propane	95.05	3.67	1.28	94.41	4.08	1.51	94.74	3.87	1.39
Sea water	95.40	3.74	0.85	96.04	3.37	0.59	95.73	3.55	0.72
Toluene	95.42	3.70	0.87	95.28	3.77	0.96	95.35	3.74	0.92
Water	95.83	3.48	0.69	95.32	3.79	0.89	95.58	3.63	0.79
Xylene	95.13	3.82	1.06	95.54	3.50	0.95	95.34	3.66	1.00

ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	4.60	6.99	1.62	1.21	0.17	0.29	0.00	0.00	0.04	0.09	0.00	0.00
Benzene	7.03	4.35	1.28	1.56	0.33	0.17	0.00	0.00	0.07	0.05	0.00	0.00
Chloroform	4.40	5.36	1.03	0.78	0.18	0.24	0.00	0.00	0.05	0.06	0.00	0.00
Creosote	5.61	5.40	1.23	1.34	0.26	0.23	0.00	0.00	0.05	0.06	0.00	0.00
Heptane	6.76	6.86	1.82	1.73	0.36	0.34	0.00	0.00	0.10	0.11	0.00	0.00
Hexane	8.79	5.25	1.76	1.99	0.41	0.25	0.00	0.00	0.10	0.07	0.00	0.00
Pentane	7.94	6.07	1.98	2.38	0.42	0.28	0.00	0.00	0.11	0.07	0.00	0.00
Propane	8.10	8.83	2.95	2.87	0.43	0.45	0.00	0.00	0.15	0.16	0.00	0.00
Sea water	5.69	5.17	1.09	1.13	0.29	0.22	0.00	0.00	0.07	0.05	0.00	0.00
Toluene	5.51	5.90	1.31	1.27	0.24	0.30	0.00	0.00	0.06	0.07	0.00	0.00
Water	6.61	4.22	1.08	1.49	0.34	0.15	0.00	0.00	0.07	0.03	0.00	0.00
Xylene	2.89	2.34	0.00	0.00	0.30	0.23	0.00	0.00	0.09	0.07	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	31.92	48.46	11.23	8.40	37.34	62.66	0.00	0.00	28.93	71.07	0.00	0.00
Benzene	49.45	30.58	9.02	10.95	66.20	33.80	0.00	0.00	60.18	39.82	0.00	0.00
Chloroform	38.03	46.34	8.86	6.77	42.89	57.11	0.00	0.00	42.06	57.94	0.00	0.00
Creosote	41.30	39.77	9.02	9.90	53.56	46.44	0.00	0.00	47.37	52.63	0.00	0.00
Heptane	39.35	39.94	10.61	10.09	51.08	48.92	0.00	0.00	47.57	52.43	0.00	0.00
Hexane	49.42	29.52	9.89	11.18	62.01	37.69	0.30	0.00	58.18	41.82	0.00	0.00
Pentane	43.24	33.06	10.76	12.94	60.03	39.97	0.00	0.00	61.93	38.07	0.00	0.00
Propane	35.60	38.83	12.97	12.60	48.86	51.03	0.00	0.11	47.56	52.44	0.00	0.00
Sea water	43.47	39.57	8.33	8.63	57.31	42.50	0.19	0.00	57.26	42.74	0.00	0.00
Toluene	39.38	42.16	9.39	9.07	44.57	55.43	0.00	0.00	45.31	54.69	0.00	0.00
Water	49.32	31.48	8.07	11.13	69.14	30.86	0.00	0.00	71.13	28.87	0.00	0.00
Xylene	55.22	44.78	0.00	0.00	56.68	43.32	0.00	0.00	57.24	42.76	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	7.86	4.18	1.20	1.65	0.41	0.18	0.00	0.00	0.10	0.06	0.00	0.00
Benzene	7.31	4.37	1.34	1.61	0.36	0.20	0.00	0.00	0.09	0.04	0.00	0.00
Chloroform	3.98	5.40	1.08	0.84	0.13	0.17	0.00	0.00	0.03	0.02	0.00	0.00
Creosote	4.49	6.24	1.45	1.08	0.16	0.26	0.00	0.00	0.03	0.04	0.00	0.00
Heptane	8.14	5.40	1.40	1.88	0.49	0.31	0.00	0.00	0.14	0.08	0.00	0.00
Hexane	8.30	5.19	1.89	2.35	0.40	0.22	0.00	0.00	0.10	0.05	0.00	0.00
Pentane	7.50	6.36	2.18	2.15	0.42	0.33	0.00	0.00	0.15	0.09	0.00	0.00
Propane	8.18	8.69	2.61	2.34	0.47	0.48	0.00	0.00	0.17	0.18	0.00	0.00
Sea water	5.99	4.98	1.20	1.27	0.25	0.23	0.00	0.00	0.05	0.04	0.00	0.00
Toluene	5.43	6.15	1.54	1.54	0.26	0.32	0.00	0.00	0.05	0.10	0.00	0.00
Water	3.84	7.36	1.30	0.94	0.15	0.39	0.00	0.00	0.03	0.10	0.00	0.00
Xylene	6.03	5.77	1.50	1.42	0.30	0.25	0.00	0.00	0.08	0.07	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	52.78	28.08	8.04	11.10	70.17	29.83	0.00	0.00	62.82	37.18	0.00	0.00
Benzene	49.96	29.89	9.14	11.02	64.45	35.55	0.00	0.00	68.61	31.39	0.00	0.00
Chloroform	35.24	47.77	9.53	7.47	44.00	56.00	0.00	0.00	57.45	42.55	0.00	0.00
Creosote	33.86	47.08	10.90	8.17	38.37	61.63	0.00	0.00	46.38	53.62	0.00	0.00
Heptane	48.39	32.13	8.33	11.15	61.36	38.64	0.00	0.00	63.35	36.65	0.00	0.00
Hexane	46.80	29.26	10.67	13.27	64.90	35.10	0.00	0.00	66.01	33.99	0.00	0.00
Pentane	41.25	34.94	11.99	11.82	56.02	43.98	0.00	0.00	60.92	39.08	0.00	0.00
Propane	37.46	39.83	11.97	10.73	49.47	50.42	0.11	0.00	48.28	51.72	0.00	0.00
Sea water	44.57	37.06	8.94	9.42	52.23	47.77	0.00	0.00	56.63	43.37	0.00	0.00
Toluene	37.03	41.97	10.52	10.48	45.17	54.66	0.17	0.00	33.33	66.67	0.00	0.00
Water	28.55	54.78	9.68	6.99	27.90	72.10	0.00	0.00	20.80	79.20	0.00	0.00
Xylene	40.98	39.19	10.20	9.62	54.63	45.37	0.00	0.00	52.38	47.62	0.00	0.00



Total number of collisions in ABM validation tests for  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	15.01	15.63	15.32	1.09
Benzene	14.82	15.33	15.07	1.07
Chloroform	12.09	11.65	11.87	0.85
Creosote	14.18	13.75	13.96	0.99
Heptane	18.08	17.83	17.95	1.28
Hexane	18.62	18.50	18.56	1.32
Pentane	19.24	19.18	19.21	1.37
Propane	23.93	23.12	23.53	1.68
Sea water	13.71	13.99	13.85	0.99
Toluene	14.66	15.39	15.03	1.07
Water	13.98	14.09	14.04	1.00
Xylene	14.40	15.41	14.91	1.06

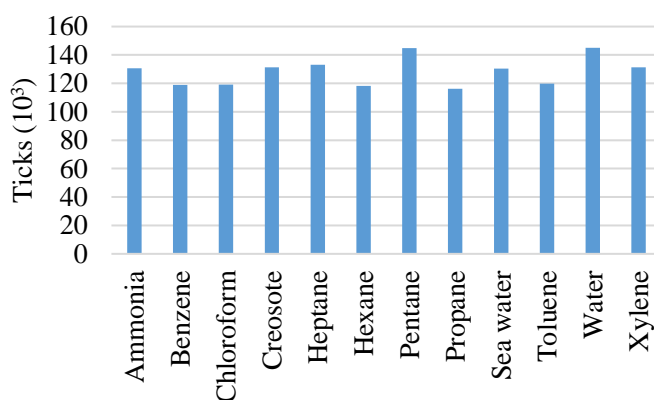
Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $5 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	4.25	4.35	4.30	1.04
Benzene	4.22	4.36	4.29	1.03
Chloroform	3.81	3.91	3.86	0.93
Creosote	4.26	4.17	4.22	1.01
Heptane	4.31	4.53	4.42	1.06
Hexane	4.44	4.57	4.51	1.08
Pentane	4.23	4.59	4.41	1.06
Propane	4.65	4.77	4.71	1.13
Sea water	4.08	4.19	4.13	1.00
Toluene	4.25	4.31	4.28	1.03
Water	4.07	4.24	4.15	1.00
Xylene	4.21	4.29	4.25	1.02

**APPENDIX 7.2 - ABM Validation Test Results for  $7.5 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $7.5 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	Average (10 <sup>3</sup> )	Ratio <sup>70</sup>
Ammonia	81.32	179.83	130.58	0.90
Benzene	59.38	178.25	118.82	0.82
Chloroform	61.75	176.53	119.14	0.82
Creosote	88.03	174.66	131.35	0.91
Heptane	85.42	180.77	133.10	0.92
Hexane	56.46	179.80	118.13	0.81
Pentane	110.77	178.83	144.80	1.00
Propane	54.43	178.16	116.30	0.80
Sea water	84.75	176.28	130.52	0.90
Toluene	60.23	179.25	119.74	0.83
Water	112.55	177.68	145.12	1.00
Xylene	86.04	176.43	131.24	0.90



Comparison of average number of ticks in ABM validation tests for  $7.5 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>70</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	40.18	1.26	0.29	41.14	1.12	0.24	40.66	1.19	0.27
Benzene	37.95	1.13	0.23	39.34	1.01	0.23	38.64	1.07	0.23
Chloroform	37.95	1.13	0.23	31.65	0.71	0.13	34.80	0.92	0.18
Creosote	32.45	1.01	0.23	35.40	1.12	0.26	33.92	1.06	0.24
Heptane	46.35	1.28	0.30	46.13	1.41	0.41	46.24	1.35	0.36
Hexane	45.88	1.48	0.38	48.08	1.48	0.41	46.98	1.48	0.40
Pentane	50.20	1.70	0.43	10.74	1.18	0.34	30.47	1.44	0.38
Propane	59.24	1.87	0.53	60.96	1.94	0.57	60.10	1.91	0.55
Sea water	35.38	1.03	0.23	36.14	1.08	0.21	35.76	1.05	0.22
Toluene	39.15	1.32	0.33	39.90	1.13	0.27	39.52	1.22	0.30
Water	36.28	1.14	0.26	36.91	1.07	0.27	36.60	1.10	0.27
Xylene	37.36	1.07	0.24	39.08	1.35	0.29	38.22	1.21	0.27

Distribution of ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Ammonia	96.28	3.02	0.70	96.80	2.63	0.57	96.54	2.82	0.64
Benzene	96.54	2.86	0.59	96.95	2.48	0.57	96.75	2.67	0.58
Chloroform	96.54	2.86	0.59	97.44	2.17	0.39	96.95	2.55	0.50
Creosote	96.34	2.98	0.67	96.25	3.03	0.71	96.30	3.01	0.69
Heptane	96.70	2.67	0.63	96.20	2.94	0.86	96.45	2.81	0.74
Hexane	96.11	3.10	0.79	96.21	2.96	0.83	96.16	3.03	0.81
Pentane	95.93	3.25	0.81	87.64	9.62	2.74	94.36	4.46	1.18
Propane	96.10	3.04	0.86	96.05	3.05	0.90	96.07	3.05	0.88
Sea water	96.56	2.81	0.64	96.55	2.88	0.57	96.55	2.84	0.60
Toluene	95.97	3.22	0.81	96.60	2.74	0.66	96.28	2.98	0.73
Water	96.30	3.02	0.68	96.49	2.80	0.71	96.39	2.91	0.70
Xylene	96.62	2.76	0.63	95.97	3.31	0.72	96.28	3.04	0.68

ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	10.76	16.51	6.96	5.95	0.41	0.84	0.01	0.00	0.10	0.19	0.00	0.00
Benzene	11.53	14.13	6.59	5.70	0.50	0.62	0.01	0.00	0.09	0.14	0.00	0.00
Chloroform	9.02	11.87	3.62	3.18	0.30	0.53	0.00	0.00	0.07	0.09	0.00	0.00
Creosote	11.50	11.90	4.60	4.44	0.48	0.52	0.00	0.00	0.11	0.12	0.00	0.00
Heptane	18.99	11.28	6.95	9.13	0.89	0.37	0.00	0.01	0.20	0.10	0.00	0.00
Hexane	16.48	14.52	7.37	7.50	0.81	0.66	0.00	0.01	0.19	0.19	0.00	0.00
Pentane	12.86	19.98	9.18	8.19	0.50	1.19	0.01	0.00	0.13	0.30	0.00	0.00
Propane	18.67	19.34	10.85	10.38	0.93	0.92	0.02	0.01	0.25	0.28	0.00	0.00
Sea water	14.24	10.22	5.02	5.91	0.67	0.36	0.00	0.00	0.15	0.08	0.00	0.00
Toluene	9.89	17.36	6.72	5.18	0.36	0.95	0.00	0.00	0.09	0.24	0.00	0.00
Water	15.47	9.66	5.12	6.03	0.78	0.36	0.00	0.00	0.18	0.08	0.00	0.00
Xylene	13.21	12.65	5.61	5.89	0.56	0.51	0.00	0.00	0.11	0.13	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	35.35	33.86	15.02	15.77	52.16	47.37	0.28	0.19	45.45	54.55	0.00	0.00
Benzene	30.39	37.23	17.37	15.01	44.36	55.02	0.44	0.18	39.06	60.94	0.00	0.00
Chloroform	32.57	42.86	13.09	11.48	35.83	63.93	0.12	0.12	43.05	56.95	0.00	0.00
Creosote	35.46	36.68	14.18	13.68	47.86	51.94	0.00	0.20	46.26	53.74	0.00	0.00
Heptane	40.96	24.34	15.00	19.70	69.77	28.98	0.16	1.09	67.67	32.33	0.00	0.00
Hexane	35.93	31.64	16.07	16.36	54.63	44.90	0.14	0.34	49.21	50.79	0.00	0.00
Pentane	25.61	39.79	18.28	16.32	29.48	69.99	0.35	0.18	30.52	69.48	0.00	0.00
Propane	31.51	32.64	18.32	17.53	49.87	48.96	0.80	0.37	47.65	52.35	0.00	0.00
Sea water	40.24	28.90	14.18	16.69	65.31	34.50	0.00	0.19	63.95	36.05	0.00	0.00
Toluene	25.27	44.34	17.15	13.24	27.45	72.09	0.23	0.23	27.88	72.12	0.00	0.00
Water	42.64	26.63	14.10	16.63	68.57	31.25	0.00	0.18	69.77	30.23	0.00	0.00
Xylene	35.35	33.86	15.02	15.77	52.16	47.37	0.28	0.19	45.45	54.55	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	10.67	16.43	7.64	6.40	0.35	0.76	0.01	0.00	0.07	0.18	0.00	0.00
Benzene	10.31	15.73	7.23	6.07	0.36	0.64	0.00	0.00	0.09	0.14	0.00	0.00
Chloroform	9.11	12.71	5.23	4.60	0.29	0.42	0.00	0.00	0.06	0.07	0.00	0.00
Creosote	11.96	12.65	5.54	5.25	0.55	0.56	0.00	0.00	0.12	0.14	0.00	0.00
Heptane	15.04	15.03	8.13	7.93	0.72	0.69	0.00	0.00	0.20	0.22	0.00	0.00
Hexane	15.90	15.57	8.14	8.47	0.71	0.76	0.01	0.00	0.19	0.22	0.00	0.00
Pentane	4.45	6.28	0.01	0.01	0.46	0.72	0.00	0.00	0.14	0.20	0.00	0.00
Propane	19.50	19.72	10.83	10.92	1.02	0.90	0.01	0.01	0.32	0.25	0.00	0.00
Sea water	14.04	10.75	5.19	6.17	0.66	0.42	0.00	0.00	0.13	0.08	0.00	0.00
Toluene	13.11	13.36	6.73	6.69	0.55	0.58	0.00	0.00	0.12	0.15	0.00	0.00
Water	10.72	14.12	6.38	5.68	0.41	0.65	0.01	0.00	0.10	0.17	0.00	0.00
Xylene	10.22	16.42	6.73	5.72	0.39	0.95	0.01	0.00	0.08	0.21	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	26.15	42.00	17.23	14.62	29.13	70.27	0.37	0.22	27.55	72.45	0.00	0.00
Benzene	26.21	39.99	18.37	15.43	36.18	63.52	0.20	0.10	39.83	60.17	0.00	0.00
Chloroform	28.80	40.16	16.51	14.53	40.99	58.87	0.00	0.14	43.75	56.25	0.00	0.00
Creosote	33.77	35.75	15.66	14.82	49.55	50.09	0.09	0.27	46.56	53.44	0.00	0.00
Heptane	32.60	32.58	17.62	17.19	50.85	48.87	0.07	0.21	47.83	52.17	0.00	0.00
Hexane	33.07	32.38	16.92	17.62	48.28	51.12	0.34	0.27	46.97	53.03	0.00	0.00
Pentane	41.37	58.44	0.10	0.08	39.10	60.90	0.00	0.00	41.67	58.33	0.00	0.00
Propane	31.98	32.35	17.76	17.91	52.73	46.28	0.31	0.67	56.29	43.71	0.00	0.00
Sea water	38.85	29.74	14.35	17.06	61.13	38.68	0.09	0.09	61.50	38.50	0.00	0.00
Toluene	32.86	33.49	16.87	16.78	48.54	51.19	0.18	0.09	43.96	56.04	0.00	0.00
Water	29.05	38.26	17.29	15.40	38.53	60.82	0.47	0.19	38.24	61.76	0.00	0.00
Xylene	26.15	42.00	17.23	14.62	29.13	70.27	0.37	0.22	27.55	72.45	0.00	0.00



Total number of collisions in ABM validation tests for  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	41.73	42.69	42.55	41.73
Benzene	39.30	40.70	40.58	39.30
Chloroform	39.30	33.01	32.59	39.30
Creosote	33.68	36.63	36.74	33.68
Heptane	47.93	47.71	47.84	47.93
Hexane	47.74	49.93	49.93	47.74
Pentane	52.33	12.87	12.35	52.33
Propane	61.64	63.36	63.43	61.64
Sea water	36.64	37.41	37.45	36.64
Toluene	40.79	41.54	41.36	40.79
Water	37.68	38.31	38.24	37.68
Xylene	38.67	40.39	40.68	38.67

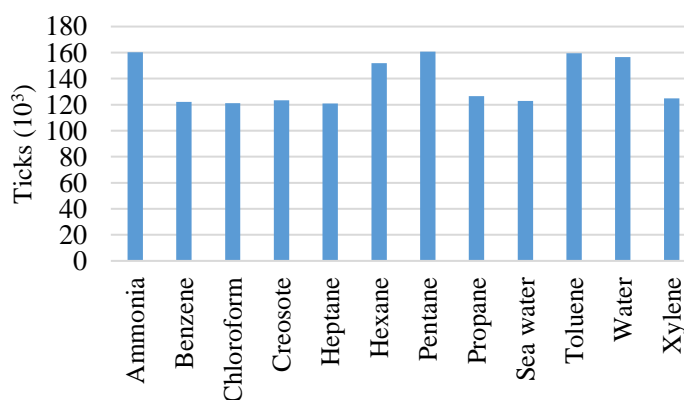
Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $7.5 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	6.42	6.94	6.68	1.02
Benzene	6.12	6.86	6.49	0.99
Chloroform	5.62	6.27	5.94	0.90
Creosote	6.21	6.63	6.42	0.98
Heptane	6.63	7.11	6.87	1.05
Hexane	6.42	7.14	6.78	1.03
Pentane	6.93	0.54	3.73	0.57
Propane	6.09	7.33	6.71	1.02
Sea water	6.17	6.70	6.43	0.98
Toluene	6.14	6.85	6.50	0.99
Water	6.40	6.74	6.57	1.00
Xylene	6.40	6.85	6.63	1.01

**APPENDIX 7.3 - ABM Validation Test Results for  $10 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $10 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (<math>10^3</math>)</b>	<b>2<sup>nd</sup> Test (<math>10^3</math>)</b>	<b>Average (<math>10^3</math>)</b>	<b>Ratio<sup>71</sup></b>
Ammonia	81.31	238.97	160.14	1.02
Benzene	79.55	164.76	122.16	0.78
Chloroform	78.05	164.46	121.26	0.77
Creosote	78.24	168.42	123.33	0.79
Heptane	76.09	165.90	121.00	0.77
Hexane	64.89	239.11	152.00	0.97
Pentane	79.45	242.20	160.83	1.03
Propane	81.47	171.59	126.53	0.81
Sea water	77.99	167.79	122.89	0.78
Toluene	79.38	239.50	159.44	1.02
Water	75.66	237.61	156.64	1.00
Xylene	81.46	168.34	124.90	0.80



Comparison of average number of ticks in ABM validation tests for  $10 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>71</sup> <sup>71</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	83.28	2.35	0.54	81.31	2.24	0.53	82.30	2.29	0.53
Benzene	77.58	2.16	0.47	16.73	1.86	0.48	47.16	2.01	0.47
Chloroform	65.38	1.39	0.21	62.70	1.63	0.29	64.04	1.51	0.25
Creosote	74.45	1.95	0.45	72.39	1.95	0.40	73.42	1.95	0.42
Heptane	91.71	2.79	0.66	90.90	2.76	0.66	91.31	2.78	0.66
Hexane	97.89	2.72	0.69	96.79	2.91	0.69	97.34	2.82	0.69
Pentane	98.76	2.93	0.78	98.62	2.99	0.74	98.69	2.96	0.76
Propane	127.52	3.79	0.94	132.81	4.01	1.01	130.16	3.90	0.97
Sea water	75.02	1.94	0.45	73.76	2.02	0.43	74.39	1.98	0.44
Toluene	82.74	2.13	0.48	77.87	2.27	0.48	80.31	2.20	0.48
Water	77.67	1.98	0.43	76.61	2.25	0.47	77.14	2.12	0.45
Xylene	81.26	2.32	0.51	78.17	2.08	0.44	79.72	2.20	0.47

Distribution of ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Ammonia	96.65	2.73	0.62	96.71	2.66	0.63	96.68	2.69	0.62
Benzene	96.73	2.69	0.58	87.72	9.76	2.52	95.00	4.05	0.95
Chloroform	97.61	2.08	0.31	97.04	2.52	0.44	97.33	2.30	0.37
Creosote	96.88	2.53	0.59	96.86	2.61	0.53	96.87	2.57	0.56
Heptane	96.38	2.93	0.69	96.37	2.93	0.70	96.37	2.93	0.70
Hexane	96.63	2.69	0.68	96.42	2.90	0.68	96.53	2.79	0.68
Pentane	96.38	2.86	0.76	96.35	2.92	0.73	96.37	2.89	0.74
Propane	96.42	2.86	0.71	96.36	2.91	0.73	96.39	2.89	0.72
Sea water	96.92	2.50	0.58	96.79	2.65	0.56	96.86	2.57	0.57
Toluene	96.94	2.50	0.56	96.59	2.82	0.60	96.77	2.65	0.58
Water	96.99	2.47	0.54	96.57	2.84	0.59	96.78	2.65	0.56
Xylene	96.63	2.76	0.61	96.88	2.58	0.54	96.75	2.67	0.57

ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	22.10	26.63	17.87	16.68	0.90	1.40	0.03	0.02	0.19	0.35	0.00	0.00
Benzene	25.17	21.41	15.58	15.42	1.24	0.88	0.02	0.02	0.28	0.19	0.00	0.00
Chloroform	22.11	16.56	12.43	14.28	0.91	0.47	0.00	0.01	0.14	0.07	0.00	0.00
Creosote	21.22	22.29	15.70	15.24	0.88	1.04	0.02	0.02	0.22	0.23	0.00	0.00
Heptane	26.27	27.38	19.45	18.61	1.35	1.39	0.02	0.02	0.33	0.33	0.00	0.00
Hexane	27.08	29.37	20.93	20.52	1.17	1.50	0.03	0.02	0.31	0.38	0.00	0.00
Pentane	28.83	29.69	20.06	20.18	1.44	1.43	0.03	0.03	0.40	0.38	0.00	0.00
Propane	39.09	35.01	26.80	26.62	2.07	1.58	0.07	0.07	0.53	0.42	0.00	0.00
Sea water	22.19	22.20	14.99	15.64	0.91	1.00	0.02	0.01	0.22	0.23	0.00	0.00
Toluene	22.35	25.99	17.64	16.77	0.86	1.24	0.02	0.01	0.20	0.28	0.00	0.00
Water	22.97	22.73	16.28	15.68	0.98	0.97	0.01	0.02	0.21	0.22	0.00	0.00
Xylene	24.60	22.81	15.97	17.88	1.20	1.08	0.02	0.02	0.26	0.25	0.00	0.00

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	30.27	28.07	19.66	22.00	51.68	46.64	0.86	0.82	51.18	48.82	0.00	0.00
Benzene	32.45	27.60	20.08	19.88	57.35	40.79	0.93	0.93	60.17	39.83	0.00	0.00
Chloroform	33.81	25.33	19.01	21.84	65.28	33.79	0.29	0.65	66.83	33.17	0.00	0.00
Creosote	28.50	29.94	21.09	20.47	44.97	53.18	1.08	0.77	48.12	51.88	0.00	0.00
Heptane	28.64	29.85	21.21	20.30	48.51	49.84	0.79	0.86	49.39	50.61	0.00	0.00
Hexane	27.66	30.00	21.38	20.96	42.89	55.05	1.18	0.88	44.33	55.67	0.00	0.00
Pentane	29.19	30.07	20.31	20.43	49.23	48.72	1.06	0.99	51.02	48.98	0.00	0.00
Propane	30.65	27.46	21.01	20.88	54.61	41.67	1.90	1.82	55.78	44.11	0.11	0.00
Sea water	29.58	29.59	19.98	20.85	46.90	51.65	0.83	0.62	48.65	51.35	0.00	0.00
Toluene	27.01	31.41	21.32	20.26	40.34	58.07	1.08	0.52	42.29	57.71	0.00	0.00
Water	29.57	29.27	20.97	20.19	49.49	49.09	0.66	0.76	49.18	50.82	0.00	0.00
Xylene	30.27	28.07	19.66	22.00	51.68	46.64	0.86	0.82	51.18	48.82	0.00	0.00

ABM second validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	23.59	24.22	16.41	17.09	1.04	1.17	0.02	0.02	0.25	0.28	0.00	0.00
Benzene	22.48	25.11	15.87	15.14	1.03	1.28	0.02	0.01	0.23	0.30	0.00	0.00
Chloroform	21.01	17.42	11.57	12.71	0.97	0.64	0.01	0.01	0.16	0.12	0.00	0.00
Creosote	25.08	18.38	13.41	15.53	1.27	0.66	0.01	0.01	0.27	0.12	0.00	0.00
Heptane	23.52	30.81	19.25	17.31	0.92	1.79	0.03	0.02	0.23	0.43	0.00	0.00
Hexane	27.19	29.44	20.67	19.50	1.32	1.53	0.03	0.04	0.31	0.38	0.00	0.00
Pentane	34.18	24.55	18.91	20.99	1.95	0.98	0.03	0.04	0.50	0.24	0.00	0.00
Propane	43.81	31.37	27.27	30.36	2.66	1.19	0.06	0.10	0.72	0.28	0.00	0.00
Sea water	17.30	27.05	16.14	13.28	0.55	1.44	0.03	0.00	0.11	0.32	0.00	0.00
Toluene	21.60	26.27	15.59	14.40	0.91	1.33	0.02	0.01	0.19	0.30	0.00	0.00
Water	18.76	27.29	15.79	14.77	0.62	1.61	0.01	0.01	0.14	0.33	0.00	0.00
Xylene	20.46	26.24	16.58	14.90	0.74	1.31	0.02	0.01	0.16	0.28	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	26.17	33.56	21.21	19.06	35.69	62.73	1.01	0.58	36.01	63.99	0.00	0.00
Benzene	28.60	31.95	20.19	19.26	44.15	54.57	0.85	0.43	43.43	56.57	0.00	0.00
Chloroform	33.50	27.78	18.45	20.27	59.64	39.07	0.49	0.80	57.54	42.46	0.00	0.00
Creosote	34.64	25.39	18.52	21.45	65.18	33.59	0.56	0.67	68.86	31.14	0.00	0.00
Heptane	25.88	33.90	21.18	19.05	33.43	64.73	1.05	0.80	35.35	64.50	0.00	0.15
Hexane	28.09	30.41	21.35	20.15	45.24	52.56	1.00	1.20	44.90	55.10	0.00	0.00
Pentane	34.66	24.89	19.17	21.28	65.18	32.81	0.84	1.17	67.56	32.30	0.00	0.13
Propane	32.98	23.62	20.53	22.86	66.31	29.57	1.52	2.60	71.74	28.16	0.00	0.10
Sea water	23.45	36.67	21.88	18.00	27.13	71.38	1.34	0.15	26.05	73.95	0.00	0.00
Toluene	27.74	33.74	20.02	18.49	39.87	58.55	1.06	0.53	38.80	61.20	0.00	0.00
Water	24.49	35.63	20.61	19.28	27.66	71.27	0.62	0.44	29.15	70.85	0.00	0.00
Xylene	26.17	33.56	21.21	19.06	35.69	62.73	1.01	0.58	36.01	63.99	0.00	0.00



Total number of collisions in ABM validation tests for  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	86.17	84.20	84.08	1.06
Benzene	80.21	19.36	19.06	0.24
Chloroform	66.98	64.30	64.54	0.81
Creosote	76.85	74.78	74.79	0.94
Heptane	95.16	94.35	94.32	1.19
Hexane	101.31	100.20	100.38	1.27
Pentane	102.47	102.33	102.39	1.29
Propane	132.25	137.54	137.76	1.74
Sea water	77.40	76.14	76.22	0.96
Toluene	85.35	80.48	80.62	1.02
Water	80.07	79.01	79.29	1.00
Xylene	84.10	81.01	80.76	1.02

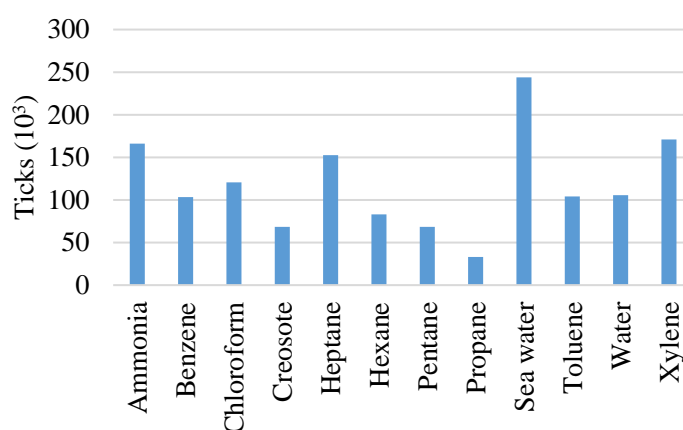
Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $10 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	9.57	8.83	9.20	1.03
Benzene	9.30	8.73	9.02	1.01
Chloroform	8.63	8.02	8.33	0.93
Creosote	9.08	8.46	8.77	0.98
Heptane	9.53	9.06	9.30	1.04
Hexane	9.76	8.94	9.35	1.04
Pentane	9.78	9.17	9.48	1.06
Propane	9.83	9.43	9.63	1.08
Sea water	9.12	8.48	8.80	0.98
Toluene	9.52	8.77	9.15	1.02
Water	9.39	8.50	8.95	1.00
Xylene	9.27	8.77	9.02	1.01

**APPENDIX 7.4 - ABM Validation Test Results for  $12.5 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $12.5 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (<math>10^3</math>)</b>	<b>2<sup>nd</sup> Test (<math>10^3</math>)</b>	<b>Average (<math>10^3</math>)</b>	<b>Ratio<sup>72</sup></b>
Ammonia	74.39	96.98	85.69	0.96
Benzene	89.50	89.15	89.33	1.00
Chloroform	91.45	83.16	87.31	0.98
Creosote	73.31	94.30	83.81	0.94
Heptane	90.94	89.48	90.21	1.01
Hexane	90.96	95.25	93.11	1.04
Pentane	83.95	93.66	88.81	0.99
Propane	93.15	95.26	94.21	1.05
Sea water	89.57	93.34	91.46	1.02
Toluene	93.67	88.26	90.97	1.02
Water	95.10	83.91	89.51	1.00
Xylene	92.78	96.00	94.39	1.05



Comparison of average number of ticks in ABM validation tests for  $12.5 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>72</sup> <sup>72</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )	2-Body Collisions ( $10^3$ )	3-Body Collisions ( $10^3$ )	4-Body Collisions ( $10^3$ )
Ammonia	141.70	4.10	0.84	144.69	4.02	0.88	143.19	4.06	0.86
Benzene	135.18	4.02	0.83	136.25	3.87	0.78	135.71	3.94	0.80
Chloroform	113.19	2.93	0.57	111.09	2.69	0.47	112.14	2.81	0.52
Creosote	126.52	3.41	0.67	126.28	3.49	0.68	126.40	3.45	0.67
Heptane	159.81	4.79	1.14	157.92	4.86	1.09	158.86	4.82	1.12
Hexane	165.40	5.14	1.19	166.81	5.54	1.35	166.11	5.34	1.27
Pentane	173.00	5.30	1.20	170.94	5.19	1.18	171.97	5.24	1.19
Propane	222.98	7.57	1.84	221.24	7.26	1.69	222.11	7.41	1.76
Sea water	128.00	3.58	0.65	128.01	3.57	0.65	128.00	3.58	0.65
Toluene	136.33	3.87	0.75	137.13	3.71	0.71	136.73	3.79	0.73
Water	127.07	3.55	0.73	128.67	3.71	0.74	127.87	3.63	0.74
Xylene	133.03	3.71	0.72	134.59	3.88	0.85	133.81	3.79	0.78

Distribution of ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	96.63	2.79	0.57	96.72	2.69	0.59	96.68	2.74	0.58
Benzene	96.54	2.87	0.59	96.70	2.74	0.55	96.62	2.81	0.57
Chloroform	97.01	2.51	0.49	97.24	2.35	0.41	97.12	2.43	0.45
Creosote	96.87	2.61	0.51	96.81	2.67	0.52	96.84	2.64	0.52
Heptane	96.42	2.89	0.69	96.37	2.96	0.67	96.40	2.92	0.68
Hexane	96.31	3.00	0.70	96.03	3.19	0.78	96.17	3.09	0.74
Pentane	96.38	2.95	0.67	96.41	2.93	0.67	96.39	2.94	0.67
Propane	95.95	3.26	0.79	96.11	3.15	0.73	96.03	3.20	0.76
Sea water	96.80	2.70	0.49	96.80	2.70	0.49	96.80	2.70	0.49
Toluene	96.72	2.75	0.53	96.88	2.62	0.50	96.80	2.68	0.52
Water	96.74	2.71	0.55	96.66	2.78	0.56	96.70	2.75	0.56
Xylene	96.78	2.70	0.53	96.61	2.79	0.61	96.69	2.74	0.57

ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	38.80	31.78	29.09	1.42	2.13	0.09	0.07	0.26	0.46	0.00	0.00	38.80
Benzene	43.02	34.02	30.87	1.42	2.43	0.14	0.10	0.26	0.58	0.00	0.00	43.02
Chloroform	36.75	30.32	29.97	2.04	1.82	0.09	0.07	0.44	0.39	0.00	0.00	36.75
Creosote	35.56	26.69	23.51	1.00	1.82	0.06	0.04	0.16	0.41	0.00	0.00	35.56
Heptane	37.34	30.75	27.47	1.32	1.94	0.09	0.06	0.24	0.43	0.00	0.00	37.34
Hexane	42.47	37.45	36.72	2.41	2.12	0.12	0.14	0.59	0.55	0.00	0.00	42.47
Pentane	46.87	40.12	39.69	2.45	2.51	0.18	0.17	0.61	0.59	0.00	0.00	46.87
Propane	65.02	52.49	51.42	2.49	4.45	0.33	0.30	0.55	1.28	0.01	0.01	65.02
Sea water	32.66	28.57	29.76	1.96	1.46	0.08	0.08	0.37	0.28	0.00	0.00	32.66
Toluene	37.38	31.06	31.06	1.85	1.85	0.08	0.08	0.39	0.36	0.00	0.00	37.38
Water	31.87	27.58	29.82	1.98	1.40	0.07	0.11	0.42	0.31	0.00	0.00	31.87
Xylene	38.80	31.78	29.09	1.42	2.13	0.09	0.07	0.26	0.46	0.00	0.00	38.80

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	29.16	23.89	21.87	38.34	57.32	2.40	1.94	36.46	63.40	0.00	0.14	29.16
Benzene	30.36	24.01	21.78	34.64	59.35	3.47	2.54	30.96	68.68	0.36	0.00	30.36
Chloroform	27.19	22.43	22.17	50.65	45.35	2.16	1.84	52.54	47.34	0.00	0.12	27.19
Creosote	31.42	23.58	20.77	34.05	62.36	2.19	1.40	28.17	71.83	0.00	0.00	31.42
Heptane	29.51	24.30	21.71	38.76	56.90	2.64	1.70	35.32	64.38	0.15	0.15	29.51
Hexane	26.57	23.44	22.97	50.28	44.31	2.55	2.86	51.23	48.25	0.35	0.18	26.57
Pentane	27.09	23.19	22.94	46.14	47.27	3.30	3.28	50.67	49.08	0.00	0.25	27.09
Propane	29.16	23.54	23.06	32.92	58.76	4.31	4.02	29.75	69.54	0.44	0.27	29.16
Sea water	25.51	22.32	23.25	54.87	40.69	2.21	2.24	56.57	43.12	0.00	0.31	25.51
Toluene	27.42	22.78	22.78	47.83	47.91	2.17	2.09	52.21	47.66	0.13	0.00	27.42
Water	25.08	21.70	23.47	55.73	39.43	1.83	3.01	58.05	41.95	0.00	0.00	25.08
Xylene	29.16	23.89	21.87	38.34	57.32	2.40	1.94	36.46	63.40	0.00	0.14	29.16

ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	42.88	35.44	32.51	33.85	2.32	1.48	0.09	0.13	0.56	0.33	0.00	0.00
Benzene	37.60	35.89	31.09	31.67	1.99	1.70	0.08	0.10	0.42	0.35	0.00	0.00
Chloroform	26.19	35.08	26.75	23.07	0.89	1.69	0.07	0.04	0.14	0.32	0.00	0.00
Creosote	32.64	35.74	29.52	28.38	1.46	1.88	0.10	0.05	0.31	0.37	0.00	0.00
Heptane	47.96	38.02	33.82	38.12	2.92	1.62	0.13	0.19	0.75	0.35	0.00	0.00
Hexane	52.91	37.75	35.62	40.53	3.70	1.50	0.14	0.20	1.02	0.33	0.00	0.00
Pentane	46.20	45.45	38.70	40.59	2.45	2.41	0.15	0.17	0.61	0.57	0.00	0.00
Propane	65.79	51.38	49.87	54.21	4.43	2.15	0.28	0.39	1.21	0.47	0.00	0.01
Sea water	37.53	32.67	27.63	30.18	2.03	1.39	0.06	0.09	0.41	0.24	0.00	0.00
Toluene	40.82	33.17	30.33	32.82	2.20	1.31	0.09	0.11	0.46	0.25	0.00	0.00
Water	39.83	30.96	27.31	30.57	2.36	1.22	0.05	0.08	0.52	0.22	0.00	0.00
Xylene	37.29	36.39	30.64	30.27	1.89	1.80	0.10	0.09	0.43	0.41	0.00	0.00

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	29.64	24.49	22.47	23.40	57.75	36.78	2.29	3.18	63.08	36.81	0.11	0.00
Benzene	27.60	26.34	22.82	23.25	51.41	43.96	2.15	2.48	54.11	45.50	0.13	0.26
Chloroform	23.57	31.58	24.08	20.76	32.99	62.84	2.76	1.41	30.62	69.38	0.00	0.00
Creosote	25.85	28.30	23.38	22.48	41.76	54.00	2.72	1.52	45.43	54.42	0.15	0.00
Heptane	30.37	24.07	21.42	24.14	60.19	33.37	2.64	3.81	68.19	31.63	0.00	0.18
Hexane	31.72	22.63	21.36	24.30	66.78	27.11	2.55	3.56	75.46	24.24	0.00	0.30
Pentane	27.03	26.59	22.64	23.75	47.24	46.51	2.93	3.32	51.23	48.44	0.17	0.17
Propane	29.74	23.22	22.54	24.50	61.12	29.65	3.89	5.35	71.83	27.57	0.06	0.53
Sea water	29.32	25.52	21.59	23.57	56.88	38.98	1.65	2.49	63.25	36.75	0.00	0.00
Toluene	29.76	24.18	22.12	23.93	59.24	35.38	2.32	3.05	64.41	35.45	0.00	0.14
Water	30.96	24.06	21.22	23.76	63.69	32.86	1.24	2.21	70.12	29.61	0.13	0.13
Xylene	27.71	27.04	22.76	22.49	48.79	46.31	2.53	2.37	50.89	48.76	0.24	0.12



Total number of collisions in ABM validation tests for  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	146.63	149.60	148.12	1.12
Benzene	140.03	140.89	140.46	1.06
Chloroform	116.69	114.24	115.46	0.87
Creosote	130.60	130.45	130.52	0.99
Heptane	165.74	163.86	164.80	1.25
Hexane	171.74	173.70	172.72	1.31
Pentane	179.50	177.31	178.40	1.35
Propane	232.38	230.19	231.29	1.75
Sea water	132.23	132.24	132.23	1.00
Toluene	140.95	141.55	141.25	1.07
Water	131.35	133.12	132.23	1.00
Xylene	137.46	139.31	138.39	1.05

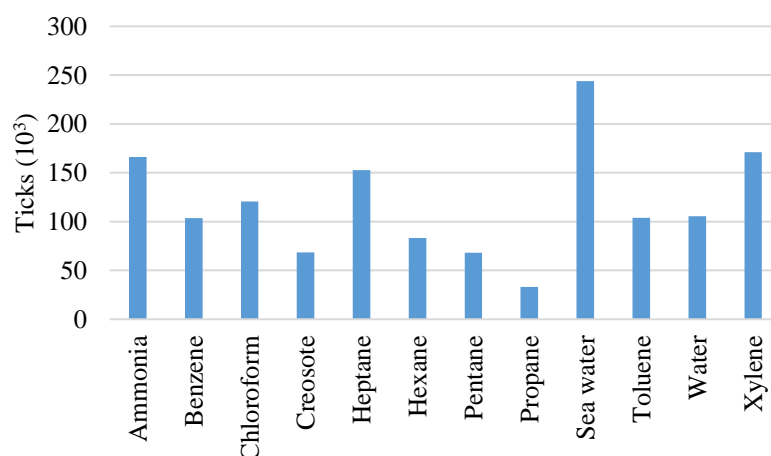
Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $12.5 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	11.30	11.45	11.37	1.02
Benzene	11.24	11.30	11.27	1.01
Chloroform	11.33	10.56	10.95	0.98
Creosote	10.83	11.09	10.96	0.98
Heptane	11.66	11.64	11.65	1.05
Hexane	11.69	11.75	11.72	1.05
Pentane	11.67	11.75	11.71	1.05
Propane	12.03	12.40	12.22	1.10
Sea water	11.12	11.14	11.13	1.00
Toluene	11.38	11.33	11.36	1.02
Water	11.19	11.09	11.14	1.00
Xylene	11.30	11.37	11.33	1.02

**APPENDIX 7.5 - ABM Validation Test Results for  $15 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) World Patch for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $15 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (<math>10^3</math>)</b>	<b>2<sup>nd</sup> Test (<math>10^3</math>)</b>	<b>Average (<math>10^3</math>)</b>	<b>Ratio<sup>73</sup></b>
Ammonia	96.03	77.99	87.01	1.53
Benzene	71.92	112.32	92.12	1.62
Chloroform	109.15	55.34	82.25	1.45
Creosote	59.71	94.66	77.19	1.36
Heptane	64.78	75.84	70.31	1.24
Hexane	111.27	52.47	81.87	1.44
Pentane	72.63	57.07	64.85	1.14
Propane	57.82	65.20	61.51	1.08
Sea water	89.57	80.25	84.91	1.49
Toluene	74.80	107.59	91.20	1.60
Water	55.84	57.86	56.85	1.00
Xylene	55.83	97.32	76.58	1.35



Comparison of average number of ticks in ABM validation tests for  $15 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>73</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	217,37	6,54	1,33	219,94	6,79	1,27	218.66	6.66	1.30
Benzene	206,20	6,32	1,21	209,60	6,42	1,21	207.90	6.37	1.21
Chloroform	180,10	4,62	0,75	172,43	4,58	0,76	176.26	4.60	0.76
Creosote	193,65	5,31	0,92	195,07	5,61	0,99	194.36	5.46	0.95
Heptane	242,84	8,29	1,73	249,16	8,31	1,77	246.00	8.30	1.75
Hexane	254,32	8,57	1,87	249,16	8,31	1,77	251.74	8.44	1.82
Pentane	262,90	9,00	1,98	259,75	8,86	1,89	261.33	8.93	1.94
Propane	347,40	12,89	2,83	344,28	12,69	2,66	345.84	12.79	2.74
Sea water	194,57	5,66	1,03	193,73	5,79	1,05	194.15	5.73	1.04
Toluene	211,25	6,66	1,37	212,62	6,40	1,25	211.93	6.53	1.31
Water	199,38	5,85	1,09	198,59	5,51	0,96	198.99	5.68	1.02
Xylene	207,81	6,49	1,17	209,88	6,52	1,29	208.85	6.50	1.23

Distribution of ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Ammonia	96.51	2.90	0.59	96.47	2.98	0.56	96.49	2.94	0.57
Benzene	96.48	2.96	0.57	96.49	2.96	0.56	96.48	2.96	0.56
Chloroform	97.10	2.49	0.41	96.99	2.58	0.43	97.05	2.53	0.42
Creosote	96.88	2.66	0.46	96.73	2.78	0.49	96.81	2.72	0.47
Heptane	96.04	3.28	0.68	96.11	3.21	0.68	96.08	3.24	0.68
Hexane	96.06	3.24	0.71	96.11	3.21	0.68	96.08	3.22	0.69
Pentane	95.99	3.29	0.72	96.03	3.27	0.70	96.01	3.28	0.71
Propane	95.67	3.55	0.78	95.73	3.53	0.74	95.70	3.54	0.76
Sea water	96.68	2.81	0.51	96.59	2.89	0.52	96.63	2.85	0.52
Toluene	96.34	3.04	0.62	96.53	2.90	0.57	96.43	2.97	0.59
Water	96.64	2.83	0.53	96.85	2.69	0.47	96.74	2.76	0.50
Xylene	96.45	3.01	0.54	96.41	2.99	0.59	96.43	3.00	0.57

ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	49.95	59.48	55.94	52.00	2.18	3.61	0.42	0.33	0.44	0.87	0.01	0.00
Benzene	52.19	52.40	51.00	50.62	2.87	2.80	0.33	0.32	0.63	0.57	0.01	0.00
Chloroform	43.39	47.06	46.56	43.09	1.85	2.36	0.24	0.16	0.31	0.44	0.00	0.01
Creosote	42.39	53.68	51.96	45.62	1.64	3.07	0.37	0.23	0.28	0.62	0.01	0.00
Heptane	63.58	61.12	58.15	59.99	3.85	3.50	0.43	0.51	0.92	0.78	0.01	0.01
Hexane	65.72	63.98	61.96	62.66	3.91	3.64	0.54	0.49	0.99	0.86	0.01	0.01
Pentane	61.60	71.08	67.94	62.28	3.19	4.60	0.70	0.52	0.76	1.18	0.02	0.02
Propane	95.30	79.63	83.87	88.60	6.79	3.79	0.98	1.34	1.91	0.85	0.03	0.05
Sea water	53.52	44.65	46.95	49.46	3.18	1.92	0.24	0.32	0.64	0.38	0.00	0.01
Toluene	59.45	48.15	49.21	54.44	3.78	2.19	0.28	0.42	0.93	0.42	0.00	0.01
Water	46.31	54.42	51.08	47.57	2.08	3.16	0.38	0.23	0.37	0.71	0.01	0.00
Xylene	54.49	51.62	50.48	51.23	3.15	2.69	0.30	0.35	0.64	0.52	0.00	0.01

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	22.98	27.36	25.74	23.92	33.30	55.23	6.39	5.08	33.38	65.64	0.83	0.15
Benzene	25.31	25.41	24.73	24.55	45.39	44.33	5.19	5.09	51.90	47.11	0.91	0.08
Chloroform	24.09	26.13	25.85	23.93	40.06	51.13	5.26	3.55	40.98	57.82	0.53	0.66
Creosote	21.89	27.72	26.83	23.56	30.89	57.76	6.96	4.39	30.71	68.20	0.77	0.33
Heptane	26.18	25.17	23.94	24.70	46.39	42.25	5.16	6.19	53.51	45.16	0.81	0.52
Hexane	25.84	25.16	24.36	24.64	45.61	42.41	6.30	5.68	52.97	45.75	0.54	0.75
Pentane	23.43	27.04	25.84	23.69	35.42	51.12	7.73	5.73	38.43	59.61	1.11	0.86
Propane	27.43	22.92	24.14	25.50	52.67	29.37	7.60	10.37	67.42	29.96	0.96	1.66
Sea water	27.51	22.95	24.13	25.42	56.11	33.92	4.29	5.69	62.09	36.84	0.39	0.68
Toluene	28.14	22.79	23.29	25.77	56.67	32.91	4.14	6.27	67.91	30.92	0.22	0.95
Water	23.23	27.30	25.62	23.86	35.50	54.09	6.45	3.97	33.67	65.13	0.92	0.28
Xylene	26.22	24.84	24.29	24.65	48.64	41.40	4.58	5.38	54.66	44.57	0.34	0.43

ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to in a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	59.19	51.44	53.30	56.02	3.55	2.51	0.35	0.39	0.75	0.50	0.01	0.01
Benzene	51.81	53.91	52.77	51.12	2.71	3.04	0.34	0.33	0.55	0.65	0.01	0.00
Chloroform	45.25	42.79	41.85	42.54	2.21	1.93	0.20	0.23	0.42	0.34	0.01	0.00
Creosote	45.97	52.28	50.04	46.79	2.08	2.98	0.32	0.23	0.40	0.58	0.01	0.01
Heptane	62.88	61.06	61.99	63.24	3.94	3.31	0.53	0.53	0.95	0.79	0.01	0.02
Hexane	62.88	61.06	61.99	63.24	3.94	3.31	0.53	0.53	0.95	0.79	0.01	0.02
Pentane	66.79	66.02	62.50	64.44	3.84	3.89	0.53	0.59	0.90	0.94	0.02	0.02
Propane	86.43	88.13	84.96	84.76	5.06	5.46	1.08	1.10	1.23	1.37	0.03	0.04
Sea water	48.52	50.50	47.20	47.51	2.48	2.81	0.25	0.26	0.49	0.55	0.01	0.00
Toluene	51.79	55.95	52.65	52.24	2.61	3.15	0.32	0.31	0.54	0.70	0.01	0.00
Water	45.38	53.68	51.60	47.93	1.94	2.96	0.37	0.25	0.32	0.62	0.01	0.00
Xylene	53.44	53.19	51.77	51.48	2.97	2.92	0.31	0.31	0.66	0.62	0.01	0.01

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	26.91	23.39	24.23	25.47	52.24	36.92	5.08	5.76	59.46	39.27	0.47	0.79
Benzene	24.72	25.72	25.18	24.39	42.21	47.38	5.34	5.06	45.26	53.75	0.74	0.25
Chloroform	26.24	24.81	24.27	24.67	48.32	42.19	4.45	5.04	54.45	44.24	0.79	0.52
Creosote	23.56	26.80	25.65	23.98	37.06	53.13	5.65	4.17	39.98	58.70	0.81	0.51
Heptane	25.24	24.50	24.88	25.38	47.39	39.86	6.43	6.33	53.68	44.57	0.68	1.07
Hexane	25.24	24.50	24.88	25.38	47.39	39.86	6.43	6.33	53.68	44.57	0.68	1.07
Pentane	25.71	25.42	24.06	24.81	43.40	43.95	6.03	6.62	47.80	49.66	1.27	1.27
Propane	25.10	25.60	24.68	24.62	39.85	43.00	8.52	8.64	46.11	51.33	0.98	1.58
Sea water	25.05	26.07	24.36	24.52	42.76	48.55	4.25	4.44	46.81	52.33	0.57	0.29
Toluene	24.36	26.31	24.76	24.57	40.87	49.25	5.02	4.86	43.19	55.69	0.80	0.32
Water	22.85	27.03	25.98	24.14	35.12	53.65	6.75	4.48	32.95	65.27	1.36	0.42
Xylene	25.46	25.34	24.67	24.53	45.60	44.85	4.73	4.82	51.20	47.71	0.62	0.46



Total number of collisions in ABM validation tests for  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	225.24	228.00	226.62	1.10
Benzene	213.73	217.23	215.48	1.05
Chloroform	185.48	177.77	181.62	0.88
Creosote	199.88	201.67	200.78	0.98
Heptane	252.86	259.24	256.05	1.24
Hexane	264.76	259.24	262.00	1.27
Pentane	273.89	270.49	272.19	1.32
Propane	363.12	359.64	361.38	1.76
Sea water	201.26	200.57	200.92	0.98
Toluene	219.28	220.26	219.77	1.07
Water	206.32	205.06	205.69	1.00
Xylene	215.47	217.69	216.58	1.05

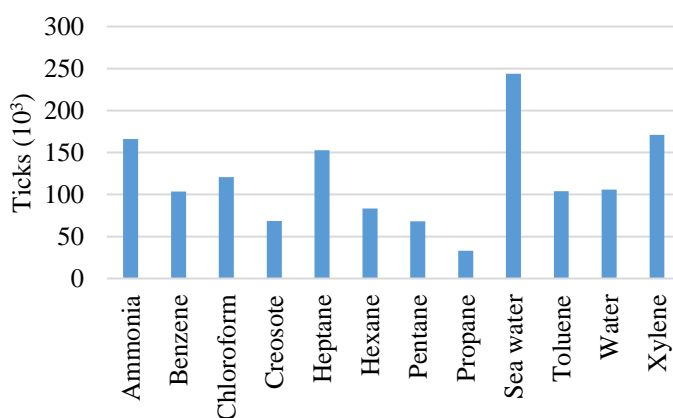
Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $15 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	13.94	13.79	13.86	1.05
Benzene	13.27	13.99	13.63	1.03
Chloroform	13.21	12.61	12.91	0.98
Creosote	13.17	13.56	13.36	1.01
Heptane	13.87	13.99	13.93	1.06
Hexane	11.36	13.99	12.67	0.96
Pentane	14.06	13.86	13.96	1.06
Propane	14.14	14.26	14.20	1.08
Sea water	13.59	13.49	13.54	1.03
Toluene	13.70	13.99	13.85	1.05
Water	13.16	13.22	13.19	1.00
Xylene	13.36	13.49	13.42	1.02

**APPENDIX 7.6 - ABM Validation Test Results for  $50 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $50 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (<math>10^3</math>)</b>	<b>2<sup>nd</sup> Test (<math>10^3</math>)</b>	<b>Average (<math>10^3</math>)</b>	<b>Ratio<sup>74</sup></b>
Ammonia	66.53	95.78	81.16	0.77
Benzene	68.78	138.05	103.42	0.98
Chloroform	71.35	134.66	103.01	0.98
Creosote	66.42	104.27	85.35	0.81
Heptane	64.49	90.41	77.45	0.74
Hexane	70.04	67.96	69.00	0.66
Pentane	63.48	64.68	64.08	0.61
Propane	49.87	58.22	54.05	0.51
Sea water	67.86	98.81	83.34	0.79
Toluene	66.99	131.56	99.28	0.94
Water	74.50	136.07	105.29	1.00
Xylene	67.81	98.27	83.04	0.79



Comparison of average number of ticks in ABM validation tests for  $50 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>74</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )	2-Body Collisions (10 <sup>3</sup> )	3-Body Collisions (10 <sup>3</sup> )	4-Body Collisions (10 <sup>3</sup> )
Ammonia	3.35	0.40	0.11	3.33	0.40	0.11	3.34	0.40	0.11
Benzene	3.20	0.37	0.10	3.17	0.37	0.10	3.18	0.37	0.10
Chloroform	2.52	0.25	0.05	2.52	0.26	0.05	2.52	0.26	0.05
Creosote	2.80	0.31	0.07	2.78	0.30	0.07	2.79	0.30	0.07
Heptane	4.19	0.55	0.18	4.22	0.55	0.18	4.20	0.55	0.18
Hexane	4.60	0.62	0.21	4.57	0.62	0.21	4.59	0.62	0.21
Pentane	4.84	0.66	0.23	4.92	0.67	0.23	4.88	0.67	0.23
Propane	12.69	2.03	0.85	12.75	2.05	0.85	12.72	2.04	0.85
Sea water	2.87	0.32	0.08	2.83	0.31	0.08	2.85	0.31	0.08
Toluene	3.20	0.38	0.10	3.23	0.38	0.10	3.21	0.38	0.10
Water	2.94	0.33	0.08	2.89	0.32	0.08	2.92	0.33	0.08
Xylene	3.15	0.37	0.10	3.17	0.37	0.10	3.16	0.37	0.10

Distribution of ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions	2-Body Collisions	3-Body Collisions	4-Body Collisions
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Ammonia	86.68	10.40	2.92	86.68	10.39	2.93	86.68	10.39	2.92
Benzene	87.10	10.16	2.75	87.06	10.17	2.76	87.08	10.17	2.75
Chloroform	89.09	8.99	1.92	89.05	9.02	1.93	89.07	9.00	1.93
Creosote	88.08	9.60	2.32	88.08	9.60	2.32	88.08	9.60	2.32
Heptane	85.22	11.19	3.59	85.18	11.20	3.61	85.20	11.20	3.60
Hexane	84.77	11.42	3.81	84.77	11.42	3.81	84.77	11.42	3.81
Pentane	84.45	11.60	3.95	84.46	11.58	3.96	84.46	11.59	3.95
Propane	81.49	13.07	5.45	81.48	13.08	5.44	81.48	13.07	5.45
Sea water	87.93	9.68	2.39	87.99	9.64	2.37	87.96	9.66	2.38
Toluene	87.00	10.21	2.79	87.00	10.22	2.78	87.00	10.22	2.78
Water	87.74	9.79	2.47	87.76	9.79	2.45	87.75	9.79	2.46
Xylene	87.12	10.17	2.72	87.09	10.18	2.73	87.10	10.17	2.72

ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	0.79	0.79	0.88	0.88	0.10	0.10	0.10	0.10	0.03	0.03	0.03	0.03
Benzene	0.75	0.76	0.84	0.85	0.09	0.09	0.10	0.10	0.02	0.02	0.03	0.03
Chloroform	0.59	0.59	0.67	0.68	0.06	0.06	0.06	0.07	0.01	0.01	0.01	0.01
Creosote	0.66	0.66	0.74	0.74	0.07	0.07	0.08	0.08	0.02	0.02	0.02	0.02
Heptane	1.00	1.00	1.09	1.09	0.13	0.13	0.14	0.14	0.04	0.04	0.05	0.05
Hexane	1.10	1.11	1.20	1.19	0.15	0.15	0.16	0.16	0.05	0.05	0.05	0.05
Pentane	1.17	1.17	1.25	1.25	0.16	0.16	0.17	0.17	0.06	0.06	0.06	0.06
Propane	3.12	3.12	3.22	3.22	0.50	0.50	0.51	0.51	0.21	0.21	0.21	0.22
Sea water	0.67	0.68	0.76	0.76	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02
Toluene	0.75	0.76	0.84	0.84	0.09	0.09	0.10	0.10	0.02	0.03	0.03	0.03
Water	0.69	0.69	0.78	0.78	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02
Xylene	0.75	0.74	0.83	0.84	0.09	0.09	0.09	0.09	0.02	0.02	0.02	0.03

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	23.69	23.71	26.35	26.25	24.31	24.36	25.71	25.62	24.52	24.29	25.69	25.50
Benzene	23.49	23.67	26.40	26.44	24.12	24.53	25.69	25.67	24.14	24.45	25.62	25.79
Chloroform	23.50	23.20	26.54	26.76	24.78	24.30	25.32	25.60	25.34	24.30	25.17	25.19
Creosote	23.55	23.39	26.48	26.58	24.53	24.47	25.37	25.63	24.98	24.83	24.99	25.19
Heptane	23.95	23.90	26.05	26.11	24.48	24.33	25.54	25.65	24.35	24.33	25.54	25.78
Hexane	23.93	24.16	26.01	25.90	24.11	24.61	25.79	25.49	24.06	24.43	25.86	25.65
Pentane	24.11	24.22	25.92	25.75	24.47	24.69	25.55	25.28	24.59	24.48	25.55	25.38
Propane	24.62	24.63	25.38	25.38	24.68	24.72	25.28	25.32	24.68	24.67	25.28	25.37
Sea water	23.34	23.64	26.64	26.38	24.30	24.69	25.72	25.29	24.55	24.96	25.38	25.11
Toluene	23.60	23.71	26.37	26.33	24.21	24.46	25.69	25.63	24.38	24.71	25.47	25.44
Water	23.60	23.55	26.39	26.47	24.45	24.39	25.53	25.64	24.97	24.88	24.86	25.29
Xylene	23.75	23.54	26.19	26.52	24.49	24.25	25.51	25.75	25.08	24.37	25.11	25.43

ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )	1 <sup>st</sup> Q. (10 <sup>3</sup> )	2 <sup>nd</sup> Q. (10 <sup>3</sup> )	3 <sup>rd</sup> Q. (10 <sup>3</sup> )	4 <sup>th</sup> Q. (10 <sup>3</sup> )
Ammonia	0.79	0.88	0.87	0.10	0.10	0.10	0.10	0.03	0.03	0.03	0.03	0.79
Benzene	0.75	0.83	0.83	0.09	0.09	0.09	0.09	0.02	0.03	0.03	0.03	0.75
Chloroform	0.59	0.67	0.67	0.06	0.06	0.06	0.07	0.01	0.01	0.01	0.01	0.59
Creosote	0.66	0.74	0.73	0.07	0.07	0.08	0.08	0.02	0.02	0.02	0.02	0.66
Heptane	1.01	1.10	1.10	0.14	0.14	0.14	0.14	0.04	0.04	0.05	0.05	1.01
Hexane	1.10	1.18	1.19	0.15	0.15	0.16	0.16	0.05	0.05	0.05	0.05	1.10
Pentane	1.19	1.27	1.27	0.17	0.16	0.17	0.17	0.06	0.06	0.06	0.06	1.19
Propane	3.14	3.23	3.24	0.51	0.51	0.52	0.52	0.21	0.21	0.21	0.22	3.14
Sea water	0.67	0.75	0.75	0.07	0.08	0.08	0.08	0.02	0.02	0.02	0.02	0.67
Toluene	0.77	0.85	0.85	0.09	0.09	0.10	0.10	0.03	0.03	0.03	0.03	0.77
Water	0.68	0.77	0.76	0.08	0.08	0.08	0.08	0.02	0.02	0.02	0.02	0.68
Xylene	0.75	0.83	0.83	0.09	0.09	0.09	0.09	0.02	0.02	0.03	0.03	0.75

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	23.82	26.44	26.15	24.24	24.48	25.81	25.48	24.11	24.72	25.72	25.46	23.82
Benzene	23.84	26.34	26.35	24.13	24.75	25.65	25.48	24.35	24.90	25.43	25.33	23.84
Chloroform	23.29	26.51	26.71	24.75	24.30	25.41	25.54	25.55	24.46	24.95	25.03	23.29
Creosote	23.61	26.57	26.37	24.36	24.73	25.64	25.26	24.44	25.23	25.42	24.91	23.61
Heptane	23.93	26.04	26.05	24.48	24.35	25.59	25.58	24.53	24.24	25.58	25.65	23.93
Hexane	24.11	25.86	25.94	24.42	24.52	25.45	25.60	24.49	24.50	25.59	25.42	24.11
Pentane	24.13	25.87	25.84	24.53	24.42	25.47	25.58	24.59	24.25	25.53	25.63	24.13
Propane	24.63	25.30	25.39	24.78	24.71	25.20	25.31	24.66	24.68	25.24	25.42	24.63
Sea water	23.59	26.56	26.42	24.16	24.75	25.66	25.42	24.34	25.16	25.51	24.99	23.59
Toluene	23.90	26.46	26.20	23.89	24.98	25.74	25.39	24.27	25.11	25.38	25.25	23.90
Water	23.59	26.58	26.33	24.30	24.66	25.52	25.53	24.40	24.83	25.51	25.25	23.59
Xylene	23.72	26.27	26.30	24.41	24.54	25.51	25.53	24.55	24.87	25.24	25.33	23.72



Total number of collisions in ABM validation tests for  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	3.86	3.84	3.84	1.16
Benzene	3.67	3.64	3.64	1.10
Chloroform	2.83	2.83	2.83	0.86
Creosote	3.18	3.16	3.15	0.96
Heptane	4.91	4.95	4.95	1.50
Hexane	5.43	5.40	5.40	1.64
Pentane	5.73	5.81	5.82	1.76
Propane	15.57	15.63	15.65	4.74
Sea water	3.26	3.22	3.22	0.98
Toluene	3.68	3.71	3.71	1.12
Water	3.35	3.30	3.30	1.00
Xylene	3.62	3.64	3.64	1.10

Cumulative number of same-charged nanoparticles at the interface of ABM validation tests for  $50 \times 10^3$  same-charged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	48.58	48.91	48.74	1.00
Benzene	48.57	49.13	48.85	1.00
Chloroform	47.76	48.41	48.09	0.99
Creosote	48.19	48.62	48.41	0.99
Heptane	48.84	49.12	48.98	1.01
Hexane	48.94	48.94	48.94	1.01
Pentane	48.92	48.92	48.92	1.00
Propane	48.93	49.09	49.01	1.01
Sea water	48.28	48.66	48.47	1.00
Toluene	48.55	49.15	48.85	1.00
Water	48.44	48.93	48.69	1.00
Xylene	48.52	48.86	48.69	1.00

## APPENDIX 8 - ABM Validation Test Results for SDS Molecules

### APPENDIX 8.1 - ABM Validation Test Results for $5 \times 10^3$ SDS Molecules in 20 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM validation tests for  $5 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio<sup>75</sup></b>
Acetic acid	154.03	67.11	110.57	0.47
Acetone	163.32	64.44	113.88	0.48
Ammonia	185.32	72.75	129.04	0.54
Benzene	205.76	76.68	141.22	0.60
Bromine	238.70	247.23	242.97	1.02
Butane	221.29	253.41	237.35	1.00
Castor oil	288.79	279.83	284.31	1.20
Chloride	275.55	245.85	260.70	1.10
Chloroform	187.39	240.77	214.08	0.90
Ether	155.32	231.38	193.35	0.81
Glycerine	186.95	247.95	217.45	0.92
Heptane	153.04	206.89	179.97	0.76
Hexane	184.39	204.30	194.34	0.82
Hexanol	196.15	227.20	211.67	0.89
Linseed oil	240.04	259.18	249.61	1.05
Methanol	210.39	262.26	236.33	1.00
Pentane	156.16	253.23	204.70	0.86
Propane	121.01	152.29	136.84	0.58
Sea water	224.81	225.46	225.14	0.95
Water	206.14	268.42	237.28	1.00

<sup>75</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 20 different solvents in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1st Test			2nd Test			Average		
	2-Body	3-Body	4-Body	2-Body	3-Body	4-Body	2-Body	3-Body	4-Body
	Collisions	Collisions	Collisions	Collisions	Collisions	Collisions	Collisions	Collisions	Collisions
	(106)	(106)	(106)	(106)	(106)	(106)	(106)	(106)	(106)
Acetic acid	32.40	23.51	17.49	17.90	12.39	8.69	25.15	17.95	13.09
Acetone	31.87	20.18	14.05	17.23	10.20	6.51	24.55	15.19	10.28
Ammonia	34.07	20.56	13.62	15.39	8.84	5.55	24.73	14.70	9.58
Benzene	27.11	16.36	10.75	13.69	7.95	4.92	20.40	12.16	7.83
Bromine	38.46	32.70	28.10	41.85	27.20	19.64	40.15	29.95	23.87
Butane	37.77	23.28	16.51	44.06	27.50	18.95	40.92	25.39	17.73
Chloride	37.14	29.58	24.21	41.16	26.15	18.34	39.15	27.87	21.27
Chloroform	28.72	22.55	17.97	33.24	26.11	21.08	30.98	24.33	19.52
Ether	28.37	18.26	12.88	36.80	24.21	17.58	32.58	21.24	15.23
Heptane	28.47	18.18	12.79	33.24	26.11	21.08	30.85	22.15	16.93
Hexane	33.26	21.48	15.34	36.09	23.26	16.54	34.68	22.37	15.94
Hexanol	38.79	24.06	16.45	39.42	24.65	17.13	39.11	24.36	16.79
Methanol	39.28	24.98	17.43	43.56	27.82	19.55	41.42	26.40	18.49
Pentane	32.51	20.43	14.24	40.39	25.88	18.53	36.45	23.16	16.38
Sea water	33.18	23.96	18.25	37.87	27.33	20.69	35.53	25.64	19.47
Water	33.92	23.81	18.18	43.87	31.26	23.97	38.89	27.54	21.08

Distribution of ABM validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 20 different solvents in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Acetic acid	44.14	32.03	23.83	45.92	31.78	22.30	44.76	31.94	23.30
Acetone	48.21	30.53	21.26	50.77	30.04	19.19	49.08	30.37	20.56
Ammonia	49.92	30.13	19.95	51.68	29.68	18.64	50.45	29.99	19.55
Benzene	50.00	30.17	19.82	51.54	29.94	18.53	50.51	30.10	19.40
Bromine	38.75	32.95	28.31	47.19	30.66	22.15	42.73	31.87	25.40
Butane	48.70	30.02	21.28	48.68	30.38	20.93	48.69	30.22	21.10
Chloride	40.84	32.53	26.63	48.06	30.53	21.41	44.34	31.56	24.10
Chloroform	41.47	32.57	25.96	41.33	32.47	26.21	41.39	32.51	26.09
Ether	47.67	30.69	21.64	46.82	30.81	22.37	47.19	30.76	22.06
Glycerine	42.23	32.36	25.42	41.86	32.23	25.92	42.03	32.29	25.68
Heptane	47.90	30.59	21.51	41.33	32.47	26.21	44.12	31.67	24.21
Hexane	47.46	30.66	21.88	47.56	30.65	21.79	47.51	30.66	21.84
Hexanol	48.91	30.34	20.74	48.55	30.36	21.09	48.73	30.35	20.92
Linseed oil	46.58	31.10	22.32	46.26	31.18	22.56	46.40	31.14	22.45
Methanol	48.08	30.58	21.34	47.91	30.59	21.50	47.99	30.58	21.43
Pentane	48.39	30.42	21.19	47.63	30.52	21.85	47.97	30.47	21.56
Propane	75.15	15.52	9.33	71.80	17.23	10.97	73.32	16.45	10.22
Sea water	44.01	31.78	24.20	44.10	31.82	24.09	44.06	31.80	24.14
Water	44.68	31.37	23.95	44.27	31.54	24.19	44.45	31.47	24.09

ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions				Three-Body Collisions				Four-Body Collisions			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Acetic acid	8.03	8.44	7.41	8.51	5.71	6.14	5.37	6.28	4.18	4.61	3.93	4.76
Acetone	8.20	8.00	8.27	7.40	5.12	5.11	5.25	4.71	3.50	3.59	3.66	3.31
Ammonia	8.79	8.57	7.01	9.70	5.27	5.20	4.23	5.87	3.45	3.48	2.80	3.89
Benzene	5.22	7.41	8.04	6.45	3.12	4.45	4.85	3.93	2.04	2.90	3.17	2.64
Bromine	9.96	9.52	9.42	9.55	8.45	8.03	8.02	8.19	7.13	6.86	6.89	7.22
Butane	8.59	7.37	11.11	10.69	5.28	4.51	6.90	6.60	3.70	3.18	4.93	4.70
Chloride	9.22	9.21	9.30	9.41	7.31	7.22	7.37	7.68	5.93	5.85	6.02	6.41
Chloroform	7.56	6.97	6.68	7.51	5.96	5.35	5.33	5.92	4.75	4.23	4.29	4.70
Ether	7.76	6.91	5.97	7.72	5.02	4.43	3.82	4.99	3.56	3.08	2.71	3.53
Heptane	6.53	7.25	7.32	7.37	4.12	4.60	4.68	4.79	2.87	3.18	3.27	3.47
Hexane	8.15	8.90	8.14	8.07	5.24	5.72	5.30	5.23	3.70	4.08	3.82	3.74
Hexanol	8.36	9.80	9.25	11.38	5.15	6.06	5.75	7.11	3.47	4.14	3.93	4.91
Linseed oil	8.06	8.40	8.35	7.94	5.37	5.61	5.58	5.31	3.80	4.04	4.00	3.85
Methanol	9.14	10.64	8.98	10.52	5.83	6.79	5.71	6.65	4.09	4.76	3.98	4.60
Pentane	8.13	8.20	6.89	9.29	5.06	5.25	4.28	5.85	3.46	3.74	2.96	4.08
Propane	9.54	9.89	11.26	10.14	2.01	1.91	2.48	2.03	1.24	1.11	1.49	1.23
Sea water	9.53	9.93	10.15	10.07	6.91	7.12	7.22	7.14	5.27	5.35	5.35	5.30
Water	7.63	8.59	8.20	9.51	5.46	5.96	5.86	6.54	4.19	4.53	4.44	5.02

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 20 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions				Three-Body Collisions				Four-Body Collisions			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Acetic acid	24.80	26.06	22.88	24.80	24.30	26.14	22.86	26.71	23.93	26.37	22.50	24.80
Acetone	25.73	25.10	25.95	25.73	25.38	25.30	25.99	23.33	24.88	25.52	26.07	25.73
Ammonia	25.80	25.14	20.58	25.80	25.61	25.27	20.56	28.57	25.37	25.53	20.56	25.80
Benzene	19.24	27.34	29.64	19.24	19.09	27.22	29.68	24.02	18.94	27.02	29.48	19.24
Bromine	25.91	24.76	24.51	25.91	25.84	24.56	24.54	25.06	25.38	24.40	24.51	25.91
Butane	22.75	19.52	29.41	22.75	22.69	19.36	29.62	28.34	22.40	19.26	29.88	22.75
Chloride	24.82	24.81	25.05	24.82	24.72	24.41	24.91	25.95	24.50	24.16	24.88	24.82
Chloroform	26.33	24.26	23.28	26.33	26.43	23.71	23.63	26.23	26.40	23.56	23.89	26.33
Ether	27.35	24.36	21.06	27.35	27.47	24.28	20.93	27.31	27.63	23.94	21.03	27.35
Heptane	22.95	25.46	25.70	22.95	22.67	25.28	25.72	26.33	22.42	24.85	25.56	22.95
Hexane	24.50	26.77	24.47	24.50	24.38	26.63	24.66	24.33	24.12	26.61	24.88	24.50
Hexanol	21.55	25.26	23.85	21.55	21.38	25.17	23.89	29.56	21.09	25.16	23.88	21.55
Linseed oil	24.62	25.64	25.50	24.62	24.55	25.67	25.51	24.27	24.20	25.76	25.47	24.62
Methanol	23.27	27.10	22.86	23.27	23.34	27.20	22.84	26.62	23.47	27.30	22.83	23.27
Pentane	25.00	25.23	21.19	25.00	24.75	25.70	20.94	28.62	24.32	26.26	20.78	25.00
Propane	23.38	24.21	27.57	23.38	23.87	22.62	29.38	24.13	24.50	21.82	29.48	23.38
Sea water	24.03	25.02	25.57	24.03	24.32	25.08	25.43	25.16	24.77	25.18	25.14	24.03
Water	22.48	25.31	24.17	22.48	22.92	25.03	24.59	27.45	23.02	24.91	24.45	22.48

ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions				Three-Body Collisions				Four-Body Collisions			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Acetic acid	4.56	4.56	3.88	4.90	3.14	3.16	2.65	3.43	2.20	2.21	1.87	2.42
Acetone	4.17	4.28	4.43	4.34	2.45	2.52	2.66	2.57	1.57	1.60	1.71	1.64
Ammonia	3.87	3.62	4.00	3.90	2.14	2.07	2.37	2.25	1.29	1.30	1.54	1.42
Benzene	3.49	3.44	3.48	3.28	2.07	2.05	1.96	1.88	1.30	1.33	1.15	1.13
Bromine	10.18	10.18	10.77	10.72	6.61	6.70	6.91	6.98	4.78	4.90	4.92	5.04
Butane	10.15	10.73	10.96	12.23	6.27	6.73	6.82	7.68	4.22	4.70	4.68	5.34
Chloride	11.16	10.31	11.10	5.39	7.11	6.52	7.14	3.77	4.99	4.52	5.06	11.16
Chloroform	7.84	7.80	8.80	8.79	6.17	6.09	6.92	6.93	4.97	4.89	5.58	5.63
Ether	9.72	9.77	8.11	9.20	6.43	6.44	5.32	6.03	4.71	4.67	3.88	4.32
Heptane	7.84	7.80	8.80	8.79	6.17	6.09	6.92	6.93	4.97	4.89	5.58	5.63
Hexane	9.79	8.59	8.64	9.08	6.33	5.52	5.61	5.80	4.51	3.89	4.05	4.09
Hexanol	8.96	10.53	9.92	6.29	5.57	6.60	6.20	4.39	3.86	4.58	4.29	8.96
Linseed oil	8.85	10.05	10.34	9.43	5.99	6.73	6.97	6.37	4.40	4.79	5.07	4.60
Methanol	11.54	10.58	10.70	10.74	7.36	6.75	6.90	6.81	5.19	4.74	4.89	4.74
Pentane	10.38	10.58	10.70	5.59	6.71	6.78	6.80	3.99	4.85	4.85	4.83	10.38
Propane	10.62	12.94	11.26	3.19	2.27	3.37	2.40	2.10	1.39	2.16	1.50	10.62
Sea water	9.61	9.09	9.88	9.29	6.93	6.52	7.22	6.65	5.32	4.97	5.49	4.92
Water	10.94	10.23	11.68	11.03	7.60	7.31	8.44	7.91	5.84	5.57	6.55	6.02

Distribution of ABM second validation test results for the two, three, and four-body collisions of  $5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions				Three-Body Collisions				Four-Body Collisions			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Acetic acid	25.47	25.46	21.67	27.39	25.37	25.52	21.43	27.67	25.29	25.40	21.47	27.84
Acetone	24.21	24.86	25.72	25.21	24.05	24.71	26.05	25.18	24.07	24.49	26.27	25.17
Ammonia	25.12	23.53	25.99	25.36	24.23	23.42	26.87	25.48	23.28	23.38	27.76	25.58
Benzene	25.47	25.10	25.43	23.99	25.99	25.74	24.60	23.67	26.46	27.11	23.40	23.03
Bromine	24.32	24.31	25.74	25.62	24.30	24.62	25.42	25.67	24.35	24.94	25.07	25.64
Butane	23.02	24.35	24.87	27.75	22.79	24.47	24.80	27.94	22.30	24.81	24.70	28.20
Chloride	29.40	27.15	29.25	14.19	28.97	26.59	29.09	15.35	19.40	17.56	19.67	43.37
Chloroform	23.59	23.47	26.49	26.45	23.61	23.32	26.52	26.54	23.59	23.20	26.49	26.72
Ether	26.41	26.54	22.05	25.00	26.54	26.60	21.96	24.90	26.77	26.59	22.07	24.57
Heptane	23.59	23.47	26.49	26.45	23.61	23.32	26.52	26.54	23.59	23.20	26.49	26.72
Hexane	27.13	23.79	23.93	25.15	27.22	23.72	24.12	24.95	27.26	23.51	24.49	24.74
Hexanol	25.09	29.50	27.79	17.62	24.46	29.00	27.27	19.28	17.81	21.13	19.79	41.28
Linseed oil	22.89	25.98	26.74	24.39	22.98	25.82	26.76	24.44	23.31	25.39	26.89	24.41
Methanol	26.49	24.29	24.57	24.66	26.46	24.25	24.79	24.49	26.54	24.22	25.01	24.23
Pentane	27.86	28.41	28.72	15.01	27.64	27.95	27.99	16.42	19.48	19.47	19.40	41.64
Propane	27.93	34.04	29.63	8.39	22.41	33.28	23.62	20.70	8.88	13.76	9.58	67.78
Sea water	25.38	24.01	26.09	24.52	25.37	23.87	26.42	24.34	25.70	24.01	26.53	23.76
Water	24.93	23.31	26.63	25.13	24.31	23.38	27.01	25.29	24.36	23.21	27.33	25.10



Total number of collisions in ABM validation tests for  $5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Acetic acid	73.39	38.99	25.15	0.64
Acetone	66.10	33.94	24.55	0.57
Ammonia	68.25	29.78	24.73	0.56
Benzene	54.21	26.56	20.40	0.46
Bromine	99.25	88.70	40.15	1.07
Butane	77.56	90.51	40.92	0.96
Chloride	90.93	85.65	39.15	1.01
Chloroform	69.24	80.42	30.98	0.86
Ether	59.51	78.59	32.58	0.79
Heptane	59.43	80.42	30.85	0.80
Hexane	70.08	75.90	34.68	0.83
Hexanol	79.31	81.20	39.11	0.92
Linseed oil	70.31	83.60	35.71	0.88
Methanol	81.69	90.94	41.42	0.99
Pentane	67.17	84.80	36.45	0.87
Propane	54.32	65.17	43.81	0.68
Sea water	75.38	85.89	35.53	0.92
Water	75.91	99.10	38.89	1.00

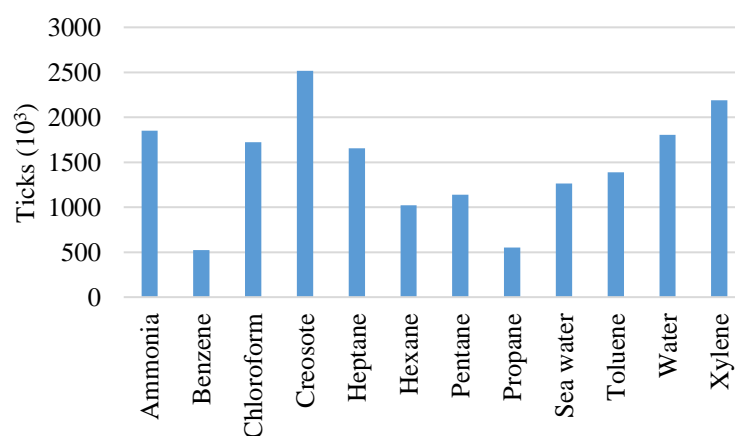
Cumulative number of SDS molecules at the interface of ABM validation tests for  $5 \times 10^3$  SDS molecules in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Acetic acid	149	90	120	0.73
Acetone	174	168	171	1.04
Ammonia	165	133	149	0.91
Benzene	124	97	111	0.67
Bromine	74	160	117	0.71
Butane	177	112	145	0.88
Chloride	96	212	154	0.94
Chloroform	103	129	116	0.71
Ether	176	181	179	1.09
Heptane	228	129	179	1.09
Hexane	206	206	206	1.26
Hexanol	163	160	162	0.98
Linseed oil	113	184	149	0.91
Methanol	195	95	145	0.88
Pentane	187	222	205	1.25
Propane	501	501	501	3.05
Sea water	137	144	141	0.86
Water	146	182	164	1.00

**APPENDIX 8.2 - ABM Validation Test Results for  $7.5 \times 10^3$  SDS Molecules in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in NetLogo models for  $7.5 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio<sup>76</sup></b>
Ammonia	111.86	107.31	109.59	1.29
Benzene	98.58	87.97	93.28	1.10
Chloroform	112.77	88.42	100.60	1.18
Creosote	100.97	79.56	90.27	1.06
Heptane	52.94	62.69	57.82	0.68
Hexane	63.83	60.98	62.41	0.73
Pentane	45.72	48.87	47.30	0.56
Propane	46.70	55.33	51.02	0.60
Sea water	86.63	73.60	80.12	0.94
Toluene	129.77	92.32	111.05	1.30
Water	77.36	92.89	85.13	1.00
Xylene	66.21	89.69	77.95	0.92



Comparison of average number of ticks in ABM validation tests for  $7.5 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<sup>76</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	41.90	26.14	18.14	38.44	24.15	16.92	40.17	25.15	17.53
Benzene	45.59	29.29	21.05	39.94	25.58	18.33	42.76	27.44	19.69
Chloroform	32.48	25.58	21.12	29.21	22.97	18.88	30.85	24.27	20.00
Creosote	36.17	27.00	21.54	31.47	23.32	18.35	33.82	25.16	19.94
Heptane	27.00	17.82	12.99	28.56	18.85	13.75	27.78	18.34	13.37
Hexane	29.76	19.51	14.21	29.49	19.31	14.03	29.63	19.41	14.12
Pentane	26.31	16.88	12.11	26.84	17.23	12.36	26.58	17.05	12.24
Propane	40.16	17.80	11.87	44.30	19.97	13.36	42.23	18.88	12.62
Sea water	34.01	24.79	19.33	31.65	23.05	17.86	32.83	23.92	18.60
Toluene	39.86	24.95	17.42	42.17	26.73	18.96	41.02	25.84	18.19
Water	33.24	23.92	18.59	36.94	26.63	20.59	35.09	25.28	19.59
Xylene	33.80	21.72	15.47	41.27	26.62	19.14	37.54	24.17	17.31

Distribution of ABM validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	48.62	30.34	21.04	48.35	30.38	21.28	48.49	30.36	21.15
Benzene	47.52	30.54	21.94	47.63	30.51	21.86	47.57	30.52	21.90
Chloroform	41.02	32.30	26.67	41.11	32.33	26.57	41.06	32.31	26.62
Creosote	42.70	31.87	25.42	43.02	31.88	25.09	42.85	31.88	25.27
Heptane	46.71	30.83	22.46	46.70	30.82	22.48	46.70	30.82	22.47
Hexane	46.88	30.74	22.38	46.94	30.73	22.32	46.91	30.74	22.35
Pentane	47.57	30.52	21.90	47.57	30.53	21.90	47.57	30.53	21.90
Propane	57.51	25.49	17.00	57.07	25.72	17.21	57.28	25.61	17.11
Sea water	43.54	31.73	24.74	43.62	31.76	24.62	43.58	31.74	24.68
Toluene	48.48	30.34	21.18	48.00	30.42	21.58	48.23	30.38	21.39
Water	43.88	31.57	24.54	43.89	31.65	24.46	43.89	31.61	24.50
Xylene	48.62	30.34	21.04	48.35	30.38	21.28	48.49	30.36	21.15

ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	10.56	9.13	10.30	11.91	6.59	5.68	6.43	7.45	4.58	3.94	4.45	5.16
Benzene	10.85	11.46	11.30	11.98	6.97	7.35	7.26	7.71	5.03	5.28	5.19	5.54
Chloroform	8.28	7.32	8.48	8.40	6.50	5.73	6.69	6.66	5.36	4.75	5.47	5.55
Creosote	9.17	8.72	9.36	8.93	6.90	6.42	7.02	6.65	5.55	5.05	5.63	5.30
Heptane	6.61	6.38	6.88	7.13	4.33	4.21	4.57	4.72	3.12	3.07	3.36	3.44
Hexane	7.47	7.27	7.24	7.78	4.87	4.80	4.77	5.08	3.51	3.53	3.49	3.68
Pentane	7.02	6.51	6.24	6.53	4.51	4.16	4.02	4.19	3.24	2.96	2.91	3.01
Propane	10.53	9.41	9.74	10.49	4.69	4.08	4.30	4.73	3.11	2.72	2.87	3.17
Sea water	8.42	8.49	8.24	8.87	6.17	6.18	5.98	6.46	4.84	4.81	4.68	5.00
Toluene	9.39	9.75	10.63	10.09	5.85	6.11	6.68	6.31	4.09	4.28	4.65	4.40
Water	8.62	8.06	8.47	8.10	6.21	5.77	6.12	5.82	4.88	4.48	4.74	4.49
Xylene	7.81	8.30	8.87	8.82	5.02	5.35	5.69	5.66	3.57	3.80	4.05	4.06

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.21	21.78	24.58	28.43	25.19	21.73	24.58	28.50	25.26	21.75	24.55	28.44
Benzene	23.80	25.13	24.79	26.27	23.81	25.09	24.77	26.33	23.89	25.11	24.67	26.33
Chloroform	25.49	22.54	26.10	25.87	25.41	22.40	26.16	26.02	25.36	22.50	25.89	26.26
Creosote	25.34	24.10	25.88	24.68	25.55	23.80	26.01	24.64	25.78	23.44	26.15	24.62
Heptane	24.49	23.62	25.47	26.42	24.27	23.61	25.66	26.46	24.02	23.64	25.86	26.49
Hexane	25.10	24.43	24.33	26.14	24.97	24.58	24.44	26.02	24.70	24.86	24.56	25.88
Pentane	26.69	24.75	23.73	24.83	26.70	24.67	23.80	24.83	26.72	24.45	23.99	24.84
Propane	26.21	23.43	24.24	26.11	26.33	22.93	24.17	26.57	26.19	22.90	24.22	26.69
Sea water	24.76	24.96	24.21	26.07	24.89	24.94	24.13	26.05	25.05	24.87	24.21	25.87
Toluene	23.56	24.46	26.67	25.30	23.44	24.49	26.76	25.31	23.51	24.55	26.67	25.26
Water	25.92	24.24	25.49	24.36	25.97	24.13	25.57	24.33	26.26	24.11	25.47	24.16
Xylene	23.12	24.56	26.25	26.08	23.11	24.62	26.18	26.08	23.10	24.54	26.16	26.21

ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	9.24	9.66	9.77	9.77	5.80	6.08	6.15	6.12	4.05	4.26	4.33	4.28
Benzene	9.71	9.72	10.36	10.15	6.22	6.22	6.64	6.50	4.46	4.46	4.76	4.65
Chloroform	7.68	6.99	7.35	7.20	6.01	5.48	5.77	5.71	4.90	4.51	4.70	4.76
Creosote	7.31	7.66	7.64	8.85	5.42	5.68	5.66	6.56	4.25	4.44	4.51	5.14
Heptane	6.79	6.91	7.20	7.65	4.49	4.54	4.76	5.07	3.29	3.30	3.47	3.69
Hexane	7.08	7.62	7.40	7.39	4.63	5.00	4.86	4.83	3.35	3.64	3.54	3.49
Pentane	6.93	6.73	6.68	6.50	4.47	4.34	4.28	4.14	3.23	3.12	3.07	2.94
Propane	11.71	10.62	11.32	10.64	5.45	4.76	5.04	4.72	3.67	3.17	3.35	3.18
Sea water	7.63	8.20	8.19	7.64	5.56	5.96	6.01	5.51	4.34	4.60	4.67	4.26
Toluene	10.99	9.93	10.42	10.84	6.97	6.29	6.59	6.87	4.94	4.46	4.67	4.88
Water	9.02	8.96	9.86	9.09	6.51	6.49	7.11	6.52	4.99	5.05	5.54	5.00
Xylene	10.21	9.37	10.93	10.76	6.57	6.03	7.03	6.99	4.75	4.33	5.01	5.05



Distribution of ABM second validation test results for the two, three, and four-body collisions of  $7.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.03	25.12	25.43	25.43	24.01	25.19	25.47	25.34	23.92	25.19	25.59	25.30
Benzene	24.31	24.34	25.95	25.40	24.32	24.32	25.96	25.40	24.34	24.34	25.96	25.36
Chloroform	26.29	23.92	25.16	24.64	26.18	23.84	25.13	24.85	25.98	23.87	24.91	25.24
Creosote	23.22	24.35	24.30	28.13	23.25	24.34	24.28	28.13	23.18	24.21	24.58	28.03
Heptane	23.79	24.20	25.22	26.79	23.80	24.10	25.23	26.87	23.95	23.97	25.23	26.85
Hexane	24.01	25.82	25.10	25.06	23.98	25.88	25.14	25.00	23.90	25.98	25.22	24.90
Pentane	25.82	25.09	24.88	24.21	25.94	25.20	24.85	24.01	26.11	25.27	24.82	23.80
Propane	26.44	23.98	25.56	24.02	27.29	23.84	25.23	23.63	27.44	23.73	25.06	23.76
Sea water	24.10	25.90	25.86	24.14	24.14	25.88	26.07	23.91	24.31	25.74	26.13	23.82
Toluene	26.05	23.55	24.70	25.70	26.09	23.52	24.67	25.72	26.08	23.54	24.62	25.77
Water	24.43	24.26	26.70	24.62	24.43	24.38	26.71	24.48	24.23	24.53	26.93	24.30
Xylene	24.73	22.70	26.49	26.08	24.69	22.66	26.41	26.25	24.80	22.64	26.19	26.37

Total number of collisions in ABM validation tests for  $7.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	38.44	24.15	31.30	0.98
Benzene	39.94	25.58	32.76	1.03
Chloroform	29.21	22.97	26.09	0.82
Creosote	31.47	23.32	27.39	0.86
Heptane	28.56	18.85	23.71	0.75
Hexane	29.49	19.31	24.40	0.77
Pentane	26.84	17.23	22.04	0.69
Propane	44.30	19.97	32.13	1.01
Sea water	31.65	23.05	27.35	0.86
Toluene	42.17	26.73	34.45	1.08
Water	36.94	26.63	31.79	1.00
Xylene	41.27	26.62	33.94	1.07

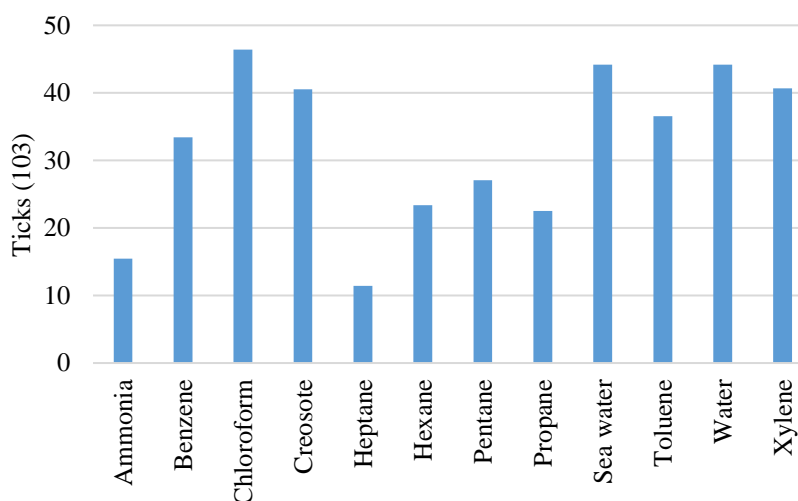
Cumulative number of SDS molecules at the interface of ABM validation tests for  $7.5 \times 10^3$  SDS molecules in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	208	152	180	0.95
Benzene	271	219	245	1.29
Chloroform	194	174	184	0.97
Creosote	198	171	185	0.97
Heptane	229	235	232	1.22
Hexane	220	240	230	1.21
Pentane	222	243	233	1.22
Propane	501	501	501	2.64
Sea water	182	250	216	1.14
Toluene	211	253	232	1.22
Water	177	203	190	1.00
Xylene	193	221	207	1.09

**APPENDIX 8.3 - ABM Validation Test Results for  $10 \times 10^3$  SDS Molecules in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $10 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	Average (10 <sup>3</sup> )	Ratio <sup>77</sup>
Ammonia	16.52	14.40	15.46	0.36
Benzene	30.93	35.89	33.41	0.78
Chloroform	49.81	42.99	46.40	1.09
Creosote	37.61	43.44	40.53	0.95
Heptane	10.51	12.30	11.41	0.27
Hexane	23.38	23.38	23.38	0.55
Pentane	26.71	27.42	27.07	0.63
Propane	24.36	20.63	22.50	0.53
Sea water	42.34	44.90	43.62	1.02
Toluene	40.26	32.85	36.56	0.86
Water	42.99	42.40	42.70	1.00
Xylene	42.76	38.86	40.81	0.96



Comparison of average number of ticks in ABM validation tests for  $10 \times 10^3$  SDS molecules in the world in a (250 x 250) patch world for 72-hours at 25°C

<sup>77</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	20.90	13.25	9.34	19.09	12.06	8.47	20.00	12.65	8.91
Benzene	29.80	19.27	13.96	32.84	21.27	15.45	31.32	20.27	14.70
Chloroform	24.34	19.28	16.38	22.45	17.83	15.13	23.40	18.56	15.76
Creosote	25.25	18.97	15.36	27.37	20.55	16.66	26.31	19.76	16.01
Heptane	13.09	8.59	6.16	14.44	9.51	6.86	13.77	9.05	6.51
Hexane	22.45	14.85	10.90	22.45	14.85	10.90	22.45	14.85	10.90
Pentane	25.40	16.57	12.10	25.48	16.59	12.10	25.44	16.58	12.10
Propane	37.60	19.30	12.94	32.76	16.71	11.15	35.18	18.01	12.04
Sea water	27.60	20.46	16.36	28.67	21.26	17.04	28.14	20.86	16.70
Toluene	35.88	23.09	16.71	31.26	20.08	14.48	33.57	21.58	15.59
Water	28.65	20.98	16.62	30.40	22.23	17.60	29.52	21.60	17.11
Xylene	36.19	23.71	17.40	33.34	21.81	15.95	34.77	22.76	16.68

Distribution of ABM validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	48.06	30.46	21.48	48.19	30.44	21.37	48.12	30.45	21.43
Benzene	47.28	30.58	22.15	47.22	30.58	22.21	47.25	30.58	22.18
Chloroform	40.57	32.14	27.29	40.52	32.17	27.31	40.55	32.15	27.30
Creosote	42.38	31.84	25.78	42.38	31.82	25.80	42.38	31.83	25.79
Heptane	47.02	30.85	22.13	46.87	30.86	22.27	46.94	30.86	22.20
Hexane	46.57	30.81	22.62	46.57	30.81	22.62	46.57	30.81	22.62
Pentane	46.97	30.64	22.38	47.04	30.62	22.34	47.00	30.63	22.36
Propane	53.84	27.64	18.52	54.04	27.56	18.40	53.93	27.60	18.46
Sea water	42.85	31.76	25.40	42.81	31.74	25.45	42.83	31.75	25.42
Toluene	47.41	30.51	22.08	47.50	30.50	22.00	47.45	30.51	22.04
Water	43.24	31.67	25.09	43.29	31.65	25.06	43.26	31.66	25.07
Xylene	46.81	30.67	22.51	46.90	30.67	22.43	46.85	30.67	22.47

ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	0.53	0.53	0.51	0.52	0.34	0.33	0.32	0.33	0.24	0.24	0.23	0.23
Benzene	0.72	0.79	0.73	0.75	0.46	0.51	0.47	0.48	0.34	0.37	0.34	0.35
Chloroform	0.60	0.60	0.60	0.63	0.47	0.48	0.48	0.50	0.40	0.40	0.41	0.42
Creosote	0.63	0.62	0.64	0.63	0.47	0.47	0.48	0.47	0.38	0.38	0.39	0.38
Heptane	0.31	0.33	0.32	0.35	0.20	0.22	0.21	0.23	0.15	0.16	0.15	0.16
Hexane	0.56	0.56	0.56	0.56	0.37	0.37	0.37	0.37	0.27	0.27	0.27	0.27
Pentane	0.65	0.62	0.64	0.63	0.42	0.41	0.42	0.41	0.31	0.30	0.30	0.30
Propane	1.02	0.89	0.91	0.94	0.53	0.46	0.46	0.48	0.36	0.31	0.31	0.32
Sea water	0.66	0.70	0.69	0.71	0.48	0.52	0.51	0.53	0.38	0.42	0.41	0.43
Toluene	0.87	0.90	0.89	0.93	0.56	0.58	0.57	0.60	0.40	0.42	0.41	0.43
Water	0.72	0.72	0.73	0.70	0.53	0.52	0.54	0.51	0.42	0.41	0.42	0.41
Xylene	0.90	0.90	0.91	0.91	0.59	0.59	0.60	0.60	0.43	0.43	0.44	0.44

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.34	25.21	24.40	25.05	25.37	25.25	24.29	25.09	25.35	25.36	24.14	25.15
Benzene	24.02	26.37	24.35	25.26	24.09	26.44	24.36	25.10	24.15	26.56	24.37	24.91
Chloroform	24.47	24.76	24.84	25.93	24.52	24.70	24.89	25.89	24.66	24.49	24.91	25.94
Creosote	25.06	24.63	25.53	24.78	25.03	24.60	25.50	24.87	24.98	24.70	25.56	24.77
Heptane	23.81	25.36	24.38	26.46	23.70	25.48	24.30	26.53	23.67	25.54	24.21	26.58
Hexane	25.08	25.10	24.81	25.01	24.97	25.11	24.90	25.01	24.79	25.16	25.02	25.04
Pentane	25.56	24.43	25.09	24.91	25.51	24.53	25.06	24.90	25.39	24.72	24.92	24.96
Propane	27.17	23.64	24.14	25.05	27.43	23.61	23.91	25.05	27.45	23.61	23.85	25.09
Sea water	23.85	25.48	25.09	25.59	23.67	25.45	25.17	25.72	23.30	25.47	25.24	25.98
Toluene	24.37	24.95	24.72	25.96	24.27	25.06	24.72	25.96	24.14	25.19	24.72	25.94
Water	25.01	25.02	25.45	24.52	25.07	24.89	25.53	24.51	25.07	24.81	25.50	24.62
Xylene	24.76	24.89	25.19	25.16	24.79	24.90	25.16	25.15	24.73	24.89	25.21	25.16

ABM first validation test results for the total number of two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules with respect to quadrants that in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C for the second model

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	0.49	0.48	0.46	0.48	0.31	0.31	0.29	0.30	0.22	0.22	0.20	0.21
Benzene	0.79	0.87	0.80	0.83	0.51	0.56	0.52	0.53	0.37	0.41	0.38	0.38
Chloroform	0.55	0.56	0.56	0.58	0.44	0.44	0.44	0.46	0.37	0.37	0.38	0.39
Creosote	0.68	0.68	0.70	0.68	0.51	0.51	0.52	0.51	0.41	0.41	0.42	0.41
Heptane	0.34	0.37	0.35	0.38	0.22	0.24	0.23	0.25	0.16	0.18	0.17	0.18
Hexane	0.56	0.56	0.56	0.56	0.37	0.37	0.37	0.37	0.27	0.27	0.27	0.27
Pentane	0.64	0.62	0.66	0.63	0.42	0.40	0.43	0.41	0.31	0.29	0.31	0.30
Propane	0.78	0.79	0.82	0.88	0.39	0.40	0.42	0.46	0.26	0.27	0.28	0.31
Sea water	0.70	0.73	0.72	0.72	0.52	0.54	0.53	0.53	0.41	0.44	0.43	0.43
Toluene	0.81	0.75	0.80	0.76	0.52	0.48	0.51	0.49	0.38	0.35	0.37	0.35
Water	0.73	0.76	0.79	0.76	0.54	0.55	0.57	0.56	0.43	0.44	0.46	0.44
Xylene	0.83	0.81	0.83	0.86	0.54	0.53	0.54	0.57	0.40	0.39	0.40	0.41



Distribution of ABM second validation test results for the two, three, and four-body collisions of  $10 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.42	25.25	24.27	25.06	25.45	25.30	24.15	25.10	25.44	25.42	23.99	25.15
Benzene	24.00	26.42	24.39	25.18	24.06	26.49	24.41	25.03	24.12	26.61	24.42	24.86
Chloroform	24.48	24.84	24.87	25.81	24.54	24.77	24.92	25.76	24.70	24.56	24.94	25.80
Creosote	24.96	24.75	25.41	24.88	24.93	24.72	25.39	24.96	24.87	24.81	25.44	24.87
Heptane	23.66	25.46	24.41	26.47	23.54	25.58	24.35	26.53	23.49	25.65	24.28	26.58
Hexane	25.08	25.10	24.81	25.01	24.97	25.11	24.90	25.01	24.79	25.16	25.02	25.04
Pentane	24.94	24.20	26.00	24.87	25.06	24.20	25.99	24.75	25.26	24.18	25.90	24.66
Propane	23.80	24.20	25.03	26.98	23.54	24.00	25.15	27.31	23.45	23.86	25.19	27.50
Sea water	24.39	25.52	25.05	25.04	24.35	25.53	25.07	25.06	24.17	25.63	25.15	25.05
Toluene	25.91	24.13	25.51	24.45	26.00	24.13	25.59	24.28	26.09	24.21	25.72	23.98
Water	24.13	24.93	25.92	25.02	24.20	24.83	25.87	25.11	24.16	24.84	25.87	25.12
Xylene	24.76	24.35	24.95	25.94	24.76	24.34	24.98	25.93	24.83	24.32	24.94	25.92

Total number of collisions in ABM validation tests for  $10 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	3.97	4.35	4.16	0.61
Benzene	6.95	6.31	6.63	0.97
Chloroform	5.54	5.99	5.77	0.84
Creosote	6.44	5.94	6.19	0.91
Heptane	3.07	2.79	2.93	0.43
Hexane	4.80	4.80	4.80	0.70
Pentane	5.42	5.41	5.42	0.79
Propane	6.06	6.99	6.53	0.96
Sea water	6.70	6.44	6.57	0.96
Toluene	6.57	7.56	7.07	1.03
Water	7.03	6.63	6.83	1.00
Xylene	7.11	7.74	7.43	1.09

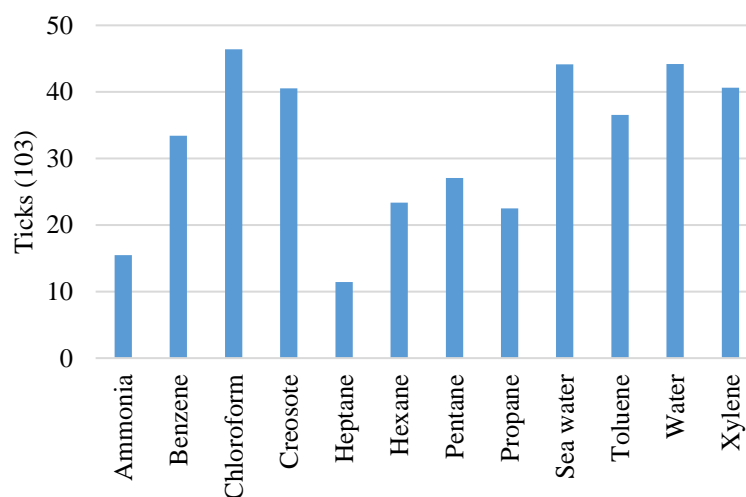
Cumulative number of SDS molecules at the interface of ABM validation tests for  $10 \times 10^3$  SDS molecules in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	224	218	221,00	1,09
Benzene	280	281	280,50	1,39
Chloroform	229	220	224,50	1,11
Creosote	232	235	233,50	1,16
Heptane	251	259	255,00	1,26
Hexane	218	218	218,00	1,08
Pentane	304	284	294,00	1,46
Propane	501	501	501,00	2,48
Sea water	186	204	195,00	0,97
Toluene	233	252	242,50	1,20
Water	249	155	202,00	1,00
Xylene	200	264	232,00	1,15

**APPENDIX 8.4 - ABM Validation Test Results for  $12.5 \times 10^3$  SDS Molecules in 12 Different Solvents in a (250 x 250) World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $12.5 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio<sup>78</sup></b>
Ammonia	54.26	28.61	41.43	1.08
Benzene	28.54	34.02	31.28	0.81
Chloroform	30.85	63.69	47.27	1.23
Creosote	74.02	55.49	64.75	1.68
Heptane	27.71	27.09	27.40	0.71
Hexane	45.39	34.97	40.18	1.04
Pentane	24.13	23.12	23.63	0.61
Propane	20.52	31.07	25.80	0.67
Sea water	42.51	56.55	49.53	1.29
Toluene	47.22	48.02	47.62	1.24
Water	35.43	41.60	38.52	1.00
Xylene	48.72	49.46	49.09	1.27



Comparison of average number of ticks in ABM validation tests for  $12.5 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<sup>78</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	42,07	27,09	19,50	28,11	17,80	12,55	35,09	22,45	16,03
Benzene	35,58	23,22	16,96	29,19	18,77	13,49	32,39	20,99	15,22
Chloroform	29,74	23,45	19,67	26,38	20,83	17,50	28,06	22,14	18,59
Creosote	34,94	26,20	21,16	29,40	22,08	17,85	32,17	24,14	19,51
Heptane	22,13	14,72	10,81	21,69	14,39	10,53	21,91	14,56	10,67
Hexane	32,03	21,24	15,65	26,66	17,62	12,94	29,34	19,43	14,29
Pentane	21,84	14,15	10,25	20,91	13,50	9,74	21,38	13,83	9,99
Propane	30,27	14,99	9,91	39,12	19,52	13,09	34,70	17,26	11,50
Sea water	26,49	19,57	15,52	31,40	23,26	18,53	28,94	21,41	17,02
Toluene	36,65	23,52	16,93	37,62	24,18	17,47	37,14	23,85	17,20
Water	24,49	17,86	14,02	27,85	20,34	15,97	26,17	19,10	14,99
Xylene	35,58	23,22	16,96	37,06	24,19	17,63	36,32	23,70	17,30

Distribution of ABM validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	47.45	30.55	22.00	48.08	30.45	21.47	47.77	30.50	21.73
Benzene	46.97	30.65	22.39	47.51	30.54	21.95	47.24	30.59	22.17
Chloroform	40.82	32.18	27.00	40.77	32.19	27.05	40.79	32.19	27.02
Creosote	42.45	31.83	25.71	42.41	31.84	25.75	42.43	31.84	25.73
Heptane	46.43	30.89	22.67	46.54	30.88	22.58	46.48	30.89	22.63
Hexane	46.47	30.82	22.71	46.60	30.79	22.61	46.53	30.80	22.66
Pentane	47.24	30.60	22.16	47.36	30.58	22.06	47.30	30.59	22.11
Propane	54.86	27.17	17.96	54.54	27.22	18.24	54.70	27.20	18.10
Sea water	43.02	31.78	25.20	42.90	31.78	25.32	42.96	31.78	25.26
Toluene	47.54	30.50	21.96	47.46	30.50	22.04	47.50	30.50	22.00
Water	43.45	31.69	24.87	43.41	31.70	24.89	43.43	31.69	24.88
Xylene	47.45	30.55	22.00	48.08	30.45	21.47	47.77	30.50	21.73

ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	10.67	10.45	9.94	11.01	6.86	6.75	6.38	7.10	4.94	4.87	4.57	5.13
Benzene	6.34	6.61	6.74	6.87	4.06	4.25	4.32	4.39	2.90	3.03	3.08	3.13
Chloroform	7.23	7.80	7.19	7.52	5.69	6.19	5.66	5.91	4.75	5.24	4.73	4.95
Creosote	8.79	8.67	8.66	8.82	6.60	6.51	6.47	6.62	5.38	5.25	5.19	5.34
Heptane	5.48	5.67	5.33	5.65	3.65	3.76	3.54	3.77	2.69	2.73	2.60	2.79
Hexane	8.11	7.79	8.24	7.88	5.39	5.17	5.46	5.21	3.97	3.82	4.03	3.83
Pentane	5.66	5.38	5.33	5.47	3.67	3.48	3.44	3.56	2.67	2.51	2.49	2.58
Propane	7.77	7.86	7.70	6.94	3.86	3.92	3.83	3.39	2.53	2.59	2.54	2.25
Sea water	6.74	6.60	6.37	6.78	5.00	4.86	4.67	5.04	3.98	3.85	3.67	4.03
Toluene	9.13	8.70	9.60	9.21	5.86	5.59	6.16	5.91	4.23	4.04	4.42	4.25
Water	0.03	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00
Xylene	8.81	8.76	9.39	8.62	5.75	5.71	6.13	5.63	4.21	4.17	4.47	4.11

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.35	24.84	23.63	26.18	25.33	24.91	23.55	26.22	25.31	24.96	23.42	26.31
Benzene	23.87	24.89	25.38	25.86	23.85	24.96	25.38	25.81	23.90	24.94	25.38	25.78
Chloroform	24.30	26.23	24.18	25.29	24.28	26.40	24.12	25.20	24.16	26.62	24.05	25.17
Creosote	25.15	24.82	24.79	25.24	25.20	24.85	24.68	25.27	25.44	24.80	24.54	25.21
Heptane	24.75	25.61	24.09	25.56	24.80	25.51	24.04	25.64	24.91	25.26	24.04	25.78
Hexane	25.33	24.33	25.73	24.60	25.39	24.36	25.71	24.53	25.38	24.40	25.77	24.46
Pentane	25.91	24.62	24.41	25.06	25.95	24.61	24.31	25.13	26.01	24.49	24.27	25.22
Propane	25.65	25.98	25.44	22.93	25.71	26.14	25.52	22.64	25.57	26.09	25.60	22.74
Sea water	25.44	24.92	24.05	25.59	25.54	24.85	23.87	25.74	25.62	24.78	23.63	25.97
Toluene	24.91	23.75	26.20	25.14	24.94	23.77	26.18	25.11	24.97	23.84	26.10	25.09
Water	25.09	24.53	25.60	24.78	25.38	23.97	26.09	24.55	25.84	23.43	25.39	25.35
Xylene	24.76	24.62	26.39	24.23	24.77	24.60	26.40	24.23	24.82	24.59	26.38	24.21

ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	7.00	6.96	6.87	7.27	4.43	4.41	4.34	4.62	3.13	3.11	3.05	3.26
Benzene	7.22	6.98	7.26	7.73	4.65	4.47	4.67	4.97	3.36	3.20	3.35	3.58
Chloroform	6.40	6.62	6.72	6.63	5.06	5.19	5.33	5.25	4.26	4.31	4.49	4.44
Creosote	7.21	7.23	7.42	7.54	5.40	5.45	5.55	5.67	4.36	4.41	4.47	4.60
Heptane	5.30	5.11	5.93	3.54	3.52	3.39	3.94	2.58	2.58	2.48	2.89	5.30
Hexane	6.70	6.34	6.66	6.96	4.42	4.20	4.41	4.60	3.23	3.10	3.25	3.36
Pentane	5.15	5.26	5.06	5.44	3.34	3.40	3.26	3.50	2.41	2.46	2.36	2.52
Propane	9.48	9.81	10.36	4.75	4.73	4.87	5.17	3.19	3.18	3.27	3.45	9.48
Sea water	7.80	7.43	8.23	7.93	5.78	5.49	6.13	5.86	4.61	4.37	4.88	4.67
Toluene	9.35	9.04	10.03	9.20	5.99	5.81	6.46	5.91	4.33	4.19	4.67	4.27
Water	6.99	6.82	7.03	7.01	5.11	4.98	5.12	5.13	4.02	3.89	4.03	4.03
Xylene	8.85	9.06	9.47	9.68	5.77	5.93	6.18	6.31	4.21	4.33	4.50	4.58



Distribution of ABM second validation test results for the two, three, and four-body collisions of  $12.5 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.89	24.78	24.45	25.88	24.89	24.76	24.41	25.94	24.91	24.82	24.30	25.97
Benzene	24.72	23.92	24.88	26.48	24.80	23.80	24.90	26.50	24.89	23.69	24.87	26.55
Chloroform	24.28	25.09	25.49	25.14	24.31	24.92	25.58	25.18	24.36	24.62	25.66	25.35
Creosote	24.52	24.61	25.24	25.63	24.44	24.70	25.16	25.70	24.45	24.72	25.06	25.76
Heptane	26.64	25.71	29.82	17.83	26.20	25.22	29.36	19.22	19.49	18.71	21.81	40.00
Hexane	25.13	23.79	24.98	26.10	25.08	23.81	25.01	26.10	24.94	23.94	25.12	26.01
Pentane	24.62	25.16	24.21	26.01	24.72	25.18	24.16	25.94	24.71	25.28	24.18	25.83
Propane	27.56	28.51	30.11	13.82	26.35	27.14	28.77	17.75	16.39	16.89	17.81	48.91
Sea water	24.83	23.68	26.23	25.26	24.84	23.61	26.34	25.21	24.87	23.61	26.31	25.22
Toluene	24.85	24.02	26.67	24.46	24.79	24.05	26.72	24.44	24.78	24.00	26.75	24.46
Water	25.10	24.50	25.24	25.16	25.14	24.47	25.15	25.24	25.15	24.38	25.24	25.22
Xylene	23.87	24.46	25.54	26.13	23.86	24.51	25.53	26.10	23.90	24.56	25.55	26.00

Total number of collisions in ABM validation tests for  $12.5 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	88.66	58.46	73.56	1.22
Benzene	75.76	61.45	68.61	1.14
Chloroform	72.86	64.71	68.79	1.14
Creosote	82.30	69.33	75.82	1.26
Heptane	47.66	46.61	47.14	0.78
Hexane	68.92	57.22	63.07	1.05
Pentane	46.24	44.15	45.20	0.75
Propane	55.17	71.73	63.45	1.05
Sea water	61.58	73.19	67.39	1.12
Toluene	77.10	79.27	78.19	1.30
Water	56.37	64.16	60.27	1.00
Xylene	75.76	78.88	77.32	1.28

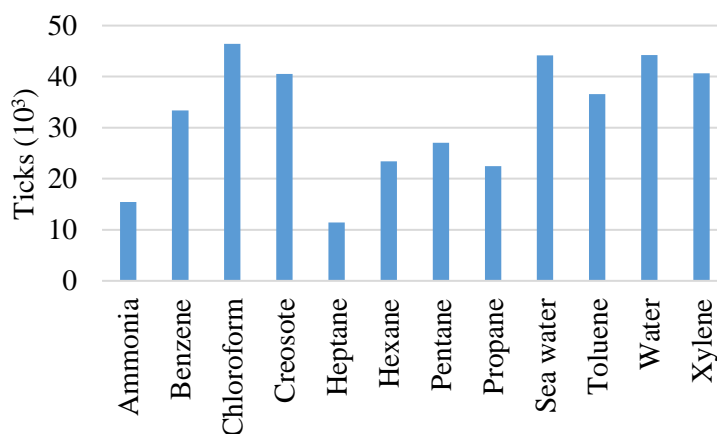
Total number of hydrophobic components  $12.5 \times 10^3$  SDS molecules at the interface for NetLogo models in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	229	296	262.50	1,47
Benzene	189	229	209.00	1,17
Chloroform	226	201	213.50	1,19
Creosote	195	154	174.50	0,97
Heptane	239	249	244.00	1,36
Hexane	231	277	254.00	1,42
Pentane	279	293	286.00	1,60
Propane	500	501	500.50	2,80
Sea water	158	184	171.00	0,96
Toluene	226	260	243.00	1,36
Water	162	196	179.00	1,00
Xylene	248	220	234.00	1,31

**APPENDIX 8.5 - ABM Validation Test Results for  $15 \times 10^3$  SDS Molecules in 12 Different Solvents in a (250 x 250) World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $15 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test (10 <sup>3</sup> )	2 <sup>nd</sup> Test (10 <sup>3</sup> )	Average (10 <sup>3</sup> )	Ratio <sup>79</sup>
Ammonia	16.52	14.40	15.46	0.35
Benzene	30.93	35.89	33.41	0.76
Chloroform	49.81	42.99	46.40	1.05
Creosote	37.61	43.44	40.53	0.92
Heptane	10.57	12.30	11.44	0.26
Hexane	23.38	23.38	23.38	0.53
Pentane	26.71	27.42	27.07	0.61
Propane	24.36	20.63	22.50	0.51
Sea water	43.34	44.99	44.17	1.00
Toluene	40.26	32.85	36.56	0.83
Water	42.99	45.40	44.20	1.00
Xylene	42.76	38.54	40.65	0.92



Comparison of average number of ticks in ABM validation tests for  $15 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<sup>79</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	20.90	13.25	9.34	19.09	12.06	8.47	20.00	12.65	8.91
Benzene	29.80	19.27	13.96	32.84	21.27	15.45	31.32	20.27	14.70
Chloroform	24.34	19.28	16.38	22.45	17.83	15.13	23.40	18.56	15.76
Creosote	25.25	18.97	15.36	27.37	20.55	16.66	26.31	19.76	16.01
Heptane	13.09	8.59	6.16	14.44	9.51	6.86	13.77	9.05	6.51
Hexane	22.45	14.85	10.90	22.45	14.85	10.90	22.45	14.85	10.90
Pentane	25.40	16.57	12.10	25.48	16.59	12.10	25.44	16.58	12.10
Propane	37.60	19.30	12.94	32.76	16.71	11.15	35.18	18.01	12.04
Sea water	27.60	20.46	16.36	28.67	21.26	17.04	28.14	20.86	16.70
Toluene	35.88	23.09	16.71	31.26	20.08	14.48	33.57	21.58	15.59
Water	28.65	20.98	16.62	30.40	22.23	17.60	29.52	21.60	17.11
Xylene	36.19	23.71	17.40	33.34	21.81	15.95	34.77	22.76	16.68

Distribution of ABM validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	48.06	30.46	21.48	48.19	30.44	21.37	48.12	30.45	21.43
Benzene	47.28	30.58	22.15	47.22	30.58	22.21	47.25	30.58	22.18
Chloroform	40.57	32.14	27.29	40.52	32.17	27.31	40.55	32.15	27.30
Creosote	42.38	31.84	25.78	42.38	31.82	25.80	42.38	31.83	25.79
Heptane	47.02	30.85	22.13	46.87	30.86	22.27	46.94	30.86	22.20
Hexane	46.57	30.81	22.62	46.57	30.81	22.62	46.57	30.81	22.62
Pentane	46.97	30.64	22.38	47.04	30.62	22.34	47.00	30.63	22.36
Propane	53.84	27.64	18.52	54.04	27.56	18.40	53.93	27.60	18.46
Sea water	42.85	31.76	25.40	42.81	31.74	25.45	42.83	31.75	25.42
Toluene	47.41	30.51	22.08	47.50	30.50	22.00	47.45	30.51	22.04
Water	43.24	31.67	25.09	43.29	31.65	25.06	43.26	31.66	25.07
Xylene	46.81	30.67	22.51	46.90	30.67	22.43	46.85	30.67	22.47

ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	5.30	5.27	5.10	5.23	3.36	3.34	3.22	3.32	2.37	2.37	2.26	2.35
Benzene	7.16	7.86	7.25	7.53	4.64	5.10	4.70	4.84	3.37	3.71	3.40	3.48
Chloroform	5.96	6.03	6.05	6.31	4.73	4.76	4.80	4.99	4.04	4.01	4.08	4.25
Creosote	6.33	6.22	6.44	6.26	4.75	4.66	4.84	4.72	3.84	3.79	3.92	3.80
Heptane	3.12	3.32	3.19	3.46	2.04	2.19	2.09	2.28	1.46	1.57	1.49	1.64
Hexane	5.63	5.63	5.57	5.61	3.71	3.73	3.70	3.71	2.70	2.74	2.73	2.73
Pentane	6.49	6.21	6.37	6.33	4.23	4.06	4.15	4.13	3.07	2.99	3.02	3.02
Propane	10.22	8.89	9.08	9.42	5.29	4.56	4.61	4.84	3.55	3.05	3.09	3.25
Sea water	6.58	7.03	6.92	7.06	4.84	5.21	5.15	5.26	3.81	4.17	4.13	4.25
Toluene	8.74	8.95	8.87	9.31	5.60	5.78	5.71	5.99	4.03	4.21	4.13	4.33
Water	7.16	7.17	7.29	7.02	5.26	5.22	5.36	5.14	4.17	4.12	4.24	4.09
Xylene	8.96	9.01	9.12	9.11	5.88	5.91	5.97	5.96	4.30	4.33	4.39	4.38

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.34	25.21	24.40	25.05	25.37	25.25	24.29	25.09	25.35	25.36	24.14	25.15
Benzene	24.02	26.37	24.35	25.26	24.09	26.44	24.36	25.10	24.15	26.56	24.37	24.91
Chloroform	24.47	24.76	24.84	25.93	24.52	24.70	24.89	25.89	24.66	24.49	24.91	25.94
Creosote	25.06	24.63	25.53	24.78	25.03	24.60	25.50	24.87	24.98	24.70	25.56	24.77
Heptane	23.81	25.36	24.38	26.46	23.70	25.48	24.30	26.53	23.67	25.54	24.21	26.58
Hexane	25.08	25.10	24.81	25.01	24.97	25.11	24.90	25.01	24.79	25.16	25.02	25.04
Pentane	25.56	24.43	25.09	24.91	25.51	24.53	25.06	24.90	25.39	24.72	24.92	24.96
Propane	27.17	23.64	24.14	25.05	27.43	23.61	23.91	25.05	27.45	23.61	23.85	25.09
Sea water	23.85	25.48	25.09	25.59	23.67	25.45	25.17	25.72	23.30	25.47	25.24	25.98
Toluene	24.37	24.95	24.72	25.96	24.27	25.06	24.72	25.96	24.14	25.19	24.72	25.94
Water	25.01	25.02	25.45	24.52	25.07	24.89	25.53	24.51	25.07	24.81	25.50	24.62
Xylene	24.76	24.89	25.19	25.16	24.79	24.90	25.16	25.15	24.73	24.89	25.21	25.16

ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	4.85	4.82	4.63	4.79	3.07	3.05	2.91	3.03	2.15	2.15	2.03	2.13
Benzene	7.88	8.68	8.01	8.27	5.12	5.63	5.19	5.32	3.73	4.11	3.77	3.84
Chloroform	5.50	5.58	5.58	5.79	4.38	4.42	4.44	4.59	3.74	3.72	3.77	3.90
Creosote	6.83	6.77	6.95	6.81	5.12	5.08	5.22	5.13	4.14	4.13	4.24	4.14
Heptane	3.42	3.68	3.53	3.82	2.24	2.43	2.32	2.52	1.61	1.76	1.67	1.82
Hexane	5.63	5.63	5.57	5.61	3.71	3.73	3.70	3.71	2.70	2.74	2.73	2.73
Pentane	6.35	6.17	6.62	6.34	4.16	4.02	4.31	4.11	3.06	2.93	3.13	2.98
Propane	7.80	7.93	8.20	8.84	3.93	4.01	4.20	4.56	2.62	2.66	2.81	3.07
Sea water	6.99	7.32	7.18	7.18	5.18	5.43	5.33	5.33	4.12	4.37	4.29	4.27
Toluene	8.10	7.54	7.97	7.64	5.22	4.84	5.14	4.88	3.78	3.51	3.72	3.47
Water	7.33	7.58	7.88	7.60	5.38	5.52	5.75	5.58	4.25	4.37	4.55	4.42
Xylene	8.26	8.12	8.32	8.65	5.40	5.31	5.45	5.65	3.96	3.88	3.98	4.13



Distribution of ABM second validation test results for the two, three, and four-body collisions of  $15 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.42	25.25	24.27	25.06	25.45	25.30	24.15	25.10	25.44	25.42	23.99	25.15
Benzene	24.00	26.42	24.39	25.18	24.06	26.49	24.41	25.03	24.12	26.61	24.42	24.86
Chloroform	24.48	24.84	24.87	25.81	24.54	24.77	24.92	25.76	24.70	24.56	24.94	25.80
Creosote	24.96	24.75	25.41	24.88	24.93	24.72	25.39	24.96	24.87	24.81	25.44	24.87
Heptane	23.66	25.46	24.41	26.47	23.54	25.58	24.35	26.53	23.49	25.65	24.28	26.58
Hexane	25.08	25.10	24.81	25.01	24.97	25.11	24.90	25.01	24.79	25.16	25.02	25.04
Pentane	24.94	24.20	26.00	24.87	25.06	24.20	25.99	24.75	25.26	24.18	25.90	24.66
Propane	23.80	24.20	25.03	26.98	23.54	24.00	25.15	27.31	23.45	23.86	25.19	27.50
Sea water	24.39	25.52	25.05	25.04	24.35	25.53	25.07	25.06	24.17	25.63	25.15	25.05
Toluene	25.91	24.13	25.51	24.45	26.00	24.13	25.59	24.28	26.09	24.21	25.72	23.98
Water	24.13	24.93	25.92	25.02	24.20	24.83	25.87	25.11	24.16	24.84	25.87	25.12
Xylene	24.76	24.35	24.95	25.94	24.76	24.34	24.98	25.93	24.83	24.32	24.94	25.92

Total number of collisions in ABM validation tests for  $15 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	43.49	39.62	41.56	0.61
Benzene	63.03	69.56	66.30	0.97
Chloroform	60.00	55.41	57.71	0.85
Creosote	59.58	64.58	62.08	0.91
Heptane	27.84	30.81	29.33	0.43
Hexane	48.20	48.20	48.20	0.71
Pentane	54.07	54.17	54.12	0.79
Propane	69.84	60.62	65.23	0.96
Sea water	64.42	66.97	65.70	0.96
Toluene	75.68	65.82	70.75	1.04
Water	66.25	70.23	68.24	1.00
Xylene	77.30	71.10	74.20	1.09

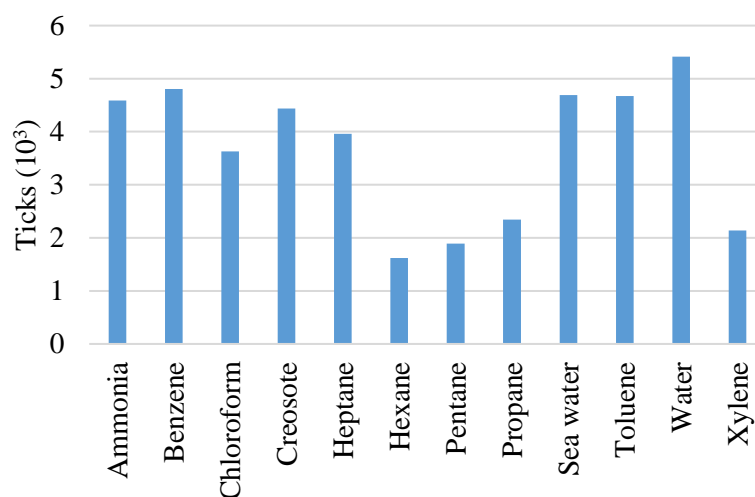
Cumulative number of SDS molecules at the interface of ABM validation tests for  $15 \times 10^3$  SDS molecules in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	224	218	221.00	1,09
Benzene	280	281	280.50	1,39
Chloroform	229	220	224.50	1,11
Creosote	232	235	233.50	1,16
Heptane	251	259	255.00	1,26
Hexane	218	218	218.00	1,08
Pentane	304	284	294.00	1,46
Propane	501	501	501.00	2,48
Sea water	186	204	195.00	0,97
Toluene	233	252	242.50	1,20
Water	249	155	202.00	1,00
Xylene	200	264	232.00	1,15

**APPENDIX 8.6 - ABM Validation Test Results for  $50 \times 10^3$  SDS Molecules in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM validation tests for  $50 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio<sup>80</sup></b>
Ammonia	6.03	3.14	4.59	0.85
Benzene	6.51	3.10	4.81	0.89
Chloroform	3.09	4.17	3.63	0.67
Creosote	3.06	5.81	4.44	0.82
Heptane	5.13	2.78	3.96	0.73
Hexane	1.97	1.27	1.62	0.30
Pentane	1.63	2.16	1.90	0.35
Propane	1.53	3.16	2.35	0.43
Sea water	7.96	1.42	4.69	0.87
Toluene	6.15	3.20	4.68	0.86
Water	7.88	2.95	5.42	1.00
Xylene	2.06	2.22	2.14	0.40



Comparison of average number of ticks in ABM validation tests for  $50 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<sup>80</sup> Ratio calculated with respect to water.

ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	16.93	11.02	8.05	10.42	6.71	4.87	13.68	8.86	6.46
Benzene	16.46	10.72	7.93	9.70	6.27	4.61	13.08	8.50	6.27
Chloroform	4.50	3.47	2.97	5.49	4.22	3.60	5.00	3.85	3.28
Creosote	5.85	4.33	3.55	9.12	6.76	5.54	7.49	5.54	4.55
Heptane	12.39	8.41	6.35	8.14	5.51	4.13	10.27	6.96	5.24
Hexane	6.68	4.44	3.29	4.90	3.24	2.39	5.79	3.84	2.84
Pentane	6.16	4.03	2.96	7.44	4.89	3.61	6.80	4.46	3.29
Propane	9.29	5.17	3.40	15.88	8.96	6.03	12.59	7.07	4.72
Sea water	12.00	8.81	7.16	3.64	2.64	2.12	7.82	5.72	4.64
Toluene	16.07	10.40	7.64	10.10	6.50	4.75	13.08	8.45	6.19
Water	12.60	9.17	7.38	6.44	4.67	3.76	9.52	6.92	5.57
Xylene	6.95	4.52	3.33	7.42	4.83	3.55	7.18	4.68	3.44

Distribution of ABM validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	47.03	30.61	22.37	47.37	30.51	22.12	47.16	30.57	22.27
Benzene	46.87	30.55	22.58	47.13	30.49	22.38	46.97	30.53	22.51
Chloroform	41.14	31.73	27.13	41.24	31.74	27.03	41.19	31.73	27.07
Creosote	42.61	31.53	25.86	42.58	31.55	25.87	42.59	31.54	25.86
Heptane	45.65	30.96	23.39	45.81	30.97	23.22	45.71	30.97	23.32
Hexane	46.36	30.80	22.83	46.52	30.81	22.66	46.43	30.81	22.76
Pentane	46.83	30.64	22.52	46.67	30.69	22.64	46.75	30.67	22.59
Propane	52.00	28.95	19.05	51.44	29.03	19.53	51.65	29.00	19.35
Sea water	42.91	31.50	25.59	43.34	31.44	25.22	43.01	31.49	25.50
Toluene	47.12	30.48	22.40	47.30	30.45	22.26	47.19	30.47	22.34
Water	43.21	31.45	25.34	43.32	31.42	25.26	43.25	31.44	25.31
Xylene	46.94	30.55	22.51	46.94	30.57	22.48	46.94	30.56	22.50

ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	4.33	4.12	4.25	4.24	2.82	2.68	2.76	2.76	2.06	1.96	2.01	2.01
Benzene	4.15	4.10	4.17	4.04	2.70	2.67	2.72	2.63	2.00	1.97	2.01	1.95
Chloroform	1.15	1.11	1.11	1.14	0.89	0.86	0.85	0.88	0.76	0.73	0.73	0.75
Creosote	1.48	1.44	1.46	1.47	1.10	1.06	1.08	1.09	0.90	0.87	0.89	0.89
Heptane	3.06	3.06	3.13	3.14	2.07	2.08	2.13	2.13	1.57	1.57	1.60	1.61
Hexane	1.65	1.68	1.64	1.71	1.10	1.11	1.09	1.14	0.82	0.83	0.80	0.85
Pentane	1.52	1.54	1.53	1.57	1.00	1.01	1.00	1.03	0.73	0.74	0.73	0.76
Propane	2.30	2.36	2.32	2.31	1.28	1.32	1.29	1.28	0.84	0.87	0.85	0.84
Sea water	2.99	2.98	3.02	3.01	2.20	2.19	2.22	2.20	1.79	1.78	1.80	1.79
Toluene	4.01	4.10	3.98	3.97	2.60	2.65	2.57	2.57	1.91	1.95	1.89	1.89
Water	3.15	3.12	3.16	3.16	2.30	2.27	2.30	2.30	1.85	1.82	1.86	1.85
Xylene	1.77	1.70	1.73	1.75	1.15	1.10	1.12	1.14	0.85	0.81	0.83	0.84

Distribution of ABM first validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.57	24.34	25.08	25.01	25.56	24.32	25.07	25.04	25.64	24.34	25.01	25.57
Benzene	25.20	24.90	25.36	24.54	25.20	24.89	25.40	24.51	25.24	24.83	25.38	25.20
Chloroform	25.46	24.66	24.63	25.25	25.50	24.63	24.60	25.26	25.57	24.74	24.46	25.46
Creosote	25.32	24.54	24.96	25.19	25.37	24.50	24.97	25.15	25.39	24.51	25.01	25.32
Heptane	24.67	24.67	25.28	25.37	24.66	24.70	25.30	25.34	24.65	24.72	25.27	24.67
Hexane	24.71	25.11	24.56	25.61	24.74	25.09	24.46	25.70	24.78	25.11	24.39	24.71
Pentane	24.72	25.00	24.82	25.47	24.76	24.95	24.82	25.47	24.76	24.97	24.78	24.72
Propane	24.77	25.43	24.97	24.83	24.81	25.56	24.90	24.74	24.82	25.60	24.86	24.77
Sea water	24.92	24.85	25.18	25.05	24.98	24.85	25.16	25.01	25.02	24.88	25.13	24.92
Toluene	24.97	25.50	24.80	24.73	24.99	25.53	24.74	24.74	25.00	25.57	24.74	24.97
Water	25.05	24.79	25.09	25.07	25.07	24.74	25.12	25.07	25.08	24.68	25.19	25.05
Xylene	25.48	24.45	24.85	25.22	25.51	24.43	24.86	25.21	25.49	24.36	24.87	25.48

ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	4.33	4.12	4.25	4.24	2.82	2.68	2.76	2.76	2.06	1.96	2.01	2.01
Benzene	4.15	4.10	4.17	4.04	2.70	2.67	2.72	2.63	2.00	1.97	2.01	1.95
Chloroform	1.15	1.11	1.11	1.14	0.89	0.86	0.85	0.88	0.76	0.73	0.73	0.75
Creosote	1.48	1.44	1.46	1.47	1.10	1.06	1.08	1.09	0.90	0.87	0.89	0.89
Heptane	3.06	3.06	3.13	3.14	2.07	2.08	2.13	2.13	1.57	1.57	1.60	1.61
Hexane	1.65	1.68	1.64	1.71	1.10	1.11	1.09	1.14	0.82	0.83	0.80	0.85
Pentane	1.52	1.54	1.53	1.57	1.00	1.01	1.00	1.03	0.73	0.74	0.73	0.76
Propane	2.30	2.36	2.32	2.31	1.28	1.32	1.29	1.28	0.84	0.87	0.85	0.84
Sea water	2.99	2.98	3.02	3.01	2.20	2.19	2.22	2.20	1.79	1.78	1.80	1.79
Toluene	4.01	4.10	3.98	3.97	2.60	2.65	2.57	2.57	1.91	1.95	1.89	1.89
Water	3.15	3.12	3.16	3.16	2.30	2.27	2.30	2.30	1.85	1.82	1.86	1.85
Xylene	1.77	1.70	1.73	1.75	1.15	1.10	1.12	1.14	0.85	0.81	0.83	0.84



Distribution of ABM second validation test results for the two, three, and four-body collisions of  $50 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.57	24.34	25.08	25.01	25.56	24.32	25.07	25.04	25.64	24.34	25.01	25.01
Benzene	25.20	24.90	25.36	24.54	25.20	24.89	25.40	24.51	25.24	24.83	25.38	24.56
Chloroform	25.46	24.66	24.63	25.25	25.50	24.63	24.60	25.26	25.57	24.74	24.46	25.23
Creosote	25.32	24.54	24.96	25.19	25.37	24.50	24.97	25.15	25.39	24.51	25.01	25.10
Heptane	24.67	24.67	25.28	25.37	24.66	24.70	25.30	25.34	24.65	24.72	25.27	25.36
Hexane	24.71	25.11	24.56	25.61	24.74	25.09	24.46	25.70	24.78	25.11	24.39	25.72
Pentane	24.72	25.00	24.82	25.47	24.76	24.95	24.82	25.47	24.76	24.97	24.78	25.48
Propane	24.77	25.43	24.97	24.83	24.81	25.56	24.90	24.74	24.82	25.60	24.86	24.72
Sea water	24.92	24.85	25.18	25.05	24.98	24.85	25.16	25.01	25.02	24.88	25.13	24.97
Toluene	24.97	25.50	24.80	24.73	24.99	25.53	24.74	24.74	25.00	25.57	24.74	24.69
Water	25.05	24.79	25.09	25.07	25.07	24.74	25.12	25.07	25.08	24.68	25.19	25.06
Xylene	25.48	24.45	24.85	25.22	25.51	24.43	24.86	25.21	25.49	24.36	24.87	25.28

Total number of collisions in ABM validation tests for  $50 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	36.00	22.00	29.00	1.32
Benzene	35.11	20.58	27.85	1.27
Chloroform	10.94	13.31	12.13	0.55
Creosote	13.73	21.42	17.58	0.80
Heptane	27.15	17.78	22.47	1.02
Hexane	14.41	10.53	12.47	0.57
Pentane	13.15	15.94	14.55	0.66
Propane	17.86	30.87	24.37	1.11
Sea water	27.97	8.40	18.19	0.83
Toluene	34.11	21.35	27.73	1.26
Water	29.15	14.87	22.01	1.00
Xylene	14.80	15.80	15.30	0.70

Cumulative number of SDS molecules at the interface of ABM validation tests for  $50 \times 10^3$  SDS molecules in 12 different solvents of the world with (250 x 250) patches for 72-hours at 25°C

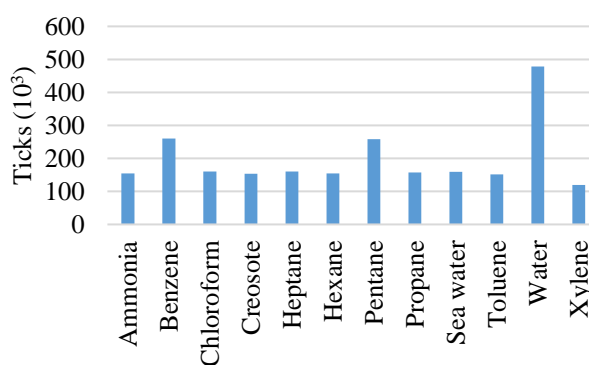
<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	232	189	210.50	1.57
Benzene	196	121	158.50	1.18
Chloroform	82	101	91.50	0.68
Creosote	123	147	135.00	1.01
Heptane	264	218	241.00	1.80
Hexane	211	174	192.50	1.44
Pentane	184	186	185.00	1.38
Propane	394	452	423.00	3.16
Sea water	154	79	116.50	0.87
Toluene	253	228	240.50	1.79
Water	145	123	134.00	1.00
Xylene	208	118	163.00	1.22

## APPENDIX 9 - ABM Load Test Results for Uncharged Nanoparticles

### APPENDIX 9.1 - ABM Load Test Results for $100 \times 10^3$ Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM load tests for  $100 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	Average ( $10^3$ )	Ratio <sup>81</sup>
Ammonia	140.86	185.17	163.01	0.93
Benzene	248.86	189.08	218.97	1.25
Chloroform	149.21	200.64	174.92	1.00
Creosote	148.54	196.10	172.32	0.98
Heptane	142.34	199.06	170.70	0.97
Hexane	292.34	193.05	242.70	1.38
Pentane	287.99	203.17	245.58	1.40
Propane	149.42	195.81	172.61	0.98
Sea water	142.37	195.50	168.94	0.96
Toluene	258.16	195.56	226.86	1.29
Water	147.60	203.41	175.51	1.00
Xylene	148.68	194.64	171.66	0.98



Comparison of average number of ticks in ABM load tests for  $100 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>81</sup> Ratio calculated with respect to water.

ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	34.82	7.34	3.04	35.80	7.38	3.07	35.31	7.36	3.06
Benzene	38.29	7.80	3.26	37.16	7.76	3.23	37.73	7.78	3.25
Chloroform	57.15	13.49	5.64	58.56	13.41	5.59	57.86	13.45	5.61
Creosote	43.28	9.68	4.03	44.73	9.80	4.07	44.00	9.74	4.05
Heptane	29.25	5.99	2.49	30.36	6.05	2.52	29.80	6.02	2.51
Hexane	29.50	5.70	2.37	30.04	5.84	2.42	29.77	5.77	2.39
Pentane	29.08	5.56	2.31	28.59	5.61	2.33	28.83	5.58	2.32
Propane	23.27	4.39	1.82	23.21	4.39	1.83	23.24	4.39	1.82
Sea water	42.33	9.38	3.89	42.89	9.28	3.85	42.61	9.33	3.87
Toluene	38.29	7.67	3.19	37.33	7.70	3.20	37.81	7.69	3.19
Water	40.65	8.98	3.73	41.49	8.92	3.71	41.07	8.95	3.72
Xylene	35.73	7.70	3.18	37.67	7.91	3.30	36.70	7.80	3.24

Distribution of ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	77.02	16.24	6.73	77.42	15.95	6.63	77.22	16.10	6.68
Benzene	77.59	15.81	6.61	77.16	16.12	6.72	77.38	15.96	6.66
Chloroform	74.92	17.68	7.39	75.51	17.29	7.20	75.22	17.49	7.30
Creosote	75.94	16.98	7.08	76.33	16.72	6.95	76.14	16.85	7.01
Heptane	77.52	15.86	6.61	77.98	15.53	6.49	77.76	15.70	6.55
Hexane	78.53	15.17	6.30	78.43	15.25	6.32	78.48	15.21	6.31
Pentane	78.71	15.04	6.25	78.25	15.36	6.39	78.48	15.20	6.32
Propane	78.93	14.90	6.16	78.88	14.91	6.21	78.91	14.91	6.19
Sea water	76.13	16.88	7.00	76.56	16.56	6.88	76.35	16.72	6.94
Toluene	77.91	15.61	6.49	77.40	15.96	6.63	77.66	15.78	6.56
Water	76.17	16.84	7.00	76.67	16.47	6.86	76.42	16.65	6.92
Xylene	76.66	16.51	6.83	77.06	16.18	6.75	76.87	16.34	6.79

ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	15.82	15.78	1.62	1.61	3.70	3.61	0.01	0.01	1.55	1.50	0.00	0.00
Benzene	16.95	16.82	2.29	2.22	3.88	3.89	0.01	0.01	1.62	1.64	0.00	0.00
Chloroform	28.21	28.08	0.40	0.47	6.73	6.75	0.00	0.00	2.82	2.82	0.00	0.00
Creosote	20.59	20.56	1.09	1.04	4.85	4.81	0.01	0.01	2.02	2.01	0.00	0.00
Heptane	12.83	12.82	1.86	1.74	2.96	3.00	0.02	0.01	1.24	1.25	0.00	0.00
Hexane	12.35	12.28	2.46	2.41	2.81	2.85	0.02	0.02	1.17	1.19	0.00	0.00
Pentane	12.15	12.00	2.46	2.47	2.76	2.76	0.02	0.02	1.15	1.16	0.00	0.00
Propane	9.61	9.38	2.13	2.15	2.20	2.15	0.02	0.02	0.92	0.90	0.00	0.00
Sea water	20.25	19.97	1.02	1.09	4.74	4.63	0.01	0.01	1.97	1.92	0.00	0.00
Toluene	16.77	16.54	2.54	2.45	3.83	3.81	0.02	0.02	1.59	1.60	0.00	0.00
Water	19.19	19.16	1.16	1.14	4.46	4.51	0.01	0.01	1.85	1.89	0.00	0.00
Xylene	16.48	16.60	1.32	1.34	3.84	3.84	0.01	0.01	1.60	1.59	0.00	0.00

Distribution of ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	45.42	45.30	4.65	4.63	18.04	41.41	40.41	0.14	0.42	50.58	49.00	0.00
Benzene	44.26	43.94	5.99	5.81	22.21	38.75	38.90	0.14	0.43	49.34	50.23	0.00
Chloroform	49.36	49.13	0.69	0.82	3.35	48.26	48.37	0.02	0.06	49.96	49.98	0.00
Creosote	47.57	47.51	2.51	2.41	9.73	45.28	44.92	0.07	0.19	50.06	49.76	0.00
Heptane	43.86	43.84	6.37	5.93	22.51	38.41	38.88	0.20	0.55	49.57	49.88	0.00
Hexane	41.87	41.63	8.33	8.16	29.76	34.74	35.29	0.22	0.71	49.25	50.04	0.00
Pentane	41.80	41.26	8.46	8.48	30.82	34.53	34.43	0.23	0.79	49.46	49.74	0.01
Propane	41.30	40.31	9.14	9.25	32.99	33.78	32.93	0.30	1.08	50.06	48.85	0.01
Sea water	47.83	47.18	2.40	2.59	10.45	45.25	44.24	0.07	0.20	50.43	49.37	0.00
Toluene	43.78	43.18	6.63	6.41	24.27	37.85	37.71	0.17	0.50	49.64	49.85	0.00
Water	47.20	47.14	2.84	2.82	11.31	44.08	44.53	0.08	0.22	49.38	50.40	0.00
Xylene	46.12	46.45	3.68	3.74	14.82	42.57	42.51	0.10	0.30	49.99	49.70	0.00

ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	15.94	15.85	1.99	2.02	3.67	3.68	0.01	0.01	1.52	1.54	0.00	0.00
Benzene	16.67	16.65	1.89	1.95	3.87	3.87	0.01	0.01	1.63	1.61	0.00	0.00
Chloroform	28.41	28.55	0.77	0.83	6.67	6.73	0.00	0.01	2.77	2.82	0.00	0.00
Creosote	20.97	20.83	1.48	1.45	4.93	4.85	0.01	0.01	2.05	2.02	0.00	0.00
Heptane	12.97	13.01	2.18	2.21	3.00	3.02	0.02	0.02	1.26	1.26	0.00	0.00
Hexane	12.64	12.79	2.28	2.33	2.87	2.93	0.02	0.02	1.20	1.22	0.00	0.00
Pentane	12.11	12.10	2.18	2.20	2.77	2.81	0.02	0.02	1.16	1.18	0.00	0.00
Propane	9.46	9.37	2.21	2.17	2.18	2.17	0.02	0.02	0.92	0.91	0.00	0.00
Sea water	20.00	19.95	1.50	1.44	4.64	4.62	0.01	0.01	1.93	1.92	0.00	0.00
Toluene	16.76	16.60	2.01	1.96	3.87	3.80	0.01	0.01	1.61	1.59	0.00	0.00
Water	19.34	18.87	1.60	1.68	4.49	4.41	0.01	0.01	1.86	1.85	0.00	0.00
Xylene	17.03	16.96	1.92	1.76	3.96	3.92	0.01	0.01	1.66	1.64	0.00	0.00



Distribution of ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	44.51	44.28	5.55	5.65	21.56	39.12	39.16	0.15	0.48	49.46	50.06	0.00
Benzene	44.87	44.80	5.10	5.24	20.09	39.87	39.91	0.14	0.45	50.03	49.52	0.00
Chloroform	48.50	48.76	1.32	1.42	5.84	46.83	47.29	0.03	0.09	49.56	50.35	0.00
Creosote	46.89	46.57	3.31	3.24	12.89	43.88	43.15	0.09	0.24	50.35	49.41	0.00
Heptane	42.71	42.84	7.19	7.26	26.77	36.37	36.66	0.20	0.65	49.63	49.72	0.00
Hexane	42.08	42.56	7.60	7.75	28.55	35.25	35.97	0.22	0.77	49.16	50.07	0.01
Pentane	42.36	42.34	7.62	7.69	28.22	35.55	36.03	0.21	0.71	49.16	50.12	0.00
Propane	40.76	40.36	9.53	9.34	33.18	33.38	33.14	0.29	1.03	49.75	49.21	0.01
Sea water	46.63	46.50	3.50	3.37	13.48	43.32	43.11	0.09	0.25	49.92	49.83	0.00
Toluene	44.90	44.46	5.39	5.24	20.30	40.13	39.42	0.15	0.43	50.07	49.50	0.00
Water	46.62	45.47	3.85	4.06	15.91	42.36	41.63	0.10	0.31	50.01	49.68	0.00
Xylene	45.20	45.03	5.09	4.68	18.25	40.99	40.62	0.14	0.36	50.02	49.61	0.00

Total number of collisions in ABM load tests for  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	45.21	46.19	46.22	0.85
Benzene	49.35	48.22	48.19	0.89
Chloroform	76.28	77.69	77.61	1.43
Creosote	56.98	58.44	58.56	1.08
Heptane	37.73	38.84	38.90	0.72
Hexane	37.57	38.11	38.25	0.71
Pentane	36.94	36.46	36.51	0.67
Propane	29.48	29.42	29.42	0.54
Sea water	55.60	56.16	56.06	1.04
Toluene	49.15	48.19	48.22	0.89
Water	53.36	54.21	54.14	1.00
Xylene	46.61	48.55	48.76	0.90

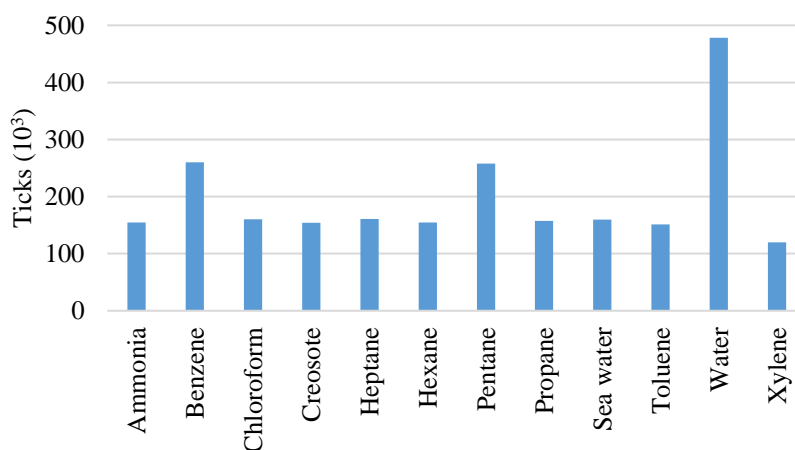
Cumulative number of uncharged nanoparticles at the interface of ABM load tests for  $100 \times 10^3$  uncharged nanoparticles in 12 different solvents of a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	96.512	97.286	96.899	1,00
Benzene	97.939	97.060	97.500	1,01
Chloroform	96.116	96.581	96.349	1,00
Creosote	96.356	96.847	96.602	1,00
Heptane	97.083	97.787	97.435	1,01
Hexane	98.758	97.824	98.291	1,02
Pentane	98.859	98.066	98.463	1,02
Propane	98.201	98.884	98.543	1,02
Sea water	96.292	96.935	96.614	1,00
Toluene	97.890	97.105	97.498	1,01
Water	96.519	97.066	96.793	1,00
Xylene	96.763	97.164	96.964	1,00

**APPENDIX 9.2 - ABM Load Test Results for  $200 \times 10^3$  Uncharged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM load tests for  $200 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	Average ( $10^3$ )	Ratio <sup>82</sup>
Ammonia	222.21	86.80	154,51	0.32
Benzene	432.00	88.68	260,34	0.54
Chloroform	234.82	85.21	160,01	0.33
Creosote	221.48	86.22	153,85	0.32
Heptane	239.97	81.55	160,76	0.34
Hexane	219.72	89.77	154,74	0.32
Pentane	433.18	83.00	258,09	0.54
Propane	228.68	85.96	157,32	0.33
Sea water	230.29	89.14	159,71	0.33
Toluene	219.32	83.55	151,44	0.32
Water	431.17	525.84	478,51	1.00
Xylene	152.15	87.36	119,75	0.25



Comparison of average number of ticks in ABM load tests for  $200 \times 10^3$  uncharged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>82</sup> Ratio calculated with respect to water.

ABM load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	129.52	25.34	10.41	108.93	24.94	10.33	119.22	25.14	10.37
Benzene	146.94	26.95	11.04	113.49	26.53	11.02	130.21	26.74	11.03
Chloroform	195.44	45.08	18.74	162.00	45.08	18.99	178.72	45.08	18.86
Creosote	154.95	33.11	13.69	129.35	32.57	13.65	142.15	32.84	13.67
Heptane	114.84	21.28	8.65	97.03	20.74	8.54	105.93	21.01	8.59
Hexane	112.36	20.25	8.18	96.06	19.90	8.12	104.21	20.07	8.15
Pentane	111.50	19.58	7.91	91.65	19.20	7.89	101.57	19.39	7.90
Propane	87.62	15.25	6.13	80.35	15.16	6.10	83.98	15.21	6.12
Sea water	152.97	32.00	13.15	126.82	31.61	13.18	139.90	31.80	13.17
Toluene	135.92	26.47	10.81	113.97	26.31	10.89	124.94	26.39	10.85
Water	163.20	30.90	12.67	166.03	30.81	12.62	164.62	30.85	12.64
Xylene	124.12	27.13	11.17	116.22	27.05	11.20	120.17	27.09	11.18

Distribution of ABM load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	78.37	15.33	6.30	75.54	17.30	7.17	77.05	16.25	6.70
Benzene	79.46	14.57	5.97	75.14	17.56	7.29	77.52	15.92	6.57
Chloroform	75.38	17.39	7.23	71.66	19.94	8.40	73.65	18.58	7.77
Creosote	76.80	16.41	6.79	73.67	18.55	7.78	75.35	17.41	7.25
Heptane	79.33	14.70	5.98	76.82	16.42	6.76	78.16	15.50	6.34
Hexane	79.81	14.38	5.81	77.42	16.04	6.54	78.69	15.16	6.15
Pentane	80.22	14.09	5.69	77.18	16.17	6.64	78.82	15.05	6.13
Propane	80.38	13.99	5.63	79.07	14.92	6.01	79.75	14.44	5.81
Sea water	77.21	16.15	6.64	73.90	18.42	7.68	75.67	17.20	7.12
Toluene	78.48	15.28	6.24	75.40	17.40	7.20	77.04	16.27	6.69
Water	78.93	14.94	6.13	79.27	14.71	6.03	79.10	14.82	6.08
Xylene	76.42	16.71	6.87	75.24	17.51	7.25	75.84	17.10	7.06

ABM first load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	52.34	51.83	12.55	12.80	12.49	12.42	0.21	0.22	5.21	5.19	0.00	0.00
Benzene	56.81	55.93	16.85	17.35	13.38	13.05	0.25	0.26	5.59	5.44	0.00	0.00
Chloroform	92.47	91.21	5.81	5.95	22.60	22.31	0.08	0.09	9.46	9.28	0.00	0.00
Creosote	68.49	67.50	9.38	9.58	16.51	16.30	0.15	0.15	6.87	6.82	0.00	0.00
Heptane	43.17	43.84	14.11	13.72	10.30	10.46	0.26	0.25	4.29	4.36	0.00	0.00
Hexane	41.34	41.87	14.93	14.22	9.84	9.87	0.28	0.26	4.08	4.09	0.00	0.00
Pentane	40.41	39.98	15.40	15.71	9.58	9.45	0.27	0.28	3.98	3.92	0.00	0.00
Propane	30.59	31.13	13.14	12.75	7.30	7.41	0.28	0.27	3.04	3.08	0.01	0.00
Sea water	65.48	65.90	11.09	10.50	15.79	15.85	0.19	0.17	6.52	6.62	0.00	0.00
Toluene	55.37	54.76	12.84	12.94	13.07	12.96	0.22	0.22	5.41	5.39	0.00	0.00
Water	64.79	64.46	17.18	16.78	15.17	15.24	0.25	0.24	6.30	6.36	0.00	0.00
Xylene	55.59	54.58	6.96	6.99	13.56	13.30	0.13	0.14	5.64	5.52	0.00	0.00

Distribution of ABM first load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	40.41	40.02	9.69	9.88	33.76	32.93	32.74	0.57	2.08	49.07	48.82	0.03
Benzene	38.66	38.06	11.47	11.81	39.40	30.38	29.63	0.58	2.34	49.46	48.16	0.03
Chloroform	47.31	46.67	2.97	3.04	11.68	44.36	43.80	0.16	0.45	50.25	49.29	0.01
Creosote	44.20	43.56	6.05	6.19	22.53	38.81	38.31	0.34	1.08	49.62	49.29	0.01
Heptane	37.59	38.17	12.29	11.95	39.50	29.65	30.10	0.76	2.86	48.16	48.93	0.05
Hexane	36.79	37.27	13.29	12.65	41.56	28.77	28.85	0.82	3.10	48.41	48.43	0.05
Pentane	36.24	35.86	13.81	14.09	44.88	27.36	26.99	0.77	3.44	48.61	47.89	0.05
Propane	34.91	35.53	15.00	14.55	45.98	26.30	26.70	1.02	4.15	47.60	48.17	0.08
Sea water	42.80	43.08	7.25	6.86	24.81	37.30	37.45	0.44	1.29	48.98	49.71	0.02
Toluene	40.74	40.29	9.45	9.52	33.02	33.35	33.07	0.56	2.02	49.08	48.88	0.03
Water	39.70	39.50	10.53	10.28	35.37	31.98	32.13	0.52	1.86	48.84	49.28	0.02
Xylene	44.79	43.98	5.60	5.63	20.56	39.91	39.13	0.40	1.20	49.89	48.89	0.02

ABM second load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	48.66	4.93	5.20	12.52	12.21	0.10	0.11	5.21	5.12	5.33	0.00	0.00
Benzene	52.02	4.46	4.53	13.26	13.09	0.09	0.09	5.55	5.46	5.12	0.00	0.00
Chloroform	80.41	0.67	0.64	22.47	22.59	0.01	0.01	9.47	9.52	7.29	0.00	0.00
Creosote	62.46	2.28	2.46	16.20	16.28	0.04	0.05	6.82	6.83	7.90	0.00	0.00
Heptane	41.24	7.28	7.28	10.18	10.25	0.16	0.16	4.26	4.27	5.73	0.00	0.00
Hexane	39.84	7.89	8.28	9.75	9.78	0.18	0.19	4.04	4.07	4.88	0.00	0.00
Pentane	37.95	7.73	7.59	9.47	9.39	0.18	0.17	3.96	3.92	5.72	0.00	0.00
Propane	30.07	9.95	9.96	7.37	7.31	0.25	0.24	3.06	3.03	3.43	0.00	0.00
Sea water	60.78	2.76	2.64	15.79	15.71	0.06	0.05	6.61	6.57	5.10	0.00	0.00
Toluene	52.22	4.91	4.92	12.98	13.12	0.10	0.10	5.41	5.48	4.89	0.00	0.00
Water	53.89	4.69	4.42	13.32	13.54	0.10	0.09	5.56	5.63	6.34	0.00	0.00
Xylene	64.89	17.77	18.58	15.06	15.24	0.24	0.26	6.27	6.35	5.61	0.00	0.00



Distribution of ABM second load test results for the two, three, and four-body collisions of  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	68.24	6.91	7.29	17.56	69.26	0.57	0.62	29.55	49.00	51.00	0.00	0.00
Benzene	70.04	6.01	6.10	17.85	69.55	0.48	0.48	29.49	51.61	48.39	0.00	0.00
Chloroform	77.18	0.64	0.61	21.57	70.42	0.03	0.03	29.52	56.63	43.37	0.00	0.00
Creosote	74.89	2.73	2.95	19.42	70.20	0.17	0.22	29.41	46.37	53.63	0.00	0.00
Heptane	62.50	11.03	11.03	15.43	69.12	1.08	1.08	28.73	42.70	57.30	0.00	0.00
Hexane	60.58	12.00	12.59	14.83	68.92	1.27	1.34	28.47	45.47	54.53	0.00	0.00
Pentane	60.49	12.32	12.10	15.09	68.54	1.31	1.24	28.91	40.66	59.34	0.00	0.00
Propane	52.43	17.35	17.37	12.85	67.31	2.30	2.21	28.18	46.90	53.10	0.00	0.00
Sea water	74.15	3.37	3.22	19.26	70.04	0.27	0.22	29.47	56.30	43.70	0.00	0.00
Toluene	69.60	6.54	6.56	17.30	70.05	0.53	0.53	28.88	52.84	47.16	0.00	0.00
Water	70.61	6.15	5.79	17.45	70.19	0.52	0.47	28.82	47.03	52.97	0.00	0.00
Xylene	55.80	15.28	15.98	12.95	69.24	1.09	1.18	28.49	53.09	46.91	0.00	0.00

Total number of collisions in ABM load tests for  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	165,27	144,20	154,73	0,74
Benzene	184,93	151,03	167,98	0,81
Chloroform	259,27	226,07	242,67	1,17
Creosote	201,75	175,57	188,66	0,91
Heptane	144,77	126,31	135,54	0,65
Hexane	140,79	124,08	132,43	0,64
Pentane	138,99	118,74	128,87	0,62
Propane	109,00	101,61	105,31	0,51
Sea water	198,12	171,62	184,87	0,89
Toluene	173,19	151,16	162,18	0,78
Water	206,77	209,45	208,11	1,00
Xylene	162,42	154,47	158,44	0,76

Cumulative number of uncharged nanoparticles at the interface of ABM load tests for  $200 \times 10^3$  uncharged nanoparticles in 12 different solvents of the world with (250 x 250) patches for 72-hours at 25°C

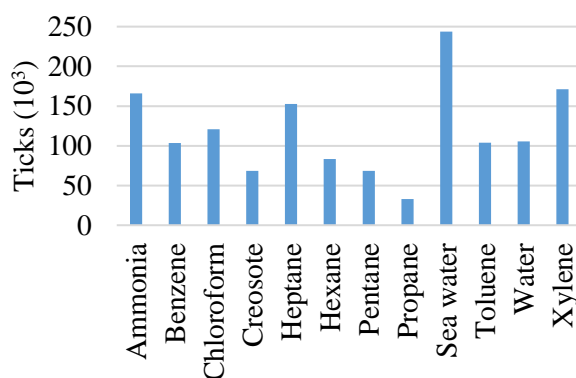
<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	193,94	189,35	191,64	1,00
Benzene	196,81	188,90	192,85	1,01
Chloroform	192,18	186,85	189,51	0,99
Creosote	192,77	188,27	190,52	0,99
Heptane	195,12	190,05	192,59	1,00
Hexane	195,81	189,97	192,89	1,01
Pentane	198,79	190,09	194,44	1,01
Propane	198,01	191,64	194,82	1,02
Sea water	192,67	188,06	190,36	0,99
Toluene	193,82	189,11	191,46	1,00
Water	195,82	188,84	192,33	1,00
Xylene	190,41	196,73	193,57	1,01

## APPENDIX 10 - ABM Load Test Results for Same-charged Nanoparticles

### APPENDIX 10.1 - ABM Load Test Results for $100 \times 10^3$ Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM load tests for  $100 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	Average ( $10^3$ )	Ratio <sup>83</sup>
Ammonia	98.39	108.48	103.43	0.60
Benzene	116.90	124.57	120.74	0.71
Chloroform	109.47	27.40	68.44	0.40
Creosote	219.22	86.13	152.68	0.89
Heptane	81.79	84.56	83.17	0.49
Hexane	72.73	63.76	68.25	0.40
Pentane	27.43	38.39	32.91	0.19
Propane	233.78	254.02	243.90	1.43
Sea water	99.76	108.26	104.01	0.61
Toluene	100.57	110.77	105.67	0.62
Water	97.72	244.44	171.08	1.00
Xylene	98.39	108.48	103.43	0.60



Comparison of average number of ticks in ABM load tests for  $100 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>83</sup> Ratio calculated with respect to water.

ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	17.46	2.95	0.87	0.47	0.10	0.03	8.97	1.53	0.45
Benzene	16.76	2.85	0.82	16.72	2.84	0.82	16.74	2.85	0.82
Chloroform	14.33	2.43	0.61	14.26	2.41	0.61	14.29	2.42	0.61
Creosote	15.17	2.58	0.70	15.23	2.59	0.70	15.20	2.59	0.70
Heptane	21.55	3.59	1.10	21.50	3.58	1.10	21.53	3.58	1.10
Hexane	23.40	3.87	1.20	17.42	2.95	0.87	20.41	3.41	1.03
Pentane	25.43	4.18	1.30	25.40	4.18	1.30	25.41	4.18	1.30
Propane	84.91	13.49	4.12	84.49	13.42	4.10	84.70	13.45	4.11
Sea water	15.50	2.64	0.72	15.45	2.63	0.72	15.48	2.63	0.72
Toluene	16.91	2.87	0.83	16.80	2.85	0.83	16.86	2.86	0.83
Water	15.70	2.67	0.74	15.76	2.69	0.74	15.73	2.68	0.74
Xylene	16.69	2.84	0.82	16.58	2.82	0.81	16.64	2.83	0.81

Distribution of ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	82.04	13.88	4.08	78.38	17.09	4.53	81.94	13.97	4.09
Benzene	82.04	13.94	4.02	82.03	13.94	4.02	82.04	13.94	4.02
Chloroform	82.48	13.99	3.54	82.50	13.97	3.54	82.49	13.98	3.54
Creosote	82.20	14.00	3.80	82.24	13.97	3.78	82.22	13.99	3.79
Heptane	82.11	13.68	4.21	82.12	13.66	4.21	82.12	13.67	4.21
Hexane	82.19	13.59	4.22	82.02	13.90	4.08	82.12	13.72	4.16
Pentane	82.25	13.53	4.22	82.24	13.55	4.21	82.24	13.54	4.22
Propane	82.82	13.15	4.02	82.83	13.15	4.02	82.83	13.15	4.02
Sea water	82.18	13.98	3.83	82.17	13.99	3.83	82.18	13.99	3.83
Toluene	82.03	13.94	4.03	82.04	13.93	4.03	82.03	13.94	4.03
Water	82.16	13.97	3.87	82.11	14.01	3.88	82.14	13.99	3.87
Xylene	82.03	13.95	4.02	82.02	13.96	4.01	82.03	13.96	4.02

ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	0.14	0.14	0.10	0.10	0.03	0.03	0.02	0.02	0.01	0.01	0.01	0.00
Benzene	4.12	4.12	4.26	4.26	0.70	0.71	0.72	0.72	0.20	0.21	0.21	0.21
Chloroform	3.52	3.51	3.64	3.65	0.60	0.60	0.61	0.61	0.15	0.15	0.15	0.16
Creosote	3.73	3.73	3.86	3.85	0.64	0.64	0.65	0.65	0.17	0.17	0.18	0.18
Heptane	5.31	5.32	5.46	5.45	0.89	0.89	0.90	0.90	0.27	0.27	0.28	0.28
Hexane	5.79	5.78	5.91	5.92	0.97	0.96	0.97	0.97	0.30	0.30	0.30	0.30
Pentane	6.30	6.29	6.42	6.42	1.04	1.04	1.05	1.05	0.33	0.32	0.33	0.33
Propane	21.15	21.15	21.30	21.31	3.37	3.36	3.38	3.38	1.03	1.03	1.03	1.03
Sea water	3.80	3.82	3.95	3.94	0.65	0.66	0.66	0.66	0.18	0.18	0.18	0.18
Toluene	3.80	3.82	3.95	3.94	0.65	0.66	0.66	0.66	0.18	0.18	0.18	0.18
Water	3.86	3.86	3.99	3.99	0.66	0.66	0.67	0.67	0.18	0.18	0.19	0.19
Xylene	4.11	4.11	4.24	4.23	0.70	0.71	0.71	0.71	0.20	0.20	0.21	0.21

Distribution of ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.61	24.63	25.40	25.36	24.83	24.88	25.18	25.11	24.73	24.87	25.19	25.22
Benzene	24.57	24.60	25.43	25.40	24.74	24.82	25.16	25.28	24.63	24.99	25.17	25.21
Chloroform	24.57	24.52	25.42	25.48	24.87	24.80	25.10	25.23	24.83	24.74	25.17	25.26
Creosote	24.58	24.58	25.43	25.40	24.82	24.86	25.16	25.16	24.90	24.82	25.16	25.12
Heptane	24.66	24.69	25.34	25.31	24.77	24.91	25.16	25.17	24.82	24.86	25.18	25.15
Hexane	24.76	24.69	25.27	25.29	24.96	24.76	25.11	25.17	24.93	24.80	25.10	25.17
Pentane	24.76	24.75	25.25	25.24	24.95	24.83	25.10	25.12	24.95	24.84	25.10	25.11
Propane	24.91	24.91	25.08	25.09	24.96	24.94	25.04	25.06	25.03	24.89	25.02	25.06
Sea water	24.52	24.62	25.46	25.40	24.76	24.84	25.20	25.19	24.81	24.86	25.22	25.12
Toluene	24.52	24.62	25.46	25.40	24.76	24.84	25.20	25.19	24.81	24.86	25.22	25.12
Water	24.60	24.61	25.41	25.38	24.77	24.89	25.19	25.14	24.81	24.95	25.11	25.13
Xylene	24.61	24.63	25.40	25.36	4.22	4.23	4.28	4.27	1.21	1.22	1.23	1.24

ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	42.85	42.96	44.24	44.19	7.32	7.35	7.45	7.41	2.15	2.15	2.19	2.18
Benzene	41.20	41.16	42.47	42.40	7.06	7.06	7.15	7.15	2.04	2.04	2.06	2.06
Chloroform	35.04	34.96	36.29	36.33	5.99	5.98	6.08	6.09	1.51	1.52	1.54	1.54
Creosote	37.43	37.41	38.71	38.75	6.43	6.41	6.52	6.52	1.75	1.74	1.76	1.76
Heptane	53.11	53.13	54.35	54.43	8.88	8.91	8.99	9.00	2.73	2.74	2.78	2.78
Hexane	42.85	42.96	44.24	44.19	7.32	7.35	7.45	7.41	2.15	2.15	2.19	2.18
Pentane	62.87	62.84	64.15	64.13	10.39	10.42	10.51	10.51	3.24	3.23	3.27	3.27
Propane	210.72	210.59	211.89	211.71	33.50	33.52	33.54	33.59	10.23	10.22	10.27	10.25
Sea water	37.98	37.95	39.26	39.30	6.53	6.53	6.62	6.63	1.79	1.79	1.81	1.81
Toluene	41.34	41.31	42.65	42.72	7.09	7.06	7.18	7.20	2.05	2.05	2.08	2.08
Water	38.70	38.79	40.04	40.06	6.65	6.68	6.79	6.76	1.85	1.85	1.88	1.87
Xylene	40.77	40.87	42.10	42.10	7.00	7.03	7.11	7.10	2.02	2.01	2.04	2.04



Distribution of ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.58	24.65	25.39	25.39	24.79	24.90	25.17	25.14	24.85	24.81	25.17	25.18
Benzene	24.63	24.62	25.40	25.35	24.84	24.84	25.17	25.15	24.84	24.89	25.15	25.12
Chloroform	24.57	24.51	25.44	25.48	24.82	24.79	25.16	25.23	24.78	24.84	25.21	25.17
Creosote	24.58	24.56	25.42	25.44	24.85	24.78	25.19	25.18	24.93	24.82	25.14	25.11
Heptane	24.70	24.71	25.28	25.31	24.83	24.90	25.12	25.14	24.77	24.85	25.16	25.21
Hexane	24.59	24.66	25.39	25.36	24.79	24.90	25.23	25.08	24.76	24.84	25.24	25.15
Pentane	24.75	24.74	25.26	25.25	24.84	24.90	25.13	25.13	24.89	24.84	25.13	25.14
Propane	24.94	24.92	25.08	25.06	24.97	24.99	25.00	25.04	24.97	24.95	25.05	25.02
Sea water	24.59	24.56	25.41	25.44	24.83	24.81	25.15	25.21	24.89	24.84	25.17	25.11
Toluene	24.61	24.59	25.39	25.42	24.86	24.74	25.17	25.24	24.82	24.78	25.15	25.25
Water	24.56	24.61	25.41	25.42	24.74	24.85	25.25	25.15	24.83	24.83	25.22	25.12
Xylene	24.58	24.65	25.39	25.39	4.22	4.24	4.29	4.28	1.22	1.21	1.23	1.23

Total number of collisions in ABM load tests for  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	21.28	4.30	1.45	0.08
Benzene	20.43	20.39	20.39	1.06
Chloroform	17.37	17.30	17.29	0.90
Creosote	18.46	18.52	18.52	0.97
Heptane	26.24	26.20	26.18	1.36
Hexane	28.47	22.49	21.58	1.12
Pentane	30.92	30.89	30.89	1.61
Propane	102.52	102.10	102.03	5.32
Sea water	18.86	18.81	18.80	0.98
Toluene	20.61	20.51	20.49	1.07
Water	19.11	19.17	19.19	1.00
Xylene	20.34	20.24	20.23	1.05

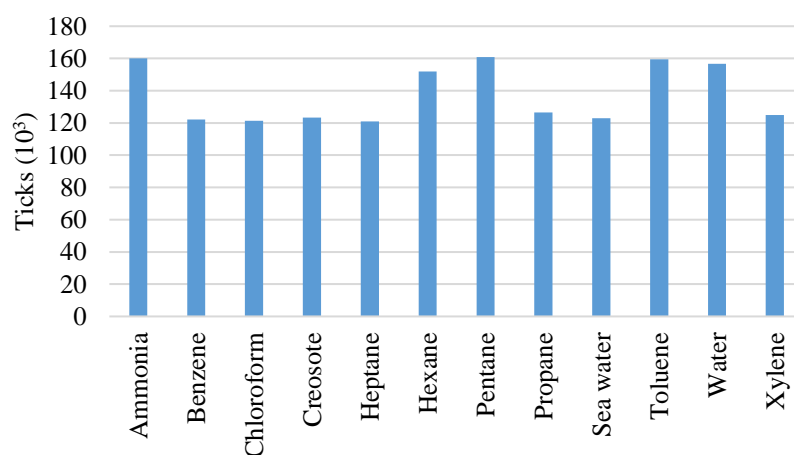
Cumulative number of same-charged nanoparticles at the interface of ABM load tests for  $100 \times 10^3$  same-charged nanoparticles in 12 different solvents of the world with (250 x 250) patches for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test</b>	<b>2<sup>nd</sup> Test</b>	<b>Average</b>	<b>Ratio</b>
Ammonia	99,533	98,985	99,259	1.01
Benzene	98,274	98,300	98,287	1.00
Chloroform	98,877	98,954	98,916	1.00
Creosote	98,674	99,232	98,953	1.00
Heptane	99,680	99,060	99,370	1.01
Hexane	99,054	99,095	99,075	1.00
Pentane	98,969	98,863	98,916	1.00
Propane	97,176	99,361	98,269	1.00
Sea water	99,293	98,179	98,736	1.00
Toluene	98,918	98,938	98,928	1.00
Water	98,678	98,760	98,719	1.00
Xylene	98,835	99,493	99,164	1.00

**APPENDIX 10.2 - ABM Load Test Results for  $200 \times 10^3$  Same-charged Nanoparticles in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C**

Total number of ticks in ABM load tests for  $200 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test	2 <sup>nd</sup> Test	Average	Ratio <sup>84</sup>
Ammonia	105.92	128.28	117.10	1.10
Benzene	110.96	87.40	99.18	0.93
Chloroform	541.56	413.12	477.34	4.49
Creosote	169.02	214.69	191.85	1.80
Heptane	88.60	118.34	103.47	0.97
Hexane	86.70	71.06	78.88	0.74
Pentane	107.49	75.43	91.46	0.86
Propane	95.50	125.72	110.61	1.04
Sea water	135.22	123.62	129.42	1.22
Toluene	112.30	81.22	96.76	0.91
Water	109.43	103.23	106.33	1.00
Xylene	97.00	121.51	109.25	1.03



Comparison of average number of ticks in ABM load tests for  $200 \times 10^3$  same-charged nanoparticles in a (250 x 250) patch world for 72-hours at 25°C

<sup>84</sup> Ratio calculated with respect to water.

ABM load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	10.51	3.47	1.08	1.01	0.35	0.11	5.76	1.91	0.60
Benzene	11.17	3.73	1.17	8.92	2.99	0.95	10.05	3.36	1.06
Chloroform	47.28	14.87	4.59	38.57	12.53	3.95	42.93	13.70	4.27
Creosote	17.09	5.79	1.86	21.25	7.12	2.27	19.17	6.45	2.07
Heptane	8.30	2.62	0.78	10.95	3.44	1.01	9.62	3.03	0.89
Hexane	7.96	2.48	0.72	6.59	2.06	0.60	7.27	2.27	0.66
Pentane	9.64	2.96	0.85	6.86	2.12	0.61	8.25	2.54	0.73
Propane	7.86	2.30	0.64	12.78	4.36	1.41	10.32	3.33	1.02
Sea water	13.86	4.72	1.52	12.78	4.36	1.41	13.32	4.54	1.47
Toluene	11.26	3.75	1.18	8.35	2.80	0.89	9.81	3.27	1.03
Water	11.33	3.86	1.25	10.73	3.66	1.19	11.03	3.76	1.22
Xylene	9.85	3.30	1.04	11.25	3.76	1.19	10.55	3.53	1.12

Distribution of ABM load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	69.77	23.06	7.18	68.70	23.59	7.71	69.67	23.10	7.22
Benzene	69.50	23.20	7.30	69.37	23.26	7.37	69.44	23.23	7.33
Chloroform	70.84	22.28	6.88	70.05	22.76	7.18	70.49	22.50	7.02
Creosote	69.07	23.40	7.53	69.35	23.24	7.41	69.23	23.31	7.46
Heptane	70.96	22.40	6.64	71.09	22.33	6.57	71.04	22.36	6.60
Hexane	71.31	22.21	6.48	71.23	22.25	6.52	71.27	22.23	6.50
Pentane	71.64	22.02	6.34	71.51	22.10	6.39	71.59	22.05	6.36
Propane	72.81	21.30	5.89	68.89	23.51	7.60	70.34	22.70	6.97
Sea water	68.96	23.47	7.57	68.89	23.51	7.60	68.93	23.49	7.58
Toluene	69.58	23.15	7.27	69.37	23.27	7.36	69.49	23.20	7.31
Water	68.92	23.48	7.59	68.88	23.51	7.61	68.90	23.50	7.60
Xylene	69.36	23.28	7.36	69.45	23.22	7.33	69.41	23.25	7.34

ABM first load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	2.64	2.64	2.62	2.62	0.87	0.88	0.86	0.86	0.27	0.27	0.27	0.27
Benzene	2.81	2.81	2.78	2.78	0.94	0.94	0.92	0.92	0.30	0.30	0.29	0.29
Chloroform	11.83	11.82	11.82	11.82	3.72	3.72	3.71	3.72	1.15	1.15	1.14	1.15
Creosote	4.28	4.28	4.26	4.26	1.45	1.45	1.44	1.44	0.47	0.47	0.46	0.46
Heptane	2.09	2.09	2.06	2.06	0.67	0.66	0.64	0.65	0.20	0.20	0.19	0.19
Hexane	2.01	2.01	1.97	1.97	0.63	0.63	0.61	0.61	0.18	0.19	0.18	0.18
Pentane	2.43	2.43	2.39	2.39	0.75	0.75	0.73	0.73	0.22	0.22	0.21	0.21
Propane	1.99	1.99	1.94	1.94	0.59	0.59	0.56	0.56	0.16	0.16	0.15	0.15
Sea water	3.48	3.48	3.45	3.45	1.19	1.19	1.17	1.17	0.38	0.38	0.38	0.38
Toluene	2.83	2.83	2.80	2.80	0.95	0.94	0.93	0.93	0.30	0.30	0.29	0.29
Water	2.84	2.84	2.82	2.82	0.97	0.97	0.96	0.96	0.32	0.31	0.31	0.31
Xylene	2.47	2.47	2.45	2.45	0.83	0.83	0.82	0.82	0.26	0.27	0.26	0.26

Distribution of ABM first load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	25.10	25.12	24.91	24.88	50.04	16.70	16.78	16.49	51.47	16.19	16.39	15.95
Benzene	25.12	25.12	24.87	24.90	49.79	16.82	16.85	16.54	51.10	16.36	16.45	16.08
Chloroform	25.01	24.99	25.00	25.00	51.46	16.19	16.19	16.17	51.92	16.05	16.05	15.98
Creosote	25.05	25.07	24.95	24.93	49.49	16.86	16.87	16.78	50.71	16.44	16.48	16.38
Heptane	25.20	25.21	24.80	24.80	51.03	16.51	16.48	15.98	52.38	16.09	16.13	15.40
Hexane	25.24	25.26	24.76	24.74	51.29	16.41	16.44	15.86	52.62	15.99	16.17	15.22
Pentane	25.21	25.20	24.79	24.80	51.69	16.26	16.25	15.80	53.03	15.86	15.89	15.22
Propane	25.34	25.33	24.64	24.69	52.76	15.98	16.01	15.25	53.79	15.74	15.74	14.73
Sea water	25.09	25.09	24.91	24.90	49.33	16.96	16.94	16.77	50.60	16.56	16.53	16.31
Toluene	25.12	25.10	24.89	24.89	49.89	16.83	16.75	16.52	51.28	16.46	16.33	15.93
Water	25.10	25.08	24.89	24.92	49.32	17.01	16.96	16.71	50.50	16.70	16.54	16.26
Xylene	25.11	25.12	24.90	24.87	49.61	16.87	16.91	16.61	50.88	16.43	16.59	16.10

ABM second load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	0.27	0.27	0.24	0.24	0.09	0.10	0.08	0.08	0.03	0.03	0.02	0.02
Benzene	2.24	2.24	2.22	2.22	0.75	0.75	0.74	0.74	0.24	0.24	0.23	0.23
Chloroform	9.64	9.64	9.64	9.64	3.13	3.14	3.13	3.13	0.99	0.99	0.99	0.99
Creosote	5.32	5.32	5.30	5.30	1.78	1.78	1.77	1.78	0.57	0.57	0.56	0.57
Heptane	2.76	2.75	2.72	2.72	0.87	0.87	0.85	0.85	0.26	0.26	0.25	0.25
Hexane	1.67	1.67	1.63	1.63	0.53	0.52	0.50	0.50	0.16	0.15	0.15	0.15
Pentane	1.73	1.74	1.69	1.69	0.54	0.54	0.52	0.52	0.16	0.16	0.15	0.15
Propane	3.20	3.20	3.18	3.19	1.10	1.09	1.08	1.09	0.36	0.35	0.35	0.35
Sea water	3.20	3.20	3.18	3.19	1.10	1.09	1.08	1.09	0.36	0.35	0.35	0.35
Toluene	2.10	2.10	2.08	2.07	0.71	0.71	0.69	0.69	0.22	0.22	0.22	0.22
Water	2.69	2.70	2.67	2.67	0.92	0.92	0.91	0.91	0.30	0.30	0.29	0.29
Xylene	2.82	2.83	2.80	2.80	0.95	0.95	0.93	0.93	0.30	0.30	0.29	0.29



Distribution of ABM second load test results for the two, three, and four-body collisions of  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	26.32	26.41	23.66	23.61	27.21	27.56	22.72	22.51	28.28	28.74	21.50	21.48
Benzene	25.15	25.12	24.85	24.89	25.24	25.18	24.77	24.81	25.41	25.28	24.58	24.74
Chloroform	25.00	25.00	24.99	25.00	25.01	25.03	24.99	24.98	24.99	25.07	24.98	24.96
Creosote	25.04	25.03	24.96	24.96	25.07	25.06	24.92	24.96	25.18	25.05	24.84	24.93
Heptane	25.18	25.16	24.82	24.85	25.32	25.26	24.66	24.76	25.51	25.49	24.41	24.59
Hexane	25.33	25.29	24.68	24.70	25.61	25.49	24.49	24.41	25.92	25.67	24.15	24.26
Pentane	25.28	25.31	24.70	24.71	25.48	25.53	24.47	24.52	25.85	25.70	24.22	24.24
Propane	25.08	25.06	24.91	24.96	25.15	25.09	24.85	24.91	25.20	25.16	24.76	24.88
Sea water	25.08	25.06	24.91	24.96	25.15	25.09	24.85	24.91	25.20	25.16	24.76	24.88
Toluene	25.15	25.15	24.88	24.82	25.27	25.25	24.74	24.74	25.36	25.40	24.59	24.64
Water	25.08	25.13	24.92	24.86	25.15	25.20	24.83	24.82	25.09	25.30	24.85	24.76
Xylene	25.09	25.11	24.88	24.91	25.21	25.22	24.78	24.79	25.27	25.40	24.64	24.69

Total number of collisions in ABM load tests for  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	15.07	1.47	8.27	0.52
Benzene	16.08	12.86	14.47	0.90
Chloroform	66.74	55.06	60.90	3.80
Creosote	24.74	30.64	27.69	1.73
Heptane	11.70	15.40	13.55	0.85
Hexane	11.16	9.25	10.20	0.64
Pentane	13.45	9.59	11.52	0.72
Propane	10.80	18.54	14.67	0.92
Sea water	20.10	18.54	19.32	1.21
Toluene	16.18	12.04	14.11	0.88
Water	16.44	15.58	16.01	1.00
Xylene	14.20	16.20	15.20	0.95

Cumulative number of same-charged nanoparticles at the interface of ABM load tests for  $200 \times 10^3$  same-charged nanoparticles in 12 different solvents of the world with (250 x 250) patches for 72-hours at 25°C

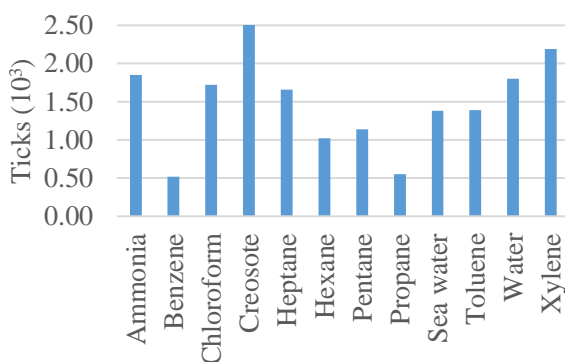
<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	13.05	1.26	7.15	1.00
Benzene	14.12	11.31	12.71	1.78
Chloroform	77.78	59.95	68.86	9.63
Creosote	23.57	29.61	26.59	3.72
Heptane	8.31	11.09	9.70	1.36
Hexane	7.24	5.83	6.53	0.91
Pentane	7.80	5.67	6.74	0.94
Propane	1.57	17.23	9.40	1.31
Sea water	18.59	17.23	17.91	2.50
Toluene	14.16	14.17	14.17	1.98
Water	14.90	14.06	14.48	2.02
Xylene	12.61	14.17	13.39	1.87

## APPENDIX 11 - ABM Load Test Results for SDS Molecules

### APPENDIX 11.1 - ABM Load Test Results for $100 \times 10^3$ SDS Molecules in 12 Different Solvents in a (250 x 250) Patch World for 72-hours at 25°C

Total number of ticks in ABM load tests for  $100 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test ( $10^3$ )	2 <sup>nd</sup> Test ( $10^3$ )	Average ( $10^3$ )	Ratio <sup>85</sup>
Ammonia	1.87	1.83	1.85	1.03
Benzene	0.53	0.52	0.52	0.29
Chloroform	0.67	2.78	1.72	0.96
Creosote	2.55	2.48	2.52	1.40
Heptane	1.67	1.64	1.66	0.92
Hexane	1.59	0.45	1.02	0.57
Pentane	0.52	1.75	1.14	0.63
Propane	0.51	0.60	0.55	0.31
Sea water	2.53	0.23	1.38	0.76
Toluene	2.01	0.77	1.39	0.77
Water	0.71	2.90	1.80	1.00
Xylene	2.08	2.30	2.19	1.21



Comparison of average number of ticks in ABM load tests for  $100 \times 10^3$  SDS molecules in a (250 x 250) patch world for 72-hours at 25°C

<sup>85</sup> Ratio calculated with respect to water.

ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )	2-Body Collisions (10 <sup>6</sup> )	3-Body Collisions (10 <sup>6</sup> )	4-Body Collisions (10 <sup>6</sup> )
Ammonia	8.60	5.56	4.06	8.42	5.44	3.96	8.51	5.50	4.01
Benzene	3.18	1.97	1.39	3.12	1.93	1.36	3.15	1.95	1.38
Chloroform	1.56	1.04	0.80	4.22	3.02	2.43	2.89	2.03	1.62
Creosote	5.42	3.84	3.05	5.25	3.72	2.94	5.34	3.78	3.00
Heptane	6.70	4.52	3.42	6.57	4.42	3.34	6.63	4.47	3.38
Hexane	1.70	1.68	1.71	2.73	1.79	1.32	2.22	1.74	1.51
Pentane	3.24	2.11	1.55	7.66	5.07	3.79	5.45	3.59	2.67
Propane	5.41	3.12	2.08	6.03	3.48	2.33	5.72	3.30	2.21
Sea water	5.78	4.08	3.22	0.03	0.02	0.07	2.90	2.05	1.64
Toluene	8.67	5.54	4.03	4.27	2.67	1.91	6.47	4.10	2.97
Water	2.50	1.67	1.27	6.88	4.85	3.81	4.69	3.26	2.54
Xylene	8.35	5.39	3.97	8.89	5.74	4.23	8.62	5.56	4.10

Distribution of ABM load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	1 <sup>st</sup> Test			2 <sup>nd</sup> Test			Average		
	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)	2-Body Collisions (%)	3-Body Collisions (%)	4-Body Collisions (%)
Ammonia	47.22	30.51	22.27	47.24	30.52	22.24	47.23	30.51	22.25
Benzene	48.61	30.11	21.28	48.68	30.08	21.24	48.65	30.10	21.26
Chloroform	45.81	30.66	23.53	43.63	31.21	25.16	44.20	31.06	24.74
Creosote	44.01	31.22	24.76	44.10	31.20	24.70	44.06	31.21	24.73
Heptane	45.76	30.89	23.35	45.83	30.86	23.31	45.80	30.87	23.33
Hexane	33.39	33.05	33.56	46.75	30.65	22.60	40.53	31.77	27.70
Pentane	46.92	30.60	22.48	46.37	30.68	22.95	46.53	30.66	22.81
Propane	51.01	29.39	19.59	50.90	29.41	19.69	50.95	29.40	19.65
Sea water	44.20	31.19	24.61	21.17	20.78	58.05	43.99	31.09	24.92
Toluene	47.53	30.36	22.11	48.25	30.18	21.57	47.76	30.30	21.94
Water	45.93	30.75	23.32	44.28	31.20	24.52	44.71	31.08	24.21
Xylene	47.17	30.42	22.40	47.12	30.44	22.44	47.15	30.43	22.42

ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	2.13	2.14	2.16	2.18	1.38	1.38	1.39	1.41	1.00	1.01	1.02	1.03
Benzene	0.79	0.79	0.80	0.80	0.49	0.49	0.49	0.50	0.35	0.34	0.35	0.35
Chloroform	0.40	0.39	0.39	0.39	0.26	0.26	0.26	0.26	0.20	0.20	0.20	0.20
Creosote	1.34	1.34	1.37	1.37	0.95	0.95	0.97	0.97	0.75	0.75	0.77	0.77
Heptane	1.68	1.65	1.66	1.72	1.13	1.11	1.12	1.16	0.86	0.84	0.85	0.88
Hexane	1.70	1.68	1.71	1.69	1.13	1.12	1.14	1.13	0.85	0.84	0.86	0.85
Pentane	0.81	0.79	0.81	0.83	0.53	0.52	0.53	0.54	0.39	0.38	0.39	0.40
Propane	1.35	1.36	1.35	1.36	0.78	0.78	0.78	0.78	0.52	0.52	0.52	0.52
Sea water	1.44	1.47	1.40	1.47	1.01	1.04	0.98	1.04	0.80	0.82	0.78	0.82
Toluene	2.22	2.15	2.16	2.14	1.42	1.38	1.38	1.37	1.03	1.00	1.00	1.00
Water	0.62	0.63	0.62	0.63	0.42	0.42	0.41	0.43	0.32	0.32	0.31	0.32
Xylene	2.09	2.08	2.07	2.12	1.34	1.34	1.33	1.37	0.99	0.99	0.98	1.01

Distribution of ABM first load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.71	24.90	25.07	25.32	24.76	24.86	25.01	25.37	24.69	24.89	25.07	25.35
Benzene	24.88	24.74	25.10	25.28	24.86	24.72	25.07	25.35	24.85	24.75	25.08	25.32
Chloroform	25.31	24.88	25.10	24.71	25.36	24.91	25.10	24.63	25.42	24.95	24.99	24.64
Creosote	24.64	24.80	25.27	25.29	24.62	24.82	25.31	25.24	24.64	24.75	25.28	25.32
Heptane	25.08	24.57	24.73	25.63	25.09	24.51	24.75	25.65	25.07	24.49	24.73	25.71
Hexane	25.08	24.83	25.21	24.89	25.07	24.84	25.19	24.89	25.03	24.81	25.23	24.93
Pentane	25.00	24.47	24.89	25.65	24.97	24.49	24.91	25.63	24.93	24.37	24.99	25.71
Propane	24.95	25.04	24.89	25.12	24.92	25.06	24.88	25.14	24.98	25.09	24.86	25.08
Sea water	24.91	25.37	24.22	25.49	24.85	25.47	24.16	25.52	24.91	25.51	24.12	25.46
Toluene	25.57	24.84	24.88	24.70	25.62	24.83	24.88	24.67	25.63	24.78	24.91	24.68
Water	24.91	25.05	24.75	25.29	24.90	25.07	24.62	25.41	24.92	25.17	24.51	25.40
Xylene	24.97	24.89	24.73	25.42	24.96	24.93	24.72	25.39	24.93	24.92	24.73	25.41

ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )	1 <sup>st</sup> Q. (10 <sup>6</sup> )	2 <sup>nd</sup> Q. (10 <sup>6</sup> )	3 <sup>rd</sup> Q. (10 <sup>6</sup> )	4 <sup>th</sup> Q. (10 <sup>6</sup> )
Ammonia	2.08	2.10	2.14	2.10	1.35	1.36	1.38	1.35	0.98	0.99	1.01	0.99
Benzene	0.77	0.78	0.78	0.79	0.48	0.49	0.48	0.49	0.34	0.34	0.34	0.34
Chloroform	1.04	1.07	1.03	1.08	0.74	0.76	0.74	0.78	0.60	0.61	0.60	0.63
Creosote	1.33	1.32	1.30	1.31	0.94	0.94	0.92	0.92	0.75	0.74	0.73	0.73
Heptane	1.61	1.65	1.65	1.66	1.08	1.11	1.11	1.12	0.82	0.84	0.84	0.85
Hexane	0.68	0.69	0.68	0.68	0.45	0.45	0.45	0.44	0.33	0.33	0.33	0.33
Pentane	1.89	1.92	1.91	1.94	1.25	1.27	1.27	1.28	0.93	0.95	0.95	0.96
Propane	1.47	1.52	1.52	1.52	0.85	0.88	0.88	0.88	0.57	0.59	0.59	0.59
Sea water	0.01	0.10	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.00	0.00
Toluene	1.07	1.07	1.06	1.07	0.67	0.67	0.67	0.67	0.48	0.48	0.48	0.48
Water	1.74	1.74	1.71	1.69	1.23	1.22	1.20	1.19	0.97	0.96	0.95	0.94
Xylene	2.26	2.16	2.25	2.21	1.46	1.40	1.45	1.43	1.08	1.03	1.07	1.06



Distribution of ABM second load test results for the two, three, and four-body collisions of  $100 \times 10^3$  SDS molecules in 12 different solvents with respect to quadrants located at a (250 x 250) patch world for 72-hours at 25°C

Solvent	Two-Body Collisions with Respect to Quadrants				Three-Body Collisions with Respect to Quadrants				Four-Body Collisions with Respect to Quadrants			
	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)	1 <sup>st</sup> Q. (%)	2 <sup>nd</sup> Q. (%)	3 <sup>rd</sup> Q. (%)	4 <sup>th</sup> Q. (%)
Ammonia	24.74	24.92	25.39	24.95	24.74	24.95	25.42	24.90	24.68	24.97	25.37	24.98
Benzene	24.76	25.03	25.00	25.21	24.76	25.14	24.92	25.18	24.74	25.13	24.92	25.20
Chloroform	24.60	25.28	24.42	25.69	24.56	25.24	24.47	25.73	24.49	25.25	24.49	25.77
Creosote	25.25	25.07	24.83	24.84	25.28	25.16	24.76	24.81	25.38	25.12	24.74	24.76
Heptane	24.53	25.13	25.05	25.30	24.53	25.12	25.06	25.29	24.47	25.14	25.06	25.32
Hexane	24.96	25.35	24.94	24.75	25.02	25.33	24.94	24.71	24.95	25.34	24.94	24.77
Pentane	24.63	25.10	24.97	25.30	24.63	25.06	25.01	25.31	24.61	25.05	25.02	25.32
Propane	24.41	25.16	25.17	25.26	24.40	25.16	25.13	25.31	24.36	25.13	25.18	25.33
Sea water	4.02	70.58	12.66	12.74	38.55	38.00	11.95	11.49	40.82	38.75	10.78	9.65
Toluene	25.07	25.02	24.90	25.01	25.02	24.97	24.96	25.06	25.06	24.96	24.99	24.99
Water	25.34	25.27	24.79	24.60	25.37	25.25	24.78	24.60	25.36	25.30	24.80	24.54
Xylene	25.44	24.34	25.30	24.92	25.49	24.30	25.30	24.91	25.47	24.21	25.35	24.96

Total number of collisions in ABM load tests for  $100 \times 10^3$  SDS molecules in 12 different solvents located at a (250 x 250) patch world for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>6</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>6</sup>)</b>	<b>Average (10<sup>6</sup>)</b>	<b>Ratio</b>
Ammonia	18.21	17.83	18.02	1.72
Benzene	6.53	6.42	6.47	0.62
Chloroform	3.41	9.66	6.54	0.62
Creosote	12.31	11.91	12.11	1.15
Heptane	14.64	14.33	14.49	1.38
Hexane	5.09	5.84	5.47	0.52
Pentane	6.90	16.52	11.71	1.12
Propane	10.61	11.84	11.23	1.07
Sea water	13.07	0.12	6.59	0.63
Toluene	18.24	8.84	13.54	1.29
Water	5.45	15.54	10.49	1.00
Xylene	17.71	18.86	18.29	1.74

Cumulative number of SDS molecules at the interface of ABM load tests for  $100 \times 10^3$  SDS molecules in 12 different solvents of the world with (250 x 250) patches for 72-hours at 25°C

<b>Solvent</b>	<b>1<sup>st</sup> Test (10<sup>3</sup>)</b>	<b>2<sup>nd</sup> Test (10<sup>3</sup>)</b>	<b>Average (10<sup>3</sup>)</b>	<b>Ratio</b>
Ammonia	196	159	178	2.73
Benzene	142	114	128	1.97
Chloroform	78	74	76	1.17
Creosote	63	65	64	0.98
Heptane	199	85	142	2.18
Hexane	193	83	138	2.12
Pentane	138	86	112	1.72
Propane	316	230	273	4.20
Sea water	99	62	81	1.24
Toluene	190	87	139	2.13
Water	76	54	65	1.00
Xylene	160	151	156	2.39

## APPENDIX 12 - The Inventory of Experiments Held at Hacettepe University Environmental Engineering Research Laboratory

1. Experiments with DI
  - $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 60^\circ$
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
  - 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
  - 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles,  $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
2. Experiments with chloroform
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 60$
  - 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
  - 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 60^\circ$
3. Experiments with methanol
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 60^\circ$
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 60^\circ$
4. Experiments with cement factory wastewater treatment plant water
  - Input water with 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
  - Input water with 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
  - Output water with 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
  - Output water with 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$ ,  $\alpha = 30^\circ$
5. Experiments with Eymir Lake water
  - 3 mg/ml SDS,  $\alpha = 30^\circ$
  - 3 mg/ml SDS,  $\alpha = 60^\circ$
  - 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles,  $\alpha = 30^\circ$
  - 3 mg/ml SDS, 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles,  $\alpha = 60^\circ$

**APPENDIX 13 - Surface Tension Experiments with MWCNT and Graphene at HUATARC**

**APPENDIX 13.1 - Surface Tension Measurement Results for DI+SDS+Graphene (0.82 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (0.82 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	50.35	50.94	49.31	50.20	4.05	3.93	3.95	3.97
0.01	50.15	50.62	49.36	50.04	4.05	3.93	3.94	3.97
0.03	50.14	50.96	49.47	50.19	4.05	3.93	3.94	3.97
0.04	50.25	50.66	49.40	50.11	4.05	3.93	3.94	3.97
0.05	50.00	50.68	49.24	49.97	4.05	3.93	3.94	3.97
0.07	50.01	50.45	49.27	49.91	4.05	3.93	3.94	3.97
0.09	49.97	50.35	49.17	49.83	4.05	3.93	3.93	3.97
0.12	50.02	50.33	49.21	49.85	4.05	3.93	3.94	3.97
0.13	50.06	50.28	49.07	49.80	4.04	3.93	3.94	3.97
0.14	49.87	50.32	49.04	49.74	4.05	3.93	3.94	3.97
0.16	49.88	49.96	49.09	49.64	4.05	3.93	3.94	3.97
0.18	49.75	50.01	48.89	49.55	4.05	3.93	3.93	3.97
0.20	49.75	50.34	49.04	49.71	4.05	3.93	3.94	3.97
0.21	49.77	49.87	49.00	49.55	4.04	3.93	3.93	3.97
0.20	49.75	50.34	49.04	49.71	4.05	3.93	3.94	3.97
0.22	49.78	50.00	48.89	49.56	4.04	3.93	3.93	3.97
0.24	48.67	49.62	48.90	49.07	4.06	3.93	3.94	3.97
0.25	49.78	50.03	48.86	49.55	4.04	3.93	3.94	3.97
0.26	49.65	49.67	48.82	49.38	4.04	3.93	3.94	3.97
0.28	49.55	49.71	48.77	49.35	4.04	3.93	3.94	3.97
0.28	49.55	49.71	48.77	49.35	4.04	3.93	3.94	3.97
0.29	49.56	49.64	48.81	49.34	4.04	3.93	3.93	3.97
0.30	49.57	49.57	48.78	49.31	4.04	3.93	3.94	3.97
0.32	49.54	49.51	48.74	49.27	4.04	3.93	3.93	3.97
0.34	49.57	49.51	48.65	49.24	4.04	3.93	3.93	3.97
0.38	49.43	49.58	48.63	49.21	4.04	3.93	3.94	3.97
0.40	49.43	49.16	48.54	49.04	4.04	3.92	3.93	3.97
0.41	49.29	49.25	48.39	48.98	4.04	3.92	3.94	3.97

continued on the next page,

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.43	49.38	49.32	48.37	49.03	4.04	3.92	3.94	3.97
0.45	49.34	49.00	48.38	48.91	4.04	3.92	3.93	3.97
0.46	49.25	48.98	48.35	48.86	4.04	3.92	3.93	3.97
0.47	49.22	48.88	48.42	48.84	4.04	3.92	3.93	3.97
0.49	49.35	49.14	48.35	48.95	4.04	3.92	3.93	3.97
0.50	49.32	48.67	48.31	48.77	4.04	3.92	3.94	3.97
0.51	49.27	49.05	48.26	48.86	4.04	3.92	3.93	3.97
0.53	49.33	48.65	48.16	48.72	4.04	3.92	3.93	3.96
0.54	49.14	48.97	48.15	48.75	4.04	3.92	3.93	3.97
0.55	49.16	48.61	48.08	48.62	4.04	3.92	3.94	3.97
0.57	49.17	48.82	48.15	48.72	4.04	3.92	3.94	3.97
0.58	49.19	48.47	48.12	48.59	4.04	3.91	3.93	3.96
0.59	49.16	48.49	48.12	48.59	4.04	3.92	3.94	3.97
0.61	49.10	48.63	48.19	48.64	4.04	3.92	3.94	3.97
0.62	49.10	48.60	47.98	48.56	4.04	3.92	3.93	3.96
0.65	49.04	48.48	47.88	48.47	4.04	3.92	3.93	3.96
0.66	49.02	48.29	48.02	48.44	4.04	3.92	3.93	3.96
0.67	49.10	48.34	47.89	48.44	4.04	3.92	3.93	3.96
0.68	48.94	48.20	47.95	48.36	4.04	3.92	3.93	3.96
0.70	48.93	48.38	47.94	48.42	4.04	3.92	3.93	3.96
0.71	48.97	48.17	47.75	48.30	4.04	3.92	3.93	3.96
0.72	48.92	48.31	47.76	48.33	4.04	3.92	3.93	3.96
0.74	48.80	48.32	47.76	48.29	4.04	3.92	3.93	3.96
0.75	48.89	48.13	47.85	48.29	4.04	3.92	3.93	3.96
0.76	48.73	48.08	47.85	48.22	4.04	3.92	3.94	3.96
0.78	48.72	48.15	47.84	48.23	4.03	3.92	3.93	3.96
0.79	48.78	48.21	47.82	48.27	4.04	3.92	3.93	3.96
0.82	48.81	48.17	47.82	48.71	4.04	3.92	3.93	3.96
0.83	48.64	48.11	47.66	48.14	4.03	3.92	3.93	3.96
0.84	48.79	48.02	47.61	48.14	4.04	3.92	3.93	3.96
0.86	48.68	47.84	47.52	48.01	4.03	3.92	3.93	3.96
0.87	48.62	47.92	47.73	48.09	4.03	3.92	3.93	3.96
0.88	48.64	48.02	47.73	48.13	4.03	3.92	3.94	3.96
0.90	48.57	47.76	47.50	47.94	4.03	3.92	3.93	3.96
0.88	48.64	48.02	47.73	48.13	4.03	3.92	3.94	3.96
0.91	48.62	47.96	47.37	47.99	4.03	3.92	3.93	3.96
0.92	48.40	47.72	47.52	47.88	4.03	3.92	3.93	3.96

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.95	48.48	47.65	47.29	47.81	4.03	3.92	3.93	3.96
0.96	48.34	47.71	47.47	47.84	4.03	3.92	3.93	3.96
0.97	48.56	47.79	47.60	47.98	4.03	3.91	3.93	3.96
0.99	48.32	47.54	47.38	47.75	4.03	3.92	3.93	3.96
1.00	48.32	47.62	47.24	47.73	4.03	3.92	3.93	3.96
1.01	48.36	47.56	47.33	47.75	4.03	3.91	3.93	3.96
1.03	48.28	47.48	47.32	47.69	4.03	3.91	3.93	3.96
1.04	48.36	47.49	47.07	47.64	4.03	3.91	3.93	3.96
1.05	48.04	47.52	47.40	47.65	4.03	3.91	3.93	3.96
1.07	48.37	47.57	47.48	47.81	4.03	3.91	3.94	3.96
1.08	48.09	47.42	47.28	47.60	4.03	3.91	3.93	3.96
1.09	48.09	47.47	47.16	47.57	4.03	3.91	3.93	3.96
1.11	48.21	47.32	47.02	47.52	4.03	3.91	4.50	4.15
1.12	48.19	47.35	47.14	47.56	4.03	3.91	3.93	3.96
1.13	48.10	47.33	46.97	47.47	4.03	3.91	3.93	3.96
1.15	48.02	47.30	47.12	47.48	4.03	3.91	3.93	3.96
1.16	48.04	47.27	47.28	47.53	4.03	3.91	3.93	3.96
1.17	47.91	47.18	47.25	47.45	4.03	3.91	3.93	3.96
1.19	47.85	47.35	47.11	47.44	4.03	3.91	3.93	3.96
1.20	47.89	47.14	47.00	47.34	4.03	3.91	3.93	3.96
1.21	47.90	47.04	47.01	47.32	4.03	3.91	3.93	3.96
1.21	47.90	47.04	47.01	47.32	4.03	3.91	3.93	3.96
1.22	47.94	47.13	46.88	47.32	4.03	3.91	3.92	3.95
1.24	47.71	47.08	47.00	47.26	4.03	3.91	3.93	3.96
1.26	47.81	47.00	47.09	47.30	4.46	3.91	3.93	4.10
1.28	47.42	46.97	46.96	47.12	4.64	3.91	3.93	4.16
1.29	47.66	46.79	46.85	47.10	4.64	3.91	3.93	4.16
1.30	47.76	46.96	46.80	47.17	4.03	3.91	3.93	3.96
1.32	47.52	47.00	46.82	47.11	4.03	3.91	3.93	3.96
1.33	47.66	46.86	46.78	47.10	4.03	3.91	3.92	3.95
1.34	47.63	46.79	46.90	47.11	4.03	3.91	3.93	3.96
1.36	47.32	46.86	46.97	47.05	4.03	3.91	3.93	3.96
1.37	47.50	46.79	46.98	47.09	4.03	3.91	3.92	3.95
1.38	47.53	46.64	46.69	46.95	4.03	3.91	3.93	3.95
1.40	47.37	46.81	46.62	46.93	4.03	3.91	3.93	3.95
1.42	47.56	46.59	46.62	46.85	4.03	3.91	3.93	3.94
1.44	47.47	46.69	46.62	46.93	4.03	3.91	3.93	3.95

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.49	47.12	46.59	46.50	46.73	4.63	3.91	3.92	4.15
1.50	47.24	46.44	46.63	46.77	4.03	3.91	3.93	3.95
1.51	47.19	46.34	46.59	46.71	4.03	3.91	3.93	3.95
1.53	47.19	46.49	46.52	46.73	4.03	3.91	3.93	3.95
1.54	47.06	46.43	46.63	46.71	4.63	3.91	3.93	4.15
1.55	47.22	46.36	46.79	46.79	4.03	3.91	3.93	3.95
1.57	47.15	46.23	46.43	46.60	4.03	3.91	3.93	3.95
1.58	47.10	46.40	46.39	46.63	4.03	3.91	3.92	3.95
1.61	47.09	46.11	46.47	46.56	4.03	3.91	3.93	3.95
1.62	47.04	46.40	46.31	46.58	4.02	3.90	3.93	3.95
1.63	46.93	46.04	46.43	46.47	4.02	3.91	3.92	3.95
1.65	46.87	46.08	46.64	46.53	4.63	3.91	3.93	4.15
1.66	47.03	46.24	46.33	46.53	4.02	3.90	3.93	3.95
1.67	46.84	45.97	46.22	46.34	4.02	3.91	3.92	3.95
1.69	46.86	46.05	46.40	46.44	4.02	3.91	3.92	3.95
1.70	46.96	45.97	46.38	46.44	4.02	3.90	3.92	3.95
1.71	46.78	45.87	46.20	46.28	4.02	3.90	3.93	3.95
1.73	46.81	45.90	46.21	46.31	4.02	3.91	3.92	3.95
1.75	46.62	45.91	46.29	46.27	4.02	3.90	3.93	3.95
1.76	46.79	45.80	46.22	46.27	4.02	3.90	3.92	3.95
1.78	46.89	45.80	46.26	46.32	4.02	3.90	3.92	3.95
1.79	46.53	45.85	46.15	46.18	4.02	3.90	3.93	3.95
1.80	46.66	45.66	46.18	46.17	4.02	3.90	3.93	3.95
1.82	46.63	45.71	45.96	46.10	4.02	3.90	4.49	4.14
1.83	46.57	45.72	46.10	46.13	4.02	3.90	3.92	3.95
1.84	46.68	45.60	46.09	46.12	4.02	3.90	3.92	3.95
1.86	46.56	45.60	46.05	46.07	4.02	3.90	3.92	3.95
1.87	46.41	45.72	45.99	46.04	4.01	3.90	3.92	3.94
1.88	46.77	45.46	45.99	46.07	4.02	3.90	3.93	3.95
1.90	45.92	45.50	46.04	45.82	4.02	3.90	3.92	3.95
1.91	46.24	45.56	45.98	45.93	4.02	3.90	3.92	3.95
1.92	47.15	45.46	45.88	46.16	4.02	3.90	3.93	3.95
1.94	45.91	45.41	45.91	45.74	4.62	3.90	3.92	4.15
1.95	46.25	45.49	46.01	45.92	4.02	3.90	3.93	3.95
1.96	46.22	45.46	45.78	45.82	4.02	3.90	4.49	4.14
1.98	46.08	45.32	45.71	45.70	4.02	3.90	3.92	3.95
1.99	46.51	45.27	45.80	45.86	4.02	3.90	3.92	3.95

**APPENDIX 13.2 - Surface Tension Measurement Results for DI+SDS+Graphene (3 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (3.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	22.71	21.43	21.56	21.90	4.15	3.96	3.84	3.98
0.01	22.70	21.41	21.56	21.89	4.15	3.91	3.84	3.97
0.03	22.71	21.41	21.56	21.90	4.20	3.95	3.80	3.98
0.04	22.70	21.42	21.55	21.89	4.15	3.91	3.84	3.97
0.05	22.71	21.42	21.55	21.89	4.27	4.02	3.85	4.05
0.07	22.69	21.44	21.55	21.89	4.15	3.91	3.84	3.97
0.08	22.68	21.42	21.54	21.88	4.15	3.95	3.85	3.98
0.09	22.67	21.43	21.56	21.88	4.15	3.91	3.84	3.97
0.11	22.69	21.43	21.57	21.89	4.15	3.96	3.84	3.99
0.12	22.67	21.42	21.57	21.89	4.16	3.96	3.84	3.99
0.13	22.67	21.41	21.56	21.88	4.20	3.96	3.84	4.00
0.14	22.68	21.41	21.56	21.89	4.15	3.91	3.84	3.97
0.16	22.68	21.40	21.56	21.88	4.15	3.95	3.84	3.98
0.17	22.66	21.41	21.54	21.87	4.16	3.96	3.81	3.97
0.18	22.67	21.42	21.55	21.88	4.15	3.95	3.84	3.98
0.20	22.67	21.42	21.55	21.88	4.15	3.91	3.84	3.97
0.21	22.65	21.43	21.54	21.88	4.20	3.91	3.80	3.97
0.22	22.65	21.44	21.56	21.89	4.20	3.90	3.84	3.98
0.24	22.65	21.42	21.56	21.88	4.15	3.91	3.84	3.97
0.25	22.64	21.42	21.57	21.88	4.20	3.91	3.84	3.98
0.28	22.66	21.41	21.56	21.88	4.21	4.02	3.84	4.02
0.29	22.67	21.43	21.55	21.88	4.21	3.91	3.84	3.99
0.30	22.67	21.43	21.52	21.87	4.20	4.02	3.84	4.02
0.32	22.67	21.42	21.53	21.87	4.11	4.02	3.84	3.99
0.33	22.64	21.43	21.53	21.87	4.15	3.90	3.80	3.95
0.34	22.66	21.42	21.56	21.88	4.21	3.95	3.84	4.00
0.38	22.66	21.41	21.56	21.88	4.15	3.91	3.80	3.95
0.40	22.68	21.41	21.56	21.88	4.15	3.95	3.81	3.97
0.38	22.66	21.41	21.56	21.88	4.15	3.91	3.80	3.95
0.42	22.66	21.42	21.51	21.86	4.15	3.90	3.84	3.97
0.43	22.66	21.44	21.53	21.88	4.15	3.95	3.84	3.98
0.45	22.64	21.43	21.54	21.87	4.15	4.02	3.84	4.00

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	22.66	21.41	21.54	21.87	4.15	3.95	3.80	3.97
0.49	22.65	21.41	21.56	21.87	4.15	4.02	3.80	3.99
0.50	22.67	21.41	21.56	21.88	4.15	3.95	3.84	3.98
0.51	22.67	21.42	21.54	21.88	4.15	3.95	3.85	3.98
0.53	22.65	21.43	21.53	21.87	4.20	4.02	3.84	4.02
0.54	22.64	21.42	21.53	21.86	4.15	3.95	3.84	3.98
0.57	22.62	21.42	21.56	21.87	4.15	3.90	3.84	3.97
0.58	22.64	21.42	21.56	21.87	4.20	4.02	3.80	4.01
0.59	22.63	21.41	21.55	21.86	4.14	3.95	3.84	3.98
0.61	22.64	21.42	21.57	21.88	4.14	4.02	3.84	4.00
0.62	22.64	21.43	21.56	21.87	4.10	3.91	3.80	3.94
0.63	22.62	21.42	21.55	21.86	4.15	3.95	3.80	3.97
0.65	22.62	21.43	21.52	21.86	4.14	4.02	3.84	4.00
0.66	22.63	21.42	21.53	21.86	4.14	3.95	3.84	3.98
0.67	22.61	21.42	21.55	21.86	4.14	3.95	3.84	3.98
0.68	22.62	21.42	21.57	21.87	4.20	3.96	3.85	4.00
0.70	22.63	21.42	21.57	21.87	4.14	3.95	3.80	3.97
0.71	22.63	21.42	21.57	21.87	4.14	3.90	3.84	3.96
0.72	22.63	21.43	21.56	21.87	4.14	3.96	3.84	3.98
0.74	22.63	21.41	21.56	21.87	4.14	4.02	3.80	3.99
0.75	22.63	21.42	21.53	21.86	4.14	4.02	3.84	4.00
0.76	22.61	21.43	21.53	21.86	4.14	3.95	3.80	3.97
0.78	22.62	21.42	21.55	21.86	4.14	3.96	3.84	3.98
0.79	22.61	21.42	21.56	21.86	4.14	4.02	3.84	4.00
0.80	22.63	21.42	21.56	21.87	4.14	3.96	3.84	3.98
0.82	22.63	21.41	21.55	21.86	4.14	3.95	3.84	3.98
0.83	22.64	21.42	21.56	21.87	4.14	4.02	3.84	4.00
0.78	22.62	21.42	21.55	21.86	4.14	3.96	3.84	3.98
0.84	22.64	21.42	21.56	21.87	4.14	3.96	3.84	3.98
0.86	22.63	21.42	21.57	21.87	4.14	4.02	3.84	4.00
0.87	22.63	21.43	21.55	21.87	4.14	4.02	3.84	4.00
0.88	22.62	21.42	21.55	21.86	4.14	3.95	3.84	3.98
0.90	22.60	21.42	21.55	21.86	4.19	4.02	3.84	4.02
0.92	22.61	21.42	21.56	21.86	4.14	3.96	3.84	3.98
0.94	22.61	21.42	21.55	21.86	4.14	4.02	3.84	4.00
0.95	22.62	21.43	21.56	21.87	4.19	3.95	3.84	4.00
0.96	22.61	21.43	21.56	21.86	4.14	4.02	3.84	4.00

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	22.59	21.43	21.53	21.85	4.19	3.96	3.84	4.00
1.00	22.60	21.43	21.53	21.85	4.19	4.02	3.84	4.02
1.01	22.60	21.43	21.54	21.86	4.10	4.02	3.84	3.99
1.03	22.59	21.42	21.55	21.85	4.19	3.90	3.84	3.98
1.04	22.59	21.42	21.55	21.85	4.10	3.96	3.81	3.95
1.05	22.57	21.43	21.55	21.85	4.14	3.96	3.80	3.97
1.07	22.60	21.42	21.55	21.85	4.10	3.91	3.84	3.95
1.08	22.59	21.42	21.55	21.85	4.14	3.96	3.84	3.98
1.09	22.60	21.43	21.54	21.86	4.14	3.96	3.84	3.98
1.11	22.59	21.42	21.52	21.85	4.10	3.96	3.84	3.97
1.12	22.59	21.43	21.53	21.85	4.14	4.02	3.84	4.00
1.15	22.59	21.43	21.56	21.86	4.14	4.02	3.84	4.00
1.16	22.58	21.42	21.56	21.85	4.14	3.95	3.84	3.97
1.17	22.60	21.42	21.56	21.86	4.14	4.02	3.84	4.00
1.19	22.59	21.42	21.56	21.86	4.14	4.02	3.84	4.00
1.20	22.59	21.42	21.55	21.85	4.14	4.02	3.84	4.00
1.21	22.59	21.43	21.53	21.85	4.14	4.02	3.84	4.00
1.22	22.59	21.43	21.54	21.85	4.14	4.02	3.84	4.00
1.24	22.59	21.43	21.54	21.85	4.14	3.96	3.84	3.98
1.25	22.58	21.42	21.55	21.85	4.14	3.96	3.80	3.97
1.26	22.59	21.43	21.55	21.86	4.14	4.02	3.84	4.00
1.28	22.59	21.41	21.54	21.85	4.14	3.95	3.80	3.96
1.30	22.60	21.41	21.55	21.85	4.13	4.02	3.84	4.00
1.32	22.59	21.41	21.55	21.85	4.14	3.90	3.84	3.96
1.33	22.59	21.42	21.53	21.85	4.09	4.02	3.84	3.98
1.34	22.59	21.43	21.54	21.85	4.09	4.02	3.84	3.98
1.36	22.57	21.43	21.55	21.85	4.09	4.02	3.84	3.98
1.37	22.57	21.44	21.55	21.85	4.13	4.02	3.80	3.98
1.38	22.59	21.44	21.55	21.86	4.13	4.02	3.84	4.00
1.40	22.57	21.42	21.55	21.85	4.09	4.02	3.84	3.98
1.41	22.58	21.41	21.54	21.84	4.14	4.02	3.84	4.00
1.41	22.58	21.41	21.54	21.84	4.14	4.02	3.84	4.00
1.42	22.57	21.43	21.55	21.85	4.13	4.02	3.84	4.00
1.44	22.57	21.42	21.54	21.84	4.09	4.02	3.84	3.98
1.45	22.56	21.41	21.54	21.84	4.13	4.02	3.84	4.00
1.46	22.57	21.43	21.54	21.84	4.13	4.02	3.84	4.00
1.48	22.57	21.44	21.53	21.84	4.09	4.02	3.84	3.98

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	22.55	21.43	21.54	21.84	4.13	4.02	3.84	4.00
1.51	22.56	21.44	21.55	21.85	4.13	3.96	3.84	3.98
1.53	22.56	21.43	21.55	21.85	4.13	4.02	3.84	4.00
1.54	22.56	21.42	21.54	21.84	4.13	4.02	3.84	4.00
1.55	22.56	21.42	21.53	21.84	4.13	4.02	3.84	4.00
1.58	22.55	21.43	21.53	21.84	4.13	4.02	3.84	4.00
1.59	22.55	21.43	21.54	21.84	4.13	3.96	3.81	3.96
1.61	22.55	21.43	21.54	21.84	4.13	4.02	3.84	4.00
1.62	22.55	21.42	21.54	21.84	4.13	3.95	3.84	3.97
1.63	22.57	21.43	21.55	21.85	4.13	4.02	3.84	4.00
1.65	22.55	21.43	21.54	21.84	4.13	3.96	3.84	3.98
1.66	22.56	21.43	21.54	21.85	4.13	3.96	3.84	3.98
1.67	22.55	21.43	21.53	21.84	4.13	4.02	3.84	4.00
1.69	22.55	21.42	21.53	21.83	4.13	3.96	3.84	3.98
1.70	22.55	21.42	21.53	21.83	4.13	3.96	3.84	3.98
1.71	22.54	21.43	21.55	21.84	4.08	4.02	3.84	3.98
1.73	22.56	21.42	21.55	21.84	4.13	4.02	3.84	4.00
1.74	22.56	21.41	21.55	21.84	4.08	4.02	3.84	3.98
1.75	22.57	21.43	21.54	21.85	4.08	3.96	3.84	3.96
1.76	22.56	21.43	21.55	21.85	4.08	3.96	3.80	3.95
1.78	22.56	21.44	21.54	21.85	4.13	3.96	3.80	3.96
1.79	22.56	21.43	21.53	21.84	4.12	3.96	3.84	3.97
1.80	22.56	21.44	21.54	21.84	4.08	3.96	3.84	3.96
1.82	22.54	21.42	21.54	21.83	4.12	3.96	3.84	3.97
1.84	22.54	21.42	21.54	21.83	4.12	4.02	3.84	3.99
1.86	22.56	21.42	21.55	21.84	4.08	3.96	3.84	3.96
1.87	22.55	21.43	21.54	21.84	4.12	4.02	3.80	3.98
1.88	22.54	21.44	21.54	21.84	4.08	4.02	3.84	3.98
1.90	22.55	21.43	21.53	21.84	4.08	4.02	3.80	3.97
1.91	22.54	21.43	21.54	21.84	4.12	4.02	3.84	3.99
1.92	22.53	21.42	21.55	21.83	4.13	3.96	3.84	3.98
1.94	22.53	21.42	21.54	21.83	4.08	4.02	3.84	3.98
1.95	22.54	21.43	21.53	21.83	4.13	3.96	3.80	3.96
1.96	22.52	21.42	21.55	21.83	4.12	4.02	3.84	3.99
1.98	22.53	21.43	21.55	21.84	4.13	3.96	3.84	3.98
1.99	22.52	21.40	21.55	21.82	4.12	3.95	3.80	3.96

**APPENDIX 13.3 - Surface Tension Measurement Results for DI+SDS+Graphene (6 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (6.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	26.38	25.10	24.22	25.24	3.89	3.97	4.50	4.12
0.01	26.43	25.11	24.20	25.25	3.89	3.97	4.57	4.14
0.03	26.41	25.08	24.20	25.23	3.89	3.97	4.57	4.14
0.04	26.42	25.05	24.20	25.22	3.89	3.97	4.64	4.17
0.05	26.40	25.05	24.22	25.22	3.89	3.97	4.50	4.12
0.07	26.44	25.06	24.20	25.23	3.89	3.97	4.49	4.12
0.08	26.41	25.07	24.20	25.23	3.89	3.97	4.56	4.14
0.09	26.37	25.06	24.21	25.21	3.89	3.97	4.65	4.17
0.11	26.34	25.07	24.21	25.20	3.89	3.97	4.57	4.14
0.12	26.40	25.07	24.21	25.22	3.89	3.97	4.56	4.14
0.13	26.37	25.06	24.20	25.21	3.89	3.97	4.65	4.17
0.14	26.29	25.02	24.21	25.18	3.89	3.97	4.56	4.14
0.16	26.37	25.03	24.20	25.20	3.89	3.97	4.50	4.12
0.17	26.35	25.04	24.19	25.19	3.89	3.97	4.56	4.14
0.18	26.36	25.04	24.18	25.19	3.89	3.97	4.56	4.14
0.20	26.32	25.06	24.19	25.19	3.89	3.97	4.65	4.17
0.21	26.34	25.05	24.17	25.18	3.89	3.97	4.56	4.14
0.22	26.24	25.05	24.18	25.16	3.89	3.97	4.56	4.14
0.24	26.22	25.05	24.18	25.15	3.89	3.97	4.56	4.14
0.25	26.31	25.05	24.18	25.18	3.89	3.97	4.56	4.14
0.28	26.30	25.01	24.18	25.16	3.89	3.97	4.56	4.14
0.29	26.28	24.99	24.16	25.14	3.89	3.97	4.56	4.14
0.30	26.28	25.03	24.17	25.16	3.89	3.97	4.56	4.14
0.32	26.27	25.02	24.16	25.15	3.89	3.97	4.56	4.14
0.33	26.29	25.03	24.18	25.17	3.89	3.97	4.56	4.14
0.34	26.25	25.03	24.19	25.15	3.89	3.97	4.56	4.14
0.37	26.17	25.03	24.18	25.13	3.89	3.97	4.64	4.17
0.38	26.21	24.98	24.18	25.12	3.89	3.97	4.56	4.14
0.41	26.23	25.00	24.15	25.13	3.89	3.97	4.55	4.14
0.42	26.18	25.01	24.17	25.12	3.89	3.97	4.56	4.14
0.43	26.18	25.01	24.16	25.12	3.89	3.97	4.57	4.14
0.45	26.19	25.02	24.14	25.12	3.89	3.97	4.56	4.14

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
P0.47	26.13	24.98	24.14	25.08	3.89	3.97	4.56	4.14
0.49	26.14	24.96	24.13	25.08	3.89	3.97	4.56	4.14
0.50	26.14	24.95	24.13	25.07	3.89	3.97	4.56	4.14
0.51	26.09	24.98	24.13	25.07	3.89	3.97	4.56	4.14
0.53	26.11	24.99	24.13	25.07	3.89	3.97	4.56	4.14
0.54	25.98	25.01	24.13	25.04	3.89	3.97	4.56	4.14
0.55	26.11	24.99	24.13	25.07	3.89	3.97	4.56	4.14
0.57	25.95	25.00	24.14	25.03	3.89	3.97	4.56	4.14
0.58	26.03	24.98	24.14	25.05	3.89	3.97	4.55	4.14
0.59	26.00	24.96	24.14	25.03	3.89	3.97	4.56	4.14
0.61	25.95	24.95	24.13	25.01	3.89	4.01	4.56	4.15
0.62	26.04	24.95	24.14	25.04	3.89	3.97	4.56	4.14
0.63	26.05	24.98	24.15	25.06	3.89	4.01	4.48	4.13
0.65	26.04	24.97	24.12	25.04	3.89	3.97	4.56	4.14
0.66	25.95	24.95	24.12	25.01	3.89	4.01	4.64	4.18
0.68	25.99	24.95	24.12	25.02	3.89	3.97	4.64	4.17
0.70	25.92	24.94	24.10	24.99	3.89	3.97	4.55	4.14
0.71	25.90	24.93	24.10	24.97	3.89	3.97	4.55	4.14
0.72	25.90	24.95	24.12	24.99	3.89	3.97	4.55	4.14
0.74	26.00	24.95	24.09	25.01	3.89	3.97	4.65	4.17
0.75	25.89	24.92	24.09	24.96	3.89	3.91	4.55	4.12
0.76	25.89	24.91	24.11	24.97	3.89	3.91	4.55	4.12
0.78	25.91	24.90	24.08	24.96	3.89	3.97	4.65	4.17
0.79	25.96	24.90	24.08	24.98	3.89	3.91	4.55	4.12
0.80	25.90	24.90	24.10	24.97	3.89	3.91	4.55	4.12
0.82	25.87	24.90	24.11	24.96	3.89	3.97	4.55	4.14
0.84	25.89	24.93	24.09	24.97	3.89	3.97	4.55	4.14
0.86	25.91	24.93	24.11	24.98	3.89	3.91	4.55	4.12
0.87	25.84	24.90	24.09	24.94	3.89	3.91	4.56	4.12
0.88	25.81	24.87	24.09	24.92	3.89	3.91	4.48	4.09
0.87	25.84	24.90	24.09	24.94	3.89	3.91	4.56	4.12
0.90	25.87	24.88	24.08	24.95	3.89	3.91	4.54	4.11
0.91	25.90	24.87	24.11	24.96	3.89	3.91	4.48	4.09
0.92	25.82	24.89	24.08	24.93	3.89	3.97	4.48	4.11
0.94	25.80	24.90	24.08	24.93	3.89	3.97	4.48	4.11
0.95	25.85	24.91	24.07	24.94	3.89	3.97	4.54	4.13
0.96	25.88	24.89	24.09	24.96	3.89	3.91	4.56	4.12

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	25.78	24.88	24.07	24.91	3.89	3.91	4.54	4.11
1.00	25.78	24.86	24.07	24.90	3.89	3.97	4.55	4.14
1.01	25.86	24.85	24.06	24.92	3.89	3.91	4.49	4.09
1.03	25.81	24.86	24.05	24.91	3.89	3.91	4.65	4.15
1.04	25.77	24.86	24.05	24.89	3.89	3.97	4.55	4.14
1.05	25.75	24.86	24.05	24.89	3.89	3.91	4.56	4.12
1.07	25.84	24.88	24.05	24.92	3.89	3.91	4.55	4.12
1.08	25.81	24.88	24.08	24.92	3.89	3.97	4.48	4.11
1.09	25.76	24.86	24.06	24.89	3.89	3.91	4.48	4.09
1.11	25.74	24.86	24.06	24.88	3.89	3.91	4.47	4.09
1.12	25.77	24.85	24.06	24.89	3.89	3.97	4.55	4.13
1.13	25.77	24.84	24.06	24.89	3.89	3.91	4.55	4.12
1.15	25.75	24.83	24.06	24.88	3.89	3.97	4.55	4.14
1.16	25.78	24.85	24.05	24.89	3.89	3.91	4.54	4.11
1.17	25.73	24.85	24.08	24.89	3.89	3.97	4.64	4.17
1.19	25.73	24.85	24.06	24.88	3.89	3.97	4.48	4.11
1.20	25.77	24.87	24.05	24.89	3.89	3.97	4.48	4.11
1.22	25.67	24.83	24.06	24.85	3.89	3.91	4.64	4.14
1.24	25.72	24.82	24.03	24.86	3.89	3.91	4.54	4.11
1.25	25.74	24.83	24.03	24.87	3.89	3.91	4.54	4.11
1.26	25.68	24.84	24.03	24.85	3.89	3.91	4.54	4.11
1.28	25.65	24.84	24.03	24.84	3.89	3.97	4.48	4.11
1.29	25.68	24.82	24.03	24.84	3.89	3.97	4.55	4.13
1.30	25.71	24.83	24.03	24.86	3.89	3.97	4.54	4.13
1.32	25.61	24.82	24.02	24.82	3.89	3.97	4.55	4.14
1.33	25.61	24.81	24.02	24.81	3.89	3.91	4.55	4.12
1.32	25.61	24.82	24.02	24.82	3.89	3.97	4.55	4.14
1.34	25.66	24.79	24.01	24.82	3.89	3.91	4.62	4.14
1.36	25.68	24.80	24.02	24.84	3.89	3.97	4.47	4.11
1.37	25.63	24.81	24.04	24.82	3.89	3.91	4.47	4.09
1.38	25.64	24.81	24.03	24.83	3.89	3.91	4.47	4.09
1.40	25.62	24.81	24.04	24.82	3.89	3.91	4.47	4.09
1.41	25.66	24.82	24.03	24.84	3.89	3.91	4.47	4.09
1.42	25.60	24.79	24.03	24.80	3.89	3.91	4.55	4.12
1.44	25.60	24.78	24.01	24.80	3.89	3.97	4.53	4.13
1.45	25.58	24.78	24.02	24.79	3.89	3.91	4.48	4.09
1.46	25.61	24.76	24.01	24.79	3.89	3.91	4.53	4.11

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.49	25.56	24.78	23.99	24.78	3.89	3.97	4.54	4.13
1.50	25.54	24.78	24.03	24.78	3.89	3.91	4.53	4.11
1.51	25.57	24.78	24.01	24.79	3.89	3.97	4.54	4.13
1.53	25.58	24.79	23.99	24.79	3.89	3.91	4.54	4.11
1.54	25.54	24.77	23.98	24.76	3.89	3.91	4.54	4.11
1.55	25.52	24.75	24.01	24.76	3.89	3.91	4.54	4.11
1.57	25.50	24.77	23.99	24.75	3.89	3.91	4.42	4.07
1.58	25.55	24.76	23.98	24.76	3.89	3.97	4.46	4.11
1.59	25.53	24.76	23.99	24.76	3.89	3.97	4.54	4.13
1.61	25.51	24.76	24.00	24.76	3.89	3.91	4.47	4.09
1.62	25.48	24.77	24.00	24.75	3.89	3.91	4.46	4.09
1.63	25.49	24.76	24.01	24.75	3.89	3.91	4.46	4.09
1.65	25.47	24.76	24.04	24.76	3.89	3.97	4.46	4.11
1.66	25.48	24.76	23.98	24.74	3.89	3.91	4.47	4.09
1.67	25.45	24.74	24.00	24.73	3.93	3.91	4.47	4.10
1.69	25.48	24.73	23.99	24.73	3.92	3.97	4.53	4.14
1.70	25.49	24.73	23.99	24.74	3.93	3.91	4.47	4.10
1.71	25.43	24.74	23.98	24.72	3.93	3.91	4.47	4.10
1.73	25.45	24.72	23.98	24.72	3.93	3.91	4.46	4.10
1.74	25.46	24.76	23.98	24.74	3.93	3.91	4.47	4.10
1.75	25.49	24.73	24.00	24.74	3.93	3.97	4.47	4.12
1.76	25.43	24.74	23.98	24.72	3.93	3.97	4.54	4.14
1.78	25.43	24.73	23.96	24.71	3.93	3.91	4.53	4.12
1.79	25.42	24.73	23.96	24.70	3.92	3.91	4.46	4.10
1.80	25.44	24.73	23.95	24.71	3.93	3.91	4.46	4.10
1.82	25.43	24.71	23.96	24.70	3.93	3.91	4.54	4.12
1.83	25.41	24.72	23.97	24.70	3.93	3.91	4.46	4.10
1.84	25.42	24.72	23.96	24.70	3.93	3.91	4.46	4.10
1.86	25.41	24.73	23.95	24.70	3.93	3.97	4.46	4.12
1.87	25.43	24.72	23.96	24.70	3.93	3.97	4.46	4.12
1.90	25.41	24.71	23.96	24.69	3.93	3.97	4.46	4.12
1.91	25.42	24.72	23.96	24.70	3.93	3.97	4.46	4.12
1.92	25.41	24.70	23.97	24.69	3.93	3.91	4.46	4.10
1.94	25.40	24.71	23.96	24.69	3.93	3.91	4.46	4.10
1.95	25.39	24.71	23.95	24.68	3.93	3.97	4.52	4.14
1.96	25.38	24.70	23.97	24.68	3.92	3.97	4.46	4.12
1.98	25.40	24.70	23.96	24.69	3.93	3.97	4.40	4.10

**APPENDIX 13.4 - Surface Tension Measurement Results for DI+SDS+Graphene (8.2mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (8.20 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	21.96	21.87	21.80	21.88	3.88	3.82	3.81	3.84
0.01	21.97	21.86	21.80	21.88	3.88	3.86	3.81	3.85
0.03	21.94	21.85	21.79	21.86	3.88	3.86	3.84	3.86
0.04	21.92	21.86	21.79	21.86	3.88	3.86	3.84	3.86
0.05	21.93	21.84	21.82	21.87	3.88	3.86	3.81	3.85
0.07	21.94	21.84	21.79	21.86	3.88	3.86	3.84	3.86
0.08	21.93	21.85	21.80	21.86	3.88	3.86	3.88	3.87
0.09	21.95	21.83	21.81	21.86	3.88	3.86	3.84	3.86
0.11	21.94	21.84	21.80	21.86	3.84	3.86	3.84	3.85
0.12	21.93	21.84	21.78	21.85	3.84	3.86	3.84	3.85
0.13	21.92	21.83	21.80	21.85	3.84	3.86	3.84	3.85
0.14	21.92	21.82	21.78	21.84	3.87	3.81	3.84	3.84
0.16	21.91	21.83	21.78	21.84	3.87	3.86	3.84	3.86
0.17	21.90	21.83	21.79	21.84	3.87	3.85	3.84	3.86
0.20	21.91	21.82	21.78	21.84	3.87	3.85	3.84	3.85
0.22	21.92	21.82	21.77	21.84	3.83	3.85	3.84	3.84
0.24	21.90	21.82	21.76	21.83	3.83	3.85	3.84	3.84
0.25	21.89	21.81	21.75	21.82	3.87	3.85	3.84	3.85
0.28	21.88	21.79	21.76	21.81	3.87	3.81	3.80	3.83
0.29	21.88	21.80	21.75	21.81	3.87	3.85	3.84	3.85
0.30	21.88	21.79	21.74	21.80	3.87	3.85	3.84	3.85
0.32	21.87	21.78	21.76	21.81	3.87	3.85	3.84	3.85
0.33	21.88	21.76	21.74	21.79	3.86	3.84	3.80	3.83
0.34	21.88	21.78	21.74	21.80	3.82	3.88	3.84	3.85
0.37	21.87	21.79	21.74	21.80	3.86	3.84	3.84	3.85
0.34	21.88	21.78	21.74	21.80	3.82	3.88	3.84	3.85
0.38	21.87	21.78	21.73	21.79	3.86	3.84	3.84	3.85
0.40	21.86	21.79	21.74	21.80	3.86	3.84	3.84	3.85
0.41	21.85	21.77	21.74	21.79	3.86	3.84	3.84	3.85
0.42	21.84	21.78	21.73	21.79	3.86	3.84	3.83	3.85
0.43	21.86	21.79	21.73	21.79	3.86	3.84	3.84	3.85
0.45	21.85	21.76	21.74	21.78	3.86	3.84	3.84	3.85

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	21.84	21.77	21.73	21.78	3.89	3.84	3.84	3.86
0.49	21.85	21.76	21.74	21.78	3.85	3.84	3.84	3.84
0.50	21.84	21.74	21.73	21.77	3.85	3.88	3.83	3.85
0.51	21.83	21.74	21.72	21.76	3.85	3.80	3.83	3.83
0.53	21.83	21.73	21.73	21.76	3.85	3.88	3.84	3.86
0.54	21.82	21.74	21.73	21.77	3.85	3.84	3.83	3.84
0.55	21.80	21.73	21.71	21.74	3.85	3.84	3.83	3.84
0.57	21.81	21.73	21.71	21.75	3.85	3.84	3.79	3.83
0.58	21.81	21.73	21.71	21.75	3.85	3.84	3.83	3.84
0.59	21.79	21.74	21.70	21.74	3.81	3.84	3.87	3.84
0.61	21.82	21.74	21.70	21.75	3.85	3.84	3.83	3.84
0.62	21.81	21.74	21.70	21.75	3.85	3.83	3.84	3.84
0.63	21.80	21.73	21.70	21.74	3.85	3.84	3.79	3.83
0.65	21.80	21.72	21.70	21.74	3.85	3.84	3.79	3.83
0.66	21.82	21.72	21.69	21.74	3.85	3.84	3.79	3.83
0.68	21.78	21.73	21.68	21.73	3.85	3.83	3.83	3.84
0.70	21.79	21.72	21.68	21.73	3.85	3.83	3.83	3.84
0.71	21.79	21.72	21.68	21.73	3.81	3.83	3.83	3.82
0.72	21.75	21.71	21.68	21.71	3.80	3.79	3.83	3.81
0.74	21.78	21.72	21.68	21.73	3.84	3.83	3.83	3.83
0.75	21.77	21.70	21.67	21.71	3.84	3.87	3.83	3.85
0.76	21.76	21.71	21.68	21.71	3.84	3.83	3.83	3.83
0.78	21.76	21.70	21.68	21.71	3.84	3.83	3.83	3.83
0.79	21.77	21.68	21.67	21.70	3.84	3.87	3.83	3.85
0.80	21.77	21.69	21.67	21.71	3.84	3.83	3.83	3.83
0.82	21.75	21.68	21.66	21.70	3.84	3.83	3.83	3.83
0.83	21.76	21.68	21.67	21.70	3.84	3.83	3.83	3.83
0.84	21.77	21.68	21.66	21.70	3.84	3.83	3.83	3.83
0.86	21.76	21.69	21.67	21.70	3.84	3.83	3.83	3.83
0.87	21.75	21.68	21.67	21.70	3.84	3.83	3.83	3.83
0.88	21.74	21.67	21.67	21.69	3.84	3.83	3.83	3.83
0.91	21.72	21.67	21.67	21.69	3.87	3.83	3.83	3.84
0.92	21.72	21.67	21.67	21.69	3.80	3.83	3.83	3.82
0.94	21.71	21.67	21.65	21.68	3.83	3.83	3.83	3.83
0.95	21.71	21.68	21.66	21.68	3.83	3.83	3.83	3.83
0.96	21.71	21.66	21.66	21.68	3.83	3.83	3.78	3.82

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	21.71	21.67	21.66	21.68	3.83	3.83	3.83	3.83
1.00	21.71	21.66	21.67	21.68	3.83	3.83	3.83	3.83
1.01	21.71	21.65	21.65	21.67	3.83	3.83	3.83	3.83
1.03	21.71	21.67	21.65	21.67	3.83	3.83	3.82	3.83
1.04	21.71	21.66	21.64	21.67	3.83	3.86	3.83	3.84
1.05	21.71	21.64	21.64	21.66	3.83	3.86	3.78	3.83
1.07	21.69	21.65	21.64	21.66	3.83	3.82	3.78	3.81
1.08	21.70	21.66	21.65	21.67	3.83	3.86	3.78	3.83
1.09	21.69	21.63	21.64	21.65	3.83	3.82	3.78	3.81
1.11	21.69	21.61	21.64	21.65	3.79	3.82	3.78	3.80
1.12	21.68	21.63	21.64	21.65	3.83	3.82	3.82	3.82
1.13	21.67	21.63	21.64	21.65	3.83	3.82	3.78	3.81
1.15	21.67	21.61	21.63	21.64	3.83	3.82	3.82	3.82
1.16	21.65	21.63	21.64	21.64	3.83	3.86	3.82	3.83
1.17	21.67	21.61	21.63	21.64	3.79	3.82	3.82	3.81
1.19	21.65	21.61	21.62	21.63	3.83	3.82	3.82	3.82
1.20	21.65	21.61	21.62	21.63	3.83	3.82	3.82	3.82
1.21	21.66	21.62	21.63	21.63	3.83	3.82	3.82	3.82
1.22	21.65	21.59	21.63	21.63	3.83	3.82	3.82	3.82
1.24	21.65	21.60	21.61	21.62	3.83	3.82	3.82	3.82
1.25	21.66	21.61	21.62	21.63	3.83	3.82	3.82	3.82
1.26	21.66	21.60	21.62	21.63	3.83	3.82	3.82	3.82
1.28	21.64	21.60	21.61	21.62	3.83	3.82	3.82	3.82
1.29	21.65	21.60	21.61	21.62	3.83	3.82	3.82	3.82
1.30	21.65	21.61	21.61	21.63	3.83	3.82	3.82	3.82
1.32	21.64	21.59	21.61	21.61	3.83	3.82	3.82	3.82
1.34	21.63	21.61	21.61	21.62	3.83	3.82	3.82	3.82
1.36	21.63	21.59	21.61	21.61	3.82	3.85	3.82	3.83
1.37	21.62	21.60	21.59	21.61	3.82	3.82	3.82	3.82
1.38	21.63	21.60	21.59	21.61	3.86	3.85	3.82	3.84
1.40	21.62	21.60	21.61	21.61	3.82	3.81	3.82	3.82
1.41	21.60	21.59	21.58	21.59	3.82	3.85	3.82	3.83
1.42	21.62	21.60	21.58	21.60	3.82	3.78	3.82	3.80
1.44	21.61	21.60	21.60	21.60	3.82	3.81	3.82	3.82
1.45	21.59	21.57	21.58	21.58	3.82	3.81	3.82	3.82
1.46	21.60	21.58	21.58	21.59	3.82	3.81	3.82	3.82

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.49	21.59	21.57	21.59	21.58	3.82	3.81	3.82	3.82
1.50	21.58	21.57	21.58	21.58	3.82	3.81	3.82	3.82
1.51	21.60	21.57	21.57	21.58	3.82	3.81	3.85	3.83
1.53	21.61	21.57	21.59	21.59	3.82	3.81	3.82	3.82
1.54	21.57	21.55	21.56	21.56	3.82	3.81	3.82	3.82
1.55	21.59	21.56	21.58	21.58	3.82	3.81	3.81	3.81
1.57	21.60	21.55	21.60	21.58	3.82	3.81	3.82	3.82
1.58	21.59	21.54	21.57	21.57	3.82	3.81	3.82	3.82
1.59	21.57	21.57	21.58	21.57	3.82	3.81	3.81	3.81
1.61	21.59	21.56	21.58	21.58	3.82	3.81	3.82	3.82
1.62	21.59	21.55	21.58	21.57	3.85	3.81	3.81	3.83
1.63	21.58	21.54	21.57	21.56	3.81	3.81	3.81	3.81
1.65	21.59	21.55	21.58	21.57	3.81	3.81	3.81	3.81
1.66	21.59	21.53	21.58	21.57	3.81	3.81	3.81	3.81
1.67	21.57	21.54	21.57	21.56	3.81	3.81	3.77	3.80
1.69	21.57	21.54	21.58	21.56	3.81	3.81	3.77	3.80
1.70	21.59	21.54	21.58	21.57	3.81	3.81	3.81	3.81
1.71	21.56	21.53	21.56	21.55	3.81	3.81	3.81	3.81
1.73	21.56	21.54	21.56	21.55	3.81	3.81	3.81	3.81
1.74	21.56	21.54	21.58	21.56	3.81	3.77	3.77	3.78
1.75	21.56	21.53	21.57	21.55	3.81	3.81	3.81	3.81
1.76	21.55	21.54	21.56	21.55	3.81	3.77	3.85	3.81
1.78	21.56	21.54	21.56	21.55	3.81	3.81	3.77	3.80
1.79	21.54	21.53	21.57	21.55	3.81	3.80	3.81	3.81
1.80	21.54	21.55	21.56	21.55	3.81	3.81	3.77	3.80
1.82	21.54	21.54	21.56	21.55	3.81	3.80	3.81	3.81
1.84	21.53	21.53	21.55	21.54	3.81	3.77	3.77	3.78
1.86	21.53	21.53	21.56	21.54	3.81	3.80	3.81	3.81
1.87	21.54	21.54	21.56	21.55	3.81	3.80	3.81	3.81
1.88	21.54	21.52	21.57	21.54	3.81	3.80	3.81	3.81
1.90	21.53	21.53	21.56	21.54	3.81	3.77	3.81	3.80
1.91	21.53	21.54	21.57	21.55	3.81	3.77	3.81	3.80
1.92	21.53	21.54	21.56	21.54	3.81	3.80	3.84	3.82
1.94	21.53	21.53	21.55	21.54	3.81	3.80	3.81	3.81
1.95	21.53	21.53	21.55	21.54	3.84	3.80	3.77	3.81
1.96	21.53	21.52	21.56	21.53	3.84	3.80	3.77	3.81
1.98	21.53	21.52	21.56	21.54	3.81	3.80	3.77	3.79

**APPENDIX 13.5 - Surface Tension Measurement Results for DI+SDS+Graphene  
(44.3 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (44.30 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	27.42	27.99	26.75	27.39	4.90	5.06	4.76	4.91
0.01	27.42	27.99	26.76	27.39	4.85	5.06	4.76	4.89
0.03	27.43	28.00	26.76	27.40	4.85	5.03	4.76	4.88
0.04	27.46	28.00	26.78	27.42	4.90	5.03	4.76	4.89
0.05	27.43	27.98	26.77	27.40	4.90	5.02	4.80	4.91
0.07	27.45	28.00	26.79	27.41	4.85	5.03	4.76	4.88
0.08	27.47	28.01	26.78	27.42	4.94	5.03	4.76	4.91
0.09	27.48	27.98	26.79	27.42	5.01	5.02	4.79	4.94
0.11	27.48	28.00	26.82	27.43	4.98	5.06	4.76	4.93
0.12	27.49	27.99	26.81	27.43	4.86	5.07	4.80	4.91
0.13	27.48	28.01	26.79	27.43	4.90	5.02	4.80	4.91
0.14	27.47	28.02	26.81	27.43	4.94	5.06	4.80	4.93
0.17	27.49	28.03	26.79	27.44	4.94	5.06	4.80	4.93
0.18	27.49	28.02	26.80	27.44	4.90	5.06	4.79	4.92
0.20	27.47	28.04	26.81	27.44	4.86	5.03	4.80	4.90
0.21	27.49	28.03	26.79	27.44	4.86	5.03	4.80	4.90
0.22	27.49	28.04	26.79	27.44	4.86	5.06	4.79	4.91
0.24	27.49	28.04	26.80	27.44	4.86	5.03	4.80	4.90
0.25	27.50	28.03	26.81	27.45	4.86	5.03	4.80	4.90
0.28	27.49	28.04	26.80	27.44	4.86	5.03	4.80	4.89
0.30	27.51	28.05	26.80	27.45	4.86	5.07	4.79	4.91
0.32	27.49	28.04	26.81	27.45	4.86	5.07	4.79	4.91
0.33	27.49	28.05	26.83	27.46	4.86	5.07	4.79	4.91
0.34	27.51	28.06	26.83	27.46	4.86	5.03	4.79	4.89
0.37	27.50	28.09	26.84	27.48	4.86	5.07	4.79	4.91
0.38	27.50	28.08	26.86	27.48	4.86	5.11	4.79	4.92
0.40	27.52	28.09	26.84	27.48	4.86	5.06	4.79	4.91
0.41	27.51	28.09	26.84	27.48	4.86	5.07	4.79	4.91
0.40	27.52	28.09	26.84	27.48	4.86	5.06	4.79	4.91
0.42	27.51	28.08	26.86	27.48	4.86	5.07	4.79	4.91
0.43	27.53	28.08	26.85	27.49	4.87	5.11	4.79	4.92
0.45	27.52	28.09	26.85	27.49	4.86	5.07	4.79	4.91

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	27.54	28.09	26.86	27.50	4.87	5.07	4.79	4.91
0.49	27.54	28.09	26.84	27.49	4.81	5.07	4.76	4.88
0.50	27.54	28.10	26.86	27.50	4.86	5.07	4.83	4.92
0.51	27.53	28.10	26.86	27.49	4.81	5.07	4.75	4.88
0.53	27.56	28.11	26.85	27.51	4.86	5.11	4.75	4.91
0.54	27.55	28.14	26.86	27.52	4.81	5.11	4.79	4.91
0.55	27.56	28.13	26.86	27.51	4.87	5.07	4.79	4.91
0.57	27.56	28.14	26.86	27.52	4.87	5.11	4.75	4.91
0.58	27.55	28.13	26.85	27.51	4.91	5.11	4.75	4.92
0.59	27.58	28.14	26.87	27.53	4.87	5.11	4.80	4.92
0.61	27.56	28.14	26.86	27.52	4.87	5.11	4.75	4.91
0.62	27.58	28.13	26.88	27.53	4.87	5.11	4.79	4.92
0.63	27.57	28.15	26.89	27.53	4.87	5.11	4.79	4.92
0.65	27.57	28.14	26.88	27.53	4.87	5.07	4.79	4.91
0.66	27.57	28.15	26.90	27.54	4.87	5.11	4.79	4.92
0.67	27.58	28.15	26.89	27.54	4.91	5.03	4.79	4.91
0.68	27.60	28.14	26.91	27.55	4.87	5.11	4.79	4.92
0.70	27.58	28.14	26.92	27.55	4.87	5.03	4.79	4.90
0.71	27.59	28.15	26.92	27.55	4.81	5.07	4.79	4.89
0.72	27.59	28.16	26.92	27.56	4.87	5.07	4.79	4.91
0.74	27.58	28.15	26.91	27.55	4.91	5.07	4.79	4.92
0.75	27.60	28.17	26.92	27.57	4.87	5.03	4.79	4.90
0.76	27.59	28.18	26.92	27.56	4.87	5.11	4.79	4.92
0.78	27.61	28.19	26.92	27.57	4.87	5.03	4.79	4.90
0.79	27.59	28.19	26.93	27.57	4.87	5.11	4.79	4.92
0.80	27.61	28.20	26.93	27.58	4.87	5.07	4.79	4.91
0.82	27.60	28.21	26.92	27.57	4.87	5.11	4.79	4.92
0.83	27.60	28.20	26.92	27.57	4.87	5.11	4.79	4.92
0.86	27.61	28.22	26.92	27.58	4.87	5.11	4.79	4.92
0.87	27.60	28.21	26.92	27.58	4.87	5.11	4.79	4.92
0.88	27.60	28.22	26.93	27.58	4.87	5.11	4.79	4.92
0.90	27.61	28.22	26.92	27.58	4.87	5.11	4.79	4.92
0.91	27.60	28.22	26.92	27.58	4.87	5.11	4.79	4.92
0.92	27.61	28.20	26.93	27.58	4.87	5.07	4.79	4.91
0.94	27.61	28.22	26.94	27.59	4.88	5.11	4.79	4.92
0.95	27.61	28.21	26.91	27.57	4.87	5.07	4.79	4.91

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.97	27.59	28.23	26.95	27.59	4.87	5.11	4.79	4.92
0.99	27.64	28.23	26.94	27.60	4.87	5.07	4.79	4.91
1.00	27.61	28.24	26.95	27.60	4.87	5.07	4.79	4.91
1.01	27.62	28.24	26.97	27.61	4.87	5.07	4.79	4.91
1.03	27.63	28.26	26.96	27.62	4.87	5.07	4.79	4.91
1.04	27.62	28.26	26.94	27.61	4.87	5.07	4.79	4.91
1.05	27.63	28.27	26.98	27.62	4.87	5.07	4.79	4.91
1.07	27.62	28.27	26.98	27.62	4.87	5.07	4.79	4.91
1.08	27.63	28.28	26.96	27.62	4.92	5.07	4.79	4.92
1.09	27.64	28.31	26.97	27.64	4.87	5.07	4.79	4.91
1.11	27.63	28.29	26.99	27.64	4.87	5.07	4.79	4.91
1.12	27.66	28.27	26.99	27.64	4.87	5.07	4.79	4.91
1.13	27.63	28.28	26.98	27.63	4.87	5.07	4.79	4.91
1.15	27.66	28.30	27.01	27.66	4.87	5.07	4.79	4.91
1.16	27.67	28.25	26.99	27.64	4.87	5.11	4.79	4.92
1.17	27.67	28.29	26.99	27.65	4.87	5.07	4.79	4.91
1.19	27.69	28.31	27.02	27.67	4.87	5.07	4.79	4.91
1.20	27.66	28.28	27.00	27.65	4.87	5.07	4.79	4.91
1.21	27.67	28.28	27.00	27.65	4.87	5.07	4.78	4.91
1.22	27.68	28.31	26.99	27.66	4.82	5.11	4.79	4.91
1.24	27.68	28.29	27.02	27.66	4.92	5.07	4.79	4.92
1.25	27.71	28.28	27.00	27.66	4.92	5.07	4.78	4.92
1.26	27.69	28.31	27.02	27.67	4.92	5.07	4.78	4.92
1.28	27.69	28.33	27.01	27.67	4.82	5.11	4.79	4.90
1.29	27.71	28.30	27.00	27.67	4.88	5.07	4.78	4.91
1.30	27.70	28.31	27.02	27.67	4.88	5.07	4.78	4.91
1.32	27.71	28.33	27.03	27.69	4.88	5.11	4.79	4.92
1.34	27.69	28.34	27.03	27.69	4.88	5.07	4.75	4.90
1.36	27.73	28.35	27.03	27.70	4.88	5.07	4.82	4.92
1.37	27.70	28.35	27.05	27.70	4.88	5.07	4.78	4.91
1.38	27.70	28.34	27.05	27.70	4.88	5.07	4.75	4.90
1.40	27.72	28.35	27.06	27.71	4.88	5.11	4.78	4.92
1.41	27.73	28.37	27.05	27.72	4.88	5.07	4.78	4.91
1.42	27.73	28.36	27.05	27.71	4.88	5.07	4.78	4.91
1.44	27.75	28.37	27.06	27.73	4.88	5.07	4.82	4.92
1.45	27.77	28.37	27.07	27.74	4.88	5.07	4.75	4.90

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.48	27.78	28.37	27.08	27.74	4.88	5.07	4.78	4.91
1.49	27.78	28.38	27.09	27.75	4.88	5.07	4.78	4.91
1.50	27.81	28.37	27.07	27.75	4.88	5.07	4.78	4.91
1.51	27.80	28.38	27.10	27.76	4.88	5.07	4.78	4.91
1.53	27.79	28.38	27.11	27.76	4.88	5.07	4.78	4.91
1.54	27.82	28.38	27.09	27.76	4.83	5.07	4.78	4.89
1.55	27.81	28.39	27.11	27.77	4.89	5.07	4.78	4.91
1.57	27.81	28.37	27.09	27.76	4.88	5.07	4.74	4.90
1.58	27.84	28.39	27.09	27.77	4.89	5.07	4.78	4.91
1.59	27.86	28.39	27.09	27.78	4.88	5.06	4.78	4.91
1.61	27.84	28.41	27.12	27.79	4.88	5.07	4.78	4.91
1.62	27.86	28.40	27.11	27.79	4.89	5.07	4.78	4.91
1.63	27.89	28.41	27.09	27.80	4.84	5.03	4.78	4.88
1.65	27.89	28.44	27.11	27.81	4.83	5.03	4.78	4.88
1.67	27.92	28.45	27.10	27.82	4.84	5.03	4.78	4.88
1.69	27.92	28.43	27.10	27.82	4.84	5.03	4.78	4.88
1.70	27.91	28.44	27.11	27.82	4.84	5.03	4.78	4.88
1.73	27.93	28.45	27.12	27.83	4.77	5.03	4.78	4.86
1.74	27.92	28.46	27.12	27.83	4.84	5.03	4.78	4.88
1.75	27.94	28.43	27.11	27.83	4.84	5.03	4.78	4.88
1.76	27.93	28.44	27.11	27.83	4.77	5.03	4.78	4.86
1.78	27.92	28.44	27.12	27.82	4.77	5.03	4.78	4.86
1.79	27.94	28.45	27.13	27.84	4.78	5.03	4.78	4.86
1.80	27.94	28.45	27.12	27.83	4.78	5.03	4.78	4.86
1.82	27.96	28.45	27.12	27.85	4.78	5.03	4.78	4.86
1.83	27.94	28.46	27.13	27.84	4.77	5.03	4.78	4.86
1.84	27.97	28.44	27.12	27.85	4.78	5.03	4.78	4.86
1.86	27.98	28.46	27.13	27.86	4.78	5.03	4.78	4.86
1.87	27.97	28.45	27.12	27.85	4.84	5.03	4.78	4.88
1.88	27.97	28.46	27.14	27.86	4.78	5.03	4.78	4.86
1.90	27.97	28.46	27.13	27.86	4.78	5.03	4.78	4.86
1.91	27.98	28.48	27.13	27.86	4.78	5.03	4.78	4.86
1.92	27.98	28.48	27.15	27.87	4.78	5.03	4.78	4.86
1.94	28.00	28.47	27.15	27.87	4.78	5.03	4.78	4.86
1.95	28.00	28.49	27.16	27.88	4.78	5.07	4.78	4.87
1.96	27.99	28.50	27.14	27.88	4.78	5.03	4.78	4.86
1.98	28.01	28.49	27.17	27.89	4.78	5.03	4.78	4.86

**APPENDIX 13.6 - Surface Tension Measurement Results for DI + SDS + Graphene  
(59.00 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (59.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	24.44	25.33	24.06	24.61	4.41	4.54	4.31	4.42
0.01	24.46	25.31	24.08	24.61	4.41	4.54	4.31	4.42
0.03	24.44	25.30	24.07	24.60	4.41	4.54	4.31	4.42
0.04	24.44	25.30	24.06	24.60	4.41	4.54	4.31	4.42
0.05	24.45	25.30	24.07	24.61	4.41	4.54	4.31	4.42
0.07	24.45	25.30	24.07	24.61	4.41	4.53	4.31	4.42
0.08	24.44	25.29	24.06	24.60	4.41	4.54	4.31	4.42
0.09	24.45	25.30	24.07	24.61	4.41	4.57	4.31	4.43
0.11	24.46	25.28	24.08	24.61	4.41	4.53	4.31	4.42
0.12	24.45	25.26	24.09	24.60	4.41	4.57	4.31	4.43
0.13	24.45	25.28	24.09	24.60	4.41	4.57	4.31	4.43
0.14	24.45	25.25	24.10	24.60	4.41	4.53	4.31	4.42
0.16	24.45	25.26	24.10	24.60	4.41	4.53	4.31	4.42
0.18	24.46	25.26	24.12	24.61	4.41	4.53	4.31	4.41
0.20	24.46	25.25	24.11	24.61	4.41	4.53	4.31	4.41
0.21	24.45	25.27	24.11	24.61	4.37	4.53	4.31	4.40
0.22	24.46	25.25	24.12	24.61	4.41	4.53	4.27	4.40
0.24	24.46	25.26	24.11	24.61	4.37	4.56	4.31	4.41
0.25	24.46	25.25	24.11	24.61	4.45	4.56	4.31	4.44
0.28	24.46	25.22	24.10	24.59	4.45	4.56	4.31	4.44
0.29	24.48	25.23	24.10	24.60	4.40	4.52	4.31	4.41
0.30	24.46	25.21	24.12	24.60	4.40	4.52	4.27	4.40
0.29	24.48	25.23	24.10	24.60	4.40	4.52	4.31	4.41
0.32	24.46	25.22	24.11	24.60	4.45	4.52	4.27	4.41
0.33	24.48	25.21	24.10	24.59	4.41	4.52	4.27	4.40
0.34	24.45	25.22	24.11	24.59	4.40	4.56	4.27	4.41
0.37	24.47	25.20	24.10	24.59	4.41	4.52	4.31	4.41
0.40	24.46	25.19	24.14	24.60	4.41	4.52	4.31	4.41
0.41	24.46	25.21	24.13	24.60	4.45	4.52	4.31	4.43
0.42	24.46	25.21	24.12	24.59	4.45	4.52	4.31	4.43
0.43	24.47	25.21	24.14	24.61	4.37	4.52	4.31	4.40
0.45	24.46	25.20	24.15	24.60	4.41	4.52	4.31	4.41

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	24.46	25.19	24.15	24.60	4.37	4.52	4.31	4.40
0.49	24.45	25.20	24.16	24.60	4.41	4.52	4.31	4.41
0.50	24.45	25.20	24.15	24.60	4.41	4.52	4.31	4.41
0.51	24.46	25.20	24.15	24.60	4.41	4.52	4.35	4.42
0.53	24.46	25.19	24.18	24.61	4.41	4.52	4.35	4.42
0.54	24.47	25.18	24.16	24.60	4.41	4.52	4.31	4.41
0.55	24.45	25.20	24.18	24.61	4.41	4.52	4.31	4.41
0.57	24.45	25.19	24.17	24.60	4.41	4.52	4.31	4.41
0.58	24.46	25.19	24.16	24.60	4.41	4.52	4.35	4.42
0.59	24.46	25.20	24.17	24.61	4.41	4.52	4.31	4.41
0.61	24.47	25.19	24.17	24.61	4.41	4.52	4.35	4.42
0.62	24.46	25.18	24.17	24.60	4.41	4.52	4.35	4.42
0.63	24.47	25.19	24.16	24.61	4.41	4.52	4.35	4.42
0.65	24.46	25.19	24.17	24.61	4.40	4.52	4.39	4.44
0.66	24.47	25.19	24.17	24.61	4.41	4.52	4.31	4.41
0.67	24.46	25.20	24.17	24.61	4.41	4.52	4.35	4.42
0.68	24.47	25.19	24.18	24.61	4.40	4.52	4.31	4.41
0.71	24.48	25.20	24.18	24.62	4.41	4.52	4.35	4.42
0.72	24.48	25.19	24.18	24.61	4.40	4.52	4.35	4.42
0.72	24.48	25.19	24.18	24.61	4.40	4.52	4.35	4.42
0.74	24.48	25.19	24.21	24.63	4.40	4.52	4.31	4.41
0.75	24.50	25.19	24.20	24.63	4.40	4.52	4.31	4.41
0.76	24.49	25.19	24.20	24.63	4.40	4.52	4.31	4.41
0.78	24.49	25.19	24.21	24.63	4.40	4.52	4.35	4.42
0.79	24.50	25.18	24.21	24.63	4.40	4.51	4.31	4.41
0.80	24.51	25.19	24.22	24.64	4.40	4.51	4.35	4.42
0.82	24.50	25.19	24.23	24.64	4.40	4.52	4.35	4.42
0.83	24.50	25.19	24.22	24.64	4.40	4.51	4.35	4.42
0.86	24.51	25.21	24.24	24.65	4.37	4.51	4.31	4.40
0.87	24.50	25.21	24.24	24.65	4.40	4.51	4.31	4.41
0.88	24.52	25.20	24.22	24.65	4.40	4.51	4.35	4.42
0.90	24.51	25.21	24.23	24.65	4.37	4.51	4.31	4.40
0.91	24.50	25.21	24.24	24.65	4.37	4.51	4.35	4.41
0.92	24.51	25.20	24.23	24.65	4.40	4.51	4.35	4.42
0.94	24.51	25.21	24.23	24.65	4.40	4.51	4.35	4.42
0.95	24.50	25.22	24.24	24.65	4.40	4.55	4.35	4.43
0.96	24.51	25.21	24.25	24.65	4.37	4.51	4.35	4.41

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0.99	24.51	25.24	24.25	24.67	4.37	4.55	4.35	4.42
1.00	24.50	25.21	24.24	24.65	4.41	4.51	4.35	4.42
1.01	24.50	25.22	24.24	24.66	4.37	4.51	4.35	4.41
1.03	24.51	25.23	24.25	24.66	4.44	4.51	4.35	4.43
1.04	24.51	25.22	24.27	24.67	4.37	4.51	4.35	4.41
1.05	24.50	25.22	24.26	24.66	4.40	4.55	4.34	4.43
1.07	24.50	25.22	24.26	24.66	4.36	4.55	4.34	4.42
1.08	24.51	25.22	24.27	24.67	4.36	4.51	4.34	4.41
1.09	24.52	25.21	24.27	24.67	4.40	4.55	4.34	4.43
1.11	24.50	25.21	24.28	24.66	4.40	4.55	4.34	4.43
1.12	24.50	25.22	24.29	24.67	4.40	4.51	4.34	4.42
1.13	24.50	25.23	24.30	24.68	4.40	4.55	4.34	4.43
1.15	24.51	25.22	24.30	24.68	4.40	4.55	4.34	4.43
1.16	24.51	25.22	24.30	24.68	4.40	4.55	4.34	4.43
1.17	24.53	25.21	24.31	24.68	4.40	4.51	4.34	4.42
1.19	24.53	25.22	24.30	24.68	4.40	4.51	4.38	4.43
1.21	24.53	25.21	24.32	24.69	4.40	4.55	4.31	4.42
1.22	24.53	25.21	24.31	24.68	4.40	4.51	4.31	4.41
1.24	24.53	25.21	24.30	24.68	4.40	4.55	4.31	4.42
1.25	24.55	25.20	24.31	24.69	4.40	4.55	4.31	4.42
1.26	24.54	25.20	24.32	24.69	4.40	4.55	4.31	4.42
1.28	24.57	25.21	24.32	24.70	4.40	4.55	4.31	4.42
1.29	24.56	25.21	24.32	24.70	4.40	4.55	4.34	4.43
1.30	24.57	25.20	24.32	24.70	4.40	4.51	4.34	4.42
1.32	24.58	25.23	24.34	24.72	4.40	4.55	4.31	4.42
1.33	24.55	25.23	24.32	24.70	4.40	4.51	4.31	4.41
1.36	24.57	25.21	24.33	24.70	4.40	4.51	4.34	4.42
1.37	24.55	25.24	24.33	24.71	4.40	4.51	4.34	4.42
1.38	24.55	25.24	24.34	24.71	4.40	4.51	4.34	4.42
1.38	24.55	25.24	24.34	24.71	4.40	4.51	4.34	4.42
1.40	24.61	25.23	24.33	24.73	4.37	4.51	4.34	4.41
1.41	24.54	25.24	24.35	24.71	4.40	4.51	4.31	4.40
1.42	24.63	25.25	24.35	24.74	4.36	4.51	4.34	4.41
1.44	24.55	25.23	24.35	24.71	4.40	4.51	4.30	4.40
1.45	24.60	25.25	24.35	24.74	4.37	4.51	4.34	4.41
1.46	24.60	25.25	24.36	24.73	4.40	4.51	4.34	4.42
1.48	24.55	25.25	24.36	24.72	4.40	4.55	4.34	4.43
1.49	24.63	25.25	24.37	24.75	4.37	4.51	4.34	4.41
1.50	24.54	25.26	24.38	24.73	4.40	4.51	4.34	4.42

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1.53	24.59	25.26	24.38	24.74	4.36	4.51	4.34	4.40
1.54	24.55	25.26	24.40	24.74	4.40	4.51	4.34	4.41
1.55	24.64	25.26	24.40	24.76	4.36	4.51	4.34	4.40
1.57	24.55	25.25	24.39	24.73	4.44	4.51	4.34	4.43
1.58	24.63	25.27	24.40	24.76	4.40	4.51	4.34	4.42
1.59	24.56	25.27	24.40	24.74	4.36	4.51	4.30	4.39
1.61	24.60	25.26	24.41	24.76	4.44	4.54	4.34	4.44
1.62	24.62	25.27	24.39	24.76	4.40	4.51	4.34	4.42
1.63	24.56	25.26	24.39	24.74	4.44	4.51	4.34	4.43
1.65	24.66	25.26	24.40	24.77	4.36	4.51	4.34	4.40
1.66	24.57	25.25	24.40	24.74	4.40	4.54	4.34	4.43
1.67	24.63	25.26	24.40	24.76	4.36	4.51	4.34	4.40
1.69	24.63	25.26	24.41	24.77	4.36	4.54	4.34	4.41
1.70	24.58	25.26	24.40	24.75	4.40	4.51	4.34	4.41
1.71	24.65	25.26	24.40	24.77	4.40	4.51	4.34	4.41
1.73	24.59	25.25	24.42	24.76	4.36	4.50	4.34	4.40
1.74	24.67	25.27	24.42	24.78	4.40	4.54	4.34	4.43
1.75	24.60	25.26	24.43	24.76	4.40	4.54	4.34	4.43
1.76	24.63	25.27	24.43	24.77	4.40	4.50	4.34	4.41
1.78	24.67	25.26	24.44	24.79	4.40	4.54	4.34	4.43
1.79	24.60	25.26	24.44	24.76	4.40	4.54	4.34	4.43
1.80	24.67	25.25	24.46	24.79	4.40	4.54	4.34	4.43
1.82	24.62	25.27	24.45	24.78	4.40	4.54	4.34	4.43
1.83	24.65	25.27	24.45	24.79	4.40	4.54	4.34	4.42
1.84	24.63	25.28	24.47	24.79	4.40	4.54	4.34	4.42
1.86	24.62	25.27	24.47	24.79	4.40	4.54	4.30	4.41
1.87	24.66	25.27	24.48	24.80	4.36	4.54	4.34	4.41
1.88	24.61	25.28	24.47	24.78	4.39	4.54	4.30	4.41
1.90	24.66	25.28	24.48	24.81	4.39	4.54	4.34	4.42
1.91	24.64	25.29	24.48	24.80	4.39	4.54	4.34	4.42
1.92	24.63	25.30	24.48	24.81	4.39	4.54	4.34	4.42
1.94	24.66	25.29	24.49	24.82	4.39	4.54	4.34	4.42
1.95	24.63	25.29	24.49	24.80	4.40	4.54	4.33	4.42
1.96	24.66	25.31	24.50	24.82	4.39	4.54	4.33	4.42
1.98	24.62	25.31	24.51	24.81	4.39	4.54	4.34	4.42
1.99	24.65	25.30	24.49	24.81	4.39	4.54	4.34	4.42

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**APPENDIX 13.7 - Surface Tension Measurement Results for DI+SDS+Graphene (82.00 mM)**

HUATARC surface tension measurement results for DI + SDS + graphene (82.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	25.88	25.96	26.10	25.98	4.72	4.68	4.87	4.76
0.01	25.85	25.94	26.12	25.97	4.83	4.68	4.73	4.75
0.03	25.86	25.94	26.07	25.96	4.78	4.73	4.81	4.77
0.04	25.87	25.93	26.09	25.96	4.72	4.68	4.81	4.74
0.05	25.88	25.93	26.08	25.97	4.72	4.73	4.81	4.75
0.07	25.85	25.91	26.08	25.95	4.83	4.73	4.81	4.79
0.08	25.85	25.95	26.07	25.96	4.83	4.72	4.81	4.79
0.09	25.84	25.95	26.08	25.96	4.77	4.73	4.81	4.77
0.11	25.84	25.91	26.08	25.95	4.77	4.73	4.86	4.79
0.13	25.87	25.93	26.07	25.96	4.77	4.72	4.81	4.77
0.14	25.84	25.97	26.07	25.96	4.77	4.72	4.81	4.77
0.16	25.85	25.94	26.06	25.95	4.77	4.72	4.81	4.77
0.17	25.87	25.96	26.08	25.97	4.77	4.72	4.81	4.77
0.18	25.83	25.97	26.09	25.96	4.77	4.72	4.81	4.77
0.20	25.84	25.95	26.07	25.95	4.77	4.72	4.81	4.77
0.21	25.86	25.95	26.07	25.96	4.77	4.72	4.66	4.72
0.22	25.83	25.97	26.07	25.96	4.77	4.72	4.66	4.72
0.24	25.85	25.99	26.07	25.97	4.76	4.72	4.66	4.71
0.25	25.84	25.94	26.07	25.95	4.77	4.72	4.81	4.77
0.28	25.86	25.98	26.09	25.98	4.76	4.72	4.69	4.72
0.29	25.87	25.97	26.07	25.97	4.76	4.72	4.81	4.76
0.30	25.87	25.97	26.05	25.96	4.76	4.72	4.66	4.71
0.32	25.83	25.98	26.09	25.97	4.67	4.72	4.80	4.73
0.33	25.90	25.98	26.06	25.98	4.67	4.72	4.66	4.68
0.37	25.88	25.97	26.09	25.98	4.67	4.72	4.69	4.69
0.38	25.87	25.96	26.10	25.98	4.67	4.72	4.70	4.69
0.37	25.88	25.97	26.09	25.98	4.67	4.72	4.69	4.69
0.40	25.88	25.97	26.08	25.98	4.67	4.72	4.86	4.75
0.41	25.84	25.99	26.11	25.98	4.71	4.72	4.69	4.71
0.42	25.90	25.97	26.11	25.99	4.71	4.72	4.69	4.71
0.43	25.85	25.96	26.10	25.97	4.67	4.72	4.69	4.69
0.45	25.88	25.98	26.10	25.99	4.71	4.72	4.69	4.71

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	25.84	25.95	26.11	25.97	4.71	4.77	4.69	4.72
0.49	25.88	25.98	26.09	25.98	4.71	4.72	4.69	4.71
0.50	25.83	25.94	26.11	25.96	4.71	4.68	4.69	4.69
0.51	25.88	25.97	26.11	25.99	4.71	4.83	4.69	4.74
0.53	25.86	25.93	26.09	25.96	4.71	4.68	4.69	4.69
0.54	25.83	25.99	26.13	25.98	4.71	4.72	4.69	4.71
0.55	25.87	25.93	26.12	25.98	4.71	4.68	4.69	4.69
0.57	25.82	25.93	26.11	25.95	4.67	4.76	4.69	4.71
0.58	25.88	25.99	26.09	25.99	4.71	4.72	4.69	4.71
0.59	25.87	25.92	26.13	25.97	4.67	4.68	4.73	4.69
0.61	25.81	25.98	26.13	25.98	4.67	4.72	4.73	4.71
0.62	25.87	25.95	26.12	25.98	4.71	4.72	4.73	4.72
0.63	25.85	25.99	26.17	26.00	4.71	4.72	4.69	4.71
0.65	25.86	25.97	26.12	25.98	4.76	4.72	4.73	4.74
0.66	25.85	25.91	26.15	25.97	4.71	4.68	4.73	4.70
0.67	25.82	25.99	26.14	25.98	4.71	4.76	4.72	4.73
0.68	25.88	25.91	26.17	25.98	4.71	4.67	4.72	4.70
0.70	25.83	25.98	26.18	26.00	4.71	4.72	4.72	4.72
0.71	25.87	25.98	26.13	25.99	4.71	4.72	4.72	4.72
0.72	25.85	25.94	26.19	25.99	4.71	4.72	4.73	4.72
0.74	25.84	26.00	26.16	26.00	4.71	4.77	4.69	4.72
0.75	25.83	25.92	26.15	25.97	4.76	4.72	4.69	4.72
0.76	25.83	26.01	26.17	26.00	4.71	4.72	4.73	4.72
0.78	25.87	25.93	26.14	25.98	4.71	4.71	4.73	4.71
0.79	25.83	26.01	26.18	26.00	4.66	4.71	4.69	4.69
0.82	25.84	25.95	26.17	25.99	4.71	4.71	4.73	4.72
0.83	25.84	25.99	26.16	26.00	4.71	4.76	4.69	4.72
0.84	25.83	25.96	26.14	25.98	4.75	4.71	4.69	4.72
0.86	25.87	25.99	26.19	26.02	4.66	4.76	4.69	4.70
0.87	25.83	25.99	26.14	25.99	4.71	4.71	4.69	4.70
0.88	25.87	25.98	26.16	26.00	4.75	4.71	4.69	4.72
0.90	25.84	26.00	26.16	26.00	4.66	4.71	4.69	4.69
0.88	25.87	25.98	26.16	26.00	4.75	4.71	4.69	4.72
0.91	25.84	25.97	26.17	25.99	4.71	4.71	4.69	4.70
0.92	25.86	26.01	26.16	26.01	4.70	4.71	4.69	4.70
0.95	25.86	25.99	26.20	26.02	4.70	4.67	4.69	4.69
0.96	25.83	25.97	26.16	25.99	4.71	4.71	4.68	4.70

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	25.85	25.97	26.19	26.00	4.70	4.75	4.68	4.71
1.00	25.84	25.99	26.20	26.01	4.66	4.71	4.68	4.69
1.01	25.86	26.01	26.16	26.01	4.66	4.71	4.68	4.68
1.03	25.85	25.94	26.19	25.99	4.66	4.71	4.68	4.68
1.04	25.85	26.01	26.19	26.02	4.70	4.71	4.68	4.70
1.05	25.84	25.98	26.19	26.00	4.70	4.71	4.68	4.70
1.07	25.86	26.00	26.20	26.02	4.66	4.71	4.68	4.68
1.08	25.86	25.96	26.20	26.01	4.70	4.71	4.68	4.70
1.09	25.84	25.99	26.20	26.01	4.66	4.71	4.71	4.69
1.11	25.82	25.97	26.20	26.00	4.70	4.71	4.72	4.71
1.12	25.85	25.99	26.20	26.01	4.70	4.71	4.72	4.71
1.13	25.87	25.96	26.22	26.01	4.70	4.71	4.71	4.71
1.15	25.81	25.97	26.20	25.99	4.70	4.76	4.72	4.72
1.16	25.86	25.99	26.21	26.02	4.70	4.76	4.76	4.74
1.17	25.85	25.99	26.23	26.02	4.70	4.71	4.76	4.72
1.20	25.86	25.97	26.21	26.01	4.70	4.71	4.76	4.72
1.21	25.83	25.96	26.21	26.00	4.70	4.71	4.76	4.72
1.22	25.87	25.99	26.19	26.02	4.70	4.76	4.76	4.74
1.24	25.83	25.99	26.20	26.01	4.70	4.71	4.76	4.72
1.25	25.85	25.98	26.19	26.00	4.70	4.71	4.76	4.72
1.26	25.86	25.97	26.21	26.01	4.70	4.71	4.76	4.72
1.28	25.83	26.01	26.20	26.01	4.70	4.75	4.75	4.74
1.29	25.83	25.97	26.20	26.00	4.70	4.70	4.76	4.72
1.30	25.87	25.98	26.20	26.01	4.66	4.71	4.76	4.71
1.32	25.84	25.99	26.20	26.01	4.70	4.71	4.75	4.72
1.33	25.84	25.97	26.19	26.00	4.70	4.71	4.75	4.72
1.34	25.84	25.98	26.21	26.01	4.70	4.70	4.75	4.72
1.36	25.87	25.98	26.20	26.02	4.70	4.70	4.75	4.72
1.34	25.84	25.98	26.21	26.01	4.70	4.70	4.75	4.72
1.38	25.85	25.94	26.20	26.00	4.70	4.70	4.76	4.72
1.40	25.84	25.94	26.21	26.00	4.70	4.70	4.75	4.72
1.41	25.85	26.00	26.19	26.01	4.70	4.70	4.75	4.72
1.42	25.85	25.91	26.18	25.98	4.70	4.70	4.75	4.72
1.44	25.86	25.98	26.20	26.01	4.70	4.75	4.75	4.73
1.45	25.85	25.94	26.19	25.99	4.69	4.70	4.75	4.72
1.46	25.86	25.96	26.18	26.00	4.70	4.70	4.75	4.72
1.48	25.84	25.97	26.18	26.00	4.70	4.70	4.75	4.72

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	25.85	25.95	26.19	26.00	4.69	4.75	4.75	4.73
1.51	25.80	25.88	26.18	25.95	4.69	4.70	4.75	4.72
1.53	25.86	25.97	26.19	26.01	4.69	4.75	4.75	4.73
1.54	25.85	25.97	26.17	25.99	4.69	4.70	4.75	4.72
1.55	25.86	25.91	26.19	25.99	4.69	4.70	4.75	4.72
1.57	25.85	25.95	26.18	25.99	4.69	4.70	4.75	4.71
1.58	25.78	25.93	26.17	25.96	4.69	4.70	4.75	4.72
1.59	25.87	25.96	26.18	26.01	4.69	4.75	4.75	4.73
1.61	25.80	25.94	26.16	25.97	4.69	4.70	4.75	4.71
1.62	25.86	25.95	26.18	26.00	4.69	4.70	4.75	4.71
1.63	25.80	25.97	26.15	25.97	4.69	4.70	4.71	4.70
1.65	25.84	25.91	26.18	25.98	4.65	4.70	4.75	4.70
1.66	25.88	25.96	26.16	26.00	4.69	4.70	4.75	4.71
1.67	25.79	25.98	26.17	25.98	4.65	4.70	4.75	4.70
1.69	25.87	25.95	26.18	26.00	4.69	4.70	4.75	4.71
1.71	25.85	25.95	26.14	25.98	4.69	4.70	4.75	4.71
1.73	25.82	25.94	26.15	25.97	4.69	4.70	4.75	4.71
1.74	25.83	25.92	26.16	25.97	4.69	4.70	4.75	4.71
1.75	25.86	25.95	26.15	25.99	4.74	4.75	4.70	4.73
1.76	25.78	25.95	26.17	25.96	4.69	4.70	4.75	4.71
1.78	25.86	25.95	26.17	25.99	4.69	4.70	4.70	4.70
1.79	25.83	25.93	26.15	25.97	4.74	4.70	4.70	4.71
1.80	25.83	25.95	26.16	25.98	4.74	4.70	4.75	4.73
1.82	25.85	25.94	26.14	25.98	4.69	4.74	4.75	4.73
1.83	25.80	25.90	26.14	25.95	4.69	4.70	4.70	4.70
1.84	25.83	25.95	26.15	25.97	4.69	4.70	4.75	4.71
1.86	25.79	25.92	26.16	25.96	4.69	4.70	4.75	4.71
1.87	25.86	25.93	26.15	25.98	4.69	4.75	4.70	4.71
1.88	25.84	25.94	26.13	25.97	4.74	4.75	4.70	4.73
1.90	25.83	25.94	26.14	25.97	4.69	4.70	4.70	4.70
1.91	25.85	25.94	26.15	25.98	4.69	4.74	4.70	4.71
1.94	25.87	25.95	26.13	25.98	4.74	4.69	4.74	4.73
1.95	25.80	25.92	26.13	25.95	4.69	4.70	4.70	4.70
1.96	25.85	25.89	26.13	25.96	4.69	4.70	4.74	4.71
1.98	25.82	25.95	26.11	25.96	4.69	4.69	4.70	4.69
1.99	25.83	25.93	26.14	25.97	4.69	4.74	4.74	4.72

**Appendix 13.8 - Descriptive Statistics for Surface Tension Measurement Results of DI + SDS + Graphene**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.82	Exp.1	45.91	50.35	1.15	1.33	-0.13	-1.12
	Exp.2	45.27	50.96	1.54	2.36	0.30	-0.91
	Exp.3	45.71	49.47	1.03	1.05	0.23	-1.05
	Average	45.70	50.20	1.23	1.52	0.15	-1.06
3.00	Exp.1	22.52	22.71	0.05	0.00	0.21	-0.95
	Exp.2	21.40	21.45	0.01	0.00	0.05	-0.04
	Exp.3	21.51	21.57	0.01	0.00	-0.22	-0.29
	Average	21.82	21.90	0.02	0.00	0.20	-0.71
6.00	Exp.1	25.38	26.44	0.32	0.10	0.28	-1.12
	Exp.2	24.70	25.11	0.12	0.01	0.10	-1.23
	Exp.3	23.95	24.22	0.08	0.01	0.11	-1.16
	Average	24.68	25.25	0.17	0.03	0.21	-1.18
8.20	Exp.1	21.53	21.97	0.13	0.02	0.16	-1.26
	Exp.2	21.51	21.87	0.10	0.01	0.25	-1.20
	Exp.3	21.55	21.82	0.08	0.01	0.32	-1.11
	Average	21.53	21.88	0.10	0.01	0.25	-1.20
44.30	Exp.1	27.42	28.02	0.17	0.03	0.63	-0.77
	Exp.2	27.98	28.50	0.15	0.02	-0.02	-1.26
	Exp.3	26.75	27.17	0.12	0.01	0.04	-1.29
	Average	27.39	27.89	0.14	0.02	0.24	-1.15
59.00	Exp.1	24.44	24.67	0.07	0.00	0.63	-0.90
	Exp.2	25.18	25.33	0.04	0.00	0.47	-0.76
	Exp.3	24.06	24.51	0.13	0.02	0.19	-1.15
	Average	24.59	24.82	0.07	0.00	0.53	-1.07
82.00	Exp.1	25.78	25.90	0.02	0.00	-0.61	0.53
	Exp.2	25.88	26.01	0.03	0.00	-0.30	-0.47
	Exp.3	26.04	26.23	0.05	0.00	-0.40	-0.96
	Average	25.94	26.02	0.02	0.00	-0.05	-0.92



**APPENDIX 13.9 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(0.82 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (0.82 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	49.92	51.23	49.06	50.07	3.96	3.89	4.01	3.95
0.01	47.54	50.46	50.52	49.51	3.95	3.89	4.01	3.95
0.03	49.65	51.06	48.85	49.85	3.95	3.88	4.01	3.95
0.04	47.56	50.63	50.64	49.61	3.96	3.88	4.01	3.95
0.05	49.71	51.03	48.87	49.87	3.95	3.89	4.01	3.95
0.07	47.64	50.64	50.75	49.68	3.95	3.89	4.01	3.95
0.08	49.50	50.84	48.60	49.64	3.95	3.88	4.01	3.95
0.09	47.66	50.83	50.83	49.77	3.96	3.89	4.01	3.95
0.11	49.57	50.87	48.81	49.75	3.95	3.88	4.01	3.95
0.13	48.81	50.88	48.69	49.46	3.95	3.89	4.01	3.95
0.14	48.08	50.90	51.09	50.02	3.95	3.88	4.01	3.95
0.16	48.63	50.86	48.65	49.38	3.95	3.88	4.01	3.95
0.17	48.50	51.01	50.96	50.16	3.95	3.89	4.01	3.95
0.18	47.93	50.78	48.57	49.10	3.96	3.88	4.01	3.95
0.20	49.07	50.93	51.29	50.43	3.95	3.89	4.01	3.95
0.21	47.83	50.80	48.24	48.95	3.95	3.89	4.01	3.95
0.22	49.32	50.99	51.52	50.61	3.95	3.89	4.01	3.95
0.25	50.11	50.93	51.53	50.86	3.95	3.88	4.01	3.95
0.28	49.98	50.86	51.58	50.80	3.95	3.88	4.01	3.95
0.29	47.24	50.79	48.29	48.77	3.96	3.89	4.01	3.95
0.30	49.92	50.88	51.45	50.75	3.94	3.88	4.01	3.95
0.32	47.37	50.78	48.38	48.85	3.95	3.88	4.01	3.95
0.33	49.90	50.86	51.40	50.72	3.95	3.89	4.01	3.95
0.34	47.45	50.92	48.48	48.95	3.96	3.89	4.01	3.95
0.37	47.52	50.94	48.75	49.07	3.96	3.88	4.01	3.95
0.38	49.63	50.80	50.67	50.37	3.95	3.88	4.01	3.95
0.40	47.62	50.84	49.06	49.17	3.95	3.89	4.01	3.95
0.38	49.63	50.80	50.67	50.37	3.95	3.88	4.01	3.95
0.41	49.01	50.75	50.20	49.98	3.95	3.89	4.01	3.95
0.42	48.01	51.03	49.39	49.48	3.95	3.89	4.01	3.95
0.43	48.84	50.90	49.58	49.78	3.95	3.88	4.01	3.95
0.45	48.26	50.85	49.76	49.62	3.95	3.89	4.00	3.95

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	48.94	50.82	50.42	50.06	3.95	3.88	4.01	3.95
0.49	47.98	50.88	48.80	49.22	3.95	3.88	4.01	3.95
0.50	48.99	50.91	50.74	50.21	3.95	3.88	4.01	3.95
0.51	47.81	50.91	48.62	49.11	3.96	3.89	4.01	3.95
0.53	49.43	50.83	51.16	50.47	3.95	3.88	4.01	3.95
0.54	47.41	50.90	48.32	48.88	3.95	3.88	4.01	3.95
0.55	49.95	50.78	51.36	50.70	3.95	3.88	4.01	3.95
0.57	47.15	50.84	48.41	48.80	3.95	3.88	4.01	3.95
0.58	50.01	50.58	51.59	50.73	3.95	3.89	4.01	3.95
0.59	47.18	51.12	48.29	48.86	3.96	3.88	4.01	3.95
0.61	49.93	50.67	51.66	50.75	3.96	3.88	4.01	3.95
0.62	47.49	51.21	48.08	48.93	3.95	3.88	4.01	3.95
0.63	49.51	50.45	51.42	50.46	3.96	3.89	4.01	3.95
0.65	47.62	51.32	48.22	49.05	3.95	3.88	4.01	3.95
0.66	49.04	50.50	51.36	50.30	3.96	3.88	4.01	3.95
0.67	48.28	51.44	48.32	49.35	3.95	3.89	4.01	3.95
0.68	48.41	50.39	51.25	50.02	3.95	3.88	4.01	3.95
0.70	48.56	51.40	48.43	49.47	3.95	3.88	4.00	3.95
0.71	48.06	50.48	50.85	49.80	3.95	3.89	4.01	3.95
0.72	49.31	51.52	48.45	49.76	3.95	3.88	4.01	3.95
0.74	47.78	50.46	50.71	49.65	3.96	3.88	4.01	3.95
0.75	49.31	51.26	48.57	49.71	3.96	3.88	4.01	3.95
0.76	47.77	50.48	50.44	49.56	4.17	3.88	4.01	4.02
0.78	49.48	51.41	48.97	49.95	3.95	3.88	4.01	3.95
0.79	47.53	50.50	50.19	49.41	3.95	3.88	4.01	3.95
0.80	49.63	51.17	49.26	50.02	3.95	3.88	4.01	3.95
0.82	47.72	50.52	49.75	49.33	3.95	3.88	4.01	3.95
0.84	47.88	50.50	49.51	49.30	3.96	3.88	4.01	3.95
0.86	48.94	51.07	49.68	49.89	3.96	3.89	4.01	3.95
0.87	48.22	50.69	49.26	49.39	3.95	3.89	4.01	3.95
0.88	48.33	51.10	49.98	49.80	3.95	3.89	4.01	3.95
0.87	48.22	50.69	49.26	49.39	3.95	3.89	4.01	3.95
0.90	48.55	50.81	49.17	49.51	3.95	3.88	4.01	3.95
0.91	48.25	50.95	49.97	49.72	3.95	3.88	4.01	3.95
0.92	48.68	50.84	49.19	49.57	3.95	3.88	4.01	3.95
0.95	49.24	50.80	48.83	49.62	3.95	3.89	4.01	3.95
0.96	47.79	50.82	50.62	49.74	3.94	3.88	4.01	3.95

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	47.65	50.77	50.44	49.62	3.95	3.88	4.01	3.95
1.00	49.66	50.77	48.65	49.69	3.95	3.88	4.01	3.95
1.01	47.44	50.86	50.88	49.72	3.95	3.88	4.01	3.95
1.03	49.33	50.84	48.72	49.63	3.95	3.88	4.01	3.95
1.04	47.86	50.62	50.63	49.70	3.95	3.88	4.01	3.95
1.05	49.13	51.02	48.48	49.55	3.95	3.89	4.01	3.95
1.07	47.53	50.86	50.62	49.67	3.96	3.88	4.01	3.95
1.08	49.52	50.91	48.70	49.71	3.95	3.88	4.01	3.95
1.09	47.58	50.73	50.62	49.64	3.95	3.88	4.01	3.95
1.11	49.33	50.95	48.97	49.75	3.95	3.89	4.01	3.95
1.12	47.75	50.88	50.03	49.55	3.96	3.88	4.01	3.95
1.13	49.04	50.77	49.19	49.66	3.95	3.88	4.01	3.95
1.15	47.99	50.80	50.37	49.72	3.95	3.88	4.01	3.95
1.16	48.66	50.94	49.01	49.54	3.95	3.88	4.01	3.95
1.17	48.18	51.02	49.94	49.71	3.95	3.88	4.01	3.95
1.19	48.30	50.67	49.11	49.36	3.95	3.88	4.01	3.95
1.20	48.58	51.01	50.05	49.88	3.95	3.88	4.01	3.95
1.21	48.24	50.68	49.26	49.39	3.95	3.88	4.01	3.95
1.22	48.73	50.99	49.92	49.88	3.95	3.88	4.01	3.95
1.24	47.95	50.74	49.17	49.29	3.95	3.88	4.01	3.95
1.26	48.02	50.63	48.93	49.19	3.95	3.88	4.01	3.95
1.28	48.87	51.00	50.46	50.11	3.95	3.88	4.00	3.95
1.29	47.96	50.70	48.69	49.11	3.95	3.88	4.01	3.95
1.30	49.31	51.06	50.94	50.44	3.95	3.88	4.01	3.94
1.32	47.71	50.65	48.46	48.94	3.95	3.88	4.01	3.95
1.33	49.24	51.08	51.33	50.55	3.95	3.88	4.00	3.95
1.34	47.94	50.68	48.12	48.91	3.95	3.88	4.01	3.95
1.37	48.04	50.74	48.09	48.96	3.95	3.88	4.01	3.95
1.38	48.76	50.85	51.71	50.44	3.95	3.88	4.01	3.95
1.40	48.33	50.89	48.00	49.07	3.95	3.88	4.01	3.95
1.41	48.52	50.83	51.57	50.31	3.95	3.88	4.01	3.95
1.42	47.90	50.96	48.27	49.05	3.95	3.88	4.01	3.95
1.44	48.68	50.80	51.32	50.27	3.95	3.88	4.01	3.95
1.45	48.33	51.10	48.28	49.24	3.95	3.88	4.01	3.95
1.44	48.68	50.80	51.32	50.27	3.95	3.88	4.01	3.95
1.46	48.37	50.59	50.99	49.99	3.95	3.88	4.01	3.95
1.48	48.31	51.12	48.63	49.36	3.95	3.88	4.01	3.95

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	48.46	51.17	49.00	49.55	3.95	3.88	4.01	3.94
1.51	48.14	50.45	50.06	49.55	3.95	3.88	4.01	3.95
1.53	48.29	51.36	49.23	49.63	3.95	3.88	4.01	3.95
1.54	48.48	50.51	49.53	49.51	3.95	3.88	4.01	3.94
1.55	48.30	51.30	49.79	49.80	3.95	3.89	4.01	3.95
1.57	48.09	50.35	49.08	49.17	3.95	3.88	4.01	3.95
1.58	49.11	51.37	50.25	50.24	3.94	3.88	4.01	3.94
1.59	47.75	50.45	48.86	49.02	3.95	3.88	4.01	3.94
1.61	49.13	51.10	50.96	50.40	3.95	3.88	4.01	3.95
1.62	47.70	50.60	48.25	48.85	3.95	3.88	4.01	3.95
1.63	49.62	51.27	51.21	50.70	3.95	3.88	4.01	3.95
1.65	47.38	50.67	48.20	48.75	3.95	3.88	4.00	3.95
1.66	49.94	51.13	51.22	50.76	3.95	3.88	4.00	3.95
1.67	47.41	50.58	47.93	48.64	3.95	3.88	4.01	3.95
1.69	49.92	50.99	51.39	50.76	3.95	3.88	4.01	3.95
1.70	47.23	50.75	48.11	48.70	4.25	3.88	4.01	4.04
1.71	50.10	51.01	51.51	50.87	3.95	3.88	4.01	3.95
1.73	47.26	50.81	48.00	48.69	3.95	3.88	4.01	3.95
1.75	47.65	51.04	47.95	48.88	3.95	3.88	4.01	3.95
1.76	49.33	50.72	51.38	50.48	3.95	3.88	4.01	3.94
1.78	47.93	50.92	48.40	49.09	3.95	3.88	4.00	3.95
1.79	48.38	50.69	50.79	49.95	3.95	3.88	4.01	3.94
1.80	48.87	51.08	48.67	49.54	3.95	3.88	4.01	3.94
1.82	47.70	50.71	50.82	49.74	3.95	3.88	4.00	3.94
1.83	49.18	50.99	48.58	49.58	3.95	3.88	4.01	3.95
1.84	47.50	50.67	50.74	49.63	3.95	3.88	4.01	3.95
1.86	49.99	51.03	48.67	49.90	3.96	3.88	4.01	3.95
1.87	46.90	50.74	50.51	49.39	3.95	3.88	4.00	3.94
1.88	50.37	51.01	48.89	50.09	3.95	3.88	4.01	3.95
1.90	46.70	50.75	50.24	49.23	3.95	3.88	4.00	3.94
1.91	50.66	51.09	49.09	50.28	3.95	3.88	4.01	3.95
1.92	46.61	50.63	50.10	49.11	4.17	3.88	4.01	4.02
1.94	50.22	51.10	48.92	50.08	3.95	3.88	4.01	3.95
1.95	47.22	50.61	50.19	49.34	3.95	3.88	4.01	3.95
1.96	50.22	50.87	48.98	50.02	3.95	3.88	4.00	3.94
1.98	47.22	50.78	50.28	49.43	3.95	3.88	4.01	3.95
1.99	49.53	51.00	48.91	49.81	3.95	3.88	4.00	3.95

**APPENDIX 13.10 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(3.00 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (3.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	21.44	22.47	21.81	21.91	3.83	3.92	3.94	3.90
0.01	21.43	22.46	21.82	21.91	3.79	3.97	3.90	3.89
0.03	21.44	22.48	21.81	21.91	3.79	3.92	3.90	3.87
0.04	21.45	22.47	21.81	21.91	3.79	3.97	3.94	3.90
0.05	21.45	22.49	21.81	21.92	3.66	3.96	3.94	3.85
0.07	21.44	22.52	21.80	21.92	3.93	3.92	3.90	3.92
0.08	21.44	22.51	21.80	21.92	3.94	3.96	3.94	3.95
0.09	21.44	22.49	21.80	21.91	4.04	3.92	3.94	3.96
0.11	21.47	22.47	21.81	21.92	4.04	3.92	3.86	3.94
0.12	21.46	22.48	21.79	21.91	4.00	3.92	3.94	3.95
0.13	21.45	22.47	21.81	21.91	4.00	3.96	3.94	3.97
0.14	21.45	22.47	21.81	21.91	4.00	3.96	3.90	3.95
0.16	21.44	22.49	21.80	21.91	4.00	3.96	3.90	3.95
0.17	21.43	22.51	21.80	21.91	4.00	3.91	3.94	3.95
0.18	21.45	22.50	21.80	21.92	4.00	3.92	3.90	3.94
0.20	21.45	22.49	21.79	21.91	4.00	3.96	3.94	3.97
0.21	21.47	22.46	21.80	21.91	4.00	3.92	3.90	3.94
0.22	21.48	22.47	21.80	21.92	3.99	3.85	3.90	3.91
0.25	21.46	22.47	21.80	21.91	4.00	3.91	3.94	3.95
0.28	21.44	22.49	21.80	21.91	4.00	3.91	3.90	3.93
0.29	21.46	22.50	21.79	21.91	3.99	3.92	3.90	3.94
0.30	21.46	22.48	21.81	21.92	4.00	3.96	3.94	3.97
0.32	21.47	22.48	21.80	21.91	3.99	3.96	3.90	3.95
0.33	21.47	22.46	21.81	21.91	4.00	3.91	3.94	3.95
0.34	21.46	22.46	21.80	21.91	3.99	3.91	3.90	3.93
0.37	21.45	22.45	21.80	21.90	4.00	3.91	3.90	3.93
0.34	21.46	22.46	21.80	21.91	3.99	3.91	3.90	3.93
0.38	21.44	22.46	21.80	21.90	3.99	3.91	3.90	3.93
0.40	21.45	22.46	21.80	21.90	3.99	3.91	3.90	3.93
0.41	21.46	22.47	21.80	21.91	3.99	3.91	3.90	3.93
0.43	21.46	22.47	21.81	21.91	3.99	3.91	3.90	3.93
0.45	21.46	22.43	21.80	21.90	4.00	3.91	3.90	3.93

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	21.46	22.43	21.81	21.90	4.00	3.96	3.90	3.95
0.49	21.45	22.43	21.80	21.89	3.99	3.91	3.90	3.93
0.50	21.44	22.45	21.80	21.90	3.99	3.96	3.90	3.95
0.51	21.47	22.48	21.82	21.92	3.99	3.91	3.90	3.93
0.53	21.47	22.47	21.82	21.92	3.99	3.91	3.90	3.93
0.54	21.45	22.46	21.81	21.91	3.99	3.84	3.90	3.91
0.55	21.45	22.44	21.81	21.90	3.99	3.91	3.90	3.93
0.57	21.46	22.44	21.81	21.90	4.00	3.96	3.90	3.95
0.58	21.43	22.43	21.79	21.88	3.99	3.91	3.90	3.93
0.59	21.45	22.45	21.80	21.90	4.00	3.96	3.90	3.95
0.61	21.45	22.45	21.80	21.90	3.99	3.91	3.89	3.93
0.59	21.45	22.45	21.80	21.90	4.00	3.96	3.90	3.95
0.62	21.46	22.47	21.81	21.91	3.99	3.85	3.90	3.91
0.63	21.46	22.48	21.80	21.92	3.99	3.91	3.89	3.93
0.66	21.45	22.45	21.80	21.90	3.99	3.91	3.89	3.93
0.67	21.47	22.44	21.80	21.90	3.99	3.84	3.90	3.91
0.68	21.45	22.44	21.80	21.90	3.99	3.96	3.89	3.95
0.70	21.43	22.44	21.81	21.89	3.99	3.91	3.90	3.93
0.71	21.47	22.44	21.79	21.90	3.99	3.90	3.90	3.93
0.72	21.47	22.45	21.81	21.91	3.99	3.91	3.90	3.93
0.74	21.47	22.47	21.81	21.92	3.99	3.90	3.90	3.93
0.75	21.46	22.46	21.79	21.91	3.99	3.85	3.90	3.91
0.76	21.47	22.46	21.79	21.91	3.96	3.90	3.90	3.92
0.78	21.46	22.44	21.79	21.90	3.99	3.91	3.90	3.93
0.80	21.45	22.43	21.78	21.89	3.96	3.91	3.89	3.92
0.82	21.45	22.43	21.80	21.89	3.99	3.90	3.90	3.93
0.83	21.45	22.44	21.79	21.89	3.99	3.91	3.89	3.93
0.84	21.45	22.43	21.79	21.89	3.99	3.90	3.90	3.93
0.86	21.46	22.45	21.79	21.90	3.99	3.85	3.89	3.91
0.87	21.47	22.46	21.79	21.91	3.96	3.85	3.90	3.90
0.88	21.46	22.44	21.78	21.89	3.96	3.90	3.90	3.92
0.90	21.45	22.43	21.79	21.89	3.99	3.91	3.90	3.93
0.91	21.45	22.42	21.79	21.89	3.96	3.96	3.90	3.94
0.92	21.44	22.41	21.79	21.88	3.99	3.85	3.89	3.91
0.94	21.45	22.40	21.79	21.88	3.99	3.91	3.90	3.93
0.95	21.45	22.42	21.79	21.88	3.99	3.90	3.89	3.93
0.96	21.47	22.43	21.78	21.89	3.99	4.00	3.90	3.96

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	21.47	22.45	21.78	21.90	3.99	3.90	3.90	3.93
1.00	21.47	22.44	21.77	21.89	3.99	3.91	3.86	3.92
1.01	21.43	22.41	21.79	21.88	3.96	4.00	3.86	3.94
1.03	21.43	22.39	21.77	21.87	3.99	3.90	3.86	3.92
1.04	21.44	22.41	21.76	21.87	3.99	3.90	3.86	3.92
1.05	21.46	22.42	21.77	21.88	3.99	3.90	3.89	3.93
1.07	21.47	22.45	21.79	21.90	3.99	3.90	3.89	3.93
1.08	21.47	22.45	21.77	21.90	3.96	3.90	3.93	3.93
1.09	21.47	22.46	21.77	21.90	3.96	3.77	3.89	3.87
1.11	21.47	22.45	21.77	21.90	3.99	3.90	3.90	3.93
1.12	21.45	22.42	21.75	21.87	3.96	3.96	3.89	3.93
1.13	21.45	22.42	21.74	21.87	3.99	3.95	3.86	3.93
1.15	21.45	22.42	21.76	21.88	3.99	3.90	3.93	3.94
1.16	21.45	22.42	21.77	21.88	3.99	3.90	3.89	3.93
1.17	21.47	22.45	21.77	21.90	3.96	3.91	3.85	3.91
1.19	21.46	22.47	21.78	21.90	3.99	3.91	3.89	3.93
1.20	21.48	22.46	21.77	21.90	3.96	3.84	3.89	3.90
1.21	21.48	22.46	21.75	21.90	3.99	4.04	3.89	3.97
1.22	21.48	22.44	21.75	21.89	3.96	3.84	3.86	3.88
1.24	21.47	22.41	21.76	21.88	3.96	3.84	3.89	3.90
1.25	21.45	22.41	21.75	21.87	3.99	3.84	3.86	3.90
1.26	21.44	22.41	21.76	21.87	3.99	3.90	3.89	3.93
1.25	21.45	22.41	21.75	21.87	3.99	3.84	3.86	3.90
1.28	21.46	22.41	21.76	21.88	3.99	3.95	3.86	3.93
1.30	21.47	22.44	21.77	21.89	3.99	3.90	3.89	3.93
1.32	21.46	22.45	21.75	21.89	3.96	3.84	3.89	3.90
1.34	21.45	22.40	21.74	21.87	3.99	3.84	3.89	3.91
1.36	21.44	22.39	21.76	21.86	3.99	3.90	3.89	3.93
1.37	21.44	22.39	21.75	21.86	3.99	4.03	3.89	3.97
1.38	21.45	22.39	21.75	21.86	3.99	3.90	3.89	3.93
1.40	21.47	22.38	21.76	21.87	3.96	3.90	3.89	3.92
1.41	21.47	22.42	21.75	21.88	3.99	3.95	3.89	3.95
1.42	21.47	22.43	21.76	21.89	3.96	3.84	3.89	3.90
1.44	21.45	22.42	21.75	21.87	3.99	4.00	3.89	3.96
1.45	21.45	22.40	21.75	21.87	3.99	3.95	3.89	3.94
1.46	21.45	22.38	21.75	21.86	3.99	3.95	3.89	3.94
1.48	21.45	22.36	21.75	21.85	3.99	4.07	3.89	3.98

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	21.47	22.38	21.76	21.87	3.99	3.99	3.89	3.96
1.51	21.47	22.38	21.74	21.87	3.96	3.94	3.89	3.93
1.53	21.48	22.40	21.77	21.88	3.95	3.95	3.89	3.93
1.54	21.47	22.43	21.75	21.88	3.99	3.95	3.89	3.94
1.55	21.46	22.42	21.75	21.87	3.96	3.99	3.89	3.94
1.57	21.45	22.40	21.74	21.86	3.99	4.07	3.89	3.98
1.58	21.44	22.38	21.75	21.86	3.99	4.07	3.89	3.98
1.59	21.46	22.37	21.74	21.86	3.99	3.99	3.89	3.96
1.61	21.46	22.38	21.74	21.86	3.95	3.94	3.89	3.93
1.62	21.46	22.37	21.77	21.87	3.99	4.11	3.89	4.00
1.63	21.49	22.41	21.74	21.88	3.99	3.94	3.89	3.94
1.65	21.46	22.42	21.76	21.88	3.99	4.03	3.89	3.97
1.66	21.45	22.43	21.76	21.88	3.96	3.94	3.89	3.93
1.67	21.45	22.41	21.75	21.87	3.99	3.99	3.89	3.96
1.70	21.46	22.37	21.76	21.87	3.95	4.07	3.89	3.97
1.71	21.46	22.37	21.75	21.86	3.99	4.03	3.89	3.97
1.73	21.46	22.37	21.75	21.86	3.99	4.07	3.89	3.98
1.74	21.46	22.39	21.75	21.87	3.96	3.99	3.89	3.94
1.75	21.45	22.41	21.75	21.87	3.99	4.07	3.89	3.98
1.76	21.45	22.42	21.74	21.87	3.96	3.94	3.89	3.93
1.78	21.45	22.41	21.74	21.87	3.99	4.07	3.89	3.98
1.80	21.45	22.38	21.74	21.86	3.96	4.06	3.89	3.97
1.82	21.46	22.38	21.75	21.86	3.99	3.94	3.89	3.94
1.83	21.46	22.37	21.75	21.86	3.96	4.10	3.89	3.98
1.84	21.45	22.37	21.77	21.86	3.95	4.02	3.89	3.96
1.86	21.45	22.37	21.75	21.86	3.96	3.98	3.89	3.94
1.87	21.46	22.37	21.75	21.86	3.95	3.94	3.89	3.93
1.88	21.46	22.38	21.74	21.86	3.96	4.06	3.89	3.97
1.90	21.47	22.38	21.73	21.86	3.95	3.98	3.89	3.94
1.91	21.47	22.36	21.74	21.85	3.96	3.98	3.89	3.94
1.92	21.45	22.36	21.74	21.85	3.95	3.98	3.85	3.93
1.94	21.44	22.36	21.75	21.85	3.99	3.98	3.89	3.95
1.95	21.45	22.36	21.76	21.85	3.95	4.06	3.89	3.97
1.96	21.46	22.35	21.75	21.85	3.99	4.06	3.89	3.98
1.98	21.46	22.35	21.74	21.85	3.95	4.06	3.89	3.97
1.99	21.46	22.35	21.74	21.85	3.95	4.06	3.89	3.97



**APPENDIX 13.11 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(6.00 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (6.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	24.35	24.51	25.34	24.73	4.20	3.86	4.31	4.13
0.01	24.36	24.51	25.34	24.74	4.20	3.86	4.31	4.13
0.03	24.36	24.50	25.34	24.73	4.20	3.86	4.31	4.13
0.04	24.35	24.52	25.33	24.74	4.20	3.86	4.31	4.13
0.05	24.33	24.46	25.34	24.71	4.20	3.86	4.31	4.13
0.07	24.33	24.42	25.34	24.69	4.20	3.86	4.31	4.13
0.08	24.32	24.42	25.33	24.69	4.20	3.86	4.31	4.13
0.09	24.34	24.46	25.33	24.71	4.20	3.86	4.31	4.13
0.11	24.32	24.43	25.34	24.70	4.20	3.86	4.31	4.13
0.12	24.33	24.52	25.32	24.72	4.20	3.86	4.31	4.13
0.13	24.35	24.50	25.34	24.73	4.20	3.86	4.31	4.13
0.14	24.34	24.50	25.35	24.73	4.20	3.86	4.31	4.13
0.16	24.32	24.48	25.34	24.71	4.20	3.86	4.31	4.13
0.17	24.34	24.45	25.35	24.71	4.20	3.86	4.31	4.13
0.18	24.33	24.44	25.34	24.70	4.20	3.86	4.31	4.13
0.20	24.33	24.49	25.35	24.72	4.20	3.87	4.31	4.13
0.21	24.33	24.50	25.34	24.72	4.20	3.87	4.31	4.13
0.22	24.34	24.48	25.33	24.72	4.20	3.87	4.31	4.13
0.25	24.32	24.42	25.36	24.70	4.20	3.86	4.31	4.13
0.28	24.33	24.44	25.33	24.70	4.20	3.89	4.31	4.14
0.29	24.32	24.47	25.33	24.71	4.20	3.89	4.31	4.14
0.30	24.32	24.47	25.34	24.71	4.20	3.89	4.31	4.14
0.33	24.31	24.40	25.34	24.68	4.20	3.89	4.31	4.14
0.34	24.31	24.40	25.33	24.68	4.20	3.89	4.31	4.14
0.37	24.31	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.38	24.32	24.42	25.34	24.69	4.20	3.89	4.31	4.14
0.37	24.31	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.40	24.33	24.46	25.33	24.71	4.20	3.89	4.31	4.14
0.41	24.31	24.43	25.33	24.69	4.20	3.89	4.31	4.14
0.42	24.30	24.42	25.34	24.68	4.20	3.89	4.31	4.14
0.43	24.31	24.43	25.32	24.69	4.20	3.89	4.31	4.14
0.45	24.31	24.40	25.34	24.68	4.20	3.89	4.31	4.14

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	24.30	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.49	24.31	24.40	25.33	24.68	4.20	3.89	4.31	4.14
0.50	24.31	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.51	24.30	24.43	25.33	24.69	4.20	3.89	4.31	4.14
0.50	24.31	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.53	24.30	24.43	25.33	24.69	4.20	3.89	4.31	4.14
0.54	24.30	24.42	25.32	24.68	4.20	3.89	4.31	4.14
0.55	24.30	24.41	25.34	24.68	4.20	3.89	4.31	4.14
0.57	24.30	24.41	25.33	24.68	4.20	3.89	4.31	4.14
0.58	24.30	24.40	25.34	24.68	4.20	3.86	4.31	4.12
0.59	24.29	24.39	25.33	24.67	4.20	3.89	4.31	4.14
0.61	24.31	24.41	25.35	24.69	4.20	3.89	4.31	4.14
0.62	24.29	24.41	25.34	24.68	4.20	3.89	4.31	4.14
0.63	24.29	24.42	25.33	24.68	4.20	3.89	4.31	4.14
0.65	24.30	24.43	25.32	24.68	4.20	3.89	4.31	4.14
0.66	24.30	24.42	25.34	24.69	4.20	3.89	4.31	4.14
0.67	24.29	24.40	25.33	24.67	4.20	3.89	4.31	4.13
0.68	24.29	24.39	25.30	24.66	4.20	3.89	4.31	4.14
0.70	24.30	24.38	25.32	24.67	4.20	3.89	4.31	4.14
0.72	24.30	24.39	25.33	24.67	4.20	3.89	4.31	4.13
0.74	24.27	24.40	25.31	24.66	4.20	3.89	4.31	4.13
0.75	24.28	24.42	25.32	24.67	4.20	3.89	4.31	4.14
0.76	24.29	24.43	25.32	24.68	4.20	3.89	4.31	4.13
0.78	24.29	24.39	25.30	24.66	4.20	3.89	4.31	4.14
0.79	24.28	24.38	25.31	24.66	4.20	3.89	4.31	4.14
0.80	24.29	24.38	25.32	24.66	4.20	3.89	4.31	4.13
0.82	24.29	24.39	25.30	24.66	4.20	3.89	4.31	4.13
0.83	24.28	24.40	25.31	24.66	4.20	3.89	4.31	4.13
0.84	24.28	24.42	25.32	24.67	4.15	3.89	4.31	4.12
0.87	24.27	24.42	25.31	24.66	4.20	3.89	4.31	4.14
0.88	24.27	24.41	25.32	24.67	4.15	3.89	4.31	4.12
0.90	24.28	24.40	25.33	24.67	4.15	3.89	4.31	4.12
0.91	24.27	24.38	25.32	24.66	4.15	3.89	4.31	4.12
0.92	24.28	24.39	25.30	24.66	4.15	3.89	4.31	4.12
0.94	24.28	24.39	25.31	24.66	4.15	3.89	4.31	4.12
0.95	24.28	24.39	25.32	24.66	4.20	3.89	4.31	4.14
0.96	24.26	24.40	25.31	24.66	4.15	3.89	4.31	4.12

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	24.26	24.40	25.31	24.66	4.15	3.89	4.31	4.12
1.00	24.28	24.40	25.30	24.66	4.15	3.89	4.31	4.12
1.01	24.27	24.39	25.30	24.65	4.15	3.89	4.31	4.12
1.03	24.27	24.40	25.31	24.66	4.15	3.89	4.31	4.12
1.04	24.26	24.39	25.31	24.65	4.15	3.89	4.31	4.12
1.05	24.27	24.40	25.30	24.66	4.20	3.89	4.31	4.13
1.07	24.27	24.39	25.32	24.66	4.15	3.89	4.31	4.12
1.08	24.28	24.41	25.32	24.67	4.15	3.89	4.31	4.12
1.09	24.25	24.40	25.33	24.66	4.15	3.89	4.31	4.12
1.11	24.27	24.40	25.30	24.66	4.15	3.89	4.31	4.12
1.12	24.27	24.39	25.31	24.66	4.15	3.89	4.31	4.12
1.13	24.26	24.39	25.31	24.65	4.15	3.89	4.31	4.12
1.15	24.25	24.39	25.32	24.65	4.15	3.89	4.31	4.12
1.16	24.26	24.37	25.32	24.65	4.15	3.89	4.31	4.12
1.19	24.24	24.38	25.28	24.64	4.15	3.89	4.31	4.12
1.20	24.26	24.38	25.31	24.65	4.15	3.89	4.31	4.12
1.21	24.27	24.40	25.28	24.65	4.15	3.89	4.31	4.12
1.22	24.26	24.39	25.29	24.65	4.15	3.89	4.31	4.12
1.24	24.26	24.36	25.27	24.63	4.15	3.89	4.31	4.12
1.25	24.25	24.38	25.30	24.64	4.15	3.89	4.31	4.12
1.26	24.25	24.38	25.28	24.64	4.15	3.89	4.31	4.12
1.28	24.24	24.37	25.29	24.63	4.15	3.89	4.31	4.12
1.28	24.24	24.37	25.29	24.63	4.15	3.89	4.31	4.12
1.29	24.25	24.38	25.30	24.65	4.15	3.89	4.31	4.12
1.30	24.26	24.39	25.28	24.64	4.15	3.89	4.31	4.12
1.32	24.25	24.40	25.28	24.64	4.15	3.89	4.31	4.12
1.33	24.24	24.39	25.28	24.64	4.15	3.89	4.31	4.12
1.34	24.23	24.38	25.29	24.64	4.15	3.89	4.31	4.12
1.36	24.24	24.38	25.30	24.64	4.15	3.89	4.31	4.12
1.37	24.24	24.39	25.28	24.64	4.15	3.86	4.31	4.10
1.38	24.23	24.37	25.29	24.63	4.15	3.89	4.31	4.12
1.41	24.26	24.39	25.28	24.64	4.15	3.89	4.31	4.12
1.42	24.26	24.39	25.27	24.64	4.15	3.89	4.31	4.12
1.44	24.25	24.39	25.30	24.65	4.15	3.89	4.31	4.12
1.45	24.23	24.38	25.29	24.63	4.15	3.89	4.31	4.12
1.46	24.22	24.39	25.28	24.63	4.15	3.89	4.31	4.12
1.48	24.22	24.37	25.27	24.62	4.15	3.89	4.31	4.12

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	24.23	24.36	25.25	24.62	4.15	3.85	4.31	4.10
1.51	24.24	24.46	25.28	24.66	4.15	3.90	4.31	4.12
1.53	24.24	24.32	25.28	24.61	4.15	3.85	4.31	4.10
1.54	24.23	24.40	25.27	24.63	4.15	3.80	4.31	4.09
1.55	24.26	24.28	25.28	24.61	4.15	3.85	4.31	4.10
1.57	24.22	24.45	25.26	24.64	4.15	3.87	4.31	4.11
1.58	24.21	24.40	25.27	24.63	4.15	3.86	4.31	4.11
1.59	24.20	24.42	25.27	24.63	4.15	3.86	4.31	4.11
1.61	24.21	24.34	25.28	24.61	4.15	3.85	4.31	4.10
1.62	24.21	24.38	25.27	24.62	4.15	3.86	4.31	4.11
1.63	24.22	24.34	25.27	24.61	4.15	3.85	4.31	4.10
1.65	24.21	24.43	25.28	24.64	4.15	3.86	4.31	4.10
1.66	24.23	24.46	25.26	24.65	4.15	3.89	4.31	4.12
1.67	24.22	24.42	25.25	24.63	4.15	3.85	4.31	4.10
1.69	24.21	24.39	25.27	24.63	4.15	3.89	4.31	4.12
1.70	24.21	24.34	25.26	24.60	4.15	3.85	4.31	4.10
1.71	24.21	24.33	25.26	24.60	4.15	3.85	4.31	4.10
1.73	24.20	24.40	25.27	24.62	4.15	3.89	4.31	4.12
1.74	24.21	24.42	25.27	24.63	4.15	3.86	4.31	4.10
1.75	24.21	24.39	25.28	24.63	4.15	3.89	4.31	4.12
1.76	24.20	24.38	25.27	24.62	4.15	3.85	4.31	4.10
1.78	24.23	24.37	25.26	24.62	4.15	3.86	4.31	4.10
1.79	24.21	24.35	25.26	24.60	4.14	3.86	4.31	4.11
1.80	24.20	24.43	25.27	24.63	4.15	3.89	4.31	4.12
1.82	24.18	24.43	25.26	24.62	4.15	3.87	4.31	4.11
1.83	24.18	24.37	25.25	24.60	4.15	3.87	4.31	4.11
1.86	24.21	24.44	25.26	24.64	4.15	3.87	4.31	4.11
1.87	24.20	24.40	25.26	24.62	4.15	3.87	4.31	4.11
1.88	24.20	24.42	25.24	24.62	4.15	3.87	4.31	4.11
1.90	24.20	24.43	25.27	24.63	4.15	3.86	4.31	4.11
1.92	24.19	24.41	25.25	24.62	4.15	3.86	4.31	4.11
1.94	24.20	24.40	25.28	24.63	4.15	3.86	4.31	4.11
1.95	24.21	24.44	25.26	24.64	4.15	3.89	4.31	4.12
1.96	24.19	24.41	25.25	24.62	4.15	3.89	4.31	4.12
1.98	24.19	24.34	25.24	24.59	4.15	3.86	4.31	4.11
1.99	24.18	24.36	25.26	24.60	4.15	3.86	4.31	4.10

**Appendix 13.12 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(8.20 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (8.20 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	21.82	21.79	21.93	21.85	3.98	4.19	4.00	4.06
0.01	21.81	21.78	21.93	21.84	3.98	4.19	4.00	4.06
0.03	21.82	21.78	21.92	21.84	3.98	4.19	4.00	4.06
0.04	21.82	21.78	21.91	21.84	4.04	4.19	4.01	4.08
0.05	21.80	21.79	21.90	21.83	3.98	4.19	4.01	4.06
0.07	21.81	21.80	21.89	21.84	3.98	4.19	3.96	4.04
0.09	21.82	21.80	21.89	21.83	3.98	4.19	3.96	4.04
0.11	21.82	21.81	21.90	21.84	3.98	4.19	4.00	4.06
0.12	21.81	21.80	21.90	21.83	3.98	4.11	3.96	4.01
0.13	21.81	21.79	21.90	21.84	3.98	4.29	3.96	4.08
0.14	21.80	21.80	21.89	21.83	3.98	4.10	3.96	4.01
0.16	21.81	21.79	21.89	21.83	3.98	4.30	3.96	4.08
0.17	21.80	21.79	21.91	21.83	3.98	4.18	4.00	4.05
0.18	21.79	21.79	21.89	21.82	3.98	4.10	4.00	4.03
0.20	21.80	21.79	21.90	21.83	3.98	4.18	3.95	4.04
0.21	21.80	21.77	21.88	21.82	3.98	4.18	3.95	4.04
0.22	21.80	21.76	21.88	21.81	3.98	4.18	3.95	4.04
0.24	21.80	21.77	21.86	21.81	3.98	4.19	3.95	4.04
0.25	21.80	21.78	21.85	21.81	3.98	4.18	3.95	4.04
0.28	21.80	21.75	21.86	21.80	3.98	4.19	3.95	4.04
0.29	21.79	21.75	21.86	21.80	3.98	4.19	3.95	4.04
0.30	21.79	21.75	21.86	21.80	3.98	4.19	4.00	4.05
0.32	21.79	21.75	21.86	21.80	3.98	4.19	3.95	4.04
0.33	21.80	21.76	21.86	21.81	3.98	4.10	3.94	4.01
0.34	21.80	21.75	21.85	21.80	3.98	4.19	3.99	4.05
0.37	21.79	21.76	21.85	21.80	3.98	4.19	3.94	4.04
0.40	21.80	21.76	21.87	21.81	3.98	4.28	4.05	4.11
0.37	21.79	21.76	21.85	21.80	3.98	4.19	3.94	4.04
0.41	21.78	21.77	21.85	21.80	3.98	4.10	3.90	3.99
0.37	21.79	21.76	21.85	21.80	3.98	4.19	3.94	4.04
0.42	21.79	21.76	21.86	21.80	3.98	4.17	3.94	4.03
0.43	21.79	21.76	21.84	21.79	3.98	4.17	3.94	4.03
0.45	21.79	21.74	21.84	21.79	3.98	4.17	3.94	4.03

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	21.78	21.74	21.84	21.79	3.98	4.17	3.99	4.05
0.49	21.78	21.74	21.83	21.78	3.98	4.18	3.94	4.03
0.50	21.79	21.75	21.82	21.79	3.98	4.18	3.94	4.03
0.51	21.79	21.73	21.82	21.78	3.98	4.18	3.94	4.03
0.53	21.79	21.75	21.83	21.79	3.98	4.09	3.90	3.99
0.55	21.79	21.73	21.83	21.78	3.98	4.17	3.90	4.02
0.57	21.78	21.73	21.84	21.78	3.98	4.09	3.90	3.99
0.58	21.78	21.71	21.83	21.77	3.98	4.09	3.94	4.00
0.59	21.80	21.72	21.82	21.78	3.98	4.18	3.94	4.03
0.61	21.78	21.73	21.83	21.78	3.98	4.18	3.94	4.03
0.62	21.79	21.72	21.82	21.78	3.97	4.18	3.98	4.04
0.63	21.78	21.72	21.82	21.77	3.97	4.18	3.98	4.05
0.65	21.78	21.71	21.82	21.77	3.97	4.09	3.94	4.00
0.66	21.77	21.71	21.81	21.76	3.97	4.09	4.04	4.03
0.67	21.79	21.72	21.81	21.77	3.97	4.09	3.93	4.00
0.68	21.81	21.71	21.81	21.78	4.03	4.18	3.94	4.05
0.70	21.79	21.71	21.80	21.77	3.97	4.16	4.04	4.06
0.71	21.79	21.72	21.80	21.77	3.97	4.09	3.89	3.99
0.72	21.79	21.71	21.79	21.76	3.97	4.09	3.94	4.00
0.74	21.79	21.71	21.80	21.77	3.97	4.09	3.94	4.00
0.75	21.79	21.71	21.77	21.76	4.03	4.09	4.04	4.05
0.76	21.80	21.71	21.79	21.77	4.03	4.09	3.89	4.00
0.78	21.80	21.71	21.79	21.77	3.97	4.16	4.04	4.06
0.79	21.79	21.71	21.78	21.76	4.03	4.17	3.89	4.03
0.80	21.80	21.72	21.78	21.76	4.03	4.09	3.98	4.03
0.82	21.79	21.71	21.78	21.76	4.03	4.17	3.89	4.03
0.84	21.79	21.71	21.77	21.76	4.03	4.08	3.93	4.01
0.86	21.80	21.71	21.79	21.76	4.03	4.17	3.89	4.03
0.87	21.79	21.72	22.86	22.12	3.98	4.17	3.97	4.04
0.88	21.79	21.71	21.77	21.76	4.02	4.17	3.89	4.03
0.90	21.79	21.71	21.79	21.76	4.03	4.17	3.93	4.04
0.88	21.79	21.71	21.77	21.76	4.02	4.17	3.89	4.03
0.91	21.79	21.71	21.78	21.76	4.03	4.08	4.03	4.05
0.92	21.78	21.71	21.77	21.75	4.02	4.17	3.93	4.04
0.94	21.79	21.70	21.79	21.76	3.98	4.08	3.93	3.99
0.95	21.78	21.71	21.78	21.75	4.03	4.09	4.10	4.07
0.96	21.78	21.70	21.77	21.75	4.02	4.17	3.93	4.04

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	21.79	21.70	21.75	21.75	3.98	4.17	4.03	4.06
1.00	21.78	21.70	21.77	21.75	3.98	4.08	3.93	3.99
1.01	21.77	21.68	21.74	21.73	3.98	4.17	3.93	4.02
1.03	21.79	21.69	21.74	21.74	3.98	4.08	3.93	3.99
1.04	21.77	21.69	21.76	21.74	3.97	4.08	3.93	3.99
1.05	21.77	21.69	21.74	21.73	3.98	4.08	3.88	3.98
1.07	21.78	21.68	21.73	21.73	3.98	4.17	4.03	4.06
1.08	21.77	21.68	21.74	21.73	3.97	4.08	3.88	3.98
1.09	21.76	21.68	21.73	21.72	3.97	4.08	4.10	4.05
1.11	21.78	21.67	21.73	21.73	3.97	4.08	3.93	3.99
1.12	21.78	21.68	21.73	21.73	3.97	4.08	3.88	3.98
1.13	21.77	21.68	21.72	21.72	3.97	4.08	4.03	4.03
1.15	21.77	21.67	21.72	21.72	3.97	4.08	3.88	3.98
1.16	21.78	21.67	21.73	21.72	3.97	4.08	4.03	4.03
1.17	21.77	21.67	21.72	21.72	3.97	4.08	3.88	3.98
1.19	21.77	21.67	21.72	21.72	3.97	4.08	3.88	3.98
1.19	21.77	21.67	21.72	21.72	3.97	4.08	3.88	3.98
1.20	21.78	21.67	21.72	21.72	3.97	4.08	3.97	4.01
1.21	21.78	21.67	21.73	21.73	3.97	4.08	3.88	3.98
1.22	21.77	21.67	21.73	21.72	3.97	4.08	3.88	3.98
1.24	21.77	21.66	21.72	21.72	3.97	4.16	3.97	4.03
1.26	21.78	21.67	21.72	21.72	3.97	4.16	3.88	4.00
1.28	21.79	21.66	21.71	21.72	4.03	4.08	4.03	4.05
1.30	21.78	21.66	21.73	21.72	4.03	4.16	3.88	4.02
1.32	21.79	21.66	21.71	21.72	3.97	4.08	3.92	3.99
1.33	21.78	21.67	21.72	21.72	4.03	4.08	3.92	4.01
1.34	21.79	21.67	21.71	21.72	4.02	4.07	3.97	4.02
1.36	21.77	21.66	21.71	21.71	4.02	4.08	4.03	4.04
1.37	21.78	21.67	21.70	21.72	4.03	4.01	3.92	3.99
1.38	21.78	21.67	21.71	21.72	4.02	4.16	4.09	4.09
1.40	21.77	21.66	21.70	21.71	4.02	4.07	3.92	4.00
1.41	21.78	21.67	21.70	21.71	4.03	4.07	4.03	4.04
1.42	21.78	21.67	21.71	21.72	4.02	4.15	3.88	4.02
1.44	21.77	21.67	21.71	21.72	4.02	4.15	3.92	4.03
1.45	21.76	21.66	21.71	21.71	4.02	4.07	3.92	4.00
1.46	21.77	21.67	21.70	21.71	3.97	4.01	4.03	4.00
1.48	21.76	21.66	21.70	21.71	4.02	4.07	3.92	4.00

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	21.77	21.66	21.68	21.71	4.02	4.15	3.92	4.03
1.51	21.77	21.66	21.70	21.71	4.02	4.07	3.92	4.00
1.53	21.76	21.67	21.69	21.71	4.02	4.15	3.88	4.02
1.54	21.76	21.65	21.69	21.70	4.02	4.16	4.02	4.07
1.55	21.77	21.66	21.69	21.70	4.02	4.07	4.09	4.06
1.57	21.76	21.66	21.68	21.70	4.02	4.08	4.03	4.04
1.58	21.76	21.66	21.69	21.70	4.02	4.07	3.88	3.99
1.59	21.76	21.66	21.69	21.70	4.02	4.07	3.92	4.00
1.61	21.77	21.66	21.69	21.71	3.97	4.15	3.92	4.01
1.62	21.76	21.66	21.69	21.70	4.02	4.07	3.87	3.99
1.63	21.77	21.65	21.69	21.70	4.02	4.07	3.91	4.00
1.65	21.77	21.64	21.68	21.70	4.02	4.07	4.09	4.06
1.66	21.76	21.65	21.67	21.70	4.02	4.01	3.91	3.98
1.67	21.76	21.66	21.68	21.70	4.02	4.00	3.91	3.98
1.69	21.77	21.64	21.69	21.70	4.02	4.00	4.02	4.01
1.71	21.78	21.66	21.66	21.70	3.97	4.07	3.91	3.98
1.73	21.76	21.65	21.68	21.70	4.02	4.00	4.09	4.04
1.74	21.78	21.65	21.68	21.71	3.97	4.16	4.09	4.07
1.75	21.77	21.66	21.66	21.70	4.02	4.06	3.87	3.98
1.76	21.78	21.65	21.67	21.70	4.02	4.07	4.09	4.06
1.78	21.78	21.65	21.67	21.70	4.02	4.06	3.91	4.00
1.79	21.78	21.65	21.65	21.69	4.02	4.07	3.91	4.00
1.80	21.78	21.65	21.66	21.70	3.97	4.07	3.91	3.98
1.82	21.79	21.65	21.67	21.70	3.97	4.07	4.03	4.02
1.83	21.78	21.66	21.65	21.70	3.97	4.07	3.87	3.97
1.84	21.78	21.65	21.65	21.69	4.02	4.00	4.02	4.02
1.86	21.77	21.64	21.66	21.69	3.97	4.06	3.91	3.98
1.87	21.78	21.65	21.65	21.69	3.97	4.07	4.02	4.02
1.90	21.78	21.64	21.66	21.69	4.02	4.07	3.87	3.99
1.91	21.78	21.64	21.65	21.69	4.02	4.07	4.02	4.04
1.92	21.79	21.63	21.64	21.69	4.02	4.07	3.87	3.99
1.94	21.79	21.64	21.65	21.69	4.02	4.06	4.02	4.03
1.95	21.79	21.64	21.65	21.69	4.02	4.06	3.91	4.00
1.96	21.79	21.64	21.64	21.69	4.02	4.06	3.87	3.98
1.98	21.79	21.64	21.64	21.69	4.02	4.06	3.91	4.00
1.99	21.78	21.64	21.64	21.68	4.02	4.06	3.91	4.00



**APPENDIX 13.14 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(44.30 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (44.30 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	27.11	26.56	26.61	26.76	4.98	4.84	4.95	4.92
0.01	27.13	26.54	26.62	26.76	4.98	4.79	4.95	4.91
0.03	27.13	26.57	26.63	26.78	4.98	4.84	4.95	4.92
0.04	27.13	26.56	26.62	26.77	4.98	4.84	4.90	4.91
0.05	27.15	26.56	26.61	26.77	4.98	4.79	4.90	4.89
0.07	27.15	26.56	26.61	26.77	4.98	4.80	4.95	4.91
0.08	27.14	26.57	26.63	26.78	4.98	4.80	4.95	4.91
0.11	27.16	26.56	26.63	26.78	4.98	4.84	4.95	4.92
0.12	27.14	26.58	26.63	26.79	4.98	4.84	4.95	4.92
0.13	27.14	26.57	26.62	26.78	4.98	4.84	4.95	4.92
0.14	27.15	26.56	26.63	26.78	4.98	4.84	4.95	4.92
0.16	27.15	26.57	26.63	26.78	4.98	4.84	4.95	4.92
0.17	27.14	26.55	26.63	26.77	4.98	4.84	4.95	4.92
0.18	27.14	26.57	26.64	26.79	4.98	4.84	4.94	4.92
0.20	27.17	26.56	26.64	26.79	4.98	4.79	4.95	4.91
0.21	27.16	26.56	26.63	26.78	4.98	4.84	4.95	4.92
0.22	27.16	26.56	26.64	26.79	4.98	4.84	4.94	4.92
0.24	27.19	26.57	26.65	26.80	4.98	4.84	4.94	4.92
0.25	27.16	26.57	26.65	26.79	4.98	4.84	4.94	4.92
0.28	27.16	26.56	26.64	26.79	4.98	4.84	4.94	4.92
0.29	27.19	26.56	26.65	26.80	4.98	4.84	4.94	4.92
0.30	27.16	26.58	26.65	26.80	4.98	4.84	4.94	4.92
0.32	27.17	26.56	26.64	26.79	4.98	4.84	4.94	4.92
0.33	27.19	26.56	26.66	26.80	4.98	4.84	4.94	4.92
0.34	27.18	26.58	26.66	26.81	4.98	4.84	4.94	4.92
0.37	27.18	26.58	26.66	26.81	4.98	4.84	4.94	4.92
0.40	27.17	26.58	26.65	26.80	4.98	4.83	4.94	4.92
0.37	27.18	26.58	26.66	26.81	4.98	4.84	4.94	4.92
0.41	27.20	26.59	26.66	26.82	4.98	4.84	4.94	4.92
0.42	27.18	26.58	26.65	26.80	4.98	4.84	4.94	4.92
0.43	27.18	26.60	26.66	26.81	4.93	4.83	4.94	4.90
0.45	27.18	26.59	26.66	26.81	4.98	4.83	4.94	4.92

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	27.21	26.60	26.65	26.82	4.97	4.83	4.90	4.90
0.49	27.19	26.59	26.66	26.81	4.98	4.79	4.94	4.90
0.50	27.19	26.63	26.64	26.82	5.04	4.80	4.90	4.91
0.51	27.20	26.61	26.63	26.81	4.97	4.89	4.90	4.92
0.53	27.19	26.61	26.63	26.81	4.97	4.79	4.94	4.90
0.54	27.19	26.61	26.65	26.82	5.04	4.84	4.90	4.93
0.55	27.19	26.61	26.64	26.81	5.04	4.79	4.95	4.93
0.57	27.20	26.62	26.64	26.82	4.97	4.88	4.94	4.93
0.58	27.19	26.61	26.65	26.82	5.04	4.84	4.94	4.94
0.59	27.17	26.63	26.65	26.82	5.04	4.89	4.99	4.97
0.61	27.18	26.61	26.66	26.82	5.04	4.83	4.99	4.95
0.61	27.18	26.61	26.66	26.82	5.04	4.83	4.99	4.95
0.62	27.19	26.63	26.65	26.82	5.04	4.79	4.94	4.93
0.63	27.19	26.62	26.66	26.82	5.04	4.88	4.99	4.97
0.65	27.18	26.63	26.66	26.83	4.97	4.84	4.94	4.92
0.66	27.19	26.63	26.66	26.83	5.04	4.88	4.94	4.95
0.67	27.19	26.64	26.66	26.83	5.04	4.84	4.94	4.94
0.68	27.18	26.63	26.65	26.82	5.04	4.84	4.94	4.94
0.70	27.20	26.61	26.66	26.82	5.04	4.88	4.99	4.97
0.71	27.19	26.61	26.67	26.83	5.04	4.79	4.94	4.92
0.72	27.16	26.63	26.68	26.83	5.04	4.84	4.94	4.94
0.74	27.18	26.63	26.67	26.83	4.98	4.83	4.94	4.92
0.76	27.19	26.63	26.69	26.84	4.98	4.79	4.94	4.91
0.78	27.18	26.63	26.68	26.83	5.03	4.83	4.94	4.94
0.79	27.20	26.63	26.68	26.84	5.04	4.83	4.94	4.94
0.80	27.20	26.63	26.69	26.84	4.98	4.84	4.94	4.92
0.82	27.20	26.61	26.69	26.83	5.03	4.83	4.94	4.94
0.83	27.21	26.63	26.68	26.84	4.98	4.83	4.94	4.92
0.84	27.22	26.63	26.69	26.85	5.03	4.83	4.94	4.94
0.86	27.19	26.63	26.69	26.84	4.98	4.83	4.94	4.92
0.87	27.19	26.63	26.68	26.83	4.98	4.83	4.94	4.92
0.88	27.23	26.62	26.69	26.85	5.03	4.83	4.94	4.94
0.90	27.20	26.65	26.68	26.84	4.98	4.83	4.94	4.92
0.91	27.21	26.62	26.68	26.84	4.98	4.83	4.94	4.92
0.92	27.21	26.65	26.69	26.85	4.98	4.83	4.94	4.92
0.94	27.21	26.64	26.69	26.84	4.98	4.83	4.94	4.92
0.95	27.22	26.65	26.68	26.85	4.98	4.83	4.94	4.92

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	27.22	26.67	26.67	26.85	4.98	4.83	4.94	4.91
1.00	27.25	26.63	26.67	26.85	4.98	4.83	4.94	4.92
1.01	27.24	26.68	26.69	26.87	4.98	4.83	4.94	4.92
1.03	27.25	26.66	26.67	26.86	5.03	4.83	4.94	4.93
1.04	27.33	26.66	26.67	26.89	4.97	4.88	4.94	4.93
1.05	27.25	26.69	26.67	26.87	5.03	4.83	4.94	4.93
1.07	27.26	26.66	26.68	26.87	4.97	4.83	4.94	4.91
1.08	27.25	26.66	26.67	26.86	4.97	4.88	4.94	4.93
1.09	27.25	26.66	26.68	26.86	4.97	4.83	4.94	4.91
1.11	27.25	26.67	26.69	26.87	4.97	4.83	4.94	4.91
1.12	27.26	26.68	26.69	26.88	5.03	4.83	4.94	4.93
1.13	27.26	26.66	26.69	26.87	4.97	4.83	4.94	4.91
1.15	27.24	26.68	26.70	26.87	4.98	4.83	4.99	4.93
1.17	27.25	26.67	26.75	26.89	4.97	4.88	4.99	4.95
1.19	27.25	26.67	26.70	26.87	4.97	4.83	4.99	4.93
1.20	27.25	26.68	26.71	26.88	4.97	4.94	4.99	4.97
1.21	27.26	26.68	26.70	26.88	4.97	4.88	4.99	4.95
1.22	27.24	26.67	26.71	26.87	4.97	4.83	4.99	4.93
1.24	27.25	26.69	26.70	26.88	4.97	4.83	4.99	4.93
1.25	27.26	26.69	26.72	26.89	5.02	4.94	4.99	4.99
1.26	27.24	26.68	26.70	26.87	4.97	4.88	4.99	4.95
1.28	27.25	26.67	26.72	26.88	4.97	4.83	4.99	4.93
1.29	27.25	26.68	26.72	26.88	4.97	4.94	4.99	4.97
1.28	27.25	26.67	26.72	26.88	4.97	4.83	4.99	4.93
1.30	27.26	26.68	26.71	26.88	4.97	4.88	4.99	4.95
1.32	27.25	26.67	26.73	26.88	4.97	4.88	4.99	4.95
1.33	27.24	26.69	26.71	26.88	4.97	4.94	4.99	4.97
1.34	27.27	26.67	26.71	26.88	4.97	4.88	4.99	4.94
1.36	27.24	26.70	26.72	26.89	4.97	4.94	4.99	4.97
1.37	27.24	26.68	26.73	26.88	4.97	4.94	4.99	4.97
1.38	27.24	26.67	26.71	26.88	4.97	4.83	4.93	4.91
1.40	27.25	26.69	26.73	26.89	4.97	4.88	4.99	4.94
1.42	27.25	26.69	26.73	26.89	4.97	4.94	4.98	4.96
1.44	27.26	26.67	26.73	26.89	4.97	4.88	4.98	4.94
1.45	27.26	26.69	26.72	26.89	4.97	4.88	4.99	4.94
1.46	27.24	26.68	26.72	26.88	4.97	4.88	4.98	4.94
1.48	27.26	26.70	26.71	26.89	4.97	4.94	4.98	4.96

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	27.26	26.69	26.73	26.89	4.97	4.94	4.98	4.96
1.51	27.26	26.72	26.71	26.90	4.97	4.94	4.98	4.96
1.53	27.28	26.69	26.73	26.90	4.97	4.88	4.98	4.94
1.54	27.26	26.72	26.73	26.90	4.97	4.87	4.98	4.94
1.55	27.26	26.71	26.72	26.90	4.97	4.94	4.98	4.96
1.57	27.27	26.74	26.72	26.91	4.97	4.93	4.98	4.96
1.58	27.28	26.72	26.72	26.91	4.97	4.87	4.98	4.94
1.59	27.27	26.71	26.73	26.90	4.96	4.94	4.98	4.96
1.61	27.26	26.73	26.72	26.90	4.97	4.87	4.98	4.94
1.62	27.29	26.71	26.72	26.91	4.97	4.94	4.98	4.96
1.63	27.27	26.73	26.71	26.90	4.96	4.94	4.98	4.96
1.66	27.28	26.74	26.73	26.92	4.96	4.94	4.98	4.96
1.67	27.29	26.74	26.71	26.91	4.96	4.93	4.98	4.96
1.69	27.27	26.72	26.72	26.90	4.96	5.02	4.98	4.99
1.70	27.31	26.75	26.73	26.93	4.96	5.01	4.98	4.99
1.71	27.31	26.74	26.73	26.93	4.96	5.02	4.98	4.99
1.73	27.29	26.74	26.71	26.92	4.96	5.01	4.98	4.98
1.74	27.31	26.73	26.73	26.92	4.96	5.01	4.98	4.99
1.75	27.30	26.76	26.73	26.93	4.96	5.01	4.98	4.99
1.76	27.29	26.74	26.72	26.92	4.96	4.93	4.98	4.96
1.78	27.29	26.73	26.73	26.92	5.03	4.93	4.98	4.98
1.79	27.30	26.77	26.73	26.93	4.96	4.93	4.98	4.96
1.80	27.32	26.73	26.73	26.93	4.96	4.93	4.93	4.94
1.82	27.30	26.75	26.73	26.92	4.96	5.01	4.93	4.97
1.83	27.31	26.76	26.75	26.94	4.96	5.01	4.93	4.97
1.84	27.31	26.75	26.74	26.93	4.96	4.93	4.99	4.96
1.86	27.30	26.74	26.74	26.93	4.96	5.01	4.99	4.99
1.87	27.29	26.75	26.74	26.93	5.03	4.93	5.04	5.00
1.88	27.31	26.76	26.72	26.93	4.96	4.93	4.98	4.96
1.90	27.31	26.73	26.73	26.92	5.02	4.93	4.99	4.98
1.91	27.31	26.76	26.74	26.94	4.96	5.01	5.04	5.00
1.92	27.30	26.75	26.75	26.93	4.96	4.87	4.99	4.94
1.94	27.31	26.73	26.75	26.93	4.96	4.93	4.98	4.96
1.95	27.32	26.75	26.76	26.94	4.96	5.01	4.93	4.97
1.96	27.30	26.74	26.76	26.93	5.02	5.01	4.98	5.01
1.98	27.31	26.76	26.74	26.94	5.02	5.01	4.93	4.99

**APPENDIX 13.15 - Surface Tension Measurement Results for DI + SDS + MWCNT  
(82.00 mM)**

HUATARC surface tension measurement results for DI + SDS + MWCNT (82.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	25.64	26.10	26.00	25.91	4.72	4.58	4.64	4.65
0.01	25.66	26.09	25.98	25.91	4.72	4.62	4.68	4.67
0.03	25.64	26.09	25.99	25.91	4.72	4.62	4.64	4.66
0.04	25.67	26.08	25.99	25.91	4.72	4.69	4.68	4.70
0.05	25.65	26.09	25.96	25.90	4.68	4.62	4.64	4.65
0.07	25.65	26.10	25.99	25.91	4.68	4.62	4.64	4.65
0.08	25.66	26.10	25.97	25.91	4.68	4.65	4.64	4.66
0.11	25.67	26.09	25.99	25.92	4.67	4.62	4.68	4.66
0.12	25.66	26.09	25.97	25.91	4.73	4.62	4.64	4.66
0.13	25.68	26.09	25.98	25.92	4.68	4.62	4.68	4.66
0.14	25.68	26.09	25.95	25.91	4.72	4.62	4.60	4.65
0.16	25.67	26.08	25.97	25.91	4.73	4.62	4.64	4.66
0.17	25.66	26.10	25.97	25.91	4.68	4.62	4.68	4.66
0.18	25.67	26.10	26.00	25.93	4.72	4.62	4.64	4.66
0.20	25.68	26.09	25.98	25.92	4.67	4.62	4.68	4.66
0.21	25.66	26.08	25.97	25.91	4.72	4.62	4.64	4.66
0.22	25.67	26.08	26.00	25.92	4.73	4.62	4.64	4.66
0.24	25.65	26.10	25.99	25.92	4.72	4.66	4.68	4.69
0.25	25.68	26.09	25.99	25.92	4.73	4.62	4.64	4.66
0.28	25.66	26.07	26.00	25.91	4.68	4.62	4.64	4.65
0.29	25.69	26.08	26.01	25.92	4.72	4.62	4.68	4.67
0.30	25.66	26.09	26.01	25.92	4.72	4.62	4.64	4.66
0.33	25.68	26.08	26.02	25.93	4.67	4.62	4.61	4.63
0.34	25.70	26.07	26.01	25.92	4.68	4.62	4.68	4.66
0.37	25.70	26.09	26.01	25.93	4.73	4.62	4.68	4.67
0.38	25.70	26.06	26.02	25.93	4.72	4.62	4.68	4.67
0.37	25.70	26.09	26.01	25.93	4.73	4.62	4.68	4.67
0.40	25.69	26.09	26.03	25.94	4.73	4.62	4.61	4.65
0.41	25.70	26.07	26.04	25.94	4.72	4.62	4.68	4.67
0.42	25.70	26.08	26.00	25.93	4.67	4.62	4.64	4.64
0.43	25.69	26.07	26.00	25.92	4.67	4.62	4.72	4.67
0.45	25.71	26.08	26.02	25.94	4.72	4.68	4.68	4.69

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	25.71	26.07	26.03	25.94	4.72	4.62	4.68	4.67
0.49	25.71	26.09	26.03	25.94	4.67	4.62	4.72	4.67
0.50	25.70	26.05	26.01	25.92	4.72	4.62	4.64	4.66
0.51	25.71	26.08	26.01	25.93	4.72	4.62	4.64	4.66
0.53	25.70	26.07	26.02	25.93	4.72	4.62	4.64	4.66
0.54	25.69	26.07	26.02	25.92	4.72	4.65	4.64	4.67
0.55	25.69	26.06	26.02	25.93	4.72	4.62	4.68	4.67
0.57	25.70	26.08	26.02	25.93	4.72	4.62	4.60	4.65
0.58	25.69	26.06	26.04	25.93	4.72	4.62	4.64	4.66
0.59	25.69	26.05	26.01	25.92	4.72	4.61	4.61	4.65
0.61	25.68	26.07	26.02	25.92	4.72	4.65	4.72	4.70
0.62	25.71	26.06	26.02	25.93	4.72	4.62	4.64	4.66
0.65	25.70	26.07	26.02	25.93	4.67	4.65	4.72	4.68
0.66	25.70	26.08	26.04	25.94	4.72	4.65	4.61	4.66
0.67	25.71	26.07	26.04	25.94	4.72	4.61	4.61	4.65
0.68	25.71	26.05	26.02	25.93	4.72	4.57	4.61	4.63
0.70	25.70	26.07	26.05	25.94	4.72	4.61	4.64	4.66
0.71	25.69	26.07	26.03	25.93	4.72	4.65	4.64	4.67
0.72	25.72	26.05	26.03	25.94	4.72	4.61	4.64	4.66
0.74	25.69	26.06	26.03	25.93	4.67	4.61	4.64	4.64
0.75	25.70	26.07	26.02	25.93	4.72	4.61	4.64	4.66
0.76	25.70	26.07	26.06	25.94	4.72	4.61	4.61	4.64
0.76	25.70	26.07	26.06	25.94	4.72	4.61	4.61	4.64
0.78	25.71	26.06	26.02	25.93	4.72	4.65	4.72	4.70
0.79	25.73	26.08	26.05	25.95	4.72	4.68	4.68	4.69
0.80	25.69	26.05	26.04	25.93	4.72	4.61	4.61	4.64
0.82	25.71	26.07	26.00	25.93	4.72	4.61	4.68	4.67
0.83	25.70	26.06	26.08	25.95	4.72	4.61	4.68	4.67
0.84	25.72	26.05	26.02	25.93	4.72	4.64	4.61	4.65
0.86	25.72	26.07	26.05	25.95	4.71	4.61	4.67	4.67
0.87	25.71	26.06	26.06	25.94	4.72	4.61	4.72	4.68
0.90	25.72	26.04	26.07	25.94	4.71	4.65	4.68	4.68
0.91	25.71	26.06	26.02	25.93	4.72	4.67	4.60	4.66
0.92	25.71	26.08	26.06	25.95	4.71	4.65	4.68	4.68
0.94	25.69	26.04	26.04	25.92	4.71	4.65	4.60	4.65
0.95	25.70	26.09	26.03	25.94	4.71	4.67	4.71	4.70
0.96	25.72	26.06	26.08	25.95	4.71	4.65	4.68	4.68

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	25.71	26.06	26.04	25.94	4.71	4.61	4.60	4.64
1.00	25.71	26.05	26.05	25.94	4.71	4.68	4.61	4.67
1.01	25.69	26.07	26.05	25.94	4.71	4.71	4.64	4.69
1.01	25.69	26.07	26.05	25.94	4.71	4.71	4.64	4.69
1.03	25.73	26.03	26.05	25.94	4.71	4.64	4.60	4.65
1.04	25.70	26.08	26.07	25.95	4.71	4.68	4.61	4.67
1.05	25.72	26.06	26.04	25.94	4.71	4.72	4.64	4.69
1.07	25.71	26.05	26.06	25.94	4.71	4.68	4.60	4.66
1.08	25.72	26.07	26.04	25.94	4.71	4.72	4.57	4.67
1.09	25.72	26.04	26.05	25.94	4.71	4.71	4.57	4.66
1.11	25.69	26.07	26.05	25.94	4.71	4.64	4.61	4.65
1.12	25.71	26.03	26.06	25.94	4.71	4.68	4.64	4.68
1.15	25.70	26.07	26.05	25.94	4.71	4.64	4.57	4.64
1.16	25.71	26.04	26.06	25.94	4.71	4.60	4.61	4.64
1.17	25.70	26.08	26.05	25.94	4.71	4.64	4.61	4.65
1.19	25.72	26.06	26.06	25.95	4.71	4.64	4.57	4.64
1.20	25.70	26.07	26.06	25.94	4.71	4.64	4.61	4.65
1.21	25.72	26.04	26.04	25.93	4.71	4.60	4.60	4.64
1.22	25.70	26.07	26.06	25.94	4.71	4.68	4.61	4.66
1.24	25.70	26.06	26.04	25.93	4.71	4.60	4.56	4.63
1.25	25.70	26.07	26.05	25.94	4.71	4.64	4.60	4.65
1.26	25.69	26.10	26.06	25.95	4.71	4.64	4.61	4.65
1.28	25.73	26.05	26.05	25.94	4.71	4.64	4.56	4.64
1.29	25.70	26.08	26.06	25.95	4.71	4.68	4.64	4.67
1.30	25.70	26.05	26.03	25.93	4.66	4.64	4.60	4.63
1.32	25.69	26.09	26.05	25.94	4.71	4.64	4.64	4.66
1.33	25.70	26.07	26.03	25.94	4.71	4.60	4.60	4.64
1.34	25.70	26.05	26.03	25.93	4.71	4.60	4.56	4.62
1.36	25.71	26.07	26.08	25.95	4.71	4.64	4.60	4.65
1.37	25.70	26.04	26.05	25.93	4.71	4.60	4.60	4.64
1.38	25.69	26.05	26.04	25.93	4.71	4.68	4.56	4.65
1.40	25.70	26.06	26.02	25.92	4.70	4.64	4.56	4.64
1.41	25.70	26.05	26.05	25.93	4.70	4.64	4.60	4.65
1.44	25.70	26.05	26.04	25.93	4.65	4.64	4.60	4.63
1.45	25.71	26.05	26.05	25.94	4.70	4.60	4.56	4.62
1.46	25.70	26.06	26.02	25.93	4.70	4.64	4.60	4.65
1.48	25.68	26.07	26.03	25.93	4.71	4.64	4.64	4.66

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	25.70	26.05	26.02	25.92	4.70	4.71	4.64	4.68
1.51	25.69	26.05	26.02	25.92	4.70	4.67	4.60	4.66
1.53	25.70	26.06	26.01	25.92	4.70	4.64	4.63	4.66
1.54	25.69	26.06	26.04	25.93	4.70	4.67	4.60	4.66
1.55	25.69	26.04	26.00	25.91	4.65	4.68	4.60	4.64
1.57	25.69	26.06	26.01	25.92	4.70	4.64	4.60	4.65
1.58	25.68	26.06	26.05	25.93	4.70	4.64	4.67	4.67
1.59	25.69	26.03	25.98	25.90	4.70	4.64	4.64	4.66
1.61	25.68	26.07	26.02	25.93	4.66	4.71	4.63	4.67
1.62	25.68	26.03	26.03	25.92	4.70	4.64	4.60	4.65
1.63	25.67	26.02	26.01	25.90	4.65	4.67	4.56	4.63
1.65	25.70	26.06	26.03	25.93	4.70	4.67	4.60	4.66
1.66	25.69	26.03	26.01	25.91	4.65	4.64	4.60	4.63
1.67	25.68	26.06	26.02	25.92	4.61	4.67	4.60	4.63
1.69	25.69	26.03	26.01	25.91	4.70	4.64	4.64	4.66
1.70	25.67	26.08	26.01	25.92	4.65	4.64	4.60	4.63
1.71	25.70	26.06	26.01	25.92	4.65	4.63	4.60	4.63
1.74	25.68	26.08	26.02	25.93	4.65	4.64	4.59	4.63
1.75	25.67	26.04	25.99	25.90	4.61	4.60	4.63	4.61
1.76	25.68	26.06	25.99	25.91	4.65	4.67	4.63	4.65
1.78	25.68	26.04	26.02	25.91	4.65	4.63	4.63	4.64
1.79	25.67	26.08	26.01	25.92	4.65	4.60	4.63	4.63
1.80	25.68	26.04	26.02	25.91	4.65	4.63	4.59	4.62
1.82	25.66	26.04	26.00	25.90	4.65	4.56	4.60	4.60
1.83	25.67	26.03	25.99	25.90	4.70	4.60	4.63	4.65
1.86	25.68	26.04	26.01	25.91	4.65	4.60	4.60	4.61
1.87	25.68	26.03	26.00	25.90	4.65	4.60	4.60	4.62
1.88	25.67	26.06	26.00	25.91	4.65	4.56	4.60	4.60
1.90	25.67	26.05	25.98	25.90	4.65	4.60	4.55	4.60
1.91	25.66	26.06	25.99	25.90	4.70	4.56	4.63	4.63
1.92	25.67	26.05	25.99	25.91	4.65	4.56	4.60	4.60
1.94	25.66	26.03	26.00	25.90	4.70	4.60	4.63	4.64
1.95	25.66	26.06	25.99	25.90	4.70	4.60	4.63	4.64
1.96	25.67	26.06	26.01	25.91	4.65	4.63	4.67	4.65
1.98	25.65	26.00	26.01	25.89	4.70	4.63	4.63	4.65
1.99	25.66	26.06	25.99	25.90	4.65	4.60	4.59	4.61



**APPENDIX 13.16 - Descriptive Statistics for Surface Tension Measurement Results of DI + SDS + MWCNT**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.82	Exp.1	46.61	50.66	0.90	0.82	0.23	-0.90
	Exp.2	50.35	51.52	0.23	0.05	0.25	0.15
	Exp.3	47.93	51.71	1.15	1.31	0.18	-1.37
	Average	48.64	50.87	0.55	0.31	0.23	-0.59
3.00	Exp.1	21.43	21.49	0.01	0.00	-0.07	-0.21
	Exp.2	22.35	22.52	0.04	0.00	-0.16	-0.75
	Exp.3	21.73	21.82	0.03	0.00	-0.07	-1.45
	Average	21.85	21.92	0.02	0.00	-0.21	-1.19
6.00	Exp.1	24.18	24.36	0.05	0.00	-0.08	-0.98
	Exp.2	24.28	24.52	0.04	0.00	0.54	1.44
	Exp.3	25.24	25.36	0.03	0.00	-0.29	-1.16
	Average	24.59	24.74	0.03	0.00	0.28	-0.48
8.20	Exp.1	21.76	21.82	0.01	0.00	0.36	-0.04
	Exp.2	21.63	21.81	0.05	0.00	0.53	-0.90
	Exp.3	21.64	22.86	0.12	0.01	4.91	42.83
	Average	21.68	22.12	0.06	0.00	2.10	11.06
44.30	Exp.1	27.11	27.33	0.05	0.00	-0.02	-0.99
	Exp.2	26.54	26.77	0.06	0.00	0.06	-1.13
	Exp.3	26.61	26.76	0.04	0.00	-0.07	-1.10
	Average	26.76	26.94	0.05	0.00	-0.02	-1.13
59.00	Exp.1	24.13	25.76	0.19	0.04	2.25	15.16
	Exp.2	23.71	23.90	0.05	0.00	0.79	-0.62
	Exp.3	23.45	23.56	0.03	0.00	0.89	-0.13
	Average	23.80	24.33	0.07	0.01	1.66	7.31
82.00	Exp.1	25.64	25.73	0.02	0.00	-0.36	-0.42
	Exp.2	25.98	26.10	0.02	0.00	-0.65	1.14
	Exp.3	25.95	26.08	0.03	0.00	-0.10	-0.49
	Average	25.88	25.95	0.02	0.00	-0.46	-0.35

**APPENDIX 13.17 - Surface Tension Measurement Results for DI+MWCNT (2.00 mg)**

HUATARC surface tension measurement results for DI+MWCNT (2.00 mg)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	69.66	69.90	70.21	69.92	5.53	6.43	8.28	6.74
0.07	70.25	69.87	69.51	69.88	5.52	6.43	8.28	6.74
0.13	69.95	69.83	69.94	69.91	5.52	6.43	8.28	6.74
0.20	70.23	69.72	70.12	70.03	5.53	6.43	8.28	6.75
0.26	69.95	69.70	69.97	69.88	5.52	6.43	8.28	6.74
0.33	70.14	69.52	69.67	69.78	5.52	6.43	8.28	6.74
0.40	69.90	69.66	70.19	69.92	5.52	6.43	8.28	6.74
0.46	70.26	69.56	70.40	70.07	5.52	6.43	8.28	6.74
0.53	70.03	69.76	69.60	69.79	5.52	6.43	8.28	6.74
0.59	70.08	69.80	69.87	69.92	5.52	6.43	8.28	6.74
0.66	70.09	70.06	70.29	70.14	5.52	6.43	8.28	6.74
0.72	69.88	70.09	69.68	69.88	5.52	6.43	8.28	6.74
0.79	70.30	70.09	69.58	69.99	5.52	6.43	8.28	6.74
0.86	69.86	70.14	70.15	70.05	5.52	6.43	8.28	6.74
0.92	70.23	69.84	70.31	70.13	5.53	6.42	8.27	6.74
0.99	69.87	69.88	69.45	69.73	5.52	6.43	8.28	6.74
1.12	69.67	69.83	70.29	69.93	5.52	6.43	8.27	6.74
1.19	70.44	70.11	69.57	70.04	5.52	6.43	8.28	6.74
1.25	69.80	69.68	69.73	69.74	5.52	6.43	8.28	6.74
1.38	69.79	69.79	69.94	69.84	5.52	6.43	8.27	6.74
1.45	70.26	69.80	69.63	69.90	5.52	6.43	8.28	6.74
1.51	69.94	70.00	70.11	70.02	5.52	6.43	8.27	6.74
1.58	70.24	69.92	70.33	70.17	5.52	6.42	8.27	6.74
1.65	69.87	70.04	69.69	69.87	5.52	6.43	8.27	6.74
1.71	70.11	69.82	69.90	69.94	5.52	6.42	8.27	6.74
1.78	70.04	69.92	70.08	70.01	5.52	6.42	8.27	6.74
1.91	69.91	69.97	69.66	69.85	5.52	6.43	8.27	6.74
1.98	70.15	70.12	70.03	70.10	5.52	6.42	8.27	6.74
2.04	69.85	70.01	70.27	70.04	5.52	6.42	8.27	6.74
2.11	70.12	69.80	69.63	69.85	5.52	6.43	8.27	6.74
2.04	69.85	70.01	70.27	70.04	5.52	6.42	8.27	6.74
2.17	69.70	69.81	70.01	69.84	5.52	6.42	8.27	6.74
2.24	70.07	69.48	70.35	69.97	5.53	6.42	8.27	6.74

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
2.37	70.05	69.75	69.86	69.89	5.53	6.42	8.27	6.74
2.44	69.89	69.88	70.24	70.00	5.53	6.42	8.27	6.74
2.50	69.97	69.90	70.02	69.96	5.53	6.42	8.27	6.74
2.57	69.86	69.90	69.71	69.83	5.52	6.42	8.27	6.74
2.63	70.10	69.95	70.23	70.09	5.52	6.42	8.27	6.74
2.70	69.68	70.13	70.24	70.02	5.53	6.37	8.27	6.72
2.77	70.09	70.33	69.75	70.06	5.53	6.42	8.27	6.74
2.83	69.75	70.11	69.95	69.94	5.53	6.42	8.27	6.74
2.90	69.80	69.84	70.25	69.96	5.53	6.42	8.26	6.74
2.96	70.03	69.81	70.04	69.96	5.53	6.42	8.27	6.74
3.03	69.53	69.62	69.65	69.60	5.53	6.42	8.27	6.74
3.10	69.77	69.83	70.22	69.94	5.52	6.42	8.26	6.73
3.16	69.60	69.94	70.25	69.93	5.53	6.42	8.26	6.74
3.23	69.72	70.05	69.59	69.79	5.52	6.42	8.27	6.74
3.29	69.56	69.98	70.18	69.91	5.52	6.42	8.26	6.73
3.36	70.55	69.95	70.30	70.26	5.53	6.42	8.26	6.74
3.49	70.19	70.06	69.91	70.05	5.52	6.42	8.26	6.73
3.56	68.97	70.21	70.42	69.87	5.52	6.41	8.26	6.73
3.62	70.31	69.92	69.99	70.07	5.52	6.37	8.26	6.72
3.56	68.97	70.21	70.42	69.87	5.52	6.41	8.26	6.73
3.69	68.87	70.00	69.78	69.55	5.52	6.41	8.26	6.73
3.75	70.76	69.99	70.36	70.37	5.53	6.41	8.26	6.73
3.89	70.53	70.19	69.73	70.15	5.53	6.41	8.26	6.73
3.95	68.93	69.98	70.04	69.65	5.52	6.41	8.26	6.73
4.02	70.51	70.12	70.41	70.35	5.52	6.37	8.26	6.72
4.08	69.86	69.97	69.85	69.89	5.52	6.42	8.26	6.73
4.15	69.79	69.95	69.75	69.83	5.52	6.41	8.26	6.73
4.21	69.87	70.09	70.48	70.15	5.52	6.41	8.26	6.73
4.28	69.18	69.94	69.98	69.70	5.52	6.41	8.26	6.73
4.35	70.49	70.05	69.67	70.07	5.52	6.41	8.26	6.73
4.41	69.22	69.93	70.32	69.82	5.52	6.41	8.26	6.73
4.48	71.39	70.23	70.29	70.64	5.52	6.41	8.26	6.73
4.54	68.51	70.18	69.81	69.50	5.52	6.41	8.26	6.73
4.61	71.22	70.21	70.10	70.51	5.52	6.36	8.26	6.72
4.68	68.25	70.14	70.29	69.56	5.52	6.41	8.26	6.73
4.74	72.16	69.90	70.14	70.74	5.52	6.42	8.26	6.73
4.81	68.04	69.97	69.76	69.26	5.52	6.41	8.26	6.73

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
4.94	68.00	69.87	70.24	69.37	5.52	6.41	8.26	6.73
5.00	71.76	69.95	69.83	70.51	5.52	6.41	8.26	6.73
5.07	68.25	70.19	70.19	69.54	5.52	6.41	8.25	6.73
5.14	71.33	70.27	70.29	70.63	5.52	6.41	8.25	6.73
5.20	68.87	70.16	69.99	69.67	5.52	6.41	8.26	6.73
5.27	70.64	69.98	69.82	70.15	5.52	6.41	8.25	6.73
5.33	69.51	70.20	70.37	70.03	5.52	6.36	8.25	6.71
5.40	69.75	70.17	70.06	69.99	5.52	6.41	8.26	6.73
5.53	69.67	69.90	70.27	69.95	5.52	6.41	8.25	6.73
5.60	70.62	69.91	70.29	70.27	5.52	6.41	8.25	6.73
5.66	69.07	69.66	70.01	69.58	5.52	6.41	8.25	6.73
5.73	70.83	69.88	69.87	70.19	5.52	6.41	8.25	6.73
5.80	68.84	70.16	70.39	69.80	5.52	6.41	8.25	6.72
5.86	70.88	70.32	70.20	70.46	5.52	6.41	8.25	6.73
5.93	68.86	70.39	69.76	69.67	5.52	6.41	8.25	6.73
5.99	70.75	70.12	70.46	70.44	5.52	6.41	8.25	6.72
6.06	69.13	70.06	70.26	69.82	5.52	6.41	8.25	6.72
6.12	70.67	70.28	69.88	70.28	5.52	6.40	8.25	6.73
6.19	69.02	69.97	70.13	69.71	5.52	6.40	8.25	6.72
6.26	70.32	69.95	70.30	70.19	5.52	6.40	8.25	6.72
6.32	69.30	69.77	70.16	69.74	5.52	6.40	8.25	6.72
6.26	70.32	69.95	70.30	70.19	5.52	6.40	8.25	6.72
6.39	70.18	69.97	69.86	70.00	5.52	6.40	8.25	6.72
6.52	69.92	70.17	70.22	70.10	5.51	6.40	8.25	6.72
6.59	69.57	70.54	69.87	69.99	5.52	6.40	8.25	6.72
6.65	69.87	70.20	70.08	70.05	5.52	6.40	8.25	6.72
6.72	69.75	70.33	70.51	70.20	5.51	6.40	8.25	6.72
6.78	69.77	70.15	69.98	69.97	5.52	6.40	8.25	6.72
6.85	69.84	70.19	69.74	69.93	5.52	6.40	8.25	6.72
6.91	69.74	70.23	70.73	70.23	5.52	6.40	8.25	6.72
6.98	69.98	69.69	70.07	69.91	5.52	6.40	8.25	6.72
7.05	69.69	69.92	69.65	69.75	5.52	6.40	8.25	6.72
7.11	69.97	70.06	70.51	70.18	5.51	6.40	8.25	6.72
7.18	69.26	70.34	70.29	69.96	5.52	6.40	8.25	6.72
7.24	70.96	70.46	69.93	70.45	5.51	6.40	8.25	6.72
7.31	68.67	70.35	70.12	69.71	5.51	6.40	8.25	6.72
7.38	72.06	70.48	70.42	70.98	5.52	6.40	8.25	6.72

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
7.51	71.82	70.30	69.65	70.59	5.51	6.40	8.25	6.72
7.57	68.01	69.98	70.49	69.49	5.50	6.40	8.25	6.72
7.64	71.68	70.02	70.18	70.62	5.51	6.40	8.24	6.72
7.71	68.65	70.22	69.80	69.56	5.50	6.40	8.24	6.72
7.77	71.29	70.00	70.22	70.50	5.51	6.41	8.25	6.72
7.84	68.92	70.52	70.44	69.96	5.50	6.41	8.24	6.72
7.90	70.70	70.17	70.06	70.31	5.50	6.40	8.24	6.72
7.97	69.33	69.95	69.95	69.74	5.50	6.41	8.24	6.72
8.03	70.19	69.84	70.42	70.15	5.50	6.41	8.24	6.72
8.10	70.02	70.09	70.09	70.07	5.50	6.42	8.24	6.72
8.17	69.74	70.32	69.91	69.99	5.50	6.42	8.24	6.72
8.23	70.29	70.49	70.39	70.39	5.50	6.41	8.24	6.72
8.30	69.28	70.41	70.33	70.01	5.50	6.41	8.24	6.72
8.36	70.44	70.09	70.02	70.18	5.50	6.41	8.24	6.72
8.43	69.23	70.04	70.03	69.77	5.50	6.41	8.24	6.72
8.50	70.99	70.19	70.52	70.57	5.50	6.41	8.24	6.72
8.56	69.03	69.98	70.08	69.70	5.50	6.40	8.24	6.71
8.69	69.07	69.94	70.46	69.83	5.50	6.40	8.24	6.71
8.76	70.75	69.66	70.17	70.19	5.50	6.40	8.24	6.71
8.82	69.15	70.17	70.03	69.78	5.50	6.40	8.24	6.71
8.89	70.47	70.44	70.26	70.39	5.50	6.40	8.24	6.71
8.96	69.29	70.68	70.35	70.11	5.50	6.40	8.24	6.71
9.02	70.59	70.26	70.00	70.28	5.50	6.40	8.24	6.71
9.09	69.07	70.23	70.00	69.77	5.50	6.40	8.24	6.71
9.15	70.83	70.10	70.42	70.45	5.50	6.40	8.24	6.71
9.22	69.20	70.26	70.18	69.88	5.50	6.40	8.24	6.71
9.29	70.75	70.38	70.04	70.39	5.50	6.40	8.24	6.71
9.35	69.46	70.25	70.30	70.00	5.50	6.40	8.24	6.71
9.48	69.72	70.36	70.20	70.10	5.49	6.40	8.24	6.71
9.55	70.02	70.36	70.07	70.15	5.49	6.40	8.24	6.71
9.61	69.87	70.50	70.35	70.24	5.49	6.40	8.24	6.71
9.68	69.62	70.28	70.19	70.03	5.49	6.40	8.24	6.71
9.75	70.01	70.38	69.97	70.12	5.49	6.40	8.24	6.71
9.81	69.76	70.38	70.29	70.14	5.49	6.40	8.24	6.71
9.88	70.00	70.33	70.32	70.22	5.49	6.39	8.23	6.71
9.94	69.78	70.52	70.18	70.16	5.49	6.40	8.23	6.71

**APPENDIX 13.18 - Descriptive Statistics for Surface Tension Measurement Results of DI+MWCNT (2.00 mg)**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.00	Exp.1	68.00	72.47	0.79	0.63	0.26	1.11
	Exp.2	69.48	70.68	0.23	0.05	0.12	-0.24
	Exp.3	69.45	70.73	0.26	0.07	-0.26	-0.72
	Average	68.98	71.29	0.43	0.25	0.04	0.05

**APPENDIX 13.19 - Surface Tension Measurement Results for DI + Graphene (2.00 mg)**

HUATARC surface tension measurement results for DI + graphene (2.00 mg)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	70.65	69.70	70.21	70.19	5.67	5.69	5.67	5.67
0.07	70.63	70.54	70.77	70.64	5.67	5.69	5.67	5.67
0.13	70.56	70.32	70.43	70.44	5.67	5.69	5.67	5.67
0.20	70.72	70.08	70.86	70.55	5.66	5.68	5.67	5.67
0.26	70.89	70.44	70.64	70.66	5.67	5.68	5.67	5.67
0.33	70.59	70.22	70.23	70.34	5.66	5.68	5.67	5.67
0.40	70.71	70.35	70.55	70.54	5.66	5.68	5.67	5.67
0.46	70.81	70.19	70.83	70.61	5.66	5.68	4.36	5.24
0.53	70.43	70.16	70.68	70.42	5.66	5.68	5.67	5.67
0.59	70.80	70.31	70.89	70.66	5.66	5.68	5.67	5.67
0.66	70.77	70.36	70.91	70.68	5.66	5.68	4.36	5.24
0.79	70.84	70.05	70.48	70.46	5.66	5.68	5.66	5.67
0.86	70.69	70.34	70.10	70.38	5.66	5.68	5.67	5.67
0.92	70.53	70.42	71.19	70.71	5.66	5.68	4.36	5.23
0.99	70.85	70.04	70.51	70.46	5.66	5.68	5.66	5.67
1.05	70.54	70.50	70.75	70.60	5.66	5.68	5.66	5.67
1.12	70.70	70.39	71.19	70.76	5.66	5.68	4.36	5.23
1.19	70.94	70.19	70.94	70.69	5.66	5.68	4.36	5.23
1.25	70.63	70.63	70.65	70.64	5.66	5.68	5.66	5.67
1.32	70.87	70.29	70.64	70.60	5.66	5.68	5.66	5.67
1.38	70.79	69.95	70.42	70.39	5.66	5.68	5.66	5.67
1.45	70.77	70.59	70.68	70.68	5.66	5.68	5.66	5.67
1.51	70.97	70.03	71.05	70.69	5.66	5.68	5.66	5.67
1.58	70.60	70.08	70.75	70.48	5.66	5.68	4.36	5.23
1.71	70.79	69.80	70.86	70.49	5.66	5.68	4.36	5.23
1.78	70.49	70.30	70.60	70.46	5.66	5.67	4.36	5.23
1.84	70.92	70.61	71.56	71.03	5.66	5.68	4.36	5.23
1.91	70.76	69.78	70.83	70.46	5.66	5.68	4.36	5.23
1.98	70.50	70.72	71.08	70.77	5.66	5.67	4.36	5.23
1.91	70.76	69.78	70.83	70.46	5.66	5.68	4.36	5.23
2.11	70.46	69.88	70.68	70.34	5.66	5.68	4.36	5.23
2.17	70.69	70.73	71.44	70.95	5.66	5.67	4.35	5.23
2.24	70.87	69.89	70.57	70.44	5.66	5.67	4.36	5.23

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
2.37	70.95	70.73	71.63	71.10	5.66	5.67	4.35	5.23
2.44	70.62	69.91	70.64	70.39	5.66	5.67	4.36	5.23
2.50	70.53	70.83	70.96	70.77	5.66	5.67	5.66	5.66
2.57	71.10	70.14	70.75	70.66	5.65	5.67	5.66	5.66
2.63	70.41	69.77	70.38	70.18	5.66	5.67	5.66	5.66
2.70	70.75	70.47	70.76	70.66	5.66	5.67	5.66	5.66
2.77	70.70	70.30	70.18	70.39	5.65	5.67	5.66	5.66
2.83	70.28	70.23	70.14	70.22	5.65	5.67	5.66	5.66
2.90	71.25	70.29	70.55	70.70	5.66	5.67	5.66	5.66
2.96	70.52	70.09	70.39	70.33	5.65	5.67	5.66	5.66
3.03	70.63	70.37	70.69	70.56	5.65	5.67	5.66	5.66
3.10	71.16	70.19	70.78	70.71	5.65	5.67	5.66	5.66
3.03	70.63	70.37	70.69	70.56	5.65	5.67	5.66	5.66
3.16	70.22	69.98	69.93	70.04	5.65	5.67	5.66	5.66
3.23	70.94	70.71	70.90	70.85	5.65	5.67	5.66	5.66
3.29	70.72	69.88	69.81	70.14	5.65	5.67	5.66	5.66
3.36	70.39	70.37	70.42	70.39	5.65	5.67	5.66	5.66
3.42	71.26	70.13	70.77	70.72	5.65	5.67	5.65	5.66
3.49	70.46	70.00	70.15	70.20	5.65	5.67	5.66	5.66
3.56	70.79	70.29	71.03	70.70	5.65	5.67	5.65	5.66
3.62	70.86	70.03	70.07	70.32	5.65	5.67	5.65	5.66
3.69	70.49	70.37	70.01	70.29	5.65	5.66	5.65	5.65
3.75	70.98	70.03	70.70	70.57	5.65	5.67	5.65	5.66
3.82	70.65	70.27	69.69	70.20	5.65	5.67	5.65	5.66
3.95	70.73	69.95	70.29	70.32	5.65	5.66	5.65	5.66
4.02	70.59	70.20	70.32	70.37	5.65	5.66	5.64	5.65
4.08	70.78	70.33	70.84	70.65	5.65	5.66	5.65	5.65
4.15	70.78	69.92	70.06	70.26	5.65	5.66	5.65	5.66
4.21	70.67	70.36	70.32	70.45	5.65	5.66	5.65	5.65
4.35	70.75	69.91	70.04	70.23	5.65	5.66	5.64	5.65
4.41	70.44	70.35	70.28	70.36	5.65	5.66	5.65	5.66
4.48	70.91	70.06	70.94	70.63	5.65	5.66	5.65	5.65
4.54	70.26	70.34	70.22	70.27	5.65	5.66	5.65	5.65
4.61	70.93	70.18	70.64	70.58	5.65	5.66	5.65	5.65
4.68	70.80	70.01	70.68	70.50	5.65	5.66	5.65	5.65
4.74	70.75	70.21	69.66	70.21	5.65	5.66	5.65	5.65
4.81	70.91	70.04	70.84	70.59	5.65	5.66	5.65	5.65

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
4.94	70.85	70.32	70.38	70.52	5.65	5.66	5.18	5.49
5.00	70.68	70.07	71.19	70.65	5.65	5.66	5.65	5.65
5.07	70.37	70.25	70.02	70.21	5.65	5.66	5.65	5.65
5.14	70.78	70.31	70.66	70.58	5.65	5.66	5.65	5.65
5.20	70.71	69.77	69.08	69.85	5.64	5.66	5.65	5.65
5.27	71.00	70.41	70.56	70.66	5.65	5.66	5.18	5.49
5.33	70.77	69.83	70.70	70.43	5.64	5.66	5.65	5.65
5.40	70.75	69.97	70.10	70.27	5.64	5.66	5.65	5.65
5.47	70.74	70.33	70.90	70.66	5.64	5.66	4.07	5.12
5.40	70.75	69.97	70.10	70.27	5.64	5.66	5.65	5.65
5.53	70.34	69.99	70.46	70.27	5.65	5.66	5.65	5.65
5.60	71.15	70.39	70.71	70.75	5.64	5.66	5.17	5.49
5.66	70.60	70.15	70.50	70.42	5.64	5.66	5.65	5.65
5.73	71.00	69.79	70.65	70.48	5.64	5.66	5.65	5.65
5.86	70.85	69.97	70.73	70.52	5.64	5.66	5.65	5.65
5.93	70.96	69.97	70.72	70.55	5.64	5.66	5.17	5.49
5.99	70.57	70.31	70.26	70.38	5.64	5.66	5.64	5.65
6.06	70.73	69.86	70.68	70.42	5.64	5.66	5.17	5.49
6.12	70.87	70.01	70.47	70.45	5.64	5.65	5.17	5.49
6.19	70.70	70.10	70.78	70.53	5.64	5.66	5.64	5.65
6.26	71.05	70.15	70.67	70.62	5.64	5.66	5.64	5.65
6.32	70.69	69.81	70.32	70.27	5.64	5.66	5.65	5.65
6.39	71.14	70.27	70.88	70.76	5.64	5.66	5.64	5.65
6.45	70.74	69.95	69.92	70.21	5.64	5.65	5.64	5.65
6.52	70.91	69.94	70.46	70.44	5.64	5.65	5.64	5.65
6.59	70.85	70.18	70.55	70.53	5.64	5.65	5.64	5.65
6.65	70.78	69.84	70.01	70.21	5.64	5.66	5.64	5.65
6.72	70.97	70.39	71.41	70.92	5.64	5.65	5.63	5.64
6.78	70.75	70.25	70.24	70.41	5.64	5.65	5.64	5.64
6.85	70.95	69.74	70.50	70.40	5.64	5.65	5.64	5.64
6.98	70.92	69.91	70.10	70.31	5.64	5.65	5.64	5.64
7.05	70.89	69.85	70.67	70.47	5.64	5.65	5.64	5.64
7.11	70.98	70.32	70.36	70.55	5.64	5.65	5.64	5.64
7.18	70.74	69.89	70.50	70.37	5.64	5.65	5.64	5.64
7.24	71.14	70.35	70.66	70.72	5.64	5.65	5.64	5.64
7.31	70.69	70.32	70.64	70.55	5.64	5.65	5.64	5.64
7.38	70.99	69.44	70.51	70.31	5.64	5.65	5.64	5.64

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
7.51	70.81	69.77	70.20	70.26	5.64	5.65	5.64	5.64
7.57	71.29	69.86	70.47	70.54	5.63	5.65	5.64	5.64
7.64	70.55	70.63	70.63	70.60	5.64	5.65	5.64	5.64
7.71	71.18	69.80	70.37	70.45	5.64	5.65	5.64	5.64
7.77	70.97	70.45	70.72	70.71	5.63	5.65	5.64	5.64
7.84	70.80	70.14	70.89	70.61	5.63	5.65	5.64	5.64
7.90	71.01	69.55	70.48	70.35	5.64	5.65	5.64	5.64
7.97	70.84	70.73	70.77	70.78	5.63	5.65	5.64	5.64
8.03	71.03	69.60	70.39	70.34	5.63	5.65	5.64	5.64
8.10	70.56	70.10	70.48	70.38	5.63	5.65	5.64	5.64
8.17	71.38	70.49	70.34	70.74	5.63	5.65	5.64	5.64
8.23	70.69	69.98	70.97	70.55	5.63	5.65	5.64	5.64
8.30	71.46	70.19	70.33	70.66	5.63	5.65	5.64	5.64
8.36	70.73	70.27	71.27	70.76	5.63	5.65	5.63	5.64
8.43	71.27	69.68	70.76	70.57	5.63	5.65	5.16	5.48
8.50	71.05	70.56	70.34	70.65	5.63	5.65	5.64	5.64
8.56	70.95	69.75	70.74	70.48	5.63	5.65	5.64	5.64
8.63	71.24	69.55	70.03	70.27	5.63	5.65	5.63	5.64
8.69	70.89	71.19	70.94	71.01	5.63	5.64	5.63	5.64
8.76	71.26	69.18	70.87	70.44	5.63	5.65	4.31	5.20
8.82	70.94	71.02	70.53	70.83	5.63	5.64	5.63	5.64
8.89	70.64	70.04	71.40	70.69	5.63	5.64	5.16	5.48
8.96	71.14	69.74	70.16	70.35	5.63	5.64	5.64	5.64
9.09	70.86	69.29	70.33	70.16	5.63	5.65	5.63	5.64
9.15	71.06	70.23	70.54	70.61	5.63	5.64	5.63	5.64
9.22	71.04	70.63	71.22	70.97	5.63	5.64	4.04	5.11
9.29	71.43	69.20	70.24	70.29	5.63	5.65	5.63	5.63
9.35	70.00	71.22	71.29	70.83	5.63	5.64	5.16	5.48
9.42	71.67	69.78	70.84	70.76	5.63	5.64	5.16	5.48
9.48	70.29	70.39	71.02	70.57	5.63	5.64	5.16	5.48
9.55	71.39	70.98	70.91	71.10	5.63	5.64	5.16	5.48
9.61	71.27	69.42	70.58	70.42	5.63	5.63	5.63	5.63
9.68	70.41	70.55	70.33	70.43	5.63	5.64	5.63	5.63
9.75	71.90	70.12	70.63	70.88	5.63	5.64	5.63	5.63
9.81	70.56	69.49	70.70	70.25	5.63	5.64	5.16	5.48
9.88	70.74	70.93	70.54	70.74	5.63	5.64	5.63	5.63

**APPENDIX 13.20 - Descriptive Statistics for Surface Tension Measurement Results of DI + Graphene (2.00 mg)**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.00	Exp.1	70.00	71.90	0.29	0.08	0.53	1.41
	Exp.2	69.18	71.22	0.36	0.13	0.11	0.63
	Exp.3	69.08	71.63	0.39	0.15	-0.22	1.20
	Average	69.85	71.10	0.22	0.05	0.09	0.04

**APPENDIX 13.21 - Surface Tension Measurement Results for Hexane + MWCNT  
(2 mg)**

HUATARC surface tension measurement results for hexane + MWCNT (2.00 mg)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	27.76	28.14	27.87	27.93	4.99	5.05	5.00	5.01
0.07	27.80	28.17	27.89	27.96	4.98	5.11	5.00	5.03
0.13	27.82	28.09	27.92	27.94	5.02	5.17	5.00	5.07
0.20	27.85	28.07	27.91	27.95	5.05	5.11	5.04	5.07
0.26	27.77	28.15	27.91	27.94	5.05	5.11	4.99	5.05
0.33	27.83	28.14	27.98	27.98	5.00	5.10	5.06	5.05
0.40	27.87	28.13	27.88	27.96	5.00	5.10	5.00	5.03
0.46	27.86	28.18	27.83	27.96	5.05	5.09	4.97	5.04
0.53	27.88	28.16	27.86	27.96	4.99	5.15	4.96	5.03
0.59	27.87	28.20	27.88	27.98	4.99	5.14	5.01	5.05
0.66	27.94	28.25	27.90	28.03	5.04	5.14	5.06	5.08
0.72	27.90	28.29	27.95	28.05	5.04	5.21	4.97	5.07
0.79	27.84	28.22	28.00	28.02	5.04	5.14	5.07	5.08
0.86	27.92	28.24	27.98	28.05	5.10	5.20	5.07	5.12
0.92	27.90	28.27	28.01	28.06	5.11	5.20	5.07	5.13
0.99	27.93	28.32	27.97	28.07	5.04	5.20	5.07	5.10
1.05	27.92	28.31	27.92	28.05	5.06	5.10	5.06	5.07
1.19	27.90	28.34	28.00	28.08	5.02	5.06	5.01	5.03
1.32	27.92	28.36	28.02	28.10	5.02	5.16	5.12	5.10
1.38	27.87	28.30	28.02	28.06	5.02	5.05	5.01	5.03
1.45	27.93	28.27	27.97	28.05	5.13	5.09	5.07	5.10
1.51	27.93	28.33	27.98	28.08	5.07	5.14	5.07	5.09
1.58	27.95	28.29	27.99	28.07	5.08	5.14	4.97	5.06
1.71	27.98	28.33	28.04	28.12	5.03	5.09	5.14	5.09
1.78	27.94	28.31	27.97	28.07	5.03	5.14	5.15	5.11
1.84	27.95	28.30	27.95	28.07	5.09	5.19	5.02	5.10
1.91	27.90	28.34	28.04	28.09	5.08	5.28	5.02	5.13
1.98	27.91	28.29	28.02	28.07	5.09	5.20	5.07	5.12
1.91	27.90	28.34	28.04	28.09	5.08	5.28	5.02	5.13
2.04	27.93	28.39	28.07	28.13	5.08	5.21	5.07	5.12
2.11	27.94	28.40	28.10	28.15	5.04	5.04	5.02	5.03
2.17	27.89	28.45	28.06	28.13	5.09	5.04	5.01	5.05
2.24	27.93	28.44	28.08	28.15	5.16	5.08	5.01	5.09

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
2.37	27.92	28.42	28.18	28.17	5.03	5.04	5.02	5.03
2.44	27.91	28.46	28.15	28.17	5.04	5.01	5.02	5.02
2.50	27.93	28.39	28.17	28.16	5.04	5.04	5.07	5.05
2.57	27.97	28.35	28.18	28.17	5.09	5.05	5.03	5.06
2.63	28.01	28.37	28.25	28.21	5.09	4.98	5.02	5.03
2.70	27.99	28.33	28.20	28.17	5.10	5.30	5.02	5.14
2.77	28.02	28.38	28.18	28.19	5.18	5.29	5.02	5.16
2.83	27.93	28.39	28.26	28.19	5.11	5.22	5.08	5.13
2.90	27.98	28.33	28.21	28.17	5.11	5.15	5.08	5.11
2.96	27.96	28.37	28.19	28.17	5.10	5.24	5.08	5.14
0.00	27.76	28.14	27.87	27.93	4.99	5.05	5.00	5.01
0.07	27.80	28.17	27.89	27.96	4.98	5.11	5.00	5.03
0.13	27.82	28.09	27.92	27.94	5.02	5.17	5.00	5.07
0.20	27.85	28.07	27.91	27.95	5.05	5.11	5.04	5.07
0.26	27.77	28.15	27.91	27.94	5.05	5.11	4.99	5.05
0.33	27.83	28.14	27.98	27.98	5.00	5.10	5.06	5.05
0.40	27.87	28.13	27.88	27.96	5.00	5.10	5.00	5.03
0.46	27.86	28.18	27.83	27.96	5.05	5.09	4.97	5.04
0.53	27.88	28.16	27.86	27.96	4.99	5.15	4.96	5.03
0.59	27.87	28.20	27.88	27.98	4.99	5.14	5.01	5.05
0.66	27.94	28.25	27.90	28.03	5.04	5.14	5.06	5.08
0.72	27.90	28.29	27.95	28.05	5.04	5.21	4.97	5.07
0.79	27.84	28.22	28.00	28.02	5.04	5.14	5.07	5.08
0.72	27.90	28.29	27.95	28.05	5.04	5.21	4.97	5.07
0.86	27.92	28.24	27.98	28.05	5.10	5.20	5.07	5.12
0.92	27.90	28.27	28.01	28.06	5.11	5.20	5.07	5.13
0.99	27.93	28.32	27.97	28.07	5.04	5.20	5.07	5.10
1.05	27.92	28.31	27.92	28.05	5.06	5.10	5.06	5.07
1.12	27.94	28.31	27.96	28.07	5.07	5.10	5.06	5.08
1.19	27.90	28.34	28.00	28.08	5.02	5.06	5.01	5.03
1.25	27.93	28.27	27.94	28.05	5.07	5.10	5.06	5.08
1.38	27.87	28.30	28.02	28.06	5.02	5.05	5.01	5.03
1.45	27.93	28.27	27.97	28.05	5.13	5.09	5.07	5.10
1.51	27.93	28.33	27.98	28.08	5.07	5.14	5.07	5.09
1.58	27.95	28.29	27.99	28.07	5.08	5.14	4.97	5.06
1.65	27.93	28.28	28.01	28.08	5.02	5.09	5.07	5.06
1.71	27.98	28.33	28.04	28.12	5.03	5.09	5.14	5.09

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.84	27.95	28.30	27.95	28.07	5.09	5.19	5.02	5.10
1.91	27.90	28.34	28.04	28.09	5.08	5.28	5.02	5.13
1.98	27.91	28.29	28.02	28.07	5.09	5.20	5.07	5.12
2.04	27.93	28.39	28.07	28.13	5.08	5.21	5.07	5.12
2.11	27.94	28.40	28.10	28.15	5.04	5.04	5.02	5.03
2.17	27.89	28.45	28.06	28.13	5.09	5.04	5.01	5.05
2.24	27.93	28.44	28.08	28.15	5.16	5.08	5.01	5.09
2.30	27.90	28.42	28.13	28.15	5.15	5.04	5.02	5.07
2.37	27.92	28.42	28.18	28.17	5.03	5.04	5.02	5.03
2.44	27.91	28.46	28.15	28.17	5.04	5.01	5.02	5.02
2.50	27.93	28.39	28.17	28.16	5.04	5.04	5.07	5.05
2.57	27.97	28.35	28.18	28.17	5.09	5.05	5.03	5.06
2.77	28.02	28.38	28.18	28.19	5.18	5.29	5.02	5.16
2.83	27.93	28.39	28.26	28.19	5.11	5.22	5.08	5.13
2.90	27.98	28.33	28.21	28.17	5.11	5.15	5.08	5.11
2.96	27.96	28.37	28.19	28.17	5.10	5.24	5.08	5.14
3.03	27.95	28.35	28.26	28.18	5.10	5.19	4.99	5.09
0.00	27.76	28.14	27.87	27.93	4.99	5.05	5.00	5.01
0.07	27.80	28.17	27.89	27.96	4.98	5.11	5.00	5.03
0.13	27.82	28.09	27.92	27.94	5.02	5.17	5.00	5.07
0.20	27.85	28.07	27.91	27.95	5.05	5.11	5.04	5.07
0.26	27.77	28.15	27.91	27.94	5.05	5.11	4.99	5.05
0.33	27.83	28.14	27.98	27.98	5.00	5.10	5.06	5.05
0.40	27.87	28.13	27.88	27.96	5.00	5.10	5.00	5.03
0.46	27.86	28.18	27.83	27.96	5.05	5.09	4.97	5.04
0.53	27.88	28.16	27.86	27.96	4.99	5.15	4.96	5.03
0.59	27.87	28.20	27.88	27.98	4.99	5.14	5.01	5.05
0.66	27.94	28.25	27.90	28.03	5.04	5.14	5.06	5.08
0.72	27.90	28.29	27.95	28.05	5.04	5.21	4.97	5.07
0.79	27.84	28.22	28.00	28.02	5.04	5.14	5.07	5.08
0.86	27.92	28.24	27.98	28.05	5.10	5.20	5.07	5.12
0.92	27.90	28.27	28.01	28.06	5.11	5.20	5.07	5.13
0.99	27.93	28.32	27.97	28.07	5.04	5.20	5.07	5.10
0.99	27.93	28.32	27.97	28.07	5.04	5.20	5.07	5.10
1.05	27.92	28.31	27.92	28.05	5.06	5.10	5.06	5.07
1.12	27.94	28.31	27.96	28.07	5.07	5.10	5.06	5.08
1.19	27.90	28.34	28.00	28.08	5.02	5.06	5.01	5.03

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.32	27.92	28.36	28.02	28.10	5.02	5.16	5.12	5.10
1.38	27.87	28.30	28.02	28.06	5.02	5.05	5.01	5.03
1.45	27.93	28.27	27.97	28.05	5.13	5.09	5.07	5.10
1.51	27.93	28.33	27.98	28.08	5.07	5.14	5.07	5.09
1.58	27.95	28.29	27.99	28.07	5.08	5.14	4.97	5.06
1.65	27.93	28.28	28.01	28.08	5.02	5.09	5.07	5.06
1.71	27.98	28.33	28.04	28.12	5.03	5.09	5.14	5.09
1.78	27.94	28.31	27.97	28.07	5.03	5.14	5.15	5.11
1.84	27.95	28.30	27.95	28.07	5.09	5.19	5.02	5.10
1.98	27.91	28.29	28.02	28.07	5.09	5.20	5.07	5.12
2.04	27.93	28.39	28.07	28.13	5.08	5.21	5.07	5.12
2.11	27.94	28.40	28.10	28.15	5.04	5.04	5.02	5.03
2.17	27.89	28.45	28.06	28.13	5.09	5.04	5.01	5.05
2.24	27.93	28.44	28.08	28.15	5.16	5.08	5.01	5.09
2.30	27.90	28.42	28.13	28.15	5.15	5.04	5.02	5.07
2.37	27.92	28.42	28.18	28.17	5.03	5.04	5.02	5.03
2.44	27.91	28.46	28.15	28.17	5.04	5.01	5.02	5.02
2.50	27.93	28.39	28.17	28.16	5.04	5.04	5.07	5.05
2.57	27.97	28.35	28.18	28.17	5.09	5.05	5.03	5.06
2.63	28.01	28.37	28.25	28.21	5.09	4.98	5.02	5.03
2.70	27.99	28.33	28.20	28.17	5.10	5.30	5.02	5.14
2.77	28.02	28.38	28.18	28.19	5.18	5.29	5.02	5.16
2.83	27.93	28.39	28.26	28.19	5.11	5.22	5.08	5.13
2.90	27.98	28.33	28.21	28.17	5.11	5.15	5.08	5.11
2.96	27.96	28.37	28.19	28.17	5.10	5.24	5.08	5.14
3.03	27.95	28.35	28.26	28.18	5.10	5.19	4.99	5.09

**APPENDIX 13.22 - Descriptive Statistics for Surface Tension Measurement Results of Hexane + MWCNT (2.00 mg)**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.00	Exp.1	27.76	28.02	0.06	0.00	-0.74	0.83
	Exp.2	28.07	28.46	0.10	0.01	-0.53	-0.38
	Exp.3	27.83	28.26	0.12	0.01	0.48	-0.79
	Average	27.93	28.21	0.08	0.01	-0.24	-0.97



**APPENDIX 13.23 - Surface Tension Measurement Results for Hexane + Graphene  
(2 mg)**

HUATARC surface tension measurement results for hexane + graphene (2.00 mg)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	27.36	27.82	28.54	27.91	4.69	4.93	4.98	4.86
0.07	27.33	27.82	28.59	27.91	4.72	4.94	4.98	4.88
0.13	27.30	27.84	28.41	27.85	4.79	4.93	4.88	4.87
0.20	27.32	27.79	28.59	27.90	4.79	4.94	4.89	4.87
0.26	27.20	27.78	28.55	27.84	4.84	5.00	4.88	4.91
0.33	26.97	27.81	28.57	27.78	4.76	4.97	4.95	4.89
0.46	27.15	27.80	28.50	27.82	4.83	4.89	4.89	4.87
0.53	27.46	27.85	28.51	27.94	4.83	4.93	4.92	4.90
0.59	27.29	27.89	28.58	27.92	4.83	4.94	4.93	4.90
0.66	27.47	27.90	28.55	27.97	5.01	4.90	4.92	4.94
0.72	27.67	27.83	28.55	28.02	5.02	4.97	4.90	4.96
0.79	27.96	27.91	28.49	28.12	5.12	4.94	4.92	4.99
0.86	27.98	27.83	28.65	28.15	5.02	4.97	5.03	5.01
0.92	27.82	27.91	28.53	28.09	4.94	4.89	4.98	4.94
0.99	28.22	27.88	28.59	28.23	4.93	4.97	4.98	4.96
1.05	27.96	27.84	28.55	28.12	4.89	4.93	4.94	4.92
1.12	28.20	27.91	28.60	28.24	4.96	4.90	4.97	4.94
1.19	28.12	27.87	28.69	28.22	5.02	4.89	4.97	4.96
1.25	28.21	27.92	28.63	28.25	4.95	5.04	4.93	4.98
1.32	28.29	27.97	28.63	28.29	5.02	4.90	4.93	4.95
1.38	28.30	27.91	28.68	28.30	5.03	4.90	5.01	4.98
1.45	28.26	27.93	28.54	28.24	4.95	5.02	4.93	4.97
1.51	28.24	27.98	28.67	28.30	4.96	5.02	4.94	4.97
1.58	28.30	27.91	28.59	28.27	4.95	4.95	4.96	4.96
1.65	28.29	27.89	28.67	28.28	4.95	4.95	4.94	4.95
1.71	28.25	27.81	28.70	28.25	4.97	4.98	4.97	4.97
1.84	28.34	27.79	28.70	28.28	4.98	4.96	4.91	4.95
1.91	28.36	27.77	28.62	28.25	5.05	4.95	4.91	4.97
1.98	28.41	27.81	28.64	28.29	4.98	4.99	4.94	4.97
1.91	28.36	27.77	28.62	28.25	5.05	4.95	4.91	4.97
2.04	28.57	27.85	28.65	28.36	5.06	4.99	4.88	4.98
2.11	28.57	27.77	28.62	28.32	5.05	4.91	4.91	4.96
2.24	28.61	27.85	28.61	28.36	5.04	5.03	4.90	4.99

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
2.37	28.55	27.88	28.56	28.33	4.96	5.02	4.91	4.96
2.44	28.56	27.98	28.69	28.41	4.96	4.99	4.94	4.96
2.50	28.41	27.92	28.76	28.36	4.97	5.03	4.90	4.97
2.57	28.47	27.96	28.67	28.37	4.91	5.03	4.90	4.95
2.63	28.41	27.96	28.69	28.36	4.98	4.99	4.88	4.95
2.70	28.55	27.91	28.68	28.38	4.97	4.99	4.91	4.96
2.77	28.41	27.96	28.71	28.36	4.92	4.96	4.89	4.92
2.83	28.47	27.99	28.67	28.38	4.91	4.92	4.86	4.90
2.90	28.50	28.02	28.67	28.40	4.90	4.92	4.92	4.92
2.96	28.40	28.01	28.73	28.38	4.91	5.04	4.93	4.96
3.03	28.49	27.97	28.76	28.41	4.91	5.03	4.94	4.96
3.10	28.48	28.00	28.75	28.41	4.87	5.07	4.97	4.97
3.16	28.54	27.97	28.68	28.40	4.90	5.00	4.91	4.94
3.10	28.48	28.00	28.75	28.41	4.87	5.07	4.97	4.97
3.29	28.49	27.98	28.73	28.40	4.87	4.97	4.95	4.93
3.36	28.47	27.94	28.71	28.37	4.86	5.01	4.92	4.93
3.42	28.46	27.92	28.69	28.36	4.88	5.04	4.96	4.96
3.49	28.42	27.89	28.72	28.34	4.89	5.08	4.95	4.97
3.56	28.32	27.99	28.78	28.36	4.89	5.01	4.99	4.96
3.62	28.42	28.00	28.74	28.38	4.94	5.01	5.03	4.99
3.69	28.48	27.95	28.72	28.38	4.93	5.00	5.04	4.99
3.75	28.44	27.98	28.70	28.37	4.93	5.04	5.03	5.00
3.82	28.43	27.96	28.72	28.37	4.93	5.00	4.93	4.95
3.89	28.37	28.03	28.74	28.38	4.90	5.04	5.00	4.98
3.95	28.42	28.01	28.73	28.39	4.94	5.05	5.00	4.99
4.02	28.36	28.04	28.72	28.38	4.94	5.01	5.03	4.99
4.08	28.42	28.03	28.74	28.40	4.90	5.01	5.00	4.97
4.15	28.42	28.05	28.74	28.40	4.90	5.02	4.94	4.95
4.21	28.43	27.99	28.73	28.39	4.94	5.02	4.97	4.98
4.28	28.40	28.02	28.72	28.38	4.94	5.01	4.95	4.97
4.35	28.37	28.01	28.74	28.38	4.90	5.02	4.98	4.97
4.41	28.37	28.03	28.64	28.35	4.95	5.01	4.94	4.97
4.54	28.43	28.06	28.72	28.41	4.95	5.05	5.05	5.02
4.61	28.43	28.10	28.82	28.45	4.95	5.05	5.05	5.02
4.68	28.40	28.11	28.79	28.43	4.91	5.02	5.05	4.99
4.74	28.39	28.08	28.80	28.42	4.96	5.05	5.02	5.01
4.81	28.37	28.13	28.80	28.44	4.97	5.02	5.02	5.00

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
4.94	28.36	28.13	28.78	28.42	5.03	5.05	5.02	5.03
5.01	28.36	28.14	28.79	28.43	4.97	5.09	5.02	5.02
5.07	28.52	28.20	28.69	28.47	4.96	5.02	5.05	5.01
5.14	28.57	28.19	28.80	28.52	4.96	5.02	5.03	5.00
5.20	28.57	28.19	28.77	28.51	4.92	5.02	5.03	4.99
5.27	28.57	28.18	28.79	28.51	4.96	5.03	4.99	4.99
5.33	28.54	28.22	28.75	28.50	4.91	5.06	4.99	4.99
5.40	28.56	28.23	28.75	28.51	4.95	4.99	5.06	5.00
5.53	28.53	28.23	28.75	28.51	4.88	5.07	5.00	4.98
5.60	28.55	28.24	28.73	28.50	4.92	5.00	5.00	4.97
5.66	28.46	28.18	28.74	28.46	4.92	5.02	5.03	4.99
5.73	28.46	28.22	28.73	28.47	4.92	5.03	5.01	4.99
5.80	28.41	28.28	28.72	28.47	4.88	5.03	5.03	4.98
5.86	28.44	28.27	28.67	28.46	4.92	5.03	5.00	4.98
5.93	28.48	28.28	28.74	28.50	4.92	5.03	4.99	4.98
5.99	28.50	28.31	28.74	28.52	4.93	5.07	5.06	5.02
6.06	28.61	28.23	28.71	28.51	4.97	4.95	5.02	4.98
6.12	28.59	28.23	28.68	28.50	4.93	5.07	5.00	5.00
6.19	28.53	28.29	28.72	28.51	4.93	5.03	5.06	5.01
6.26	28.59	28.27	28.67	28.51	4.94	5.04	4.98	4.98
6.32	28.59	28.30	28.62	28.51	4.99	5.04	4.96	4.99
6.39	28.55	28.27	28.67	28.50	4.98	5.07	5.03	5.03
6.45	28.58	28.27	28.72	28.52	4.94	5.08	5.01	5.01
6.59	28.55	28.26	28.67	28.49	4.99	5.07	5.04	5.03
6.65	28.55	28.28	28.73	28.52	4.94	5.07	5.01	5.01
6.72	28.56	28.25	28.65	28.49	4.94	5.07	5.07	5.03
6.78	28.51	28.32	28.67	28.50	4.99	5.16	5.01	5.05
6.85	28.50	28.36	28.68	28.51	4.95	5.16	5.08	5.06
6.91	28.50	28.29	28.67	28.49	5.00	5.01	5.01	5.01
6.98	28.45	28.28	28.71	28.48	5.00	5.09	5.09	5.06
6.98	28.45	28.28	28.71	28.48	5.00	5.09	5.09	5.06
7.05	28.41	28.32	28.67	28.47	5.00	5.10	5.08	5.06
7.11	28.35	28.24	28.64	28.41	5.07	5.05	5.08	5.07
7.18	28.29	28.19	28.69	28.39	4.98	5.09	5.08	5.05
7.24	28.22	28.18	28.70	28.37	5.08	5.05	5.05	5.06
7.31	28.34	28.18	28.62	28.38	5.09	5.05	5.08	5.07
7.38	28.05	28.10	28.68	28.28	4.99	5.00	5.05	5.01

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
7.51	28.23	28.18	28.71	28.37	4.89	5.05	5.06	5.00
7.57	28.33	28.15	28.68	28.39	4.92	5.09	5.06	5.02
7.64	28.44	28.14	28.74	28.44	4.88	5.05	5.10	5.01
7.71	28.48	28.18	28.64	28.43	4.91	5.01	5.04	4.99
7.77	28.49	28.17	28.73	28.47	4.84	5.05	5.06	4.98
7.84	28.50	28.10	28.59	28.40	4.88	5.04	5.05	4.99
7.90	28.49	28.15	28.64	28.43	4.91	5.05	5.01	4.99
7.97	28.50	28.13	28.75	28.46	4.88	5.05	5.06	5.00
8.03	28.49	28.20	28.77	28.49	5.07	5.05	5.03	5.05
8.10	28.68	28.11	28.61	28.47	4.98	5.05	4.98	5.00
8.17	28.68	28.14	28.73	28.52	5.02	5.05	5.05	5.04
8.23	28.67	28.11	28.71	28.50	5.02	5.05	5.05	5.04
8.36	28.69	28.22	28.73	28.55	4.97	5.06	5.01	5.01
8.43	28.61	28.22	28.69	28.51	4.94	5.10	5.05	5.03
8.50	28.61	28.14	28.72	28.49	4.94	5.02	5.08	5.01
8.56	28.62	28.21	28.73	28.52	4.94	5.03	5.02	5.00
8.63	28.51	28.12	28.74	28.46	4.95	5.10	5.06	5.04
8.69	28.57	28.15	28.72	28.48	4.96	5.10	5.10	5.05
8.76	28.55	28.18	28.68	28.47	4.92	5.07	5.07	5.02
8.82	28.65	28.16	28.61	28.47	4.99	5.10	4.99	5.03
8.89	28.66	28.14	28.74	28.52	5.03	5.10	5.06	5.06
8.96	28.60	28.13	28.73	28.49	4.99	5.06	5.14	5.06
9.02	28.64	28.05	28.71	28.47	4.99	5.05	5.07	5.04
9.09	28.60	28.17	28.74	28.50	4.99	5.05	5.11	5.05
9.15	28.63	28.18	28.66	28.49	4.99	5.09	5.11	5.06
9.22	28.64	28.08	28.68	28.47	5.04	5.08	5.04	5.05

**APPENDIX 13.24 - Descriptive Statistics for Surface Tension Measurement Results of Hexane + Graphene (2.00 mg)**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
2.00	Exp.1	26.97	28.69	0.35	0.12	-2.34	5.12
	Exp.2	27.77	28.36	0.15	0.02	-0.21	-1.11
	Exp.3	28.41	28.82	0.07	0.01	-0.84	0.84
	Average	27.78	28.55	0.17	0.03	-1.93	3.34

## APPENDIX 13.25 - Surface Tension Measurement Results for DI + SDS (0.82 mM)

HUATARC surface tension measurement results for DI + SDS (0.82 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	41.80	41.08	40.71	41.20	3.97	4.04	3.56	3.86
0.01	41.98	41.13	40.67	41.26	3.96	4.04	3.55	3.85
0.03	42.27	41.20	40.72	41.40	3.97	4.04	3.63	3.88
0.04	42.28	41.11	40.94	41.44	3.97	4.06	3.55	3.86
0.05	42.07	41.07	40.77	41.30	4.23	4.06	3.93	4.07
0.07	42.04	41.07	40.85	41.32	4.05	4.06	3.63	3.91
0.08	42.09	41.07	40.92	41.36	4.01	4.06	3.55	3.87
0.09	42.20	40.99	41.12	41.44	4.01	4.06	3.63	3.90
0.11	41.96	41.04	41.25	41.42	3.97	4.06	3.55	3.86
0.12	41.84	41.18	41.16	41.39	4.01	4.06	3.88	3.98
0.13	41.69	41.18	41.04	41.30	4.22	4.06	3.55	3.94
0.14	41.47	41.25	40.87	41.20	4.33	4.06	3.97	4.12
0.16	41.63	41.18	40.88	41.23	4.01	4.06	3.63	3.90
0.17	41.63	41.15	40.64	41.14	4.01	4.06	4.16	4.08
0.21	41.45	41.15	40.80	41.13	4.01	4.06	3.55	3.87
0.22	41.45	41.17	40.68	41.10	4.22	4.05	3.55	3.94
0.24	41.48	41.16	40.64	41.09	4.22	4.06	3.97	4.08
0.25	41.59	41.06	40.81	41.15	3.96	4.06	3.63	3.88
0.26	41.51	41.14	40.71	41.12	4.00	4.05	3.93	3.99
0.28	41.60	41.05	41.04	41.23	4.01	4.05	3.55	3.87
0.29	41.43	41.12	40.96	41.17	4.20	4.06	3.55	3.94
0.30	41.46	41.09	40.84	41.13	3.99	4.06	3.97	4.01
0.33	41.65	41.10	40.67	41.14	4.00	4.05	4.00	4.02
0.34	41.58	41.03	40.94	41.18	3.96	4.03	3.55	3.85
0.36	41.54	41.12	40.84	41.17	4.00	4.05	3.62	3.89
0.37	41.69	41.10	40.88	41.22	3.99	4.05	3.54	3.86
0.38	41.43	41.15	40.85	41.14	4.22	4.03	3.62	3.96
0.40	41.52	41.08	40.71	41.10	4.22	4.05	4.00	4.09
0.41	41.47	41.05	40.81	41.11	4.00	4.03	3.55	3.86
0.42	41.61	41.06	40.67	41.11	3.96	4.05	3.92	3.98
0.41	41.47	41.05	40.81	41.11	4.00	4.03	3.55	3.86

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.45	41.46	41.06	40.73	41.08	4.22	4.05	3.62	3.96
0.46	41.63	41.01	40.82	41.15	3.99	4.05	3.54	3.86
0.47	41.59	41.09	40.61	41.10	4.22	4.05	4.00	4.09
0.49	41.74	40.97	40.79	41.17	4.00	4.05	4.00	4.02
0.50	41.72	41.08	40.82	41.21	3.96	4.05	3.54	3.85
0.51	41.84	41.05	40.76	41.22	3.96	4.05	3.87	3.96
0.53	41.69	41.06	40.93	41.23	4.00	4.05	3.62	3.89
0.54	41.45	41.08	40.78	41.10	4.32	4.05	3.54	3.97
0.55	41.69	41.04	40.81	41.18	4.21	4.05	3.55	3.94
0.57	41.56	41.12	40.65	41.11	3.96	4.05	4.00	4.00
0.58	41.58	40.87	40.90	41.12	3.95	4.03	3.54	3.84
0.59	41.26	41.01	40.83	41.03	4.29	4.05	3.54	3.96
0.61	41.53	41.06	40.76	41.12	4.00	4.05	3.61	3.89
0.62	41.28	40.97	40.67	40.97	4.21	4.05	3.54	3.93
0.63	41.08	41.12	40.61	40.94	4.31	4.05	3.62	3.99
0.66	41.21	41.04	40.77	41.01	3.96	4.05	3.54	3.85
0.67	41.26	40.93	40.85	41.01	3.99	4.05	3.54	3.86
0.68	41.17	41.04	40.84	41.02	3.98	4.05	3.54	3.86
0.70	41.35	41.01	40.73	41.03	3.98	4.05	3.54	3.86
0.71	41.26	41.03	40.66	40.98	4.21	4.05	3.54	3.93
0.72	41.19	41.10	40.60	40.96	4.21	4.05	3.99	4.08
0.74	41.46	40.83	40.72	41.00	3.99	4.04	3.61	3.88
0.75	41.40	40.92	40.55	40.96	4.00	4.02	3.92	3.98
0.78	41.24	40.97	40.75	40.99	4.31	4.05	3.54	3.97
0.79	41.33	40.95	40.69	40.99	4.31	4.05	3.61	3.99
0.80	41.35	40.98	40.63	40.99	3.99	4.05	3.61	3.88
0.79	41.33	40.95	40.69	40.99	4.31	4.05	3.61	3.99
0.82	41.30	41.04	40.68	41.01	3.99	4.04	3.54	3.86
0.83	41.47	40.88	40.81	41.05	3.99	4.02	3.54	3.85
0.84	41.37	40.97	40.69	41.01	3.99	4.04	3.53	3.85
0.86	41.36	40.93	40.73	41.01	3.99	4.05	3.53	3.86
0.87	41.20	40.94	40.66	40.93	4.31	4.04	3.54	3.96
0.88	41.42	40.96	40.65	41.01	3.98	4.05	3.62	3.88
0.90	41.40	40.93	40.59	40.97	3.99	4.04	3.54	3.86
0.91	41.27	40.95	40.63	40.95	3.99	4.04	3.53	3.85
0.92	41.35	40.91	40.70	40.99	3.99	4.02	3.53	3.85
0.94	41.25	40.99	40.65	40.96	4.19	4.04	3.53	3.92

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.96	41.21	40.94	40.55	40.90	4.31	4.04	3.61	3.99
0.97	41.34	41.01	40.65	41.00	3.97	4.04	3.54	3.85
0.99	41.30	40.94	40.61	40.95	3.95	4.02	3.53	3.83
1.00	41.28	40.93	40.57	40.93	3.95	4.04	3.91	3.97
1.01	41.26	40.84	40.67	40.92	3.97	4.04	3.53	3.85
1.03	41.18	40.91	40.50	40.86	4.31	4.04	3.61	3.99
1.04	41.32	40.84	40.44	40.87	3.97	4.04	3.53	3.85
1.05	41.21	40.95	40.43	40.86	4.03	4.04	3.61	3.89
1.07	41.31	40.85	40.61	40.92	3.99	4.04	3.53	3.85
1.08	41.32	40.84	40.51	40.89	3.99	4.04	3.53	3.85
1.09	41.30	40.95	40.59	40.95	3.94	4.04	3.53	3.84
1.11	41.20	40.89	40.58	40.89	4.22	4.04	3.53	3.93
1.12	41.11	40.92	40.45	40.83	4.27	4.04	3.98	4.10
1.13	41.23	40.92	40.62	40.92	3.99	4.04	3.53	3.85
1.16	41.19	40.78	40.58	40.85	3.98	4.02	3.53	3.84
1.17	41.30	40.83	40.54	40.89	3.98	4.04	3.53	3.85
1.19	41.24	40.90	40.47	40.87	4.20	4.04	3.53	3.92
1.20	41.13	40.84	40.42	40.80	4.20	4.04	3.53	3.92
1.21	41.02	40.91	40.41	40.78	4.01	4.04	3.61	3.89
1.22	41.33	40.84	40.49	40.89	3.98	4.04	3.53	3.85
1.24	41.13	40.91	40.40	40.81	3.94	4.04	3.53	3.84
1.25	41.22	40.77	40.57	40.85	3.98	4.04	3.60	3.87
1.26	41.10	40.88	40.51	40.83	4.20	4.04	3.60	3.95
1.28	41.14	40.90	40.47	40.84	4.20	4.04	3.53	3.92
1.29	41.07	40.89	40.43	40.80	4.30	4.04	3.60	3.98
1.30	41.14	40.94	40.46	40.85	3.98	4.04	3.60	3.87
1.32	41.24	40.75	40.52	40.84	3.94	4.01	3.52	3.82
1.33	41.13	40.90	40.37	40.80	3.94	4.04	3.52	3.83
1.34	41.10	40.83	40.42	40.78	4.20	4.04	3.52	3.92
1.36	41.06	40.93	40.43	40.81	4.20	4.04	3.61	3.95
1.34	41.10	40.83	40.42	40.78	4.20	4.04	3.52	3.92
1.37	41.15	40.88	40.36	40.80	4.20	4.03	3.60	3.94
1.38	41.18	40.86	40.38	40.81	3.96	4.03	3.53	3.84
1.40	41.03	40.89	40.45	40.79	3.98	4.03	3.52	3.84
1.41	41.27	40.82	40.48	40.86	3.94	4.03	3.52	3.83
1.44	41.09	40.78	40.35	40.74	4.00	4.03	3.52	3.85
1.45	41.02	40.92	40.33	40.76	4.30	4.03	3.98	4.10

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.48	41.13	40.84	40.38	40.78	3.98	4.03	3.52	3.84
1.49	41.03	40.78	40.32	40.71	3.98	4.04	3.52	3.85
1.50	41.14	40.74	40.38	40.75	3.98	4.03	3.90	3.97
1.51	41.04	40.85	40.23	40.71	4.19	4.03	3.60	3.94
1.53	41.05	40.74	40.26	40.68	4.00	4.03	3.52	3.85
1.55	41.14	40.81	40.44	40.80	3.97	4.03	3.52	3.84
1.57	41.09	40.78	40.33	40.73	3.98	4.03	3.52	3.84
1.58	41.08	40.81	40.32	40.74	3.98	4.01	3.52	3.84
1.59	41.07	40.73	40.28	40.69	3.96	4.03	3.52	3.84
1.61	40.88	40.81	40.23	40.64	4.29	4.01	3.97	4.09
1.62	41.12	40.73	40.24	40.70	3.96	4.03	3.52	3.84
1.63	40.97	40.83	40.16	40.65	3.97	4.03	3.89	3.96
1.65	41.08	40.68	40.23	40.66	3.93	4.03	3.52	3.83
1.66	41.14	40.75	40.33	40.74	3.97	4.03	3.51	3.84
1.67	40.97	40.75	40.24	40.65	3.96	4.03	3.52	3.84
1.69	40.99	40.73	40.24	40.65	4.19	4.03	3.59	3.94
1.70	40.87	40.81	40.26	40.65	4.19	4.03	3.60	3.94
1.71	41.17	40.72	40.23	40.71	3.96	4.03	3.52	3.84
1.74	41.06	40.79	40.26	40.70	3.93	4.03	3.59	3.85
1.75	40.97	40.76	40.29	40.67	3.96	4.03	3.52	3.84
1.76	40.88	40.67	40.16	40.57	4.20	4.03	3.52	3.92
1.78	40.95	40.70	40.19	40.61	3.96	4.03	3.59	3.86
1.79	40.96	40.73	40.14	40.61	3.97	4.03	3.60	3.87
1.80	41.03	40.63	40.17	40.61	3.95	4.03	3.51	3.83
1.82	40.85	40.71	40.10	40.55	3.93	4.00	3.51	3.81
1.83	40.83	40.80	40.14	40.59	3.95	4.03	3.51	3.83
1.84	40.81	40.66	40.11	40.53	4.19	4.03	3.97	4.06
1.86	40.91	40.75	40.12	40.59	3.96	4.03	3.52	3.84
1.87	40.82	40.63	40.16	40.54	3.95	4.03	3.52	3.83
1.88	40.77	40.77	40.08	40.54	3.97	4.03	3.51	3.84
1.90	40.97	40.61	40.10	40.56	3.95	4.00	3.59	3.85
1.92	40.90	40.63	40.10	40.54	3.95	4.03	3.52	3.83
1.94	40.74	40.68	40.10	40.51	4.29	4.02	3.93	4.08
1.95	40.83	40.77	40.12	40.57	4.18	4.03	3.59	3.93
1.96	40.88	40.76	40.11	40.58	3.97	4.03	3.51	3.84
1.98	40.82	40.72	40.06	40.53	3.96	4.00	3.51	3.82

## APPENDIX 13.26 - Surface Tension Measurement Results for DI + SDS (3.00 mM)

HUATARC surface tension measurement results for DI + SDS (3.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	21.82	21.41	21.87	21.70	3.89	3.91	3.93	3.91
0.01	21.80	21.42	21.87	21.70	3.89	3.91	3.89	3.90
0.03	21.80	21.41	21.84	21.68	3.94	3.91	3.93	3.93
0.04	21.80	21.41	21.84	21.68	3.90	3.91	3.93	3.91
0.05	21.82	21.41	21.85	21.69	3.94	3.91	3.89	3.91
0.07	21.83	21.41	21.83	21.69	3.93	3.91	3.93	3.92
0.08	21.83	21.41	21.85	21.70	3.90	3.91	3.89	3.90
0.11	21.82	21.42	21.85	21.70	3.90	3.86	3.89	3.88
0.12	21.80	21.40	21.85	21.68	3.90	3.91	3.89	3.90
0.13	21.80	21.41	21.84	21.69	3.90	3.86	3.89	3.88
0.14	21.81	21.40	21.83	21.68	3.93	3.91	3.85	3.90
0.16	21.80	21.41	21.84	21.68	3.93	3.86	3.93	3.91
0.17	21.81	21.40	21.83	21.68	3.90	3.91	3.93	3.91
0.18	21.81	21.40	21.85	21.69	3.93	3.86	3.89	3.89
0.20	21.81	21.41	21.85	21.69	3.90	3.86	3.89	3.88
0.21	21.81	21.41	21.85	21.69	3.90	3.91	3.93	3.91
0.24	21.81	21.41	21.84	21.69	3.93	3.91	3.89	3.91
0.25	21.80	21.41	21.84	21.68	3.90	3.91	3.93	3.91
0.26	21.80	21.40	21.83	21.68	3.90	3.91	3.89	3.90
0.28	21.80	21.40	21.84	21.68	3.90	3.86	3.93	3.89
0.29	21.81	21.40	21.84	21.68	3.93	3.86	3.89	3.89
0.30	21.81	21.41	21.84	21.69	3.90	3.91	3.93	3.91
0.32	21.81	21.41	21.84	21.69	3.93	3.91	3.93	3.92
0.33	21.81	21.42	21.86	21.70	3.93	3.86	3.93	3.91
0.34	21.82	21.42	21.84	21.69	3.93	3.91	3.89	3.91
0.37	21.80	21.39	21.84	21.68	3.93	3.91	3.89	3.91
0.38	21.80	21.39	21.85	21.68	3.93	3.91	3.89	3.91
0.40	21.80	21.41	21.84	21.68	3.90	3.91	3.89	3.90
0.41	21.80	21.40	21.85	21.68	3.93	3.86	3.89	3.89
0.42	21.81	21.42	21.86	21.69	3.93	3.86	3.89	3.89
0.41	21.80	21.40	21.85	21.68	3.93	3.86	3.89	3.89
0.43	21.81	21.41	21.86	21.69	3.93	3.86	3.89	3.89
0.45	21.81	21.42	21.86	21.69	3.90	3.86	3.89	3.88

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	21.80	21.40	21.85	21.68	3.90	3.91	3.89	3.90
0.49	21.79	21.39	21.84	21.68	3.93	3.91	3.89	3.91
0.50	21.79	21.39	21.84	21.67	3.93	3.86	3.89	3.89
0.51	21.79	21.41	21.85	21.68	3.93	3.91	3.89	3.91
0.53	21.80	21.41	21.86	21.69	3.93	3.91	3.89	3.91
0.54	21.80	21.40	21.86	21.69	3.93	3.86	3.89	3.89
0.55	21.80	21.39	21.85	21.68	3.93	3.86	3.89	3.89
0.57	21.81	21.40	21.86	21.69	3.93	3.86	3.89	3.89
0.58	21.79	21.40	21.86	21.68	3.93	3.86	3.89	3.89
0.59	21.79	21.40	21.85	21.68	3.93	3.91	3.89	3.91
0.61	21.80	21.41	21.85	21.68	3.93	3.91	3.89	3.91
0.62	21.79	21.41	21.84	21.68	3.89	3.91	3.89	3.90
0.63	21.80	21.39	21.86	21.68	3.93	3.91	3.89	3.91
0.65	21.78	21.39	21.87	21.68	3.89	3.86	3.93	3.89
0.66	21.80	21.39	21.86	21.68	3.93	3.91	3.89	3.91
0.68	21.79	21.41	21.84	21.68	3.86	3.91	3.93	3.90
0.70	21.78	21.41	21.84	21.68	3.93	3.91	3.89	3.91
0.71	21.79	21.40	21.84	21.68	3.86	3.90	3.89	3.88
0.72	21.77	21.40	21.84	21.67	3.89	3.90	3.89	3.89
0.74	21.76	21.39	21.86	21.67	3.89	3.86	3.89	3.88
0.75	21.77	21.40	21.86	21.68	3.89	3.86	3.89	3.88
0.76	21.79	21.40	21.86	21.69	3.86	3.90	3.89	3.88
0.78	21.78	21.40	21.86	21.68	3.89	3.90	3.92	3.91
0.79	21.78	21.40	21.86	21.68	3.93	3.85	3.89	3.89
0.80	21.78	21.39	21.85	21.67	3.89	3.86	3.89	3.88
0.82	21.77	21.40	21.85	21.67	3.89	3.86	3.89	3.88
0.80	21.78	21.39	21.85	21.67	3.89	3.86	3.89	3.88
0.83	21.76	21.39	21.85	21.67	3.93	3.86	3.89	3.89
0.84	21.76	21.39	21.86	21.67	3.89	3.86	3.93	3.89
0.86	21.77	21.40	21.86	21.68	3.89	3.86	3.89	3.88
0.87	21.77	21.40	21.87	21.68	3.89	3.91	3.89	3.89
0.88	21.78	21.40	21.86	21.68	3.89	3.86	3.89	3.88
0.90	21.77	21.40	21.85	21.68	3.89	3.91	3.89	3.89
0.91	21.77	21.40	21.84	21.67	3.89	3.91	3.89	3.89
0.92	21.76	21.39	21.84	21.66	3.89	3.90	3.89	3.89
0.94	21.76	21.39	21.84	21.66	3.89	3.86	3.92	3.89
0.96	21.75	21.39	21.86	21.67	3.89	3.86	3.92	3.89

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	21.77	21.41	21.86	21.68	3.89	3.86	3.92	3.89
1.00	21.77	21.40	21.85	21.67	3.89	3.85	3.92	3.89
1.01	21.76	21.40	21.86	21.68	3.89	3.91	3.89	3.89
1.03	21.76	21.40	21.84	21.67	3.89	3.86	3.92	3.89
1.04	21.77	21.39	21.85	21.67	3.89	3.86	3.89	3.88
1.05	21.75	21.38	21.84	21.66	3.89	3.86	3.92	3.89
1.07	21.75	21.39	21.85	21.66	3.89	3.91	3.89	3.89
1.08	21.77	21.41	21.85	21.68	3.89	3.86	3.89	3.88
1.09	21.76	21.40	21.85	21.67	3.89	3.85	3.89	3.88
1.11	21.76	21.41	21.85	21.67	3.89	3.91	3.92	3.91
1.13	21.76	21.40	21.85	21.67	3.89	3.86	3.89	3.88
1.15	21.76	21.40	21.84	21.66	3.89	3.91	3.92	3.90
1.16	21.76	21.39	21.84	21.66	3.89	3.91	3.89	3.89
1.17	21.77	21.39	21.84	21.67	3.89	3.90	3.92	3.91
1.19	21.75	21.39	21.84	21.66	3.89	3.90	3.92	3.91
1.20	21.76	21.41	21.83	21.66	3.89	3.90	3.92	3.91
1.21	21.75	21.41	21.84	21.67	3.89	3.86	3.92	3.89
1.22	21.77	21.40	21.84	21.67	3.89	3.86	3.92	3.89
1.24	21.76	21.40	21.83	21.66	3.89	3.85	3.92	3.89
1.25	21.75	21.39	21.84	21.66	3.89	3.91	3.92	3.91
1.26	21.77	21.39	21.83	21.66	3.89	3.90	3.92	3.91
1.28	21.76	21.39	21.83	21.66	3.89	3.86	3.92	3.89
1.29	21.76	21.38	21.84	21.66	3.89	3.90	3.92	3.90
1.30	21.76	21.40	21.85	21.67	3.89	3.86	3.92	3.89
1.32	21.76	21.40	21.84	21.66	3.89	3.90	3.89	3.89
1.33	21.76	21.39	21.84	21.66	3.89	3.86	3.92	3.89
1.32	21.76	21.40	21.84	21.66	3.89	3.90	3.89	3.89
1.34	21.77	21.39	21.83	21.66	3.89	3.90	3.92	3.90
1.37	21.77	21.40	21.84	21.67	3.89	3.91	3.92	3.90
1.38	21.77	21.40	21.83	21.67	3.89	3.90	3.89	3.89
1.40	21.77	21.40	21.82	21.66	3.89	3.90	3.92	3.91
1.41	21.75	21.38	21.82	21.65	3.89	3.85	3.92	3.89
1.42	21.76	21.40	21.82	21.66	3.89	3.90	3.92	3.90
1.44	21.76	21.39	21.83	21.66	3.89	3.85	3.92	3.89
1.45	21.77	21.39	21.84	21.67	3.89	3.91	3.92	3.91
1.46	21.76	21.40	21.83	21.66	3.89	3.90	3.92	3.90
1.48	21.75	21.40	21.83	21.66	3.89	3.90	3.92	3.90

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	21.75	21.39	21.81	21.65	3.85	3.90	3.92	3.89
1.51	21.76	21.39	21.80	21.65	3.89	3.85	3.92	3.89
1.53	21.76	21.38	21.82	21.65	3.85	3.90	3.92	3.89
1.54	21.76	21.40	21.81	21.66	3.89	3.85	3.92	3.89
1.55	21.76	21.39	21.82	21.66	3.85	3.90	3.92	3.89
1.57	21.77	21.40	21.82	21.66	3.85	3.90	3.92	3.89
1.58	21.76	21.40	21.82	21.66	3.89	3.85	3.92	3.89
1.59	21.76	21.41	21.82	21.66	3.89	3.86	3.92	3.89
1.61	21.76	21.39	21.81	21.66	3.89	3.85	3.92	3.89
1.62	21.76	21.40	21.81	21.66	3.85	3.90	3.92	3.89
1.63	21.77	21.39	21.80	21.65	3.89	3.85	3.92	3.89
1.65	21.75	21.39	21.81	21.65	3.85	3.85	3.92	3.87
1.66	21.77	21.38	21.80	21.65	3.85	3.85	3.92	3.87
1.67	21.75	21.40	21.82	21.66	3.85	3.90	3.92	3.89
1.69	21.76	21.40	21.81	21.66	3.85	3.90	3.92	3.89
1.70	21.76	21.39	21.81	21.66	3.85	3.85	3.92	3.87
1.71	21.76	21.39	21.81	21.65	3.85	3.91	3.92	3.89
1.73	21.76	21.40	21.80	21.65	3.85	3.85	3.92	3.87
1.74	21.75	21.39	21.79	21.65	3.85	3.85	3.92	3.88
1.75	21.75	21.38	21.80	21.64	3.85	3.85	3.92	3.87
1.76	21.75	21.38	21.80	21.65	3.85	3.90	3.92	3.89
1.78	21.76	21.39	21.79	21.65	3.85	3.90	3.92	3.89
1.80	21.76	21.39	21.80	21.65	3.85	3.85	3.92	3.87
1.82	21.76	21.40	21.81	21.66	3.85	3.85	3.92	3.87
1.83	21.77	21.40	21.79	21.65	3.85	3.85	3.92	3.87
1.84	21.74	21.39	21.80	21.64	3.85	3.90	3.92	3.89
1.86	21.76	21.38	21.80	21.65	3.85	3.86	3.92	3.87
1.87	21.75	21.38	21.80	21.65	3.85	3.90	3.92	3.89
1.88	21.76	21.39	21.79	21.65	3.85	3.90	3.92	3.89
1.91	21.77	21.39	21.80	21.65	3.85	3.85	3.92	3.87
1.92	21.76	21.40	21.80	21.65	3.85	3.85	3.92	3.87
1.94	21.76	21.39	21.81	21.65	3.85	3.90	3.92	3.89
1.95	21.76	21.39	21.80	21.65	3.85	3.85	3.92	3.87
1.96	21.75	21.40	21.82	21.66	3.88	3.90	3.92	3.90
1.98	21.75	21.39	21.80	21.65	3.85	3.90	3.92	3.89
1.99	21.75	21.38	21.81	21.65	3.85	3.90	3.92	3.89

**APPENDIX 13.27 - Surface Tension Measurement Results for DI + SDS (6.00 mM)**

HUATARC surface tension measurement results for DI + SDS (6.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	23.72	24.15	24.17	24.01	4.50	4.48	4.45	4.48
0.01	23.73	24.16	24.16	24.02	4.41	4.49	4.45	4.45
0.03	23.73	24.16	24.15	24.01	4.61	4.48	4.45	4.51
0.04	23.71	24.20	24.17	24.03	4.50	4.48	4.40	4.46
0.05	23.71	24.18	24.17	24.02	4.50	4.48	4.45	4.48
0.07	23.71	24.19	24.16	24.02	4.50	4.49	4.45	4.48
0.09	23.73	24.18	24.17	24.02	4.50	4.48	4.45	4.48
0.11	23.72	24.15	24.16	24.01	4.50	4.43	4.45	4.46
0.12	23.71	24.16	24.17	24.01	4.50	4.48	4.45	4.48
0.13	23.72	24.17	24.16	24.02	4.50	4.49	4.45	4.48
0.14	23.73	24.16	24.17	24.02	4.50	4.48	4.40	4.46
0.16	23.73	24.18	24.15	24.02	4.50	4.48	4.45	4.48
0.17	23.72	24.19	24.16	24.02	4.50	4.48	4.45	4.48
0.18	23.70	24.18	24.16	24.01	4.51	4.48	4.40	4.47
0.20	23.69	24.17	24.15	24.01	4.50	4.48	4.40	4.46
0.21	23.72	24.16	24.16	24.01	4.51	4.49	4.40	4.47
0.22	23.76	24.15	24.16	24.02	4.51	4.48	4.40	4.46
0.24	23.74	24.16	24.16	24.02	4.43	4.48	4.40	4.44
0.25	23.76	24.13	24.14	24.01	4.51	4.48	4.45	4.48
0.26	23.70	24.16	24.16	24.01	4.51	4.49	4.40	4.47
0.28	23.72	24.14	24.15	24.01	4.43	4.49	4.40	4.44
0.29	23.69	24.16	24.16	24.00	4.43	4.48	4.40	4.44
0.30	23.71	24.17	24.15	24.01	4.43	4.49	4.40	4.44
0.32	23.72	24.16	24.16	24.01	4.36	4.49	4.45	4.43
0.33	23.69	24.15	24.16	24.00	4.36	4.48	4.40	4.41
0.34	23.66	24.14	24.15	23.98	4.36	4.49	4.40	4.41
0.36	23.73	24.13	24.15	24.00	4.36	4.49	4.40	4.41
0.37	23.68	24.13	24.14	23.98	4.43	4.43	4.40	4.42
0.38	23.72	24.12	24.15	24.00	4.43	4.49	4.40	4.44
0.42	23.67	24.13	24.14	23.98	4.36	4.49	4.40	4.41
0.38	23.72	24.12	24.15	24.00	4.43	4.49	4.40	4.44
0.43	23.65	24.14	24.15	23.98	4.36	4.49	4.40	4.41
0.45	23.70	24.12	24.14	23.99	4.36	4.43	4.40	4.39

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	23.66	24.10	24.13	23.96	4.43	4.49	4.40	4.44
0.49	23.66	24.11	24.12	23.96	4.43	4.49	4.40	4.44
0.50	23.66	24.11	24.13	23.97	4.43	4.49	4.40	4.44
0.51	23.68	24.11	24.13	23.97	4.42	4.49	4.40	4.44
0.53	23.71	24.13	24.14	23.99	4.43	4.49	4.40	4.44
0.54	23.68	24.12	24.13	23.98	4.36	4.48	4.40	4.41
0.55	23.68	24.12	24.12	23.97	4.36	4.48	4.40	4.41
0.57	23.70	24.11	24.12	23.98	4.43	4.49	4.40	4.44
0.58	23.70	24.11	24.12	23.98	4.43	4.43	4.40	4.42
0.59	23.65	24.09	24.12	23.96	4.43	4.49	4.40	4.44
0.61	23.65	24.11	24.13	23.96	4.43	4.43	4.40	4.42
0.62	23.65	24.10	24.12	23.96	4.43	4.49	4.40	4.44
0.63	23.70	24.12	24.13	23.98	4.43	4.43	4.40	4.42
0.65	23.70	24.12	24.11	23.98	4.43	4.43	4.40	4.42
0.67	23.68	24.11	24.11	23.97	4.36	4.43	4.40	4.39
0.68	23.70	24.09	24.10	23.96	4.30	4.49	4.40	4.39
0.70	23.67	24.10	24.11	23.96	4.36	4.49	4.40	4.42
0.71	23.63	24.09	24.11	23.94	4.43	4.43	4.35	4.40
0.70	23.67	24.10	24.11	23.96	4.36	4.49	4.40	4.42
0.72	23.64	24.10	24.12	23.95	4.43	4.49	4.44	4.45
0.74	23.65	24.09	24.11	23.95	4.36	4.49	4.35	4.40
0.75	23.70	24.10	24.12	23.97	4.36	4.43	4.35	4.38
0.76	23.70	24.11	24.11	23.97	4.36	4.43	4.40	4.39
0.78	23.67	24.12	24.11	23.97	4.36	4.43	4.44	4.41
0.79	23.67	24.10	24.10	23.96	4.36	4.43	4.44	4.41
0.80	23.68	24.10	24.10	23.96	4.43	4.43	4.44	4.43
0.83	23.64	24.08	24.11	23.94	4.43	4.43	4.40	4.42
0.84	23.64	24.09	24.10	23.95	4.43	4.43	4.39	4.42
0.86	23.63	24.08	24.11	23.94	4.43	4.43	4.35	4.40
0.87	23.69	24.11	24.10	23.97	4.43	4.43	4.44	4.43
0.88	23.65	24.10	24.12	23.96	4.36	4.43	4.44	4.41
0.90	23.64	24.12	24.11	23.96	4.36	4.43	4.39	4.39
0.91	23.65	24.10	24.10	23.95	4.30	4.42	4.44	4.39
0.92	23.69	24.09	24.11	23.96	4.43	4.43	4.39	4.42
0.94	23.64	24.08	24.10	23.94	4.43	4.43	4.39	4.42
0.95	23.63	24.09	24.10	23.94	4.43	4.43	4.39	4.42
0.96	23.62	24.09	24.10	23.93	4.43	4.43	4.39	4.42

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	23.67	24.11	24.10	23.96	4.43	4.43	4.39	4.41
1.00	23.65	24.10	24.11	23.95	4.36	4.43	4.39	4.39
1.01	23.65	24.11	24.09	23.95	4.36	4.43	4.39	4.39
1.03	23.68	24.10	24.09	23.96	4.35	4.43	4.39	4.39
1.04	23.69	24.08	24.10	23.96	4.36	4.43	4.39	4.39
1.05	23.62	24.07	24.11	23.93	4.35	4.43	4.39	4.39
1.07	23.62	24.08	24.11	23.94	4.43	4.43	4.39	4.42
1.08	23.63	24.08	24.10	23.94	4.36	4.43	4.39	4.39
1.09	23.68	24.10	24.10	23.96	4.36	4.43	4.39	4.39
1.11	23.67	24.10	24.10	23.95	4.35	4.43	4.39	4.39
1.12	23.63	24.08	24.11	23.94	4.36	4.38	4.39	4.37
1.13	23.66	24.09	24.10	23.95	4.30	4.42	4.39	4.37
1.16	23.66	24.08	24.09	23.94	4.35	4.43	4.39	4.39
1.17	23.62	24.07	24.09	23.93	4.30	4.42	4.39	4.37
1.19	23.64	24.08	24.09	23.94	4.36	4.43	4.35	4.38
1.20	23.65	24.07	24.09	23.94	4.35	4.43	4.39	4.39
1.21	23.67	24.06	24.09	23.94	4.35	4.43	4.39	4.39
1.22	23.65	24.07	24.09	23.94	4.36	4.43	4.39	4.39
1.24	23.65	24.08	24.09	23.94	4.36	4.38	4.39	4.38
1.25	23.67	24.06	24.08	23.94	4.30	4.42	4.39	4.37
1.24	23.65	24.08	24.09	23.94	4.36	4.38	4.39	4.38
1.26	23.67	24.07	24.10	23.95	4.36	4.42	4.39	4.39
1.28	23.64	24.06	24.09	23.93	4.35	4.43	4.39	4.39
1.29	23.64	24.06	24.11	23.94	4.35	4.38	4.39	4.37
1.30	23.64	24.05	24.08	23.93	4.36	4.48	4.39	4.41
1.32	23.66	24.05	24.09	23.93	4.35	4.48	4.35	4.39
1.33	23.68	24.06	24.07	23.94	4.35	4.43	4.39	4.39
1.34	23.66	24.05	24.08	23.93	4.30	4.42	4.39	4.37
1.36	23.65	24.05	24.07	23.92	4.36	4.43	4.39	4.39
1.37	23.67	24.04	24.08	23.93	4.35	4.42	4.39	4.39
1.38	23.66	24.04	24.07	23.93	4.35	4.42	4.39	4.39
1.40	23.64	24.02	24.07	23.91	4.35	4.42	4.39	4.39
1.41	23.64	24.04	24.07	23.92	4.36	4.42	4.39	4.39
1.42	23.64	24.04	24.07	23.92	4.35	4.42	4.39	4.39
1.45	23.66	24.04	24.07	23.92	4.30	4.42	4.39	4.37
1.46	23.64	24.04	24.08	23.92	4.35	4.42	4.35	4.37
1.48	23.65	24.04	24.07	23.92	4.35	4.42	4.39	4.39

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	23.66	24.03	24.05	23.91	4.36	4.48	4.39	4.41
1.51	23.63	24.04	24.06	23.91	4.35	4.42	4.35	4.37
1.53	23.63	24.04	24.07	23.91	4.35	4.37	4.39	4.37
1.54	23.63	24.03	24.06	23.91	4.35	4.42	4.39	4.39
1.55	23.65	24.03	24.07	23.92	4.36	4.42	4.39	4.39
1.57	23.66	24.02	24.05	23.91	4.35	4.42	4.39	4.39
1.58	23.64	24.03	24.06	23.91	4.35	4.42	4.39	4.39
1.59	23.63	24.04	24.05	23.91	4.35	4.42	4.39	4.39
1.61	23.65	24.02	24.05	23.91	4.36	4.42	4.39	4.39
1.62	23.64	24.02	24.06	23.91	4.35	4.29	4.39	4.35
1.65	23.63	24.02	24.05	23.90	4.35	4.42	4.35	4.37
1.66	23.62	24.02	24.05	23.90	4.35	4.37	4.39	4.37
1.67	23.64	24.03	24.04	23.91	4.36	4.42	4.43	4.40
1.69	23.62	24.03	24.04	23.90	4.30	4.42	4.38	4.37
1.70	23.62	24.06	24.05	23.91	4.36	4.42	4.35	4.37
1.71	23.61	24.04	24.05	23.90	4.36	4.42	4.35	4.37
1.73	23.64	24.04	24.06	23.91	4.35	4.42	4.38	4.39
1.74	23.61	24.03	24.05	23.90	4.35	4.42	4.39	4.39
1.75	23.60	24.04	24.05	23.90	4.36	4.42	4.35	4.37
1.76	23.62	24.03	24.06	23.90	4.35	4.42	4.38	4.39
1.78	23.62	24.03	24.05	23.90	4.36	4.42	4.43	4.40
1.79	23.63	24.02	24.05	23.90	4.35	4.37	4.38	4.37
1.80	23.61	24.02	24.06	23.89	4.36	4.37	4.35	4.36
1.82	23.60	24.02	24.06	23.89	4.36	4.37	4.38	4.37
1.83	23.61	24.03	24.05	23.90	4.35	4.42	4.35	4.37
1.84	23.62	24.03	24.05	23.90	4.36	4.42	4.43	4.40
1.86	23.60	24.03	24.05	23.89	4.36	4.42	4.38	4.39
1.87	23.61	24.04	24.07	23.90	4.36	4.29	4.38	4.34
1.88	23.59	24.02	24.06	23.89	4.36	4.37	4.38	4.37
1.90	23.60	24.03	24.06	23.90	4.36	4.37	4.38	4.37
1.91	23.58	24.02	24.05	23.88	4.36	4.37	4.35	4.36
1.94	23.59	24.03	24.05	23.89	4.36	4.37	4.38	4.37
1.95	23.60	24.02	24.05	23.89	4.36	4.42	4.38	4.39
1.98	23.58	24.01	24.06	23.88	4.36	4.37	4.39	4.37
1.99	23.59	24.01	24.06	23.89	4.36	4.29	4.34	4.33

## APPENDIX 13.28 - Surface Tension Measurement Results for DI + SDS (8.20 mM)

HUATARC surface tension measurement results for DI + SDS (0.82 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	21.89	21.92	21.88	3.94	3.98	4.02	3.98	21.82
0.01	21.90	21.92	21.87	3.96	3.96	4.00	3.97	21.80
0.03	21.88	21.92	21.87	3.98	3.98	4.00	3.99	21.80
0.04	21.90	21.92	21.87	4.00	3.98	3.98	3.99	21.79
0.05	21.89	21.90	21.87	4.00	3.97	3.98	3.98	21.81
0.07	21.88	21.92	21.86	3.98	3.97	3.98	3.98	21.79
0.08	21.87	21.90	21.85	3.98	3.97	3.99	3.98	21.79
0.09	21.88	21.90	21.86	3.97	3.98	3.99	3.98	21.80
0.11	21.87	21.89	21.85	3.98	4.00	3.99	3.99	21.79
0.12	21.86	21.89	21.84	3.96	3.95	4.01	3.97	21.77
0.13	21.87	21.88	21.85	3.97	3.99	3.97	3.98	21.79
0.14	21.84	21.90	21.84	3.95	3.95	3.99	3.96	21.79
0.16	21.85	21.89	21.83	3.95	3.97	3.99	3.97	21.76
0.18	21.83	21.88	21.83	3.95	3.99	3.99	3.98	21.78
0.20	21.82	21.88	21.82	3.95	3.99	3.99	3.98	21.77
0.21	21.82	21.88	21.82	3.95	3.96	3.99	3.97	21.76
0.22	21.81	21.86	21.81	3.95	3.97	3.98	3.97	21.76
0.25	21.81	21.87	21.81	3.95	3.99	3.98	3.97	21.75
0.26	21.80	21.87	21.81	3.97	3.98	3.98	3.98	21.76
0.28	21.79	21.86	21.81	3.97	4.01	3.98	3.99	21.77
0.29	21.80	21.84	21.80	3.97	3.96	3.98	3.97	21.75
0.30	21.80	21.84	21.80	3.97	3.98	3.98	3.98	21.76
0.32	21.79	21.85	21.80	3.93	3.96	3.96	3.95	21.75
0.33	21.80	21.85	21.80	3.94	3.96	4.00	3.97	21.74
0.34	21.80	21.84	21.79	3.95	4.00	4.00	3.98	21.74
0.36	21.79	21.84	21.79	3.97	3.98	3.96	3.97	21.73
0.37	21.77	21.84	21.78	3.99	3.98	3.98	3.98	21.72
0.38	21.79	21.83	21.77	3.94	3.98	3.98	3.97	21.70
0.40	21.78	21.83	21.78	3.96	3.94	3.96	3.95	21.72
0.41	21.77	21.84	21.77	3.92	3.97	3.98	3.96	21.71
0.40	21.78	21.83	21.78	3.96	3.94	3.96	3.95	21.72
0.43	21.78	21.82	21.78	3.94	3.97	4.00	3.97	21.73
0.45	21.76	21.82	21.77	3.92	3.97	3.98	3.96	21.72

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	21.76	21.81	21.76	3.94	3.96	3.97	3.96	21.72
0.49	21.75	21.82	21.77	3.94	3.95	3.97	3.95	21.73
0.50	21.74	21.82	21.76	3.94	3.95	3.97	3.95	21.72
0.51	21.75	21.81	21.76	3.92	3.97	3.97	3.95	21.72
0.53	21.75	21.80	21.75	3.94	3.95	3.97	3.95	21.71
0.54	21.75	21.81	21.75	3.96	3.97	3.95	3.96	21.70
0.55	21.73	21.80	21.75	3.96	3.97	3.97	3.97	21.71
0.57	21.74	21.80	21.76	3.96	3.97	3.97	3.97	21.73
0.58	21.72	21.79	21.75	3.92	3.99	3.97	3.96	21.74
0.59	21.73	21.79	21.75	3.94	3.94	3.99	3.96	21.72
0.61	21.72	21.78	21.73	3.96	3.94	3.97	3.96	21.70
0.62	21.72	21.79	21.73	3.94	3.96	3.95	3.95	21.69
0.63	21.71	21.78	21.72	3.94	3.96	3.95	3.95	21.68
0.65	21.72	21.77	21.72	3.96	3.96	3.97	3.96	21.68
0.66	21.71	21.79	21.73	3.94	3.96	3.95	3.95	21.69
0.67	21.70	21.77	21.72	3.95	3.96	3.97	3.96	21.68
0.68	21.71	21.76	21.71	3.93	3.96	3.94	3.94	21.66
0.70	21.72	21.76	21.72	3.93	3.94	3.94	3.94	21.68
0.71	21.70	21.76	21.71	3.94	3.94	3.99	3.96	21.68
0.72	21.71	21.75	21.71	3.93	3.96	3.96	3.95	21.66
0.75	21.69	21.77	21.72	3.95	3.92	3.94	3.94	21.69
0.76	21.70	21.77	21.71	3.95	3.96	3.96	3.96	21.67
0.78	21.70	21.75	21.71	3.95	3.93	3.94	3.94	21.67
0.79	21.68	21.76	21.70	3.93	3.94	3.96	3.94	21.67
0.80	21.69	21.76	21.70	3.97	3.96	3.94	3.96	21.66
0.82	21.68	21.75	21.69	3.97	3.98	3.96	3.97	21.65
0.83	21.68	21.75	21.70	3.95	3.96	3.94	3.95	21.66
0.84	21.67	21.75	21.69	3.93	3.96	3.96	3.95	21.65
0.86	21.67	21.74	21.69	3.93	3.93	3.96	3.94	21.66
0.87	21.67	21.74	21.69	3.91	3.93	3.94	3.93	21.66
0.88	21.66	21.75	21.69	3.91	3.95	3.94	3.93	21.65
0.90	21.67	21.74	21.69	3.91	3.95	3.96	3.94	21.66
0.92	21.66	21.74	21.68	3.94	3.93	3.94	3.94	21.65
0.94	21.66	21.74	21.69	3.92	3.93	3.94	3.93	21.66
0.92	21.66	21.74	21.68	3.94	3.93	3.94	3.94	21.65
0.95	21.68	21.72	21.68	3.95	3.93	3.96	3.95	21.65
0.96	21.67	21.72	21.68	3.92	3.95	3.96	3.94	21.64

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	21.66	21.72	21.67	3.93	3.93	3.93	3.93	21.64
1.00	21.67	21.73	21.68	3.95	3.95	3.96	3.95	21.64
1.01	21.65	21.73	21.67	3.90	3.93	3.96	3.93	21.63
1.03	21.65	21.72	21.67	3.92	3.93	3.96	3.94	21.64
1.04	21.64	21.72	21.66	3.90	3.93	3.96	3.93	21.63
1.05	21.64	21.72	21.66	3.92	3.93	3.93	3.93	21.63
1.07	21.64	21.72	21.66	3.92	3.89	3.96	3.92	21.61
1.08	21.63	21.72	21.66	3.88	3.93	3.93	3.91	21.63
1.09	21.65	21.73	21.67	3.92	3.95	3.96	3.94	21.64
1.12	21.66	21.71	21.67	3.90	3.93	3.95	3.93	21.63
1.13	21.64	21.71	21.66	3.94	3.92	3.95	3.94	21.63
1.15	21.63	21.71	21.66	3.92	3.92	3.97	3.94	21.63
1.16	21.64	21.69	21.65	3.94	3.92	3.93	3.93	21.61
1.15	21.63	21.71	21.66	3.92	3.92	3.97	3.94	21.63
1.17	21.62	21.70	21.65	3.92	3.94	3.95	3.94	21.64
1.19	21.63	21.71	21.66	3.92	3.94	3.93	3.93	21.63
1.20	21.64	21.70	21.66	3.92	3.92	3.95	3.93	21.63
1.21	21.63	21.70	21.65	3.92	3.92	3.93	3.92	21.63
1.22	21.61	21.69	21.64	3.94	3.94	3.93	3.94	21.63
1.24	21.63	21.69	21.65	3.92	3.92	3.95	3.93	21.62
1.25	21.62	21.70	21.65	3.92	3.94	3.93	3.93	21.62
1.26	21.61	21.70	21.64	3.94	3.90	3.93	3.92	21.62
1.28	21.60	21.70	21.63	3.94	3.92	3.93	3.93	21.60
1.29	21.62	21.70	21.64	3.92	3.96	3.95	3.94	21.60
1.30	21.61	21.85	21.69	3.96	3.90	3.94	3.93	21.61
1.32	21.61	21.71	21.65	3.94	3.92	3.93	3.93	21.62
1.33	21.61	21.69	21.64	3.92	3.94	3.95	3.94	21.62
1.34	21.60	21.69	21.63	3.90	3.92	3.93	3.92	21.61
1.36	21.60	21.70	21.64	3.91	3.94	3.95	3.93	21.61
1.37	21.60	21.70	21.64	3.91	3.92	3.95	3.93	21.61
1.38	21.61	21.69	21.64	3.92	3.92	3.93	3.92	21.61
1.40	21.60	21.68	21.62	3.92	3.91	3.95	3.93	21.59
1.41	21.60	21.68	21.62	3.94	3.92	3.91	3.92	21.59
1.42	21.60	21.68	21.63	3.94	3.92	3.95	3.94	21.60
1.45	21.60	21.69	21.63	3.91	3.95	3.95	3.94	21.59
1.46	21.60	21.68	21.63	3.92	3.94	3.94	3.93	21.60
1.48	21.59	21.68	21.62	3.94	3.93	3.91	3.93	21.60

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	21.60	21.68	21.62	3.94	3.89	3.92	3.92	21.58
1.51	21.60	21.68	21.62	3.91	3.94	3.94	3.93	21.59
1.53	21.58	21.67	21.61	3.93	3.93	3.97	3.94	21.58
1.54	21.60	21.67	21.62	3.91	3.94	3.93	3.93	21.58
1.55	21.60	21.67	21.62	3.91	3.91	3.93	3.92	21.59
1.57	21.58	21.67	21.61	3.91	3.91	3.93	3.92	21.58
1.58	21.57	21.67	21.60	3.89	3.93	3.93	3.92	21.56
1.59	21.58	21.66	21.61	3.93	3.93	3.94	3.93	21.58
1.61	21.58	21.67	21.61	3.93	3.93	3.94	3.93	21.58
1.63	21.59	21.66	21.61	3.91	3.91	3.92	3.91	21.57
1.65	21.57	21.67	21.61	3.91	3.93	3.92	3.92	21.59
1.66	21.56	21.68	21.61	3.91	3.93	3.93	3.92	21.59
1.67	21.57	21.67	21.60	3.91	3.89	3.94	3.91	21.57
1.69	21.57	21.67	21.61	3.92	3.91	3.94	3.92	21.58
1.70	21.56	21.68	21.61	3.91	3.93	3.92	3.92	21.58
1.71	21.57	21.66	21.60	3.93	3.95	3.94	3.94	21.58
1.73	21.57	21.67	21.60	3.93	3.95	3.92	3.93	21.57
1.74	21.56	21.66	21.60	3.91	3.91	3.94	3.92	21.58
1.75	21.55	21.67	21.60	3.96	3.91	3.92	3.93	21.58
1.76	21.56	21.66	21.60	3.91	3.93	3.94	3.93	21.58
1.78	21.55	21.67	21.60	3.91	3.93	3.94	3.93	21.59
1.79	21.55	21.66	21.60	3.93	3.91	3.92	3.92	21.58
1.80	21.55	21.66	21.60	3.89	3.93	3.92	3.91	21.58
1.82	21.55	21.66	21.60	3.91	3.95	3.92	3.93	21.58
1.83	21.55	21.67	21.60	3.89	3.93	3.92	3.91	21.57
1.84	21.55	21.64	21.59	3.93	3.91	3.92	3.92	21.58
1.86	21.53	21.63	21.58	3.93	3.91	3.96	3.93	21.58
1.87	21.54	21.64	21.58	3.91	3.90	3.95	3.92	21.57
1.88	21.55	21.63	21.58	3.91	3.90	3.92	3.91	21.56
1.90	21.54	21.62	21.58	3.91	3.93	3.94	3.93	21.57
1.91	21.53	21.63	21.58	3.93	3.95	3.94	3.94	21.57
1.94	22.40	21.62	21.87	3.91	3.92	3.96	3.93	21.58
1.95	21.53	21.63	21.58	3.91	3.94	3.94	3.93	21.58
1.96	21.53	21.64	21.58	3.93	3.90	3.92	3.92	21.56
1.98	21.53	21.63	21.57	3.91	3.90	3.92	3.91	21.56
1.99	21.52	21.64	21.57	3.95	3.92	3.92	3.93	21.56

## APPENDIX 13.29 - Surface Tension Measurement Results for DI + SDS (44.30 mM)

HUATARC surface tension measurement results for DI + SDS (44.30 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	26.40	26.63	27.08	26.70	4.70	4.74	4.83	4.76
0.01	26.37	26.62	27.06	26.68	4.74	4.77	4.83	4.78
0.03	26.38	26.59	27.05	26.67	4.74	4.74	4.83	4.77
0.04	26.48	26.62	27.07	26.72	4.74	4.74	4.87	4.78
0.05	26.36	26.62	27.06	26.68	4.74	4.74	4.83	4.77
0.07	26.41	26.62	27.05	26.70	4.74	4.74	4.83	4.77
0.08	26.37	26.61	27.07	26.69	4.74	4.78	4.83	4.78
0.09	26.39	26.61	27.06	26.69	4.74	4.78	4.83	4.78
0.11	26.39	26.60	27.04	26.68	4.74	4.78	4.83	4.78
0.12	26.37	26.59	27.05	26.67	4.74	4.78	4.87	4.80
0.13	26.40	26.62	27.07	26.70	4.74	4.78	4.83	4.78
0.14	26.39	26.62	27.07	26.70	4.74	4.78	4.87	4.80
0.16	26.39	26.62	27.06	26.69	4.74	4.78	4.83	4.78
0.17	26.39	26.60	27.06	26.69	4.74	4.78	4.83	4.78
0.18	26.37	26.59	27.07	26.68	4.74	4.78	4.83	4.78
0.20	26.39	26.59	27.07	26.69	4.74	4.78	4.83	4.78
0.21	26.39	26.59	27.06	26.68	4.74	4.78	4.83	4.78
0.24	26.39	26.59	27.07	26.68	4.74	4.78	4.87	4.80
0.25	26.38	26.59	27.07	26.68	4.74	4.78	4.87	4.80
0.26	26.39	26.60	27.05	26.68	4.74	4.78	4.87	4.80
0.28	26.40	26.61	27.07	26.69	4.74	4.78	4.83	4.78
0.29	26.39	26.61	27.07	26.69	4.74	4.78	4.87	4.80
0.30	26.39	26.60	27.06	26.68	4.74	4.78	4.83	4.78
0.32	26.40	26.62	27.07	26.70	4.74	4.78	4.87	4.79
0.33	26.39	26.62	27.07	26.69	4.74	4.78	4.87	4.79
0.34	26.40	26.63	27.07	26.70	4.74	4.78	4.87	4.79
0.37	26.42	26.66	27.06	26.71	4.74	4.78	4.87	4.79
0.38	26.41	26.66	27.07	26.71	4.74	4.78	4.87	4.79
0.40	26.40	26.64	27.06	26.70	4.74	4.78	4.83	4.78
0.41	26.43	26.66	27.06	26.72	4.74	4.78	4.83	4.78
0.40	26.40	26.64	27.06	26.70	4.74	4.78	4.83	4.78
0.43	26.41	26.66	27.06	26.71	4.74	4.78	4.87	4.79
0.45	26.42	26.66	27.06	26.71	4.74	4.78	4.83	4.78

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	26.42	26.66	27.07	26.72	4.74	4.74	4.83	4.77
0.49	26.44	26.65	27.05	26.72	4.74	4.82	4.83	4.79
0.50	26.44	26.67	27.08	26.73	4.70	4.81	4.83	4.78
0.51	26.44	26.66	27.08	26.73	4.73	4.78	4.83	4.78
0.53	26.42	26.67	27.08	26.72	4.74	4.82	4.86	4.81
0.54	26.44	26.67	27.08	26.73	4.74	4.82	4.83	4.80
0.55	26.44	26.68	27.07	26.73	4.74	4.81	4.86	4.81
0.57	26.45	26.69	27.07	26.73	4.70	4.81	4.87	4.79
0.58	26.44	26.66	27.05	26.71	4.74	4.78	4.86	4.79
0.59	26.49	26.69	27.08	26.75	4.73	4.78	4.83	4.78
0.61	26.43	26.69	27.07	26.73	4.73	4.82	4.86	4.80
0.62	26.44	26.68	27.08	26.73	4.78	4.78	4.83	4.79
0.63	26.43	26.69	27.08	26.73	4.74	4.78	4.86	4.79
0.65	26.44	26.70	27.07	26.74	4.70	4.78	4.86	4.78
0.66	26.43	26.71	27.09	26.74	4.74	4.78	4.83	4.78
0.67	26.45	26.69	27.06	26.73	4.74	4.78	4.83	4.78
0.68	26.43	26.70	27.09	26.74	4.70	4.78	4.83	4.77
0.70	26.44	26.73	27.08	26.75	4.74	4.78	4.83	4.78
0.71	26.45	26.70	27.08	26.75	4.74	4.78	4.83	4.78
0.72	26.45	26.71	27.11	26.76	4.74	4.77	4.83	4.78
0.74	26.45	26.71	27.10	26.76	4.74	4.78	4.83	4.78
0.75	26.46	26.73	27.10	26.76	4.74	4.77	4.83	4.78
0.76	26.46	26.70	27.09	26.75	4.74	4.77	4.83	4.78
0.78	26.47	26.72	27.10	26.76	4.77	4.78	4.83	4.79
0.79	26.45	26.71	27.10	26.76	4.74	4.78	4.83	4.78
0.80	26.48	26.69	27.08	26.75	4.74	4.78	4.83	4.78
0.79	26.45	26.71	27.10	26.76	4.74	4.78	4.83	4.78
0.84	26.49	26.71	27.10	26.77	4.74	4.78	4.83	4.78
0.86	26.49	26.70	27.10	26.76	4.73	4.77	4.83	4.78
0.87	26.49	26.71	27.12	26.77	4.74	4.78	4.82	4.78
0.88	26.49	26.70	27.10	26.76	4.74	4.77	4.82	4.78
0.90	26.49	26.70	27.09	26.76	4.73	4.77	4.83	4.78
0.91	26.49	26.73	27.10	26.77	4.73	4.78	4.82	4.78
0.92	26.49	26.71	27.11	26.77	4.74	4.77	4.82	4.78
0.94	26.49	26.71	27.10	26.77	4.74	4.77	4.82	4.78
0.95	26.48	26.73	27.10	26.77	4.73	4.77	4.82	4.78
0.96	26.50	26.72	27.12	26.78	4.74	4.77	4.82	4.78

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	26.49	26.71	27.09	26.77	4.73	4.77	4.82	4.78
1.00	26.49	26.74	27.10	26.78	4.73	4.77	4.82	4.78
1.01	26.51	26.73	27.10	26.78	4.74	4.77	4.82	4.78
1.03	26.50	26.72	27.10	26.78	4.73	4.77	4.82	4.78
1.04	26.49	26.74	27.10	26.78	4.73	4.77	4.82	4.78
1.05	26.49	26.73	27.10	26.77	4.73	4.81	4.82	4.79
1.07	26.50	26.73	27.11	26.78	4.73	4.81	4.82	4.79
1.08	26.50	26.75	27.11	26.79	4.73	4.81	4.82	4.79
1.09	26.50	26.77	27.11	26.79	4.73	4.81	4.82	4.79
1.12	26.50	26.77	27.11	26.79	4.73	4.81	4.86	4.80
1.13	26.51	26.78	27.09	26.79	4.73	4.81	4.82	4.79
1.15	26.52	26.77	27.11	26.80	4.73	4.77	4.82	4.77
1.16	26.52	26.77	27.12	26.80	4.73	4.81	4.82	4.79
1.17	26.53	26.78	27.11	26.81	4.73	4.81	4.82	4.79
1.19	26.55	26.78	27.12	26.82	4.73	4.81	4.86	4.80
1.20	26.54	26.77	27.13	26.81	4.73	4.81	4.82	4.79
1.21	26.54	26.79	27.13	26.82	4.77	4.81	4.82	4.80
1.22	26.55	26.78	27.13	26.82	4.73	4.81	4.82	4.79
1.24	26.55	26.78	27.14	26.82	4.73	4.81	4.86	4.80
1.25	26.54	26.78	27.14	26.82	4.73	4.81	4.86	4.80
1.26	26.56	26.79	27.11	26.82	4.73	4.81	4.82	4.79
1.28	26.55	26.77	27.12	26.81	4.73	4.81	4.86	4.80
1.29	26.56	26.76	27.15	26.82	4.73	4.81	4.86	4.80
1.30	26.55	26.79	27.15	26.83	4.73	4.81	4.86	4.80
1.32	26.56	26.78	27.14	26.83	4.73	4.81	4.82	4.79
1.33	26.57	26.78	27.15	26.84	4.73	4.81	4.86	4.80
1.36	26.56	26.80	27.15	26.84	4.77	4.81	4.86	4.81
1.37	26.55	26.79	27.15	26.83	4.77	4.81	4.86	4.81
1.36	26.56	26.80	27.15	26.84	4.77	4.81	4.86	4.81
1.38	26.55	26.78	27.17	26.83	4.77	4.81	4.86	4.81
1.40	26.55	26.79	27.16	26.83	4.77	4.81	4.86	4.81
1.41	26.55	26.80	27.16	26.84	4.77	4.81	4.86	4.81
1.42	26.55	26.79	27.16	26.84	4.73	4.81	4.86	4.80
1.44	26.55	26.81	27.15	26.84	4.77	4.81	4.86	4.81
1.45	26.56	26.81	27.16	26.84	4.77	4.81	4.86	4.81
1.46	26.55	26.80	27.16	26.84	4.77	4.77	4.86	4.80
1.48	26.56	26.82	27.16	26.85	4.77	4.81	4.86	4.81

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	26.57	26.83	27.15	26.85	4.77	4.81	4.86	4.81
1.51	26.58	26.83	27.15	26.85	4.77	4.77	4.86	4.80
1.53	26.57	26.85	27.16	26.86	4.77	4.77	4.86	4.80
1.54	26.57	26.85	27.16	26.86	4.77	4.77	4.86	4.80
1.55	26.57	26.84	27.15	26.85	4.77	4.77	4.86	4.80
1.57	26.59	26.83	27.16	26.86	4.77	4.81	4.85	4.81
1.58	26.59	26.84	27.16	26.86	4.77	4.77	4.86	4.80
1.59	26.59	26.85	27.16	26.87	4.77	4.77	4.86	4.80
1.61	26.61	26.84	27.18	26.87	4.77	4.77	4.85	4.80
1.62	26.60	26.84	27.16	26.87	4.77	4.77	4.85	4.80
1.63	26.61	26.84	27.17	26.87	4.76	4.77	4.85	4.80
1.65	26.61	26.84	27.17	26.87	4.77	4.81	4.85	4.81
1.66	26.62	26.83	27.18	26.88	4.77	4.81	4.85	4.81
1.67	26.62	26.83	27.19	26.88	4.76	4.81	4.85	4.81
1.69	26.62	26.86	27.17	26.88	4.77	4.81	4.85	4.81
1.70	26.64	26.83	27.19	26.89	4.77	4.81	4.85	4.81
1.71	26.62	26.83	27.18	26.88	4.77	4.81	4.85	4.81
1.74	26.63	26.85	27.18	26.89	4.73	4.81	4.85	4.80
1.75	26.64	26.83	27.19	26.89	4.77	4.81	4.82	4.80
1.76	26.63	26.87	27.20	26.90	4.76	4.81	4.82	4.80
1.78	26.63	26.87	27.19	26.89	4.77	4.81	4.85	4.81
1.79	26.64	26.84	27.20	26.89	4.73	4.81	4.85	4.80
1.80	26.61	26.87	27.21	26.90	4.76	4.81	4.85	4.81
1.82	26.64	26.87	27.20	26.90	4.73	4.81	4.81	4.78
1.83	26.63	26.88	27.20	26.90	4.76	4.80	4.85	4.81
1.86	26.63	26.90	27.22	26.91	4.73	4.81	4.82	4.78
1.87	26.63	26.88	27.19	26.90	4.73	4.80	4.85	4.79
1.88	26.64	26.88	27.22	26.91	4.73	4.80	4.82	4.78
1.90	26.64	26.90	27.21	26.92	4.73	4.80	4.81	4.78
1.91	26.65	26.89	27.22	26.92	4.73	4.81	4.81	4.78
1.92	26.64	26.90	27.22	26.92	4.73	4.80	4.81	4.78
1.94	26.63	26.91	27.20	26.91	4.76	4.80	4.82	4.79
1.95	26.64	26.92	27.21	26.92	4.76	4.80	4.81	4.79
1.96	26.64	26.91	27.20	26.92	4.73	4.80	4.81	4.78
1.98	26.64	26.89	27.21	26.91	4.72	4.80	4.85	4.79
1.99	26.65	26.93	27.20	26.93	4.73	4.80	4.81	4.78

### APPENDIX 13.30 - Surface Tension Measurement Results for DI + SDS (59.00 mM)

HUATARC surface tension measurement results for DI + SDS (59.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	26.86	26.61	25.78	26.41	4.91	4.87	4.74	4.84
0.01	26.84	26.60	25.79	26.41	4.97	4.87	4.74	4.86
0.03	26.85	26.62	25.79	26.42	4.96	4.94	4.74	4.88
0.04	26.86	26.61	25.80	26.42	4.96	4.94	4.68	4.86
0.05	26.85	26.61	25.80	26.42	4.97	4.93	4.74	4.88
0.07	26.85	26.62	25.81	26.43	4.96	4.93	4.74	4.88
0.09	26.84	26.62	25.81	26.43	4.96	4.87	4.74	4.86
0.11	26.85	26.62	25.81	26.43	4.96	4.87	4.74	4.86
0.12	26.88	26.65	25.82	26.45	4.91	4.93	4.74	4.86
0.13	26.88	26.63	25.83	26.44	4.97	4.87	4.74	4.86
0.16	26.88	26.66	25.84	26.46	4.91	4.87	4.74	4.84
0.17	26.88	26.65	25.86	26.46	4.97	4.87	4.74	4.86
0.18	26.89	26.67	25.85	26.47	4.97	4.87	4.74	4.86
0.20	26.86	26.67	25.87	26.47	4.97	4.87	4.73	4.86
0.21	26.88	26.68	25.88	26.48	4.96	4.87	4.73	4.86
0.22	26.87	26.67	25.90	26.48	5.04	4.93	4.73	4.90
0.24	26.87	26.68	25.89	26.48	4.97	4.87	4.73	4.86
0.25	26.88	26.69	25.88	26.49	4.96	4.87	4.73	4.85
0.26	26.89	26.68	25.90	26.49	5.03	4.87	4.73	4.88
0.28	26.91	26.70	25.89	26.50	5.03	4.87	4.73	4.88
0.29	26.89	26.69	25.89	26.49	4.91	4.87	4.73	4.84
0.30	26.92	26.69	25.91	26.50	4.97	4.86	4.73	4.86
0.32	26.91	26.70	25.90	26.51	5.03	4.87	4.73	4.88
0.33	26.91	26.69	25.90	26.50	4.97	4.87	4.73	4.86
0.34	26.91	26.70	25.91	26.51	4.97	4.86	4.69	4.84
0.37	26.91	26.71	25.93	26.51	4.97	4.87	4.68	4.84
0.38	26.90	26.71	25.93	26.51	4.97	4.87	4.73	4.85
0.40	26.92	26.71	25.95	26.53	5.11	4.86	4.68	4.89
0.41	26.90	26.71	25.97	26.53	5.04	4.87	4.68	4.86
0.42	26.91	26.71	25.96	26.53	5.04	4.86	4.68	4.86
0.43	26.93	26.72	25.99	26.55	5.04	4.86	4.68	4.86
0.42	26.91	26.71	25.96	26.53	5.04	4.86	4.68	4.86
0.45	26.92	26.72	25.98	26.54	5.04	4.92	4.68	4.88

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	26.94	26.73	25.99	26.55	5.03	4.86	4.68	4.86
0.49	26.96	26.75	25.99	26.57	5.03	4.86	4.68	4.86
0.50	26.94	26.77	26.01	26.57	5.03	4.86	4.72	4.87
0.51	26.96	26.74	25.99	26.57	5.03	4.86	4.68	4.86
0.53	26.98	26.78	26.00	26.59	5.03	4.86	4.68	4.86
0.54	26.95	26.76	26.00	26.57	5.03	4.86	4.68	4.86
0.55	26.95	26.77	26.00	26.58	4.97	4.86	4.68	4.84
0.57	26.95	26.78	26.02	26.58	4.97	4.86	4.68	4.84
0.58	26.95	26.78	26.02	26.58	4.97	4.86	4.68	4.84
0.59	26.95	26.78	26.03	26.59	4.97	4.86	4.72	4.85
0.61	26.97	26.78	26.04	26.60	4.97	4.86	4.68	4.84
0.62	26.96	26.79	26.05	26.60	5.04	4.86	4.68	4.86
0.63	26.94	26.79	26.05	26.59	5.11	4.86	4.68	4.88
0.66	26.97	26.79	26.07	26.61	5.04	4.86	4.68	4.86
0.67	26.98	26.80	26.06	26.61	5.03	4.86	4.67	4.86
0.68	26.98	26.79	26.08	26.62	5.03	4.86	4.68	4.86
0.70	26.99	26.79	26.10	26.63	5.03	4.86	4.68	4.86
0.71	27.01	26.81	26.10	26.64	5.03	4.86	4.67	4.86
0.72	27.00	26.80	26.11	26.63	5.03	4.86	4.67	4.85
0.74	27.00	26.80	26.12	26.64	5.03	4.81	4.68	4.84
0.75	27.01	26.81	26.11	26.64	5.03	4.93	4.67	4.88
0.76	27.00	26.81	26.11	26.64	5.03	4.86	4.67	4.85
0.78	27.00	26.81	26.11	26.64	5.03	4.86	4.67	4.85
0.76	27.00	26.81	26.11	26.64	5.03	4.86	4.67	4.85
0.79	27.01	26.81	26.13	26.65	5.03	4.86	4.67	4.85
0.80	27.01	26.82	26.12	26.65	5.03	4.86	4.67	4.85
0.82	27.00	26.80	26.13	26.64	5.03	4.92	4.67	4.88
0.83	27.00	26.83	26.13	26.65	5.03	4.92	4.67	4.88
0.84	27.01	26.82	26.14	26.66	4.97	4.92	4.67	4.85
0.86	27.01	26.84	26.14	26.66	5.11	4.86	4.67	4.88
0.87	27.02	26.85	26.15	26.67	5.03	4.81	4.67	4.84
0.88	27.02	26.85	26.14	26.67	5.11	4.92	4.67	4.90
0.90	27.02	26.85	26.15	26.67	5.04	4.85	4.67	4.85
0.91	27.03	26.85	26.16	26.68	5.04	4.86	4.67	4.86
0.92	27.04	26.86	26.17	26.69	5.03	4.86	4.67	4.85
0.95	27.05	26.87	26.18	26.70	5.11	4.92	4.67	4.90
0.96	27.05	26.88	26.19	26.71	5.03	4.92	4.67	4.87

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	27.07	26.88	26.21	26.72	5.03	4.86	4.72	4.87
1.00	27.07	26.89	26.22	26.73	5.03	4.86	4.72	4.87
1.01	27.06	26.90	26.21	26.72	5.03	4.86	4.67	4.85
1.03	27.06	26.88	26.23	26.73	5.11	4.92	4.67	4.90
1.04	27.07	26.89	26.25	26.74	5.03	4.86	4.67	4.85
1.05	27.07	26.89	26.23	26.73	5.03	4.92	4.72	4.89
1.07	27.06	26.88	26.25	26.73	5.03	4.86	4.67	4.85
1.08	27.06	26.90	26.26	26.74	5.03	4.86	4.67	4.85
1.09	27.06	26.90	26.25	26.73	4.97	4.86	4.72	4.85
1.11	27.07	26.90	26.25	26.74	5.03	4.86	4.72	4.87
1.12	27.06	26.90	26.26	26.74	5.03	4.85	4.67	4.85
1.13	27.08	26.90	26.26	26.75	5.04	4.91	4.72	4.89
1.15	27.07	26.91	26.26	26.75	5.11	4.86	4.72	4.90
1.16	27.08	26.90	26.27	26.75	5.11	4.85	4.72	4.89
1.17	27.11	26.92	26.27	26.77	5.11	4.85	4.72	4.89
1.20	27.10	26.91	26.26	26.76	5.11	4.85	4.72	4.89
1.21	27.12	26.92	26.28	26.77	5.11	4.85	4.72	4.89
1.22	27.12	26.91	26.29	26.78	5.04	4.85	4.72	4.87
1.24	27.13	26.92	26.28	26.77	5.03	4.85	4.67	4.85
1.25	27.12	26.91	26.30	26.78	5.03	4.85	4.72	4.87
1.26	27.13	26.94	26.27	26.78	5.11	4.85	4.72	4.89
1.29	27.13	26.94	26.30	26.79	5.03	4.85	4.72	4.87
1.30	27.13	26.95	26.31	26.79	5.03	4.85	4.72	4.87
1.32	27.11	26.95	26.32	26.79	5.11	4.85	4.71	4.89
1.33	27.13	26.95	26.31	26.80	5.03	4.85	4.66	4.85
1.34	27.13	26.93	26.33	26.80	5.03	4.85	4.72	4.87
1.36	27.13	26.97	26.32	26.81	5.03	4.85	4.72	4.87
1.37	27.13	26.96	26.35	26.81	5.03	4.85	4.72	4.87
1.37	27.13	26.96	26.35	26.81	5.03	4.85	4.72	4.87
1.38	27.15	26.98	26.35	26.83	5.10	4.85	4.71	4.89
1.40	27.13	26.98	26.35	26.82	5.03	4.85	4.66	4.85
1.41	27.13	26.97	26.35	26.82	5.12	4.85	4.71	4.89
1.42	27.14	26.98	26.37	26.83	5.11	4.85	4.71	4.89
1.44	27.16	26.99	26.37	26.84	5.03	4.85	4.71	4.86
1.45	27.17	26.99	26.37	26.84	5.03	4.85	4.71	4.86
1.46	27.16	26.98	26.38	26.84	5.10	4.85	4.71	4.89
1.48	27.19	26.99	26.37	26.85	5.03	4.85	4.71	4.86

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	27.17	27.00	26.40	26.86	5.11	4.85	4.71	4.89
1.51	27.20	26.99	26.39	26.86	5.11	4.85	4.71	4.89
1.53	27.18	27.01	26.39	26.86	5.11	4.85	4.71	4.89
1.54	27.20	27.01	26.41	26.87	5.11	4.85	4.71	4.89
1.55	27.19	27.00	26.41	26.86	5.11	4.85	4.71	4.89
1.57	27.20	27.01	26.40	26.87	5.02	4.85	4.71	4.86
1.58	27.20	27.00	26.40	26.87	5.10	4.85	4.71	4.89
1.59	27.20	27.00	26.41	26.87	5.03	4.85	4.71	4.86
1.61	27.22	27.00	26.41	26.87	5.10	4.85	4.71	4.89
1.62	27.20	27.01	26.42	26.88	5.03	4.85	4.71	4.86
1.63	27.19	27.02	26.40	26.87	5.11	4.84	4.71	4.89
1.65	27.20	27.02	26.42	26.88	5.03	4.85	4.71	4.86
1.66	27.20	27.02	26.40	26.87	5.03	4.85	4.71	4.86
1.67	27.19	27.02	26.42	26.88	5.10	4.84	4.71	4.89
1.69	27.20	27.01	26.42	26.88	5.10	4.84	4.71	4.89
1.70	27.21	27.02	26.42	26.89	5.10	4.84	4.71	4.89
1.71	27.18	27.01	26.43	26.87	5.03	4.84	4.71	4.86
1.73	27.22	27.03	26.44	26.90	5.10	4.84	4.71	4.88
1.74	27.22	27.01	26.43	26.89	5.10	4.84	4.71	4.88
1.75	27.24	27.04	26.44	26.91	5.03	4.84	4.71	4.86
1.78	27.24	27.04	26.47	26.91	5.10	4.84	4.71	4.88
1.79	27.25	27.06	26.45	26.92	5.03	4.84	4.71	4.86
1.80	27.25	27.06	26.48	26.93	5.10	4.84	4.71	4.88
1.82	27.26	27.07	26.47	26.93	5.03	4.84	4.71	4.86
1.84	27.29	27.08	26.50	26.95	5.02	4.84	4.70	4.86
1.86	27.28	27.07	26.50	26.95	5.10	4.84	4.70	4.88
1.87	27.27	27.07	26.50	26.95	5.11	4.84	4.70	4.88
1.88	27.29	27.08	26.49	26.95	5.11	4.84	4.70	4.88
1.90	27.30	27.10	26.50	26.97	5.20	4.84	4.66	4.90
1.91	27.30	27.10	26.51	26.97	5.11	4.84	4.70	4.88
1.92	27.28	27.08	26.51	26.96	5.09	4.84	4.66	4.86
1.94	27.30	27.11	26.53	26.98	5.11	4.84	4.66	4.87
1.95	27.30	27.09	26.53	26.97	5.11	4.84	4.66	4.87
1.96	27.28	27.09	26.52	26.97	5.11	4.84	4.70	4.88
1.98	27.29	27.10	26.52	26.97	5.11	4.84	4.70	4.88
1.99	27.28	27.12	26.54	26.98	5.11	4.84	4.66	4.87

### APPENDIX 13.31 - Surface Tension Measurement Results for DI + SDS (82.00 mM)

HUATARC surface tension measurement results for DI + SDS (82.00 mM)

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	22.79	22.88	23.07	22.91	4.12	4.11	4.35	4.19
0.01	22.80	22.90	23.08	22.93	4.10	4.11	4.35	4.19
0.03	22.80	22.87	23.07	22.91	4.12	4.13	4.39	4.21
0.04	22.79	22.87	23.05	22.90	4.12	4.09	4.35	4.19
0.05	22.79	22.88	23.06	22.91	4.11	4.11	4.39	4.20
0.07	22.80	22.85	23.06	22.90	4.10	4.11	4.35	4.19
0.08	22.79	22.86	23.06	22.90	4.12	4.09	4.39	4.20
0.09	22.79	22.85	23.05	22.90	4.13	4.13	4.34	4.20
0.11	22.79	22.86	23.07	22.91	4.12	4.12	4.35	4.20
0.13	22.78	22.84	23.04	22.89	4.10	4.11	4.39	4.20
0.14	22.78	22.82	23.05	22.88	4.09	4.12	4.39	4.20
0.16	22.77	22.82	23.05	22.88	4.09	4.11	4.39	4.20
0.17	22.77	22.83	23.04	22.88	4.11	4.12	4.34	4.19
0.18	22.76	22.82	23.04	22.87	4.11	4.12	4.39	4.21
0.20	22.78	22.82	23.05	22.88	4.11	4.10	4.34	4.18
0.22	22.78	22.81	23.04	22.88	4.09	4.16	4.39	4.21
0.24	22.76	22.81	23.05	22.87	4.09	4.14	4.34	4.19
0.25	22.77	22.80	23.04	22.87	4.13	4.16	4.34	4.21
0.26	22.76	22.82	23.04	22.87	4.11	4.14	4.34	4.20
0.29	22.76	22.80	23.04	22.87	4.11	4.12	4.34	4.19
0.30	22.76	22.80	23.03	22.86	4.09	4.14	4.39	4.21
0.32	22.76	22.80	23.05	22.87	4.11	4.12	4.39	4.21
0.33	22.74	22.79	23.05	22.86	4.09	4.14	4.34	4.19
0.34	22.74	22.79	23.03	22.85	4.10	4.14	4.34	4.19
0.36	22.74	22.80	23.04	22.86	4.05	4.14	4.34	4.18
0.37	22.74	22.77	23.03	22.85	4.09	4.14	4.39	4.21
0.38	22.74	22.77	23.03	22.85	4.10	4.14	4.34	4.19
0.40	22.74	22.77	23.03	22.85	4.10	4.16	4.34	4.20
0.38	22.74	22.77	23.03	22.85	4.10	4.14	4.34	4.19
0.41	22.73	22.77	23.05	22.85	4.10	4.16	4.38	4.21
0.42	22.71	22.77	23.03	22.84	4.08	4.14	4.30	4.17
0.43	22.72	22.76	23.05	22.84	4.10	4.18	4.34	4.21
0.45	22.74	22.76	23.04	22.85	4.10	4.16	4.34	4.20

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	22.71	22.75	23.03	22.83	4.10	4.18	4.34	4.21
0.49	22.71	22.75	23.02	22.83	4.10	4.16	4.34	4.20
0.50	22.72	22.74	23.03	22.83	4.10	4.16	4.34	4.20
0.51	22.69	22.74	23.02	22.82	4.10	4.13	4.30	4.18
0.53	22.72	22.73	23.02	22.82	4.10	4.16	4.30	4.19
0.54	22.71	22.73	23.03	22.82	4.10	4.15	4.34	4.20
0.55	22.71	22.72	23.02	22.82	4.08	4.15	4.34	4.19
0.57	22.70	22.74	23.01	22.82	4.10	4.21	4.34	4.22
0.58	22.71	22.71	23.03	22.82	4.08	4.18	4.34	4.20
0.59	22.70	22.72	23.03	22.82	4.10	4.18	4.34	4.21
0.62	22.72	22.71	23.01	22.81	4.06	4.13	4.34	4.18
0.63	22.69	22.71	23.02	22.81	4.10	4.13	4.34	4.19
0.65	22.69	22.70	23.01	22.80	4.09	4.18	4.34	4.20
0.66	22.68	22.73	23.02	22.81	4.10	4.13	4.33	4.19
0.67	22.69	22.69	23.04	22.81	4.08	4.18	4.34	4.20
0.68	22.68	22.71	23.03	22.81	4.09	4.16	4.33	4.19
0.70	22.68	22.71	23.02	22.80	4.09	4.15	4.33	4.19
0.71	22.70	22.70	23.02	22.81	4.10	4.18	4.34	4.21
0.72	22.69	22.70	23.02	22.80	4.09	4.13	4.33	4.18
0.74	22.67	22.70	23.02	22.80	4.09	4.18	4.33	4.20
0.75	22.67	22.71	23.01	22.80	4.07	4.15	4.33	4.18
0.76	22.67	22.69	23.03	22.80	4.09	4.15	4.33	4.19
0.78	22.68	22.70	23.01	22.80	4.09	4.15	4.33	4.19
0.80	22.68	22.68	23.02	22.79	4.11	4.17	4.33	4.20
0.82	22.67	22.70	23.02	22.80	4.11	4.18	4.33	4.21
0.83	22.67	22.68	23.02	22.79	4.09	4.18	4.33	4.20
0.84	22.66	22.69	23.02	22.79	4.11	4.20	4.33	4.21
0.86	22.65	22.69	23.02	22.79	4.09	4.15	4.37	4.20
0.87	22.67	22.68	23.00	22.78	4.07	4.15	4.33	4.18
0.88	22.66	22.69	23.02	22.79	4.05	4.17	4.33	4.18
0.87	22.67	22.68	23.00	22.78	4.07	4.15	4.33	4.18
0.90	22.67	22.67	23.02	22.79	4.07	4.17	4.38	4.21
0.91	22.66	22.70	23.00	22.79	4.09	4.23	4.33	4.22
0.92	22.67	22.68	23.02	22.79	4.09	4.17	4.33	4.20
0.94	22.65	22.68	23.02	22.78	4.11	4.17	4.33	4.20
0.95	22.66	22.67	23.01	22.78	4.07	4.15	4.33	4.18
0.96	22.67	22.66	23.01	22.78	4.11	4.20	4.33	4.21

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	22.65	22.68	22.99	22.77	4.11	4.17	4.33	4.20
1.00	22.66	22.68	23.02	22.79	4.09	4.23	4.29	4.20
1.01	22.66	22.66	23.03	22.78	4.11	4.19	4.33	4.21
1.03	22.65	22.67	23.00	22.77	4.08	4.17	4.37	4.21
1.04	22.67	22.67	23.00	22.78	4.08	4.17	4.33	4.19
1.05	22.67	22.66	23.01	22.78	4.09	4.17	4.33	4.20
1.07	22.66	22.67	23.00	22.78	4.08	4.16	4.37	4.20
1.08	22.64	22.67	23.00	22.77	4.09	4.17	4.33	4.20
1.09	22.65	22.67	23.01	22.78	4.08	4.19	4.33	4.20
1.11	22.64	22.66	23.01	22.77	4.06	4.17	4.33	4.19
1.12	22.65	22.66	23.00	22.77	4.08	4.17	4.33	4.19
1.13	22.66	22.65	23.01	22.77	4.07	4.17	4.37	4.20
1.15	22.65	22.65	23.00	22.77	4.06	4.17	4.33	4.19
1.16	22.63	22.66	23.00	22.76	4.10	4.17	4.37	4.21
1.17	22.64	22.66	22.99	22.76	4.08	4.17	4.32	4.19
1.19	22.65	22.65	23.00	22.77	4.08	4.19	4.33	4.20
1.20	22.65	22.66	23.01	22.77	4.04	4.17	4.32	4.18
1.21	22.65	22.66	23.00	22.77	4.10	4.17	4.32	4.20
1.22	22.65	22.65	23.00	22.77	4.06	4.19	4.32	4.19
1.25	22.64	22.66	23.00	22.77	4.08	4.17	4.37	4.21
1.26	22.65	22.65	23.00	22.77	4.06	4.17	4.28	4.17
1.28	22.64	22.64	23.01	22.76	4.08	4.19	4.32	4.20
1.30	22.65	22.64	22.99	22.76	4.08	4.14	4.37	4.20
1.32	22.65	22.64	23.00	22.76	4.08	4.19	4.37	4.21
1.33	22.64	22.65	23.00	22.76	4.08	4.19	4.32	4.20
1.34	22.64	22.64	23.01	22.76	4.06	4.19	4.32	4.19
1.34	22.64	22.64	23.01	22.76	4.06	4.19	4.32	4.19
1.36	22.63	22.63	22.99	22.75	4.06	4.14	4.32	4.17
1.37	22.63	22.63	22.99	22.75	4.10	4.17	4.37	4.21
1.38	22.65	22.63	22.99	22.76	4.09	4.19	4.32	4.20
1.40	22.64	22.64	23.00	22.76	4.12	4.16	4.37	4.22
1.41	22.63	22.63	23.00	22.75	4.08	4.16	4.32	4.19
1.42	22.63	22.63	22.99	22.75	4.06	4.19	4.32	4.19
1.44	22.64	22.62	23.00	22.75	4.09	4.19	4.36	4.21
1.45	22.63	22.61	23.01	22.75	4.09	4.14	4.32	4.18
1.46	22.63	22.63	23.00	22.75	4.09	4.19	4.32	4.20
1.48	22.64	22.61	23.00	22.75	4.07	4.16	4.36	4.20

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	22.62	22.63	23.00	22.75	4.05	4.19	4.36	4.20
1.51	22.63	22.62	23.00	22.75	4.06	4.21	4.36	4.21
1.53	22.64	22.61	23.01	22.75	4.08	4.16	4.32	4.19
1.54	22.63	22.60	23.00	22.74	4.09	4.19	4.40	4.23
1.55	22.62	22.61	23.00	22.74	4.07	4.19	4.32	4.19
1.57	22.64	22.61	23.00	22.75	4.06	4.16	4.36	4.19
1.58	22.61	22.62	23.00	22.74	4.03	4.18	4.36	4.19
1.59	22.62	22.62	23.00	22.75	4.05	4.16	4.31	4.17
1.61	22.63	22.61	22.99	22.74	4.06	4.18	4.32	4.19
1.62	22.62	22.61	23.00	22.74	4.09	4.18	4.32	4.20
1.63	22.61	22.61	22.99	22.74	4.07	4.19	4.31	4.19
1.66	22.63	22.61	23.00	22.75	4.09	4.18	4.36	4.21
1.67	22.61	22.62	22.99	22.74	4.05	4.18	4.32	4.18
1.69	22.62	22.62	22.98	22.74	4.07	4.18	4.35	4.20
1.70	22.62	22.59	23.00	22.74	4.09	4.18	4.32	4.20
1.71	22.63	22.58	23.00	22.74	4.07	4.18	4.36	4.20
1.73	22.62	22.60	22.99	22.74	4.07	4.18	4.31	4.19
1.74	22.63	22.61	22.99	22.74	4.05	4.18	4.31	4.18
1.75	22.62	22.60	23.00	22.74	4.03	4.18	4.36	4.19
1.76	22.61	22.62	22.98	22.74	4.07	4.22	4.31	4.20
1.78	22.62	22.61	22.99	22.74	4.07	4.18	4.31	4.19
1.79	22.63	22.59	22.99	22.74	4.07	4.18	4.36	4.20
1.80	22.62	22.60	22.97	22.73	4.09	4.18	4.31	4.19
1.82	22.62	22.61	22.98	22.74	4.07	4.21	4.36	4.21
1.83	22.61	22.61	22.98	22.73	4.07	4.18	4.36	4.20
1.86	22.62	22.60	22.99	22.74	4.05	4.18	4.31	4.18
1.87	22.61	22.60	22.98	22.73	4.07	4.18	4.31	4.19
1.88	22.62	22.59	22.98	22.73	4.06	4.18	4.31	4.18
1.90	22.63	22.60	22.97	22.73	4.09	4.21	4.31	4.20
1.91	22.62	22.60	22.98	22.73	4.05	4.18	4.31	4.18
1.92	22.63	22.61	22.98	22.74	4.03	4.18	4.35	4.19
1.94	22.62	22.60	22.98	22.73	4.05	4.18	4.31	4.18
1.95	22.64	22.59	22.98	22.74	4.07	4.18	4.31	4.19
1.96	22.63	22.59	22.98	22.73	4.06	4.18	4.35	4.20
1.98	22.62	22.59	22.97	22.73	4.05	4.18	4.35	4.19
1.99	22.64	22.60	22.99	22.74	4.01	4.20	4.35	4.19

**APPENDIX 13.32 - Descriptive Statistics for Surface Tension Measurement Results of DI + SDS**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.82	Exp.1	40.71	42.28	0.32	0.10	0.78	0.67
	Exp.2	40.61	41.25	0.15	0.02	-0.06	-0.90
	Exp.3	39.92	41.25	0.27	0.08	-0.08	-0.68
	Average	40.32	41.44	0.23	0.06	0.03	-0.64
3.00	Exp.1	21.74	21.83	0.02	0.00	0.58	-0.93
	Exp.2	21.38	21.42	0.01	0.00	0.20	-0.35
	Exp.3	21.79	21.87	0.02	0.00	-0.54	-0.68
	Average	21.64	21.70	0.01	0.00	0.09	-0.94
6.00	Exp.1	21.55	21.82	0.07	0.01	0.51	-0.93
	Exp.2	21.52	22.40	0.12	0.01	1.78	7.87
	Exp.3	21.62	21.92	0.08	0.01	0.51	-0.88
	Average	21.57	21.88	0.09	0.01	0.52	-0.87
8.20	Exp.1	23.58	23.76	0.04	0.00	0.20	-0.56
	Exp.2	24.01	24.20	0.05	0.00	0.30	-0.95
	Exp.3	24.04	24.17	0.04	0.00	0.19	-1.13
	Average	23.88	24.03	0.04	0.00	0.23	-0.99
44.30	Exp.1	26.36	26.66	0.09	0.01	0.14	-1.23
	Exp.2	26.59	26.93	0.09	0.01	0.08	-1.06
	Exp.3	27.04	27.22	0.05	0.00	0.45	-1.06
	Average	26.67	26.93	0.08	0.01	0.20	-1.19
59.00	Exp.1	26.84	27.30	0.14	0.02	0.12	-1.17
	Exp.2	26.60	27.12	0.14	0.02	-0.12	-1.11
	Exp.3	25.78	26.54	0.22	0.05	-0.20	-1.19
	Average	26.41	26.98	0.17	0.03	-0.10	-1.18
82.00	Exp.1	22.61	22.80	0.06	0.00	0.80	-0.64
	Exp.2	22.58	22.90	0.08	0.01	0.74	-0.48
	Exp.3	22.97	23.08	0.02	0.00	0.46	-0.33
	Average	22.73	22.93	0.05	0.00	0.74	-0.56

### APPENDIX 13.33 - Surface Tension Measurement Results for Hexane

HUATARC surface tension measurement results for hexane

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	28.30	27.67	27.97	27.98	4.96	4.78	4.88	4.87
0.07	28.31	27.68	28.01	28.00	4.96	4.76	4.87	4.86
0.13	28.29	27.69	28.09	28.02	4.94	4.79	4.88	4.87
0.20	28.28	27.77	28.16	28.07	4.96	4.75	4.87	4.86
0.26	28.35	27.82	28.19	28.12	4.96	4.77	4.88	4.87
0.33	28.30	27.74	28.16	28.07	4.96	4.76	4.86	4.86
0.40	28.33	27.75	28.10	28.06	4.96	4.79	4.84	4.86
0.46	28.35	27.76	28.11	28.07	4.96	4.76	4.86	4.86
0.53	28.30	27.75	28.06	28.04	4.96	4.75	4.88	4.86
0.59	28.35	27.81	28.09	28.08	4.98	4.77	4.87	4.87
0.66	28.35	27.88	28.11	28.11	4.96	4.76	4.86	4.86
0.72	28.38	27.91	28.14	28.14	4.96	4.77	4.87	4.87
0.79	28.39	27.92	28.15	28.15	4.96	4.75	4.87	4.86
0.86	28.41	27.93	28.22	28.19	4.96	4.78	4.86	4.87
0.92	28.41	27.97	28.20	28.19	4.96	4.76	4.87	4.86
0.99	28.39	27.97	28.21	28.19	4.96	4.78	4.87	4.87
1.05	28.44	27.97	28.28	28.23	4.96	4.76	4.89	4.87
1.25	28.45	27.95	28.32	28.24	4.96	4.76	4.87	4.86
1.32	28.43	27.99	28.33	28.25	4.96	4.78	4.88	4.87
1.45	28.44	27.99	28.32	28.25	4.95	4.76	4.86	4.86
1.51	28.46	27.98	28.33	28.26	4.98	4.76	4.88	4.87
1.58	28.45	27.97	28.29	28.24	4.96	4.77	4.86	4.86
1.65	28.44	27.94	28.28	28.22	4.98	4.78	4.87	4.88
1.71	28.42	27.85	28.22	28.16	4.94	4.77	4.88	4.86
1.78	28.44	27.80	28.20	28.15	4.96	4.78	4.88	4.87
1.84	28.43	27.76	28.16	28.12	4.97	4.76	4.88	4.87
1.91	28.46	27.69	28.14	28.10	4.98	4.78	4.86	4.87
1.98	28.45	27.71	28.19	28.12	4.95	4.78	4.88	4.87
2.04	28.43	27.71	28.15	28.10	4.97	4.78	4.86	4.87
2.11	28.42	27.72	28.20	28.11	4.97	4.79	4.86	4.87
2.04	28.43	27.71	28.15	28.10	4.97	4.78	4.86	4.87
2.17	28.41	27.72	28.19	28.11	4.95	4.78	4.86	4.86
2.24	28.46	27.71	28.23	28.13	4.99	4.80	4.86	4.88

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
2.37	28.41	27.61	28.22	28.08	4.87	4.78	4.87	4.84
2.44	28.40	27.65	28.17	28.07	4.96	4.79	4.90	4.88
2.50	28.38	27.66	28.11	28.05	4.94	4.78	4.85	4.86
2.57	28.37	27.67	28.13	28.06	4.91	4.80	4.89	4.87
0.00	28.30	27.67	27.97	27.98	4.96	4.78	4.88	4.87
0.07	28.31	27.68	28.01	28.00	4.96	4.76	4.87	4.86
0.13	28.29	27.69	28.09	28.02	4.94	4.79	4.88	4.87
0.20	28.28	27.77	28.16	28.07	4.96	4.75	4.87	4.86
0.26	28.35	27.82	28.19	28.12	4.96	4.77	4.88	4.87
0.33	28.30	27.74	28.16	28.07	4.96	4.76	4.86	4.86
0.40	28.33	27.75	28.10	28.06	4.96	4.79	4.84	4.86
0.46	28.35	27.76	28.11	28.07	4.96	4.76	4.86	4.86
0.53	28.30	27.75	28.06	28.04	4.96	4.75	4.88	4.86
0.59	28.35	27.81	28.09	28.08	4.98	4.77	4.87	4.87
0.79	28.39	27.92	28.15	28.15	4.96	4.75	4.87	4.86
0.86	28.41	27.93	28.22	28.19	4.96	4.78	4.86	4.87
0.92	28.41	27.97	28.20	28.19	4.96	4.76	4.87	4.86
0.99	28.39	27.97	28.21	28.19	4.96	4.78	4.87	4.87
1.05	28.44	27.97	28.28	28.23	4.96	4.76	4.89	4.87
1.12	28.40	27.96	28.28	28.21	4.98	4.74	4.84	4.85
1.19	28.43	27.96	28.28	28.22	4.96	4.76	4.86	4.86
1.25	28.45	27.95	28.32	28.24	4.96	4.76	4.87	4.86
1.32	28.43	27.99	28.33	28.25	4.96	4.78	4.88	4.87
1.38	28.42	28.02	28.31	28.25	4.97	4.76	4.85	4.86
1.45	28.44	27.99	28.32	28.25	4.95	4.76	4.86	4.86
1.51	28.46	27.98	28.33	28.26	4.98	4.76	4.88	4.87
1.58	28.45	27.97	28.29	28.24	4.96	4.77	4.86	4.86
1.65	28.44	27.94	28.28	28.22	4.98	4.78	4.87	4.88
1.71	28.42	27.85	28.22	28.16	4.94	4.77	4.88	4.86
1.78	28.44	27.80	28.20	28.15	4.96	4.78	4.88	4.87
1.84	28.43	27.76	28.16	28.12	4.97	4.76	4.88	4.87
1.91	28.46	27.69	28.14	28.10	4.98	4.78	4.86	4.87
1.98	28.45	27.71	28.19	28.12	4.95	4.78	4.88	4.87
2.04	28.43	27.71	28.15	28.10	4.97	4.78	4.86	4.87
2.11	28.42	27.72	28.20	28.11	4.97	4.79	4.86	4.87
2.17	28.41	27.72	28.19	28.11	4.95	4.78	4.86	4.86
2.24	28.46	27.71	28.23	28.13	4.99	4.80	4.86	4.88

APPENDIX 13.34 - Descriptive Statistics for Surface Tension Measurement Results of Hexane

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.00	Exp.1	28.28	28.46	0.05	0.00	-0.73	-0.58
	Exp.2	27.61	28.02	0.13	0.02	0.13	-1.55
	Exp.3	27.97	28.33	0.09	0.01	-0.25	-0.14
	Average	27.98	28.26	0.08	0.01	0.11	-0.96

## APPENDIX 13.35 - Surface Tension Measurement Results for DI

HUATARC surface tension measurement results for DI

Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.00	69.64	69.71	71.11	70.15	3.86	3.83	3.83	3.84
0.01	69.82	70.66	70.91	70.46	3.86	3.84	3.83	3.84
0.03	69.98	70.93	72.00	70.97	3.86	3.83	3.83	3.84
0.04	70.20	70.07	70.45	70.24	3.86	3.84	3.83	3.84
0.05	70.06	69.95	70.07	70.03	3.86	3.84	3.83	3.84
0.07	70.08	70.45	70.96	70.50	3.86	3.84	3.83	3.84
0.08	70.14	70.97	71.27	70.79	3.87	3.84	3.83	3.85
0.11	69.66	69.71	70.31	69.89	3.87	3.83	3.83	3.84
0.12	69.68	70.53	70.63	70.28	3.87	3.84	3.83	3.85
0.14	70.12	70.51	70.59	70.41	3.86	3.84	3.83	3.84
0.16	70.49	69.99	70.15	70.21	3.86	3.83	3.83	3.84
0.17	70.34	70.05	70.68	70.36	3.86	3.84	3.83	3.84
0.18	69.88	70.52	71.47	70.62	3.86	3.84	3.83	3.84
0.20	69.81	70.30	71.28	70.46	3.86	3.83	3.83	3.84
0.21	70.00	70.22	70.64	70.29	3.86	3.83	3.83	3.84
0.22	70.31	70.29	70.09	70.23	3.86	3.84	3.83	3.84
0.25	70.16	70.64	70.79	70.53	3.86	3.83	3.82	3.84
0.26	69.91	70.24	70.44	70.20	3.86	3.83	3.82	3.84
0.28	70.24	70.06	70.65	70.32	3.86	3.83	3.82	3.84
0.29	70.42	70.27	71.39	70.69	3.86	3.79	3.82	3.82
0.30	70.05	70.61	71.19	70.62	3.86	3.83	3.82	3.84
0.32	69.85	70.30	70.60	70.25	3.86	3.83	3.83	3.84
0.33	69.90	70.16	70.53	70.20	3.86	3.83	3.82	3.84
0.36	70.46	70.90	71.00	70.79	3.86	3.83	3.82	3.84
0.37	70.51	70.67	70.72	70.63	3.86	3.83	3.82	3.84
0.38	70.02	70.19	70.58	70.26	3.86	3.83	3.82	3.84
0.40	69.69	70.30	70.96	70.32	3.86	3.83	3.82	3.84
0.41	70.05	70.71	70.69	70.48	3.86	3.83	3.82	3.84
0.40	69.69	70.30	70.96	70.32	3.86	3.83	3.82	3.84
0.43	70.45	70.40	70.63	70.49	3.85	3.79	3.82	3.82
0.45	70.02	70.41	70.81	70.41	3.85	3.83	3.82	3.83

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.47	70.24	70.68	70.86	70.59	3.86	3.83	3.82	3.84
0.49	70.44	70.27	70.86	70.52	3.85	3.83	3.82	3.83
0.50	70.47	70.19	70.80	70.49	3.86	3.79	3.82	3.82
0.51	69.92	70.58	70.77	70.42	3.86	3.83	3.82	3.84
0.53	69.88	70.63	70.78	70.43	3.85	3.83	3.82	3.83
0.54	70.05	70.46	70.69	70.40	3.85	3.83	3.82	3.83
0.55	70.52	70.35	70.98	70.62	3.85	3.83	3.82	3.83
0.57	70.36	70.70	70.91	70.66	3.85	3.83	3.82	3.83
0.58	70.24	70.70	70.84	70.59	3.85	3.82	3.82	3.83
0.59	70.07	70.40	70.96	70.48	3.85	3.83	3.82	3.83
0.61	70.07	70.47	70.64	70.39	3.85	3.79	3.82	3.82
0.62	70.35	70.56	70.55	70.49	3.85	3.82	3.82	3.83
0.63	70.37	70.72	70.85	70.65	3.85	3.82	3.82	3.83
0.65	70.24	70.28	71.10	70.54	3.85	3.83	3.82	3.83
0.67	70.42	70.74	70.79	70.65	3.85	3.78	3.82	3.82
0.68	70.51	70.68	70.86	70.68	3.85	3.82	3.82	3.83
0.70	70.16	70.41	70.71	70.43	3.85	3.82	3.82	3.83
0.71	69.97	70.49	70.66	70.37	3.85	3.82	3.82	3.83
0.72	70.12	70.71	70.60	70.48	3.85	3.82	3.82	3.83
0.74	70.49	70.59	70.72	70.60	3.85	3.82	3.82	3.83
0.75	70.60	70.70	70.92	70.74	3.84	3.78	3.82	3.81
0.76	70.30	70.49	70.91	70.57	3.85	3.79	3.82	3.82
0.78	70.20	70.76	71.08	70.68	3.84	3.82	3.82	3.83
0.79	70.21	70.53	71.03	70.59	3.84	3.82	3.82	3.83
0.80	70.36	70.53	70.57	70.49	3.85	3.82	3.82	3.83
0.82	70.37	70.92	70.63	70.64	3.85	3.82	3.82	3.83
0.83	70.36	70.49	70.79	70.55	3.84	3.82	3.82	3.83
0.84	70.10	70.71	70.85	70.55	3.84	3.82	3.82	3.83
0.86	70.16	70.81	70.95	70.64	3.85	3.82	3.82	3.83
0.87	70.43	70.74	70.80	70.66	3.84	3.82	3.82	3.83
0.88	70.51	70.57	70.94	70.67	3.84	3.82	3.82	3.83
0.88	70.51	70.57	70.94	70.67	3.84	3.82	3.82	3.83
0.91	70.03	70.81	70.85	70.56	3.84	3.78	3.82	3.81
0.92	70.18	70.55	70.92	70.55	3.84	3.82	3.82	3.83
0.94	70.55	70.73	70.89	70.72	3.84	3.82	3.81	3.82
0.95	70.56	70.75	70.83	70.71	3.84	3.82	3.81	3.82
0.96	70.27	70.81	71.03	70.70	3.84	3.82	3.82	3.83

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
0.99	70.36	70.61	70.88	70.62	3.84	3.78	3.81	3.81
1.00	70.30	70.72	70.55	70.52	3.84	3.82	3.82	3.83
1.01	70.20	70.74	70.64	70.53	3.85	3.82	3.81	3.83
1.03	69.89	70.74	71.04	70.56	3.84	3.82	3.81	3.82
1.04	70.32	70.63	70.86	70.60	3.84	3.82	3.81	3.82
1.05	70.52	70.58	70.91	70.67	3.84	3.78	3.81	3.81
1.07	70.39	70.56	71.07	70.67	3.84	3.82	3.81	3.82
1.08	70.25	70.70	70.97	70.64	3.84	3.82	3.81	3.82
1.09	70.28	70.67	70.61	70.52	3.84	3.78	3.81	3.81
1.11	70.26	70.73	70.45	70.48	3.84	3.81	3.81	3.82
1.12	70.42	70.97	70.98	70.79	3.83	3.78	3.81	3.81
1.13	70.45	70.75	71.01	70.74	3.83	3.77	3.81	3.80
1.15	70.15	70.58	70.52	70.42	3.84	3.81	3.81	3.82
1.16	70.20	70.67	70.70	70.52	3.84	3.78	3.81	3.81
1.17	70.43	70.87	71.18	70.83	3.84	3.81	3.81	3.82
1.19	70.45	70.82	70.72	70.66	3.84	3.81	3.81	3.82
1.20	70.64	70.60	70.67	70.64	3.83	3.81	3.81	3.82
1.22	70.11	71.13	70.89	70.71	3.84	3.81	3.81	3.82
1.24	70.29	70.81	70.80	70.63	3.84	3.81	3.81	3.82
1.25	70.52	70.38	70.78	70.56	3.83	3.81	3.78	3.81
1.26	70.37	70.78	70.80	70.65	3.84	3.77	3.81	3.81
1.28	70.48	70.77	70.93	70.73	3.83	3.77	3.81	3.80
1.29	70.38	70.21	70.68	70.42	3.84	3.77	3.81	3.81
1.30	70.28	70.37	70.65	70.43	3.83	3.81	3.81	3.82
1.32	70.05	71.12	71.00	70.72	3.84	3.77	3.81	3.81
1.33	70.03	71.55	70.84	70.81	3.83	3.81	3.81	3.82
1.34	70.53	70.76	71.03	70.77	3.83	3.81	3.81	3.82
1.36	70.63	70.58	70.66	70.62	3.84	3.77	3.81	3.81
1.37	70.52	70.62	71.17	70.77	3.83	3.77	3.81	3.80
1.38	70.46	70.69	70.81	70.65	3.83	3.77	3.81	3.80
1.40	70.27	70.50	70.69	70.49	3.83	3.81	3.81	3.82
1.41	70.44	70.47	70.87	70.59	3.83	3.81	3.81	3.82
1.44	70.39	71.05	70.80	70.75	3.83	3.81	3.81	3.82
1.44	70.39	71.05	70.80	70.75	3.83	3.81	3.81	3.82
1.45	70.32	70.44	70.51	70.42	3.83	3.81	3.81	3.82
1.46	70.47	70.54	70.92	70.64	3.83	3.81	3.81	3.82
1.48	70.36	70.61	70.73	70.57	3.83	3.81	3.81	3.82

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Time (s)	Surface Tension (dynes/cm)				Volume (ml)			
	Exp.1	Exp.2	Exp.3	Avg.	Exp.1	Exp.2	Exp.3	Avg.
1.50	70.38	70.47	70.81	70.55	3.83	3.81	3.81	3.82
1.51	70.27	70.90	71.14	70.77	3.83	3.81	3.81	3.82
1.53	70.29	71.09	70.87	70.75	3.83	3.81	3.80	3.81
1.54	70.37	71.00	70.45	70.61	3.82	3.77	3.81	3.80
1.55	70.43	70.44	70.78	70.55	3.82	3.81	3.81	3.81
1.57	70.53	70.65	70.90	70.69	3.83	3.80	3.81	3.81
1.58	70.62	71.06	70.81	70.83	3.82	3.77	3.80	3.80
1.59	70.46	70.57	71.11	70.71	3.82	3.77	3.81	3.80
1.61	70.34	70.82	70.61	70.59	3.83	3.80	3.81	3.81
1.62	70.30	70.91	70.78	70.66	3.83	3.80	3.80	3.81
1.63	70.25	71.14	70.61	70.67	3.82	3.81	3.80	3.81
1.65	70.80	70.61	70.64	70.68	3.82	3.80	3.80	3.81
1.66	70.83	70.49	70.94	70.75	3.82	3.77	3.80	3.80
1.67	70.50	70.63	70.48	70.54	3.83	3.81	3.80	3.81
1.69	70.54	70.79	70.54	70.62	3.82	3.80	3.80	3.81
1.70	70.40	70.78	70.68	70.62	3.82	3.80	3.80	3.81
1.71	70.35	70.70	70.73	70.59	3.82	3.81	3.80	3.81
1.73	70.35	71.00	71.22	70.86	3.82	3.80	3.80	3.81
1.74	70.78	70.97	70.86	70.87	3.82	3.80	3.80	3.81
1.75	70.42	70.67	70.48	70.52	3.82	3.77	3.80	3.80
1.78	70.46	70.79	70.85	70.70	3.82	3.80	3.80	3.81
1.79	70.75	70.90	70.91	70.85	3.82	3.80	3.80	3.81
1.80	70.66	70.99	70.52	70.72	3.82	3.80	3.80	3.81
1.82	70.47	70.72	70.93	70.71	3.82	3.76	3.80	3.79
1.83	70.51	70.98	70.83	70.77	3.82	3.80	3.80	3.81
1.84	70.56	71.08	70.64	70.76	3.82	3.77	3.80	3.80
1.86	70.40	70.66	71.06	70.71	3.82	3.80	3.80	3.81
1.87	70.57	70.79	71.19	70.85	3.82	3.80	3.80	3.81
1.88	70.87	71.17	71.02	71.02	3.82	3.80	3.80	3.81
1.90	70.70	70.81	70.62	70.71	3.82	3.80	3.80	3.81
1.92	70.39	70.77	70.85	70.67	3.82	3.76	3.80	3.79
1.94	70.31	70.85	70.80	70.65	3.82	3.80	3.80	3.81
1.95	70.68	70.67	71.01	70.79	3.82	3.80	3.80	3.81
1.96	70.59	70.85	70.85	70.76	3.82	3.76	3.80	3.79
1.98	70.60	70.82	71.43	70.95	3.82	3.80	3.80	3.81
1.99	70.66	70.93	70.85	70.81	3.82	3.80	3.80	3.81

**APPENDIX 13.36 - Descriptive Statistics for Surface Tension Measurement Results of DI**

Concentration (mM)	Experiment	Surface Tension (dynes/cm)					
		Min.	Max.	Standard Deviation	Variance	Skewness	Kurtosis
0.00	Exp.1	69.47	70.87	0.25	0.06	-0.58	0.41
	Exp.2	69.71	71.55	0.28	0.08	-0.40	1.30
	Exp.3	70.07	72.00	0.25	0.06	0.48	3.09
	Average	69.89	71.02	0.18	0.03	-0.78	1.30

**APPENDIX 14 - Experimental Results for DI from Hacettepe University Environmental Engineering Research Laboratory**

**APPENDIX 14.1 - Experimental Results for DI in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Avg. (mm)
1	2.04	4.29	11.32	5.88
2	35.79	20.53	28.68	28.33
3	30.00	34.21	23.68	29.30
4	25.26	29.47	18.68	24.47

Relative change in the height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

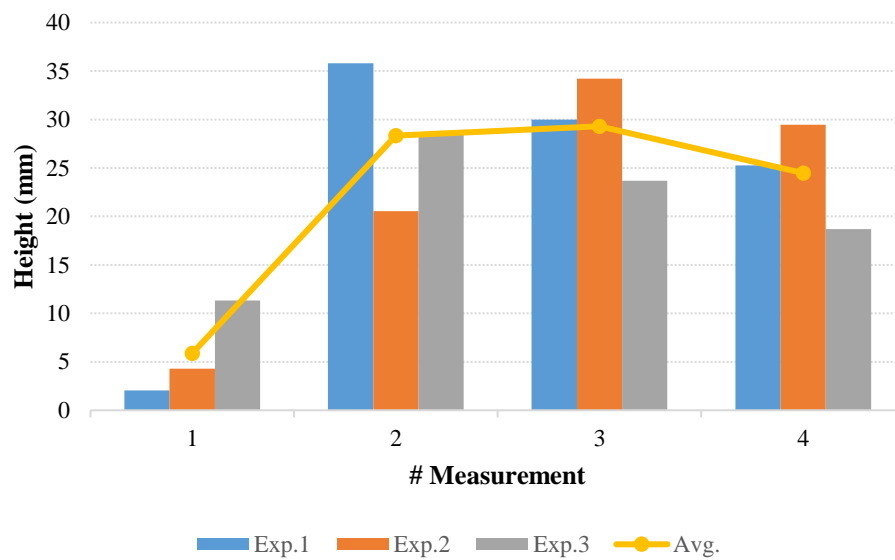
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Avg. (%)
1	-	-	-	-
2	1,657.14	378.95	153.49	729.86
3	-16.18	66.67	-17.43	11.02
4	-15.79	-13.85	-21.11	-16.92

Calculated perpendicular relative height for DI and SDS solution ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Avg. (mm)
1	31.00	17.78	24.84	24.54
2	25.98	29.63	20.51	25.37
3	21.88	25.52	16.18	21.19
4	31.00	17.78	24.84	24.54

Descriptive statistics for DI ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Err. of Mean	Median	Std. Variation	Kurtosis	Range
<b>Exp.1</b>	23.27	7.40	27.63	14.80	2.49	33.75
<b>Exp.2</b>	22.13	6.59	25.00	13.17	0.38	29.92
<b>Exp.3</b>	20.59	3.70	21.18	7.41	-0.46	17.36



Measured height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 14.2 - Experimental Results for DI with 3 mg/ml SDS in V-Shaped Pasteur Pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	-3.15	-1.37	2.69	0.49	4.90	0.71
2	-2.39	1.36	4.23	2.51	9.29	3.00
3	0.00	1.71	6.94	4.76	10.70	4.82
4	1.55	3.54	7.75	5.88	12.23	6.19
5	2.93	4.27	12.13	7.20	11.03	7.51

Relative change in the height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

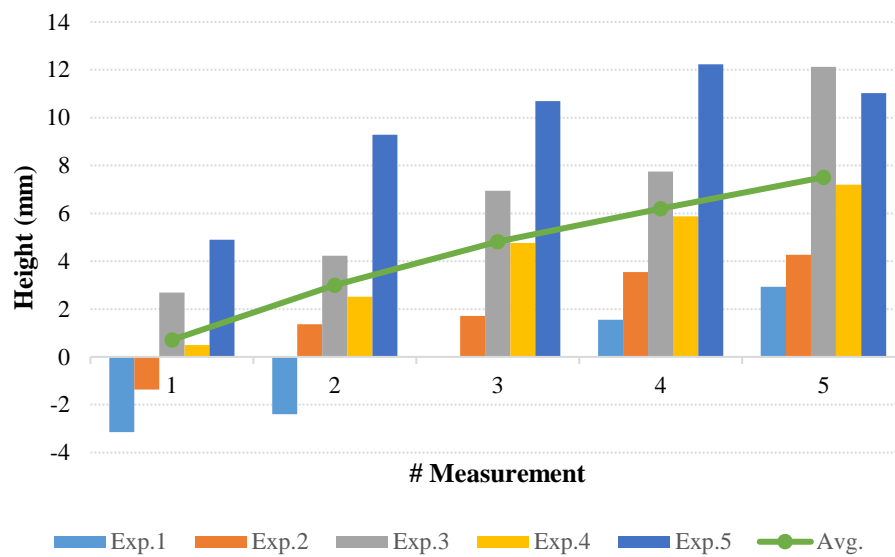
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	-24.07	-199.61	57.04	413.65	89.76	67.35
3	-100.00	25.10	64.17	89.83	15.20	18.86
4	155.00	107.52	11.74	23.52	14.29	62.41
5	88.23	20.47	56.45	22.47	-9.84	35.56

Calculated perpendicular relative height for DI ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.3 (mm)	Exp.5 (mm)	Avg. (mm)
1	-1.58	-0.69	1.35	0.25	2.45	0.36
2	-1.20	0.68	2.12	1.26	4.65	1.50
3	0.00	0.86	3.47	2.38	5.35	2.41
4	0.78	1.77	3.88	2.94	6.12	3.10
5	1.47	2.14	6.07	3.60	5.52	3.76

Descriptive statistics for DI for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Err. of Mean	Median	Std. Variation	Kurtosis	Range
<b>Exp.1</b>	-0.21	1.15	0.00	2.57	0.02	-2.14
<b>Exp.2</b>	1.90	0.98	1.71	2.20	-0.69	0.21
<b>Exp.3</b>	6.75	1.63	6.94	3.63	0.64	0.26
<b>Exp.4</b>	4.17	1.20	4.76	2.68	-0.46	-1.13
<b>Exp.5</b>	9.63	1.27	10.70	2.84	-1.53	2.54



Measured height of DI in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 14.3 - Experimental Results for DI with 3 mg/ml SDS in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI and 3 mg/ml SDS solution in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	19.47	20.24	15.71	12.20	13.20	16.16
2	18.78	38.54	24.63	15.12	13.11	22.04
3	18.17	38.78	24.76	15.53	19.03	23.25
4	18.41	41.10	23.54	16.85	25.62	25.10
5	18.41	41.90	22.44	15.53	21.56	23.98

Relative change in the height of DI and 3 mg/ml SDS solution in both cones with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

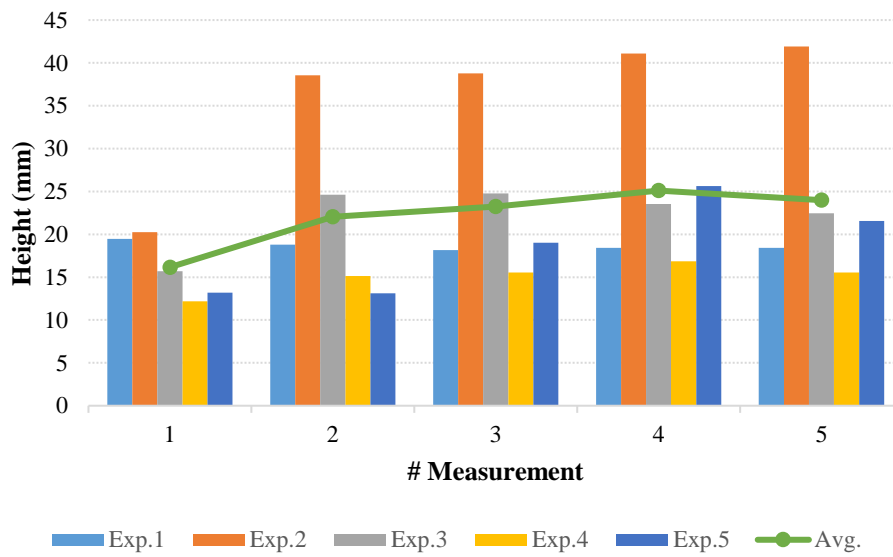
# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (%)
1	-	-	-	-	-	-
2	-3.54	90.42	56.78	23.93	-0.68	33.38
3	-3.25	0.62	0.53	2.71	45.16	9.15
4	1.32	5.98	-4.93	8.50	34.63	9.10
5	0.22	1.95	-4.67	-7.83	-15.85	-5.24

Calculated perpendicular relative height for DI and 3 mg/ml SDS solution ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	16.86	17.53	13.61	10.57	8.20	13.35
2	16.26	33.38	21.33	13.09	23.02	21.42
3	15.74	33.58	21.44	13.45	21.88	21.22
4	15.94	35.59	20.39	14.59	21.43	21.59
5	15.94	36.29	19.43	13.45	19.82	20.99

Descriptive statistics for DI and 3 mg/ml SDS solution for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Err. of Mean	Median	Std. Variation	Kurtosis	Range
<b>Exp.1</b>	18.65	0.23	18.41	0.51	1.33	1.63
<b>Exp.2</b>	36.11	4.02	38.78	8.99	-2.09	4.49
<b>Exp.3</b>	22.22	1.68	23.54	3.76	-1.91	3.75
<b>Exp.4</b>	15.05	0.77	15.53	1.72	-1.39	2.91
<b>Exp.5</b>	21.79	3.14	24.74	7.01	-2.04	4.29



Measured height of DI and 3 mg/ml SDS solution with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)



**APPENDIX 14.4 - Experimental Results for DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	12.56	25.98	27.73	19.76	25.00	22.21
2	8.41	17.07	18.05	19.51	20.85	16.78
3	11.22	15.61	13.05	15.85	19.76	15.10
4	17.44	13.54	17.95	14.51	17.80	16.25
5	17.56	13.29	15.12	14.15	15.00	15.02

Relative change in the height of DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

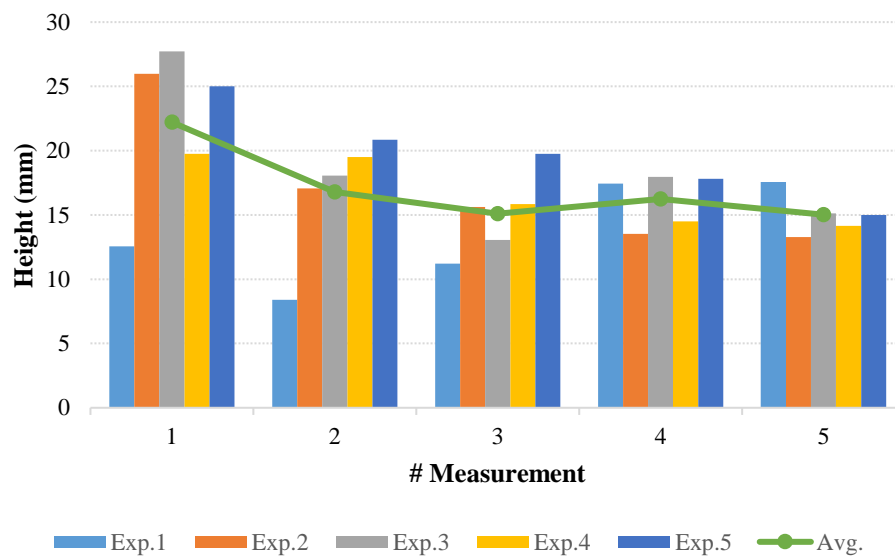
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	-33.01	-34.27	-34.92	-1.23	-16.59	-24.00
3	33.33	-8.57	-27.70	-18.75	-5.26	-5.39
4	55.43	-13.28	37.57	-8.46	-9.88	12.28
5	0.70	-1.80	-15.76	-2.52	-15.75	-7.03

Calculated perpendicular relative height for DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	10.88	22.50	24.01	17.11	21.65	19.23
2	7.28	14.78	15.63	16.90	18.06	14.53
3	9.72	13.52	11.30	13.73	17.11	13.08
4	15.10	11.73	15.55	12.57	15.42	14.07
5	15.21	11.51	13.09	12.25	12.99	13.01

Descriptive statistics for DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	13.44	1.79	12.56	4.00	-0.03	-2.09
<b>Exp.2</b>	17.10	2.33	15.61	5.20	1.77	3.26
<b>Exp.3</b>	18.38	2.52	17.95	5.63	1.47	2.66
<b>Exp.4</b>	16.76	1.21	15.85	2.70	0.38	-3.07
<b>Exp.5</b>	19.68	1.66	19.76	3.71	0.35	0.52



Measured height of DI with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 14.5 - Experimental Results for DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	19.18	10.34	22.50	17.18	19.22	17.68
2	14.74	13.95	17.50	16.24	23.12	17.11
3	17.11	16.80	15.05	12.11	21.33	16.48
4	18.42	16.39	14.69	13.90	18.90	16.46
5	15.56	15.63	11.58	12.56	15.35	14.14

Relative change in the height of DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

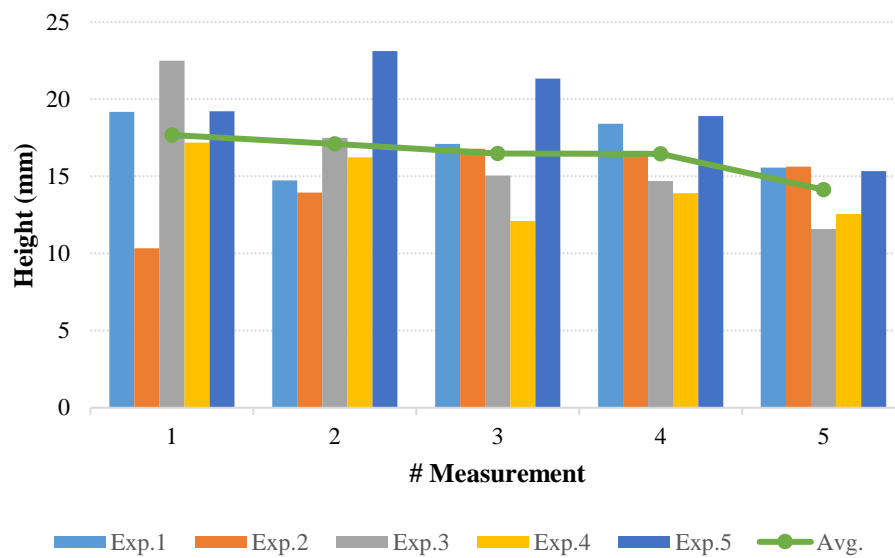
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	-23.18	34.89	-22.22	20.29	-3.26	1.30
3	16.07	20.43	-13.99	-7.74	-3.68	2.22
4	7.69	-2.43	-2.42	-11.39	-0.12	-1.73
5	-15.56	-4.66	-21.16	-18.78	-14.13	-14.86

Calculated perpendicular relative height for DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	9.59	5.17	11.25	8.59	9.61	8.84
2	7.37	6.98	8.75	8.12	11.56	8.56
3	8.56	8.40	7.53	6.06	10.67	8.24
4	9.21	8.20	7.35	6.95	9.45	8.23
5	7.78	7.82	5.79	6.28	7.68	7.07

Descriptive statistics for DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	17.00	0.84	17.11	1.87	-0.09	-2.15
<b>Exp.2</b>	14.62	1.18	15.63	2.63	-1.42	1.66
<b>Exp.3</b>	16.26	1.82	15.05	4.07	0.84	1.12
<b>Exp.4</b>	14.40	1.00	13.90	2.24	0.35	-2.48
<b>Exp.5</b>	19.58	1.31	19.22	2.92	-0.45	0.39



Measured height of DI with 3 ml/mg SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 14.6 - Experimental Results for DI with 3 mg/ml SDS in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of DI with 3 mg/ml SDS and 1 mg/ml Ag nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	16.43	14.63	1.59	-5.00	-5.00	4.53
2	17.14	13.66	34.26	22.68	22.68	22.08
3	12.16	16.46	39.27	10.85	10.85	17.92
4	17.79	16.71	35.24	16.34	16.34	20.48
5	15.17	17.20	34.39	28.78	28.78	24.86

Relative change in the height of DI with 3 mg/ml SDS and 1 mg/ml Ag nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

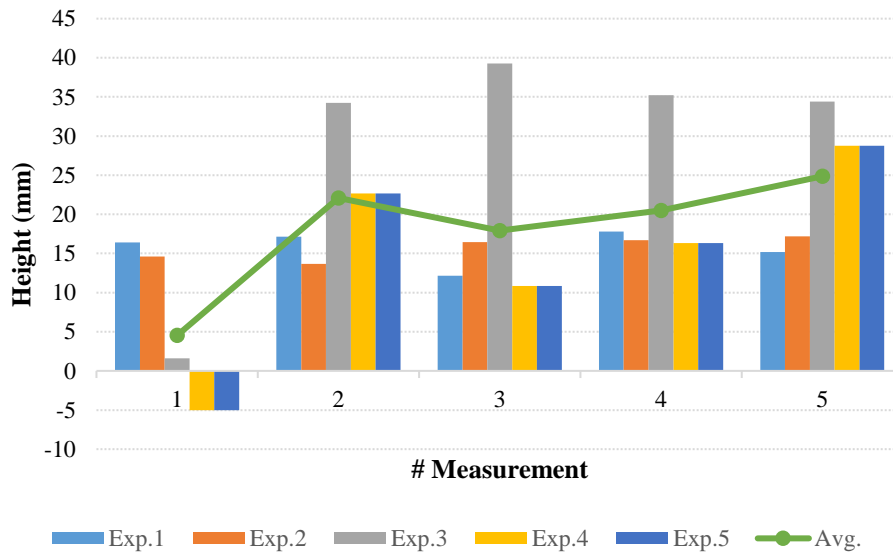
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	4.35	4.35	4.35	4.35	4.35	4.35
3	-29.05	-29.05	-29.05	-29.05	-29.05	-29.05
4	46.29	46.29	46.29	46.29	46.29	46.29
5	-14.75	-14.75	-14.75	-14.75	-14.75	-14.75

Calculated perpendicular relative height for DI with 3 mg/ml SDS and 1 mg/ml Ag nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	14.23	12.67	1.38	-4.33	10.93	6.98
2	14.84	11.83	29.67	19.64	13.84	17.96
3	10.53	14.25	34.01	9.40	14.37	16.51
4	15.41	14.47	30.52	14.15	14.58	17.83
5	13.14	14.90	29.78	24.92	14.63	19.47

Descriptive statistics for DI with 3 mg/ml SDS and 1 mg/ml Ag nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	18.65	0.23	18.41	0.51	1.33	1.63
<b>Exp.2</b>	36.11	4.02	38.78	8.99	-2.09	4.49
<b>Exp.3</b>	22.22	1.68	23.54	3.76	-1.91	3.75
<b>Exp.4</b>	15.05	0.77	15.53	1.72	-1.39	2.91
<b>Exp.5</b>	21.79	3.14	24.74	7.01	-2.04	4.29



Measured height of DI with 3 mg/ml SDS and 1 mg/ml Ag nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 15 - Experimental Results for Methanol from Hacettepe University  
Environmental Engineering Research Laboratory**

**APPENDIX 15.1 - Experimental Results for Methanol with 3 mg/ml SDS in V-  
Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	9.02	7.56	9.02	9.02	9.75	8.87
2	11.46	9.27	12.44	13.90	10.24	11.46
3	14.15	13.29	13.90	10.98	12.62	12.99
4	17.32	15.37	14.39	9.76	15.12	14.39
5	16.10	17.07	15.08	9.02	16.31	14.72

Relative change in the height methanol with 3 mg/ml SDS with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

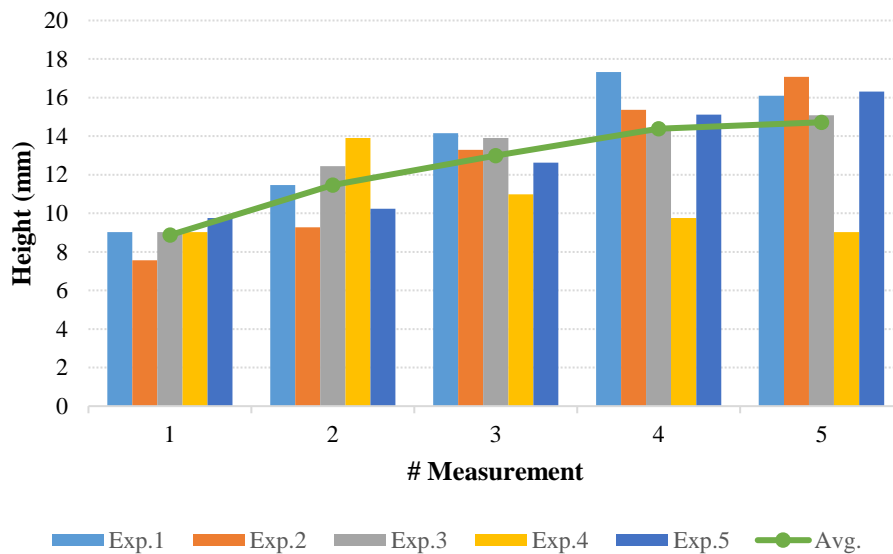
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	27.03	22.58	37.84	54.05	5.03	29.31
3	23.40	43.42	11.76	-21.05	23.19	16.14
4	22.41	15.60	3.51	-11.11	19.84	10.05
5	-7.04	11.11	4.78	-7.50	7.89	1.85

Calculated perpendicular relative height for methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	7.81	6.55	7.81	7.81	8.44	7.68
2	9.92	8.03	10.77	12.04	8.87	9.93
3	12.25	11.51	12.04	9.51	10.93	11.25
4	15.00	13.31	12.46	8.45	13.09	12.46
5	13.94	14.78	13.06	7.81	14.12	12.74

Descriptive statistics for methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	13.61	1.52	14.15	3.39	-0.43	-1.43
<b>Exp.2</b>	12.51	1.80	13.29	4.02	-0.24	-2.20
<b>Exp.3</b>	12.97	1.08	13.90	2.41	-1.44	1.92
<b>Exp.4</b>	10.54	0.91	9.76	2.04	1.50	1.96
<b>Exp.5</b>	12.81	1.30	12.62	2.90	0.17	-2.51



Measured height of methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)



**APPENDIX 15.2 - Experimental Results for Methanol with 3 mg/ml SDS in V-Shaped Pasteur Pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)**

Measured height of methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	5.12	7.32	5.85	6.83	6.20	6.26
2	7.44	7.07	6.59	8.66	8.66	7.68
3	10.49	10.37	11.46	13.17	12.68	11.63
4	13.05	13.29	13.29	14.27	13.54	13.49
5	15.61	13.90	15.61	15.00	15.73	15.17

Relative change in the height methanol with 3 mg/ml SDS with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	45.24	-3.33	12.50	26.78	39.77	24.19
3	40.98	46.55	74.07	52.11	46.48	52.04
4	24.42	28.23	15.96	8.33	6.73	16.73
5	19.63	4.59	17.43	5.13	16.22	12.60

Calculated perpendicular relative height for methanol with 3 mg/ml SDS for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	2.56	3.66	2.93	3.42	3.10	3.13
2	3.72	3.54	3.30	4.33	4.33	3.84
3	5.25	5.19	5.73	6.59	6.34	5.82
4	6.53	6.65	6.65	7.14	6.77	6.75
5	7.81	6.95	7.81	7.50	7.87	7.59

**APPENDIX 15.3 - Experimental Results for Methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	7.62	8.00	8.60	13.59	11.35	9.83
2	1.33	11.20	11.76	14.00	16.00	10.86
3	2.11	15.56	16.00	12.50	18.33	12.90
4	-2.16	12.89	18.61	11.30	20.29	12.19
5	-2.17	15.95	19.50	11.47	20.00	12.95

Relative change in the height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

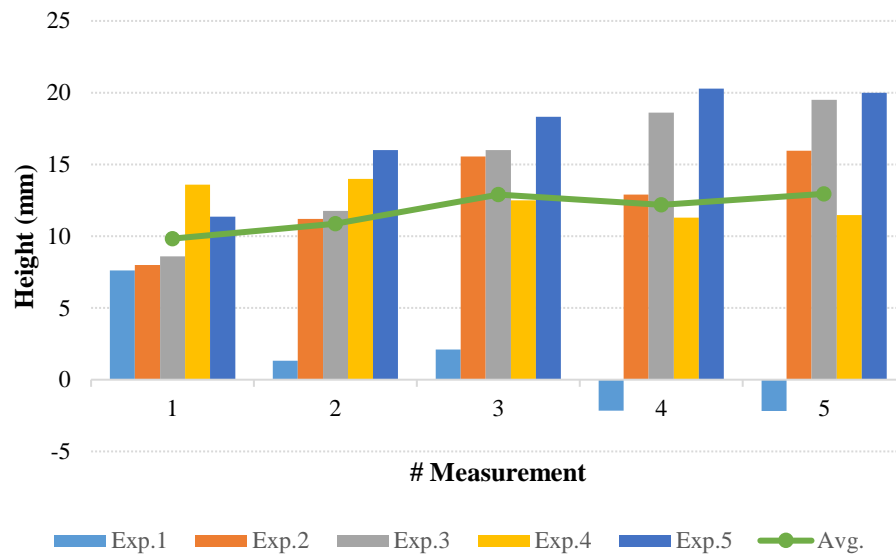
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	-82.50	40.00	36.71	3.00	40.95	7.63
3	57.90	38.89	36.09	-10.71	14.58	27.35
4	-202.70	-17.11	16.32	-9.57	10.65	-40.48
5	0.54	23.66	4.78	1.47	-1.41	5.81

Calculated perpendicular relative height for methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	6.60	6.93	7.45	11.77	9.83	8.52
2	1.15	9.70	10.18	12.12	13.86	9.40
3	1.83	13.48	13.86	10.83	15.87	11.17
4	-1.87	11.16	16.12	9.79	17.57	10.55
5	-1.88	13.81	16.89	9.93	17.32	11.21

Descriptive statistics for methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	1.35	1.80	1.33	4.02	1.03	0.88
<b>Exp.2</b>	12.72	1.47	12.89	3.28	-0.61	-0.73
<b>Exp.3</b>	14.89	2.07	16.00	4.63	-0.55	-1.71
<b>Exp.4</b>	12.57	0.54	12.50	1.22	0.13	-2.67
<b>Exp.5</b>	17.19	1.65	18.33	3.69	-1.23	0.97



Measured height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 15.4 - Experimental Results for Methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> in V-Shaped Pasteur Pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)**

Measured height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	5.24	6.22	4.63	5.24	5.00	5.27
2	9.76	9.02	7.44	7.80	7.56	8.32
3	10.24	10.24	9.76	9.88	11.71	10.37
4	12.32	13.17	12.68	11.95	13.05	12.63
5	12.80	15.37	14.76	13.90	15.00	14.37

Relative change in the height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

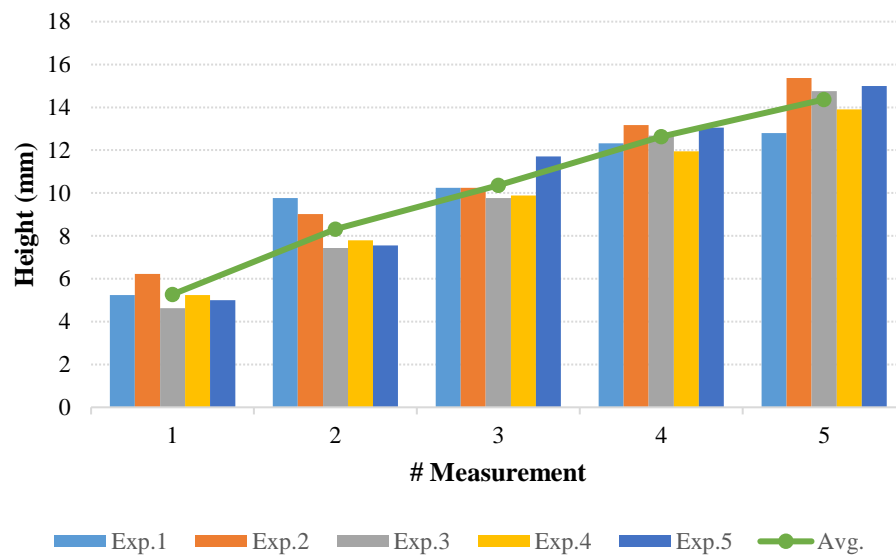
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	86.05	45.10	60.53	48.84	51.22	86.05
3	5.00	13.51	31.15	26.56	54.84	5.00
4	20.24	28.57	30.00	20.99	11.46	20.24
5	3.96	16.67	16.35	16.33	14.95	3.96

Calculated perpendicular relative height for methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	2.62	3.11	2.32	2.62	2.50	2.63
2	4.88	4.51	3.72	3.90	3.78	4.16
3	5.12	5.12	4.88	4.94	5.86	5.18
4	6.16	6.59	6.34	5.98	6.53	6.32
5	6.40	7.69	7.38	6.95	7.50	7.18

Descriptive statistics for methanol with 3 mg/ml SDS and 1 mg/ml nanoparticles Fe<sub>2</sub>O<sub>3</sub> for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	10.07	1.34	10.24	3.00	-1.25	1.68
<b>Exp.2</b>	10.80	1.60	10.24	3.57	0.06	-0.93
<b>Exp.3</b>	9.85	1.81	9.76	4.04	-0.10	-1.31
<b>Exp.4</b>	9.75	1.52	9.88	3.40	-0.19	-0.99
<b>Exp.5</b>	10.46	1.83	11.71	4.10	-0.46	-1.64



Measured height of methanol with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 16 - Experimental Results for Cement Factory Wastewater Treatment Plant from Hacettepe University Environmental Engineering Research Laboratory**

**APPENDIX 16.1 - Experimental Results for Cement Factory Wastewater Treatment Plant Input with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60s$ )**

Measured height for cement factory wastewater treatment plant input with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60 s$ )

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Avg. (mm)
1	4.67	20.00	5.14	9.94
2	-1.89	12.90	6.67	5.89
3	-7.00	6.76	4.55	1.44
4	-11.39	6.89	7.16	0.89
5	-15.26	4.00	11.25	0.00

Relative change in the height of cement factory wastewater treatment plant input with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60 s$ )

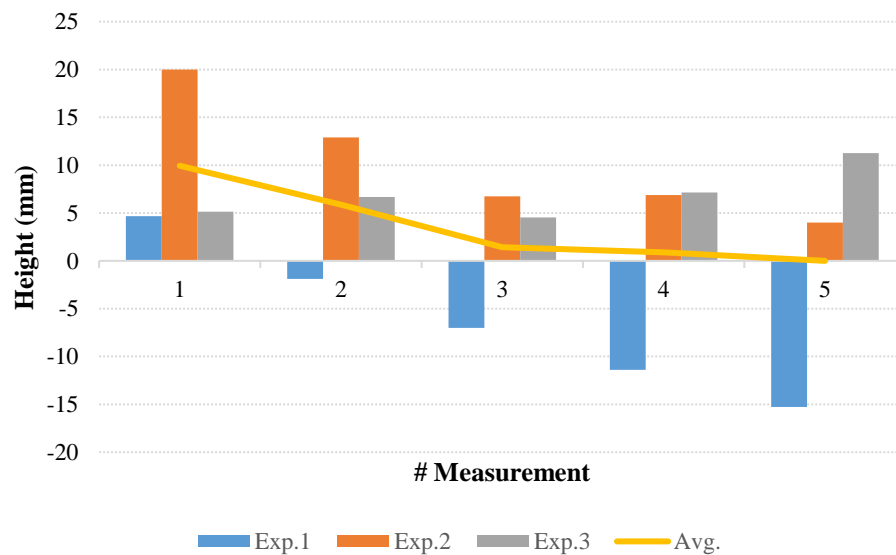
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Avg. (%)
1	-	-	-	-
2	4.67	20.00	5.14	-48.73
3	-1.89	12.90	6.67	63.66
4	-7.00	6.76	4.55	40.67
5	-11.39	6.89	7.16	16.39

Calculated perpendicular relative height for cement factory wastewater treatment plant input with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Avg. (mm)
1	2.34	10.00	2.57	4.97
2	0.95	6.45	3.34	3.58
3	3.50	3.38	2.28	3.05
4	5.70	3.45	3.58	4.24
5	7.63	2.00	5.63	5.09

Descriptive statistics for cement factory wastewater treatment plant input with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	-61.74	350.99	-70.00	784.84	0.40	-.84
<b>Exp.2</b>	101.10	286.81	68.90	641.33	1.09	0.32
<b>Exp.3</b>	69.54	117.58	66.70	262.91	1.36	2.07



**APPENDIX 16.2 - Experimental Results for Cement Factory Wastewater Treatment Plant Input with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height for cement factory wastewater treatment plant input with 3 mg/ml SDS and 1 mg/ml nanoparticles Fe<sub>2</sub>O<sub>3</sub> for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	4.21	9.47	11.76	7.22	8.92	8.32
2	8.65	12.84	10.95	9.79	12.03	10.85
3	9.46	12.25	9.52	10.00	12.70	10.79
4	8.61	12.50	9.00	12.22	12.89	11.04
5	10.81	12.22	8.59	11.35	13.06	11.21

Relative change in the height of cement factory wastewater treatment plant input with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	105.41	35.51	-6.84	35.59	34.85	40.90
3	9.38	-4.58	-13.04	2.12	5.62	-0.10
4	-8.97	2.04	-5.50	22.22	1.47	2.25
5	25.54	-2.22	-100.00	-7.12	1.29	-16.50

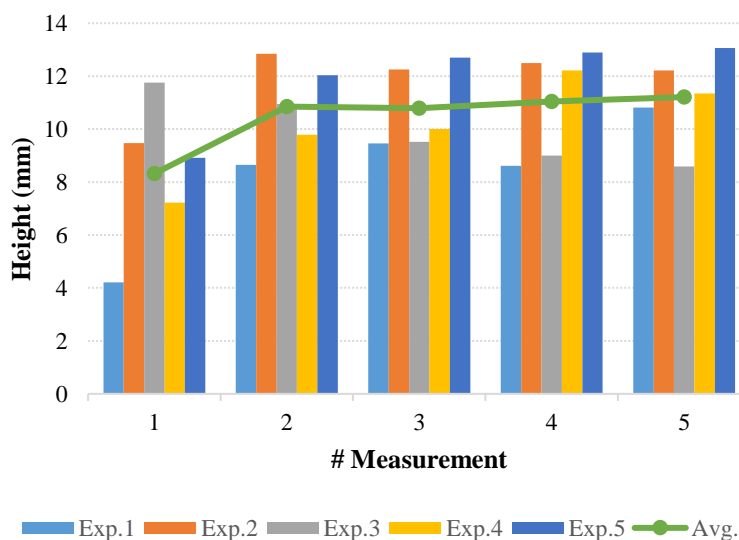


Calculated perpendicular relative height for cement factory wastewater treatment plant input with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	3.65	8.20	10.18	6.25	7.72	7.20
2	7.49	11.12	9.48	8.48	10.42	9.40
3	8.19	10.61	8.24	8.66	11.00	9.34
4	7.46	10.83	7.79	10.58	11.16	9.56
5	9.36	10.58	7.44	9.83	11.31	9.70

Descriptive statistics for cement factory wastewater treatment plant input 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	83.48	110.86	86.50	247.896	-1.49	2.97
<b>Exp.2</b>	118.56	0.61	122.50	135.681	-2.04	4.38
<b>Exp.3</b>	103.08	0.64	102.35	127.178	0.20	-3.34
<b>Exp.4</b>	101.16	0.85	100.00	190.106	-0.80	0.83
<b>Exp.5</b>	119.20	0.08	127.00	172.199	-1.97	3.93



Measured height for cement factory wastewater treatment plant input with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 16.3 - Experimental Results for Cement Factory Wastewater Treatment Plant Output with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height for cement factory wastewater treatment plant output with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	9.72	7.57	4.47	6.58	4.51	6.57
2	10.00	2.41	1.03	-3.00	6.08	3.30
3	9.72	-4.47	-7.88	-8.91	2.89	-1.73
4	8.33	-10.30	-11.06	-13.00	9.25	-3.36
5	7.23	-13.79	-10.43	-17.00	4.50	-5.90

Relative change in the height of cement factory wastewater treatment plant output with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

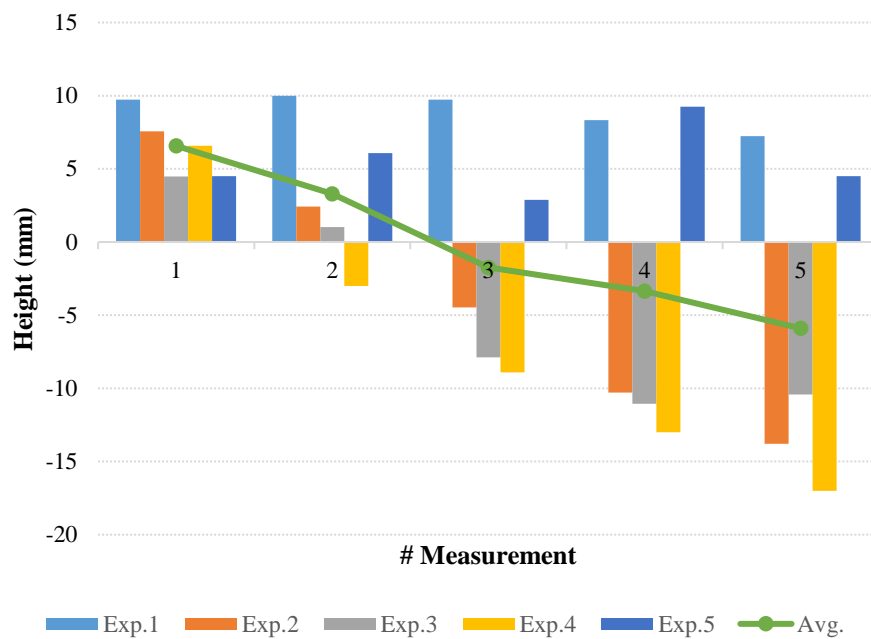
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	2.86	-68.10	-76.88	-145.60	34.84	-50.58
3	-2.78	-285.32	-861.60	197.00	-52.40	-201.02
4	-14.28	130.30	40.38	45.90	219.55	84.37
5	-13.24	33.82	-5.66	30.77	-51.35	-1.13

Calculated perpendicular relative height for cement factory wastewater treatment plant output with 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	4.86	3.79	2.24	3.29	2.26	3.29
2	5.00	1.21	0.52	1.50	3.04	2.25
3	4.86	2.24	3.94	4.46	1.45	3.39
4	4.17	5.15	5.53	6.50	4.63	5.19
5	3.62	6.90	5.22	8.50	2.25	5.30

Descriptive statistics for cement factory wastewater treatment plant output with 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	9.00	0.53	9.72	1.19	-1.03	-0.68
<b>Exp.2</b>	-3.72	3.94	-4.47	8.81	0.22	-1.81
<b>Exp.3</b>	-4.77	3.16	-7.88	7.08	0.62	-2.46
<b>Exp.4</b>	-7.07	4.12	-8.91	9.22	0.75	-0.05
<b>Exp.5</b>	5.45	1.08	4.51	2.41	1.10	1.45



Measured height for cement factory wastewater treatment plant output with 1 mg/ml  $\text{Fe}_2\text{O}_3$  nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 16.4 - Experimental Results for Cement Factory Wastewater Treatment Plant Output with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles in V-Shaped Pasteur Pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height for cement factory wastewater treatment plant output 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	3.75	7.21	5.56	9.35	8.95	6.96
2	10.00	10.00	8.06	12.84	-3.68	7.44
3	14.00	12.67	11.32	10.91	7.86	11.35
4	13.33	11.84	11.32	12.57	10.79	11.97
5	14.00	15.72	13.23	13.44	12.89	13.86

Relative change in the height of cement factory wastewater treatment plant output 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

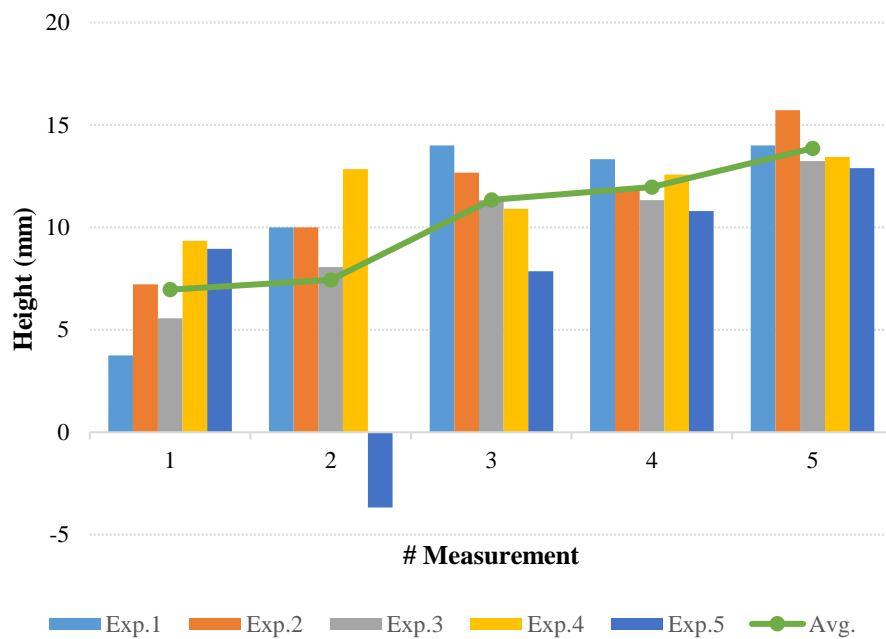
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	166.92	38.69	45.00	37.33	-141.18	29.35
3	40.00	26.67	40.47	-15.02	-313.26	-44.23
4	-4.76	-6.51	0.00	15.20	37.32	8.25
5	5.00	32.75	16.92	6.98	19.47	16.22

Calculated perpendicular relative height for cement factory wastewater treatment plant output with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	3.25	6.24	4.82	8.10	7.75	6.03
2	8.66	8.66	6.98	11.12	-3.19	6.45
3	12.12	10.97	9.80	9.45	6.81	9.83
4	11.54	10.25	9.80	10.89	9.34	10.36
5	12.12	13.61	11.46	11.64	11.16	12.00

Descriptive statistics for cement factory wastewater treatment plant output with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	11.02	1.96	13.33	4.39	-1.57	2.04
<b>Exp.2</b>	11.49	1.41	11.84	3.16	-0.05	0.30
<b>Exp.3</b>	9.90	1.37	11.32	3.06	-0.66	-0.87
<b>Exp.4</b>	11.82	0.75	12.57	1.67	-0.91	-0.56
<b>Exp.5</b>	7.36	2.89	8.95	6.46	-1.75	3.43



Measured height for cement factory wastewater treatment plant output with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 17 - Experimental Results for Eymir Lake Water from Hacettepe University Environmental Engineering Research Laboratory**

**APPENDIX 17.1 - Experimental Results for Eymir Lake with 3 mg/ml SDS ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of Eymir lake water with 3 mg/ml SDS in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

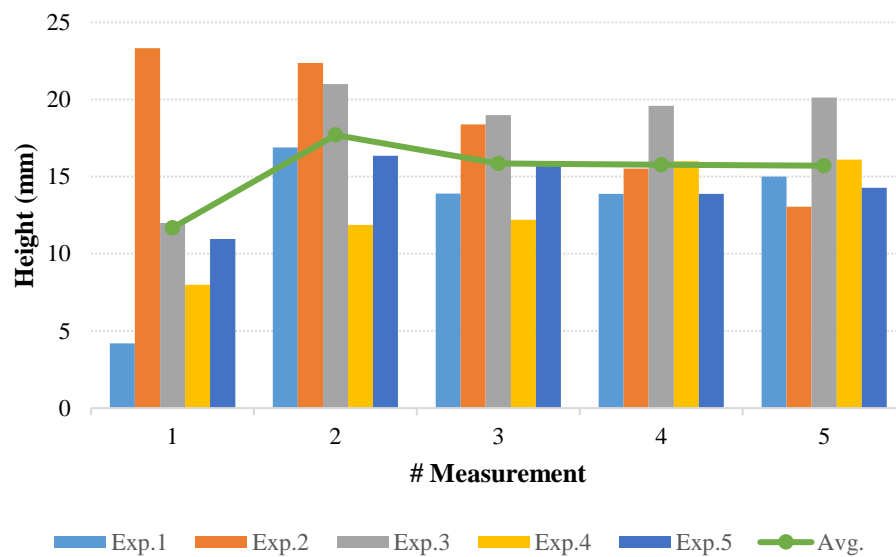
# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	4.19	23.33	12.00	8.00	10.95	11.69
2	16.90	22.38	21.00	11.88	16.35	17.70
3	13.91	18.38	19.00	12.20	15.83	15.86
4	13.89	15.53	19.60	16.00	13.89	15.78
5	15.00	13.06	20.14	16.11	14.29	15.72

Relative change in the height of Eymir lake water with 3 mg/ml SDS with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	303.34	-4.07	75.00	48.52	49.30	94.42
3	-17.69	-17.90	-9.52	2.68	-3.17	-9.12
4	-0.14	-15.52	3.16	31.15	-12.28	1.27
5	7.99	-15.91	2.77	0.69	2.86	-0.32

Descriptive statistics for Eymir lake water with 3 mg/ml SDS ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	12.78	2.22	13.91	4.95	-1.88	3.94
<b>Exp.2</b>	18.54	1.96	18.38	4.38	-0.12	-2.14
<b>Exp.3</b>	18.35	1.62	19.60	3.62	-2.01	4.22
<b>Exp.4</b>	12.84	1.51	12.20	3.37	-0.52	-0.60
<b>Exp.5</b>	14.26	0.95	14.29	2.12	-1.03	1.05



Measured height of Eymir lake water with 3 mg/ml SDS in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 17.2 - Experimental Results for Eymir Lake with 3 mg/ml SDS ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)**

Measured height of Eymir lake water with 3 mg/ml SDS in V-Shaped Pasteur Pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	2.24	0.81	1.52	0.89	2.22	1.54
2	2.00	1.44	2.89	4.43	4.50	3.05
3	2.63	2.86	2.63	4.41	5.44	3.59
4	4.10	2.50	3.10	5.29	5.95	4.19
5	4.90	2.38	3.00	5.48	6.39	4.43

Relative change in the height of Eymir lake water with 3 mg/ml SDS with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	66.66	77.47	91.04	398.21	102.50	147.18
3	31.25	98.56	-9.09	-0.38	20.99	28.27
4	2.95	-12.50	17.62	20.00	9.33	7.48
5	20.76	-4.76	-3.08	3.44	7.33	4.74

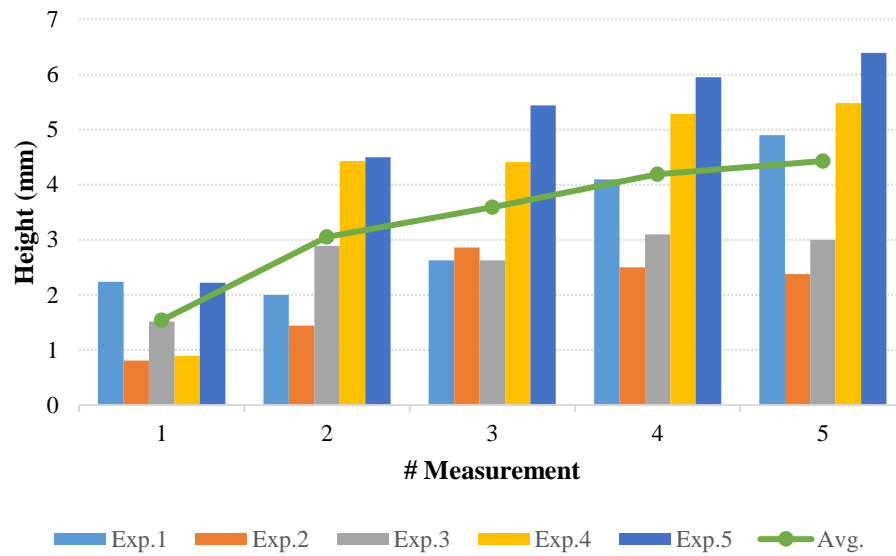
Calculated perpendicular relative height for of Eymir lake water with 3 mg/ml SDS ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	1.12	0.41	0.76	0.45	1.11	0.77
2	1.00	0.72	1.45	2.22	2.25	1.53
3	1.32	1.43	1.32	2.21	2.72	1.80
4	2.05	1.25	1.55	2.65	2.98	2.10
5	2.45	1.19	1.50	2.74	3.20	2.22



Descriptive statistics for Eymir lake water with 3 mg/ml SDS ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	2.24	0.34	2.50	0.75	-0.67	0.14
<b>Exp.2</b>	2.00	0.38	2.38	0.85	-0.71	-1.35
<b>Exp.3</b>	2.63	0.29	2.89	0.64	-1.85	3.51
<b>Exp.4</b>	4.10	0.83	4.43	1.86	-1.86	3.69
<b>Exp.5</b>	4.90	0.74	5.44	1.66	-1.35	1.64



Measured height of Eymir lake water with 3 mg/ml SDS in V-Shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 17.3 - Experimental Results for Eymir Lake Water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)**

Measured height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	6.03	7.78	4.47	14.52	4.44	7.45
2	11.90	12.78	10.22	14.74	11.11	12.15
3	12.62	12.11	10.00	15.78	11.33	12.37
4	14.72	14.29	13.00	14.50	15.00	14.30
5	12.78	15.00	12.63	12.57	14.29	13.45

Relative change in the height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

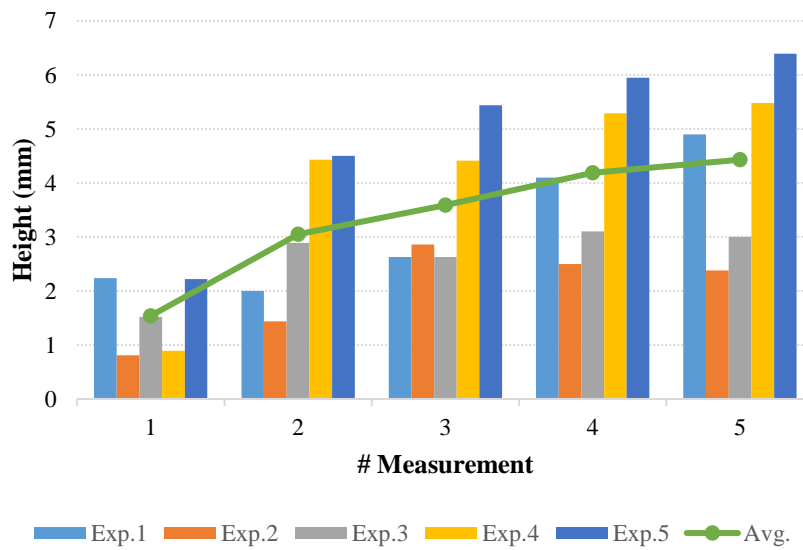
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	97.57	64.29	128.50	1.47	150.02	88.37
3	6.00	-5.26	-2.17	7.06	2.00	1.53
4	16.67	18.01	30.00	-8.10	32.35	17.79
5	-13.20	5.00	-2.83	-13.33	-4.76	-5.82

Calculated perpendicular relative height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	5.22	6.74	3.87	12.57	3.85	6.45
2	10.31	11.07	8.85	12.77	9.62	10.52
3	10.93	10.49	8.66	13.67	9.81	10.71
4	12.75	12.38	11.26	12.56	12.99	12.39
5	11.07	12.99	10.94	10.89	12.38	11.65

Descriptive statistics for Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	11.61	1.47	12.62	3.29	-1.65	3.38
<b>Exp.2</b>	12.39	1.26	12.78	2.82	-1.36	2.05
<b>Exp.3</b>	10.06	1.53	10.22	3.41	-1.40	2.13
<b>Exp.4</b>	14.42	0.52	14.52	1.16	-1.02	2.44
<b>Exp.5</b>	11.23	1.87	11.33	4.17	-1.33	1.96



Measured height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 30^\circ$ ,  $\Delta t = 60$  s)

**APPENDIX 17.4 - Experimental Results for Eymir Lake Water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> Nanoparticles Results for ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)**

Measured height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	5.79	0.79	3.71	4.22	6.02	4.11
2	6.29	2.63	6.65	4.90	6.32	5.36
3	6.84	4.35	7.25	5.77	7.10	6.26
4	7.50	5.00	7.43	6.10	7.48	6.70
5	7.80	5.29	8.06	7.32	7.98	7.29

Relative change in the height of Eymir lake water 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles with respect to ground for V-shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

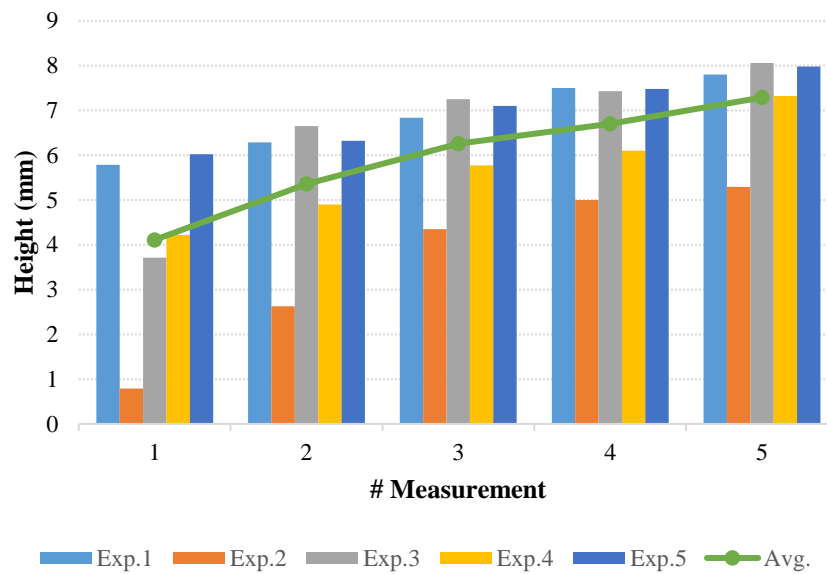
# Measurement	Exp.1 (%)	Exp.2 (%)	Exp.3 (%)	Exp.4 (%)	Exp.5 (%)	Avg. (%)
1	-	-	-	-	-	-
2	8.57	233.32	79.14	16.11	4.98	68.42
3	8.85	65.22	8.96	17.76	12.34	22.63
4	9.62	15.00	2.52	5.72	5.34	7.64
5	4.00	5.88	8.06	9.06	10.06	7.41

Calculated perpendicular relative height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

# Measurement	Exp.1 (mm)	Exp.2 (mm)	Exp.3 (mm)	Exp.4 (mm)	Exp.5 (mm)	Avg. (mm)
1	2.90	0.40	1.86	2.11	3.01	2.06
2	3.15	1.32	3.33	2.45	3.16	2.68
3	3.42	2.18	3.63	2.89	3.55	3.13
4	3.75	2.50	3.72	3.05	3.74	3.35
5	3.90	2.65	4.03	3.66	3.99	3.65

Descriptive statistics for Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

	Mean	Std. Error of Mean	Median	Std. Deviation	Skewness	Kurtosis
<b>Exp.1</b>	6.84	0.37	6.84	0.83	-0.13	-1.84
<b>Exp.2</b>	3.61	0.84	4.35	1.89	-0.97	-0.45
<b>Exp.3</b>	6.62	0.76	7.25	1.70	-1.76	3.39
<b>Exp.4</b>	5.66	0.53	5.77	1.18	0.30	-0.22
<b>Exp.5</b>	6.98	0.36	7.10	0.81	-0.04	-1.88



Measured height of Eymir lake water with 3 mg/ml SDS and 1 mg/ml Fe<sub>2</sub>O<sub>3</sub> nanoparticles in V-Shaped Pasteur pipette ( $\alpha = 60^\circ$ ,  $\Delta t = 60$  s)

## APPENDIX 18 - SQL Script Generated by MATLAB

Selected part of the automatically created structured query language (SQL) [443] script by MATLAB [283] represented below,

```
INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',1,121,'0000001.png',288,512,
    '2018.06.18-11:00:46',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',2,121,'0000002.png',288,512,
    '2018.06.18-11:00:46',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',3,121,'0000003.png',288,512,
    '2018.06.18-11:00:46',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',4,121,'0000004.png',288,512,
    '2018.06.18-11:00:46',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',5,121,'0000005.png',288,512,
    '2018.06.18-11:00:47',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',6,121,'0000006.png',288,512,
    '2018.06.18-11:00:47',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',7,121,'0000007.png',288,512,
    '2018.06.18-11:00:47',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',8,121,'0000008.png',288,512,
    '2018.06.18-11:00:48',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');

INSERT INTO phddb.extractavi
  VALUES(NULL,1,'2018.06.18',9,121,'0000009.png',288,512,
    '2018.06.18-11:00:48',user1,
    'WIN32','SERVER01','127.0.0.1','8.5.0.197613 (R2015a)');
```

## **APPENDIX 19 - Computer Configurations**

### **APPENDIX 19.1 - Hardware Configuration for the Computers with Windows OS**

- Intel Core i7 4785T @ 2.20 GHz CPU, 4 cores, 8 logical processors
- Intel HD Graphics 4600 GPU, Haswell GT2, 1 GB
- 16 GB SDRAM Dual-Channel DDR3 @ 798 MHz
- Toshiba MQ01ABD100 ATA Device (SATA), 1 TB
- Fujitsu D3334-A1 motherboard and Intel Q87 (Lynx Point) chipset

### **APPENDIX 19.2 - Software Configuration for the Computers with Windows OS**

- Arduino IDE 1.6.12
- Auto Screen Capture 2016
- Filezilla 3.22.2.2
- Glogg 0.9.2.1
- HeidiSQL 9.4
- HWiNFO64 5.42-3050
- IBM SPSS 21.0.0.0
- Macrium Reflect Free 6.2.1549
- MATLAB R2013a with the following toolboxes,
  - Image Acquisition Toolbox 4.5
  - Image Processing Toolbox 8.2
  - Neural Network Toolbox 8.0.1
  - Statistics Toolbox 8.2
- Microsoft Visio Professional 2013
- Microsoft Visual Studio Ultimate 2013
- Microsoft Windows 10 Enterprise version 1803 (64 bit)
- MySQL
  - Community Server 5.7.16
  - Utilities 1.6.4
  - Workbench 6.3.8
- NetLogo 5.3.1 (64 bit)





### **APPENDIX 19.3 - Hardware Configuration for the Computers with Linux OS**

- Intel Xeon @ 2.10 GHz CPU, 8 cores, 16 logical processors
- 16 GB SDRAM Dual-Channel DDR4 @ 1200 MHz
- Toshiba MQ01ABD100 ATA Device (SATA), 300 GB, RAID 1
- Fujitsu D3334-A1 motherboard and Intel Q87 (Lynx Point) chipset

### **APPENDIX 19.4 - Software Configuration for the Computers with Linux OS**

- Ubuntu 16.04.2 LTS (64 bit)
- NetLogo 5.3.1 (64 bit)

## APPENDIX 20 - Descriptive Statistics for Agent-Based Model

### APPENDIX 20.1 - Descriptive Statistics of Nanoparticles at the Interface

Test	Min.	Max.	Mean	Std. Error	Std. Deviation	Skewness	Kurtosis
Test 1	41	1443	1356	2.55	254.59	-3.37	10.48
Test 2	57	1448	1368	2.52	251.54	-3.47	11.14
Test 3	58	1382	1295	2.38	238.43	-3.41	10.83
Test 4	52	1417	1329	2.42	241.91	-3.46	11.13
Test 5	61	1399	1306	2.44	243.80	-3.36	10.42
<b>Avg.</b>	<b>54</b>	<b>1418</b>	<b>1331</b>	<b>2.46</b>	<b>245.96</b>	<b>-3.42</b>	<b>10.81</b>

### APPENDIX 20.2 - Descriptive Statistics of Time to Reach to the Interface

Test	Min.	Max.	Mean	Std. Error	Std. Deviation	Skewness	Kurtosis
Test 1	1.95	2528.01	1164.55	7.32	732.43	0.17	-1.17
Test 2	0.99	2198.21	975.39	6.41	641.11	0.23	-1.15
Test 3	0.75	2336.68	1107.87	7.18	717.55	0.13	-1.29
Test 4	1.24	2052.86	818.42	5.70	570.22	0.38	-0.94
Test 5	1.16	1349.65	600.89	3.61	360.51	0.33	-0.88
<b>Avg.</b>	<b>1.22</b>	<b>2093.08</b>	<b>933.43</b>	<b>6.04</b>	<b>603.62</b>	<b>0.22</b>	<b>-1.13</b>