Adsorption of Non-Ionic Surfactants on Organoclays in Drilling Fluid Investigated by Markov Chain Monte Carlo (MCMC) based Random Walk

By

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DECLARATION OF ORIGINALITY AND EXCLUSIVENESS

I hereby declare that the contents of this report are based on my original work except for only quotations and citations which I have acknowledged. I also declare that it has not been previously taken or concurrently submitted for any other degree at UCSI or other institutions.

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Date: 30th JULY 2021

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TABLE OF CONTENTS

		PAGE
ACKNOWLEDGEMENT		ii
DECLARATION OF ORIGINALITY AND EXCLUSIVENESS		iii
LIST OF FIGURES		vi
LIST OF TABLES		vi
CHAPTER I		1
INTRODUCTION		1
1.1	BACKGROUND	1
1.2	OBJECTIVES	3
1.3	PROBLEM STATEMENT	3
1.4	SCOPE OF STUDY	4
1.5	SIGNIFICANCE OF STUDY	4
CHAPTER II		5
LITERATURE REVIEW		5
2.1	INTRODUCTION	5
2.2	ADSORPTION	7
2.3	MEASUREMENT OF SURFACE-ACTIVE PROPERTIES OF NON-IONIC	8
2.4	MONTE CARLO SIMULATIONS OF THE ADSORPTION	9
2.5	SURFACE INHIBITIVE QUALITIES	10
2.6	LIQUID MISFORTUNE INHIBITIVE ATTRIBUTES	11
2.7	SEDIMENTATION SCATTERING INHIBITIVE ATTRIBUTES	13
2.8	SURFACTANT	15
2.9	TYPES OF SURFACTANTS	16
2.9.1	ANIONIC SURFACTANTS	17

2.9.2 NON-IONIC SURFACTANTS 17

2.10 USE OF CLAY 17

2.11 SUMMERY OF THE FOLLOWING RESEARCHERS/INVESTIGATOR 18

2.11.1 The investigation discovered the following 18

CHAPTER III 20

METHODOLOGY 20

3.1 OVERVIEW OF METHODOLOGY 20

3.2 RESEARCH FLOWCHART 21

3.3 MATLAB 22

3.4 MARKOV CHAIN MONTE CARLO (MCMC) 24

REFERENCES 26

LIST OF FIGURES

FIGURE		Page
2.6.1	Fluid Loss of CO and DEIONISED Water (Bol G.M.,1994)	11
2.6.2	Segmentation Test Analysis of CO/KCL(Cheatham J.B.1984)	13
2.7	Scattering Inhibitive Attributes (Friedheim J.,2011) graph of adsorption amount vs equilibrium concentration (Fritz Steven J.2014)	14
2.8	graph of adsorption amount vs equilibrium concentration (Fritz Steven J.2014)	16
3.2	Flowchart of the methodology	21

LIST OF TABLES

Table No.		
Table 3.2	shows a summary of the MATLAB in built functions that can be used in MCMC	23

LIST OF EQUATIONS

Equation No.		Page
1.0	$CO\ adsorption, D = \frac{m_t\ x\ (c_b - c_e)}{m_s} \times\ 10^{-3}\ \ (\mathrm{mg/g - shale\ powder})$	9
2.0	$AF = min\left[1, \frac{\pi(P^*\|Y)p\left(P^{(t-1)}\|P^*\right)}{\pi\left(P^{(t-1)}\|Y\right)p\left(P^*\|P^{(t-1)}\right)}\right]$	25

CHAPTER I

INTRODUCTION

1.1 BACKGROUND

Organoclays are hydrophobic materials made by incorporating organic compounds into clays and clay minerals. To improve the viscosity of synthetic-based muds, organoclays are routinely used as rheological additives in drilling fluids (SBM). Interfacial and interparticle interactions contribute to the viscosity of organoclays particles. As a result of contamination with specific cations such as calcium or a low pH state during wellbore drilling, clay layers interact and produce a flocculated structure, resulting in high rheological qualities and a large volume of fluid loss. In these cases, chemical thinners are used to neutralise the positive charge on the clay layers' edges and prevent particle flocculation. (Kania et al. 2021)

Drilling fluids are classified as either water-based mud or oil-based mud based on their primary materials. Water-based drilling fluid is the most common drilling mud in the oil industry because it is less expensive and more environmentally friendly than oil-based drilling fluid. Water-based mud, on the other hand, is recognized for having poor rheological and filtration capabilities when exposed to high temperatures and other harsh circumstances.

The surfactant has been used as an additive as they are good in reducing the rheology, risk of water blockage and filtrate volume that loss into the formation. Some types of surfactants might also be used as a lubricant and prevent the formation of in-situ water/oil emulsion. Non-ionic surfactants have been employed in drilling fluids as a rheology control ingredient to keep particles like organoclays from flocculating and preserve mud dispersion. (Yunita, Irawan, and Kania 2016).

To achieve the best results, the mud rheology must be maintained at suitable levels. Viscosity and gel strength are two of the qualities. Measuring and creating these features helps to make a good mud that removes cuttings, holds cuttings and weight material in suspension while not circulating, minimizes any negative effects on the well bore, and releases cuttings.

Molecular descriptors are currently commonly employed to predict chemical substance quantitative structural relationships. Molecular descriptors generate a variety of structure representations, atom/bond weighting systems, and mathematical functions in order to represent molecules. Non-ionic polymer adsorption can be identified using molecular descriptors.

The random walk method was used to model the adsorption of non-ionic surfactants and polymers. The van der Waal interaction is responsible for the adsorption of non-ionic surfactants onto a surface, which results in the formation of a random monolayer. A simple but accurate model was used to describe molecule deposition. (Budinski-Petkovi and Kozmidis-Luburi) investigated the irreversible adsorption of directed self-avoiding random walks of various lengths on a square lattice with equal deposition probability using Monte Carlo simulations.

The structural and physicochemical descriptors were used to classify and explain the linked structural features of different non-ionic surfactants that influence their adsorption processes on a hydrophobic surface. The influence of non-ionic surfactant branching structure on their adsorption to organoclays was then investigated using the Monte Carlo random walk method. (Kania et al. 2021).

1.2 OBJECTIVES

1. To investigate the mechanisms of surfactant adsorption on organoclays using the Random Walk method; Uniform sampling vs MCMC sampling.

2. To evaluate the adsorption rate by implementing two different sampling.

3. To evaluate the adsorption rate based on the two different sampling methods.

1.3 PROBLEM STATEMENT

Drilling mud is a complicated fluid that contains a number of additives. The drilling method and the type of reservoir being drilled determine the type and number of additives used. Drilling mud comes in a variety of forms, including water-based mud (WBM), oil-based mud (OBM), synthetic-based mud (SBM), emulsions, and so on. It is difficult to measure the self-assembly of surfactants in the mud in the laboratory, as the drilling fluids are very thick, and many other chemicals and solid additives are also presented in the system. (Bridges et al. 2020)

1.4 SCOPE OF STUDY

The aim of this research is to investigate the adsorption of non-ionic surfactants on organoclays in drilling fluid using a Markov Chain Monte Carlo (MCMC) based Random Walk. By implementing and optimising recently developed models, the study aimed to improve understanding of non-ionic surfactant adsorption on organoclays in drilling fluid. Intercalating various organic compounds into clays and clay minerals produces organoclays, which are hydrophobic materials. Organoclays are widely used in drilling fluids as rheological additives to increase the viscosity of synthetic-based mud (SBM). Interfacial and interparticle interactions cause the viscosity of organoclay particles. (Kania et al. 2021).

1.5 SIGNIFICANCE OF STUDY

The use of adsorption to both simple and complicated porous materials spans a wide range of scientific and industrial fields, with a particular focus on selective components created using lithographic patterning techniques. With the inclusion of molecular interfaces with enforced periodic boundary conditions, a series of Markov Chain Monte Carlo simulations written in the contemporary Julia language offered significant information linked to the mechanism of preferred adsorption sites. MCMC also helps to understand the distribution of the catalysis over the drilling fluid to know whether the distribution is uniform or non-uniform in the fluid and prevent the over dosage or wastage of expensive catalyst in the process drilling fluid besite of that it even helps us to save the time and use of proper method of finding of fluid that are good with certain catalyst.

CHAPTER II

LITERATURE REVIEW

2.1 INTRODUCTION

Non-ionic shampoos have been employed in lubricants as a plasticity control ingredient to keep particles like said the from flocculating and preserve mud distribution. The fundamental processes of non-ionic surfactant absorption on advantage with respect, as well as how it influences the rheology of polymer produced water, were investigated using molecular dynamics and Molecular Dynamics. The hydrophobicity and molecular weight of – anti surfactant hydrocarbon chains were discovered to have the greatest impact on non-ionic detergent adsorbed on advantage with respect using Naïve Bayes machine learning engine application. Hydrophobic contact and van der Waals interactions are the primary components, according to chemical description estimates.

The empirical influence of non-ionic surfactants hydrophilic molecules on personality to advantage with respect was then determined by Computations. Due to their small size, compounds with two chains are easily attracted to the surface, whereas compounds with 4 and 5 chains occupied more locations and interact with one another more often, resulting in an increased cluster. Non-ionic cleansers with more hydrophilic molecules were recommended to rise drilled fluid morphology and generate stable mud emulsions as a result. This method is useful for predicting the effects of a new drilling fluid additive.

Many experiments and mathematical studies have been conducted on the adsorption of carboxylic acids of the ethylene glycol moonily ether or polymer glycol ethanol type there at air electrode. The adsorption of carboxylic acids increases the aqueous solubility of the granules in total. It's one of the reasons why these chemicals are so widely used. Polymer composites, with exception of polar compounds, can not transform water molecules into repelling nanostructures rapidly, and can only be used as a collecting medium at very different levels.

Hole stabilization is among the most challenging problems to overcome amongst many difficulties and challenges experienced during oil exploration. More research is being done in drilling mud technology to develop more useable, environmentally acceptable water base muds. These muds are used in ecologically conscious places all over the world to address economic, technological, and legal challenges. According to the science, shales (which account for more than 75% of drilling deposits) are the primary cause of over 90% of wellbore instability issues. This is because the formation's primary ingredient (75 percent) is terracotta metamorphic rocks. Extensive research have also shown the difficulty of developing a low-cost, renewable, eco sustainable water - based drilling systematic way of reducing or eliminating well instabilities.

The correlation of swell and dispersal qualities of responsive clays was studied by Durgapur et al. (2012). Moisture rock (shale) swells as the drilled portion hits the shale zones due to water adsorption, resulting in reduced in strength properties finding patterns to higher stiffness and other operational problems. Such concerns have resulted to the full abandonment of many boreholes. The interplay of sandstone and liquid has been thoroughly researched, with the general notion that the type of mud used affects capillary pressure in fracking to a great amount. Physical, physiological, and chemical processes are the most common causes of forming instabilities (Al-saba M.T, 2018).

Clay's negatively surface (-ve) ions, non-ionic lubricants can diffuse onto the edges of hydrated expanding clay. The clay hydrated is suppressed as a result of this procedure. Flowers that could have been employed in the fracking inhibiting procedure have been studied in the past. To our information, no studies have looked at the influence of these synthetic flavonoid non-ionic WBDF detergents on the connections of non-ionic detergent suppression, stable, toughness, and Particles Bridge on real field peering.

There has been a lot of research on the composition of natural lubricants in reducing shale moisture and edema, but not much has been done on the possibility of ionic chemicals and aluminum sulfate in reducing shale soreness. Due to its low cost, low carbon impact, and ubiquity, the quest for suitable non-ionic polymers to limit shale hydrated is a hot topic.

2.2 ADSORPTION

The attachment of atoms, ions, or macromolecules from a gas, liquid, or soluble solid to a surface known as adsorption. This procedure forms an adsorbate coating on the adsorbent's interface. This varies from absorption, which occurs when a hydrogen dissolves or permeating a fluid (the absorbate). Adsorbate molecules, whereas absorption affects the entire area of the substance, but adsorption frequently occurs before absorbing. Both activities are referred to as sorption, while ablation is the opposite.

Adsorption can be found in a variety of organic, physiological, physiological, and toxicological profile, and it is affected by many factors such as adsorbents, caustic

soda, trying to capture while using waste heat and provide cool air for central heating and other applicable standards (adsorption chillers), organic polymers, expanding stainless steal carbons processing power, and wastewater treatment. Certain company to gain are selectively transported first from fluid phase to the face of insoluble, hard molecular diffusion in a vessel or packed in a row in adsorption studies such as adsorption, membrane filtration, and electrophoresis. Adsorption is less well-known in the biopharmaceutical industry, where it is used to extend cerebral exposure to a variety medications or components of drugs. (American Petroleum Institute, 1998)

2.3 MEASUREMENT OF SURFACE-ACTIVE PROPERTIES OF NON-IONIC

The ground behavior of the non-ionic detergent was investigated using three components. The crucial vesicle quantity was the first (CMC). CMC assessment can be done in a variety of ways. In CMC investigations, the resistance method was utilized according to the actual reference standards NSRDS-NBS 36. A solution with a high master concentration was created. This was accomplished by mixing powdered Cromulent odorata with de-ionized water in a homogeneous manner. For 2 hours, the mixture was agitated continuously using the Stuart magnets hot-plate agitator. (An Yuxiu,2018)

The adsorption properties of CO were the second surface-active attribute investigated. The desorption test was carried out utilizing a resistivity approach with various Concentration levels. CO absorption on pulverized shale is assessed in this test by determining the concentration of CO in water before and after the shale absorbs CO. On crushed shale, the amount of Sufficient quantity over the test period was estimated. A directly address by Moslemabad was used to analyses adsorb predictions. Aqueous CO solutions containing were created, and the liquids' resistivity coefficients were determined using an OAKION CON 700 workstation. For each of the values, a plot of resistance vs intensity was created. After measuring 15g of shale dust using a large

Toledo multivariate regression, the Degree Celsius International oven (UFE800-UK) was set to 120°C for 2 hours. Following adding 10 g of dry shale dust, 50 ml of each CO solutions was reweighed as mt. To achieve equilibrium, the mixture was agitated for 24 hours with a mechanical stirring. All of the cultures were placed into individual glass vials in equal volumes, and the materials were centrifuged for 4 hours at 4500 rpm.

After pouring all of the dregs into a receptacle and calculating the conductance advantages of different combinations. Subsequently, and use the equation following, the quantity of CO absorbed was estimated.

Equation 1.0

$$CO\ adsorption, D = \frac{m_t\ x\ (c_b - c_e)}{m_s} \times\ 10^{-3}\ \ (\mathrm{mg/g - shale\ powder})$$

As adequately represented earlier, the resistivity methods used in the adsorb had been done as anticipated of experiment reference standards NSRDS-NBS 36. .(Asadi M.S., Rahman K.,2017)

2.4 MONTE CARLO SIMULATIONS OF THE ADSORPTION

Modeling adsorption phenomenon of interest on smooth materials is a useful tool for predicting and correlating physical adsorption in membrane-based separation methodologies, as well as understanding vitamins and antioxidants (adsorption on solutes with a wide range of energies and weld zone trends) in heterogeneous catalysis. Because of the wide range of solids employed in these processes, there are numerous sorption models. These terms are also used to characterise various adsorption features that have been found. Because of the variability of solids, surface topography is particularly essential. (Bani G., Le Gall P. 1992.)

The adsorption of CO2 gas on the MgO (100) crystal interface is investigated using grand canonical Monte Carlo simulations. This enables us to acquire combined effect that can be correlated to experiment and to investigate the development of monolayers of various densities. Our common currency matches the existing results of the experiment fairly well. On the MgO surface, we discover a low-density adsorption monolayer in which each CO2 molecules is linked to two Mg2+ ions. We also see the creation of relatively high monolayers, where a few CO2 molecules have twisted and inclined to reveal more signaling pathways. Low-temperature calculations of either the low- and medium monolayers reveal that their hysteresis loops are remarkably similar at T=5K, with bond lengths of around 7kcalmol. Our model's high-density monolayer has a thickness that is substantially lower than the originally announced measured result. This gap is discussed, as well as solutions for overcoming it.

2.5 SURFACE INHIBITIVE QUALITIES

Because with the formation of microcapsules, CO's viable large prohibitive ability diminishes over the CMC, even while fixing increases. There is a rapid transformation in viscous lines in varying temperature mix groups of Tion in solid restrictive frames. The holes between both the viscous line multiply from start as the CO concentrate expands, as shown in Fig. 4. It was still limited as the structure advanced towards its CO CMC, demonstrating the link with CO constraint strength and its fixing. In comparison to the CMC, it was clear from the results presented that the CO's prohibitive ability had not increased significantly. 30 mass percent CO was discovered to be the highest stacking Itong for 3.5 mass percent. Tiong adsorbent thicknesses increased from 1.1 mg/g to 46.98 mg/g when CO emphases were 0.5 mass percent to a most intense CO confluence of 4.0 mass percent for shale-1 desorption and 0.5 mass percent to 3.5 mass percent for shale-2 absorption. Aside from that, for shale-1 and shale-2, there was a clear link between adsorbent dose and minerals. For shale delay, the maximum measurement of layered Into for 3.5 mass percent KCl was 27.5 mass percent. This result demonstrates the capabilities of the non-ionic rough

concentration surfactants CO 2 and KCl, which are both novel non-ionic rough concentration surfactants. (Blachier C.,2009)

2.6 LIQUID MISFORTUNE INHIBITIVE ATTRIBUTES

The filter test findings also revealed the exceptional CO focus. When compared to plan 2, description 1 (Itong in du nord water) provided a lower level of filtering (CO details). The many operating components, such as the influence of freshwater and CO on the environment. Dirts have an extended realm of public shape similar to nature, small molecular size, and a high extending limit of kaolinite. (Bol G.M.,1994)

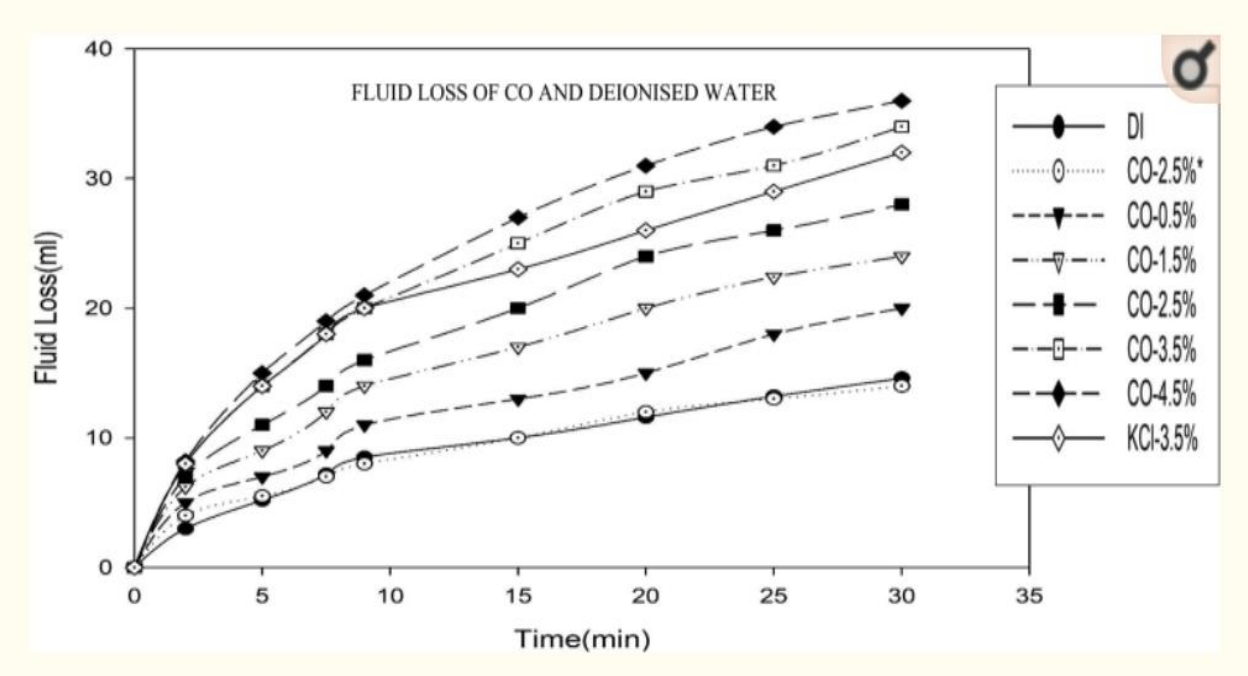

Figure 2.6.1 : Fluid Loss of CO and DEIONISED Water (Bol G.M.,1994)

It is also undeniable that desorption played a role. The absorption was discovered to be a constituent of the shale's mud composition. This could be due to the fact that the dirt component contrasts with the qualities of the two sedimentary rocks and the rock. Higher smectites levels indicate a preference for absorption of water. XRD analysis revealed that shale-1 was more abundant in elite than shale-2, giving it a more hydrophilic nature and thus a higher level of absorption, which affects filtering capabilities. Within the first 30 minutes of the test, the volume of the supernatant was measured at 14.6 mL. However, as concentrate I was increased, CO yield increased. 0.5, 1.5, 2.5, 3.5, and 4.5 mass percent parameters yielded 20 ml, 24 ml, 28 ml, 34 ml, and 38 ml gaseous carbon, respectively.

One of the possible motivations for the CO's high fluid absorption outcome is the concept of molecular deformation due to the readjustment of muck grains and the dehydration restrictions of the dirt. When extensible muds absorb water, they have a high molecular liberty, develop a waterproof tube cake quickly, and have a low API water pain value. Monomer deformation can also be thought of as the effect of quasi surfactants on the's water of kaolinite through their effect on the payment organisations of the dirts and the electromagnetic thick effect. The presence of CO on mud substrates affects the development of the electrified a double layer, changing the omega potential for a variety of degree programmes of fixing applied, based on zeta guesstimates, as evidenced by information on take important, two-fold kernel size, interparticle qualities, and point of low potential. The high zeta potential of dust tiny flecks was used to assess the reliability of colloidal scatterings. (Cheatham J.B.1984)

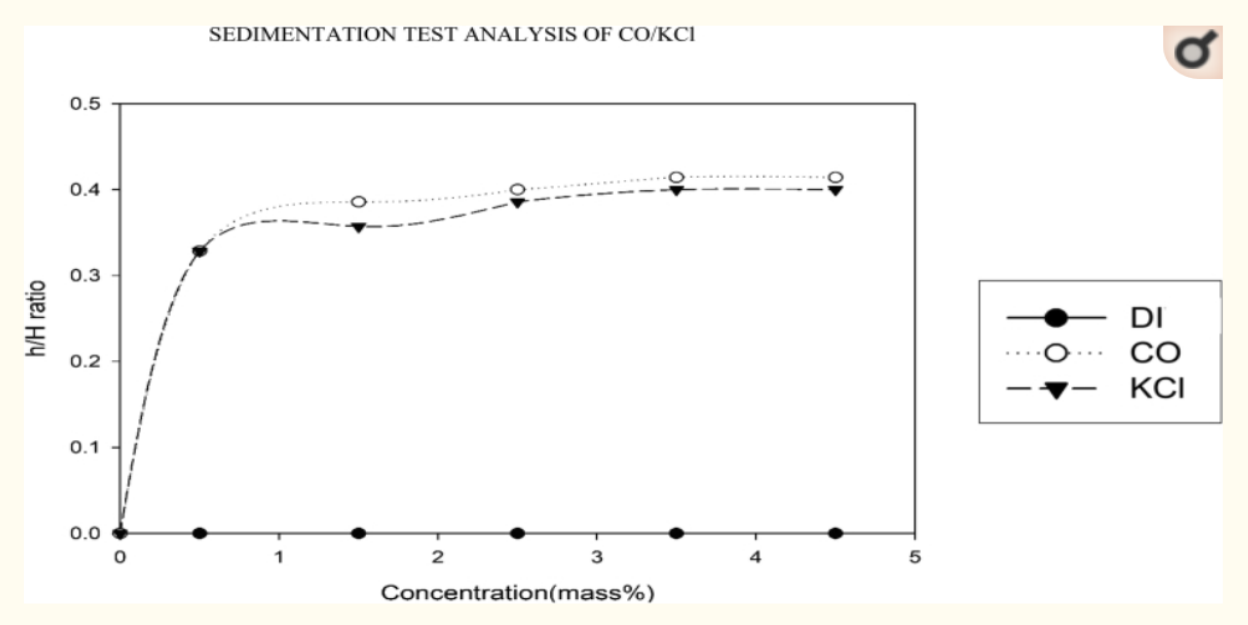

Figure 1.6.2 : Segmentation Test Analysis of CO/KCL(Cheatham J.B.1984)

2.7 SEDIMENTATION SCATTERING INHIBITIVE ATTRIBUTES

The granules of kaolin assimilated water in the por water astonishingly well when used without CO and KCl, as shown in Figure 2.6.1. This ushered in a new era of uniform hydrated dispersion dispersing all over the place. Regardless, the kaolin nanoparticles flocculated and formed dregs when exposed to CO. Increases in CO localization resulted in more significant coagulation and a faster rate of particles sinking at the bottom, resulting in dense silt formation. When KCl was used as a barrier agent, same phenomenon also occurred. When compared to KCl, CO has a higher impediment capability. The degree of persistent dispersion is a factor in the high fluid retention and expansion restriction of Nito. DI's aftereffects revealed a strong homogenous growth of permanent scattered consistent with concept, however the 3.5 mass percent CO version delivered dregs. The relationship between the CO concentrate and the dispersing strength formed was noted. CO groupings of 0.5 percent–4.5 percent revealed a drop in the h/H fraction to somewhere around 0.34–0.421 independently within the first two

days. After this time, there was no discernible difference. This was also in line with the idea that CO constraint increases as focus is increased until CMC is reached. (Dehghanpour H.,2012)

The outcomes of the dispersion experiments are shown in Exhibit. The rate of recovery in DI is 25%, reflecting a significant rate of water absorption and shale scatter. Isolated measurements of 41.5 percent –59.5 percent and 54.15 percent were reported when CO and KCl were connected. The more notable restriction and dispersing level of CO to drying of shale blades than the more typical KCl resulted in this result. When CO was communicated with other item advancement mixtures as shown in Fig. 2.6.2, the solvent strategy essays (definition 1(FF1), water tailoring (FF2), and solvent plan 3(FF3) on various WBDFs coordination of shale-1 and shale-2 were in the ranges of 77.5 percent –91.8 percent and 65.6 percent –79.8 percent for shale-1 and shale-2 separately. (Friedheim J.,2011)

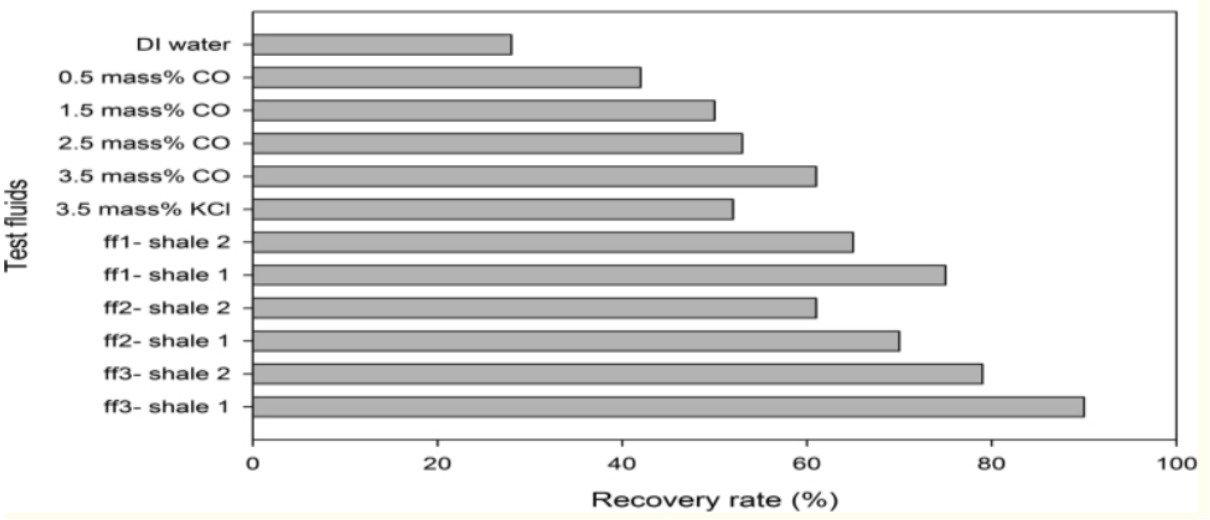

Figure 2.7: Scattering Inhibitive Attributes (Friedheim J.,2011)

2.8 SURFACTANT

Oils and lipids are a subject of surfactant adsorption in cosmetic formulation. Surfactants adsorb to these substrates, altering their properties and improving distribution in both the gas and liquid phases. Emulsifiers and surface treatment agents are two types of surfactants that have these properties. Skin and hair are the subjects of surfactant adsorption in aesthetics, with the former focusing on irritant and the latter on nourishing effect, both focused on absorption characteristics. Most of the adsorption research is focused on standalone surfactants, with only a few studies that focused on combined samples were diluted. However, there are some fascinating indications on their adsorption behavior from the days when solvents were being used as fiber proposed by researchers, and these data suggests that anionic/cationic mixed corrosion inhibitor systems have a distinct adsorption behavior.

The adsorbents of NaLMA, STAC, and the mashed framework of these two surfactants on collagen powder at 40°C are shown in the figure below. The measurement that can be applied continues to rise when the combination ratio of STAC to NaLMA rises. The adsorption quantity is greater in the combined systems of STAC:NaLMA = 6:4 and 7:3, comparing to when STAC is employed alone, with the maximum adsorption quantity at 7:3. A mixed mixture with a larger cation ratio has a higher permanent contact with keratin powdered, and according to equilibrium adsorption patterns. (Fritz Steven J.2014)

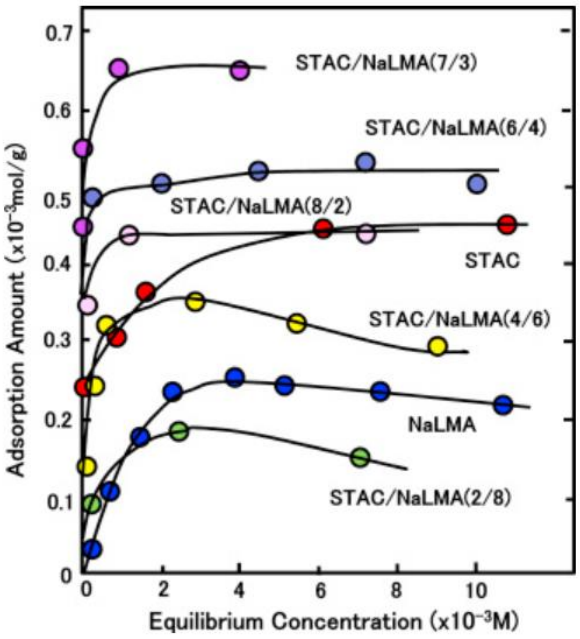

Figure 2.8 : graph of adsorption amount vs equilibrium concentration (Fritz Steven J.2014)

2.9 TYPES OF SURFACTANTS

All surfactants have an electric current on its hydrocarbon chain. Negative, negative, or balanced charges are all possibilities. Surfactants are classed as anionic, zwitterionic, charged, or anionic based on the charge of their hydrophilic heads.

2.9.1 ANIONIC SURFACTANTS

On its hydrophilic end, carboxylic acids produce a negative charge. The surfactant proteins' electrostatic repulsion aids in lifting and suspending soils in micelles. Organic compounds are commonly employed in soaps and detergents even though they may target a broad array of soils. When radioactive tracers are combined, they produce a lot of foam. Carboxylic acids are great at raising and floating particle soils, but they struggle to emulsion oily soils. (Hall Carl W,1988)

2.9.2 NON-IONIC SURFACTANTS

Natural polymers have no charges on the mutagenic effect and are hence neutral. Natural polymers are superior than aliphatic hydrocarbons at foaming oils and eliminating inorganic soils. These two ingredients are typically used to generate a double, micro cleansers that really can remove and suspend particle dirt as well as emulsion oily soils.

2.10 USE OF CLAY

The use of clay minerals in native and usage of traditional for the removal of various hazardous organic and inorganic contaminants has been a new trend in study during the last 30 years. Clay minerals, both natural and artificial, have a remarkable option to extract various pollutants. Structure composed, on the other hand, can increase

the adsorption capabilities of clay minerals, resulting in additional adsorption sites and hydroxyl group to adsorb numerous ecological toxins. This review emphasizes the significance of modifying procedures and expanding the use of innovative clay preparations nanotechnology - based to improve pollution management. (Hall Carl W.2018)

Polymeric clays, such as canopied clays and porosity clays semiconducting, have been synthesised, resulting in a novel class of heterojunction material with excellent adsorbent dosage, ability, and sensitivity. This study includes more literature of research related to health preservation issues related to the suitable qualities of nanostructured materials, such as excellent mechanical properties, tribological durability, and the inclusion of multifunction groups to extractive distillation. However, a deeper knowledge of the adsorbent surface, regeneration, and healing process of these substances is predicted to attract a huge amount of attention.

2.11 SUMMERY OF THE FOLLOWING RESEARCHERS/INVESTIGATOR

2.11.1 The investigation discovered the following

1. The degree of restriction in CO raw concentrated with tannins is equivalent to electromechanical KCl in all obstacle qualities.(Israelachvili Jacob. 2011.2011)

2. Using harsh ou pas surfactant, UCS established a link between rising temperatures and the shale's hardness.

3. The results of SEM confirmed the practical relationship between concentration and the ability of coarse non-ionic detergents to remove muds. As the planet

warms, the impediment structure, such as the shale's sturdiness, expands due to the constraint of the unprocessed concentration.

4. With a concentrate range of 2.5–3.5 mass percent, CO could be used as an antagonist component in WBDFs with a CMC of 3.5 mass percent as an optimal fixing to increase the restrictive properties.

5. When used in conjunction with the standard WBDFs synthetic concoctions, CO unprocessed concentrates was quite viable, and it also provided security to Tiong granules in the CO liquid solution.(Ji Lujun, Geehan Tomas, 2013)

6. CO unpolished start focusing can be extracted at a low cost and is readily available as an alternative for corporate KCl.

CHAPTER III

METHODOLOGY

3.1 OVERVIEW OF METHODOLOGY

In this chapter the methodology to investigate the adsorption of non-ionic surfactants will be discussed in more detail and the procedure for using Markov Chain Monte Carlo Method to determine the distribution of the surfactants on the surface of the drilling fluid. The software that can be used to simulate the adsorption of non-ionic surfactants in drilling fluid are coding software are Matlab, Python…etc. and any other coding software. However, MATLAB will be chosen for this study because it is user friendly and also the user is more familiar with MATLAB compared to the other coding software.

3.2 RESEARCH FLOWCHART

The flow chart below is a summary of the steps undertaken during the simulation to obtain the distribution of the non-ionic surfactants in the drilling fluids at different times. The steps of the process are as shown below.

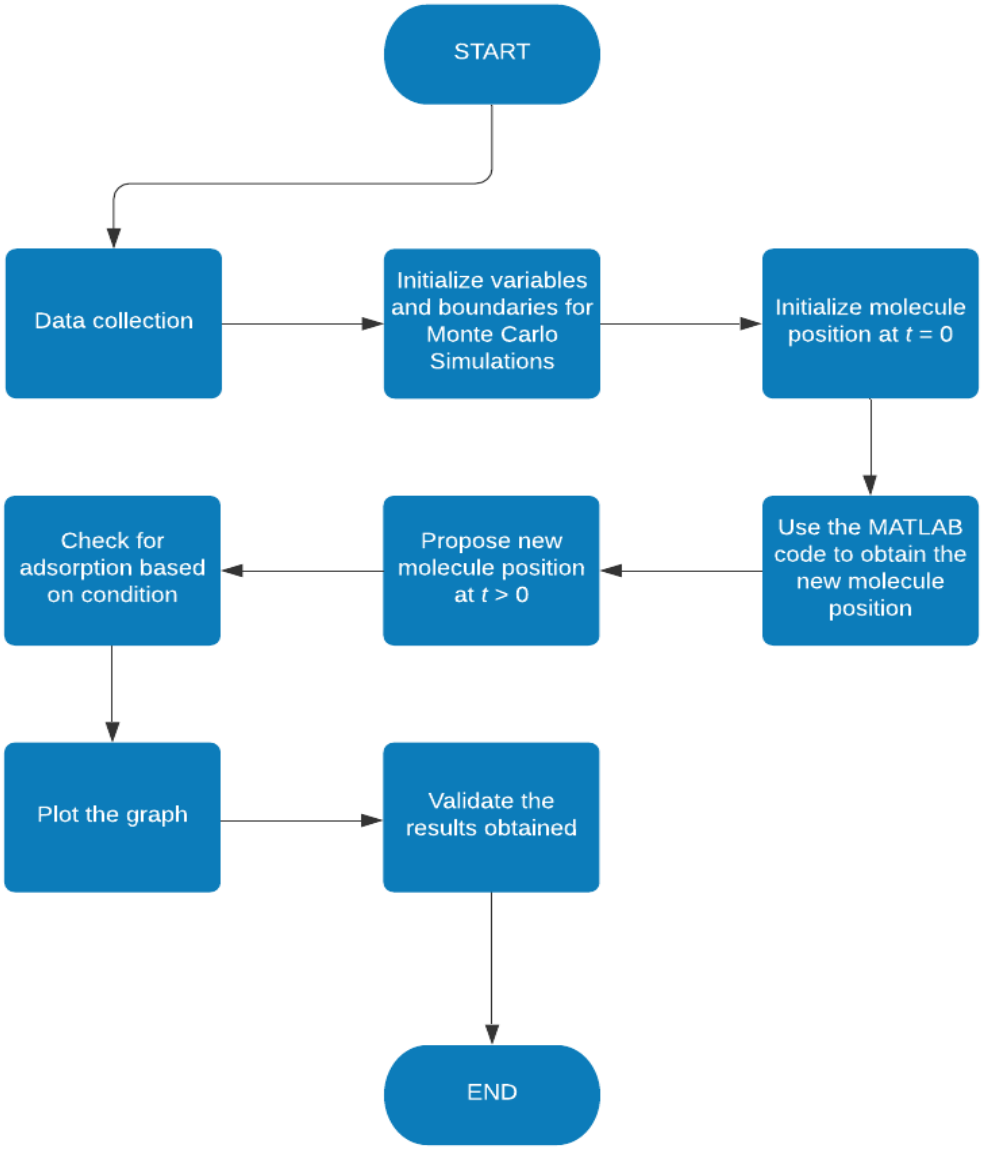

Figure 3.2 : Flowchart of the methodology

3.3 MATLAB

Matlab is programming software with versatile tools and numerical computing environment. It has the ability to allow matrix manipulation, plotting functions and data implementation of algorithms, creation of user interfaces. Matlab has in built tools that are very useful when dealing with Markov Chain Monte Carlo method.

There are three parts of MATLAB that can be used in Markov Chain Monte Carlo Techniques.

1. ***[rnd,pdf,lpr].m** - distribution function tools to complement MATLAB's

2. **mcmc*.m** - routines to calculate and display summaries of MCMC output

3. **other** - other useful routines

Table 3.2 shows a summary of the MATLAB in built functions that can be used in MCMC

1. **Distribution Function Tools**

   These functions help in various calculations involving density functions and random number generation.

- randrand - randomize both random number chains off the clock
- mvnormrnd - random multivariate normal - different from MATLAB's mvnrnd
- wishrnd - random Wishart value
- wishirnd - random Wishart value - integer df only
- invwishrnd - random inverse Wishart value
- invwishirnd - random inverse Wishart value - integer df only
- invwishpdf - inverse Wishart density
- metrop - a general Metropolis-Hastings step
- betalpr - log probability ratio for beta distribution
- gamlpr - log probability ratio for gamma distribution
- invwishlpr - log probability ratio for inverse wishart distribution
- mvnormlpr - log probability ratio for multivariate normal distribution

2. **MCMC Summaries**

- mcmclt - lower triangle - for symmetric matricies to use with mcmctrace
- mcmcsumm - calculate summary statistics(includes autocorrelations and

Gelman-Rubin statistics)

- mcmctrace - matrix of trace plots
- mcmcacf - to plot autocorrelations
- mcmcgr - Gelman-Rubin R statistic for convergence
- mcmcdemo - short demonstration program

3. Other

- ltvec - convert a lower-triangular matrix into a vector
- veclt - convert a vector into a lower-triangular matrix
- ltindex - convert row and column index into lt-index

3.4 MARKOV CHAIN MONTE CARLO (MCMC)

Markov Chain Monte Carlo (MCMC) is a method that stands out among others. Metropolis, Metropolis-Hastings, Gibbs-Sampler, and hybrids are some of the algorithms used to define Markov Chains and are suited for Bayesian inference. In this research, both Random Walk Metropolis (RWM) and Metropolis-Hasting will be used to determine the distribution of the adsorbing non-ionic surfactants in the drilling fluid.

The one of the most commonly used MCMC methods is the Metropolis-Hastings algorithm, which is the method that will be presented in this project. The implementation of the Metropolis-Hastings algorithm begins with the initial choosing of a proposal distribution $\mathbf{p(P^*,P^{(t-1)})}$, which is then used to come-up with a new candidate state $\mathbf{P^*}$, given the current state $P^{(t-1)}$ of the Markov chain. After selection of the first distribution, the Metropolis-Hastings sampling algorithm can be used by repeating the following steps:

I. Sample a Candidate Point from the proposal distribution

II. Calculate the acceptance factor:

Equation 2.0

$$AF = min\left[1, \frac{\pi(P^*|Y)p\left(P^{(t-1)}|P^*\right)}{\pi(P^{(t-1)}|Y)p(P^*|P^{(t-1)})}\right]$$

III. Generate a random value U, which is uniformly distributed on (0, 1).

IV. If $U \leq AF$, set $P^{(t)} = P^*$. Otherwise, set $P^{(t)} = P^{(t-1)}$.

V. Return to step 1 while some convergence criteria is not satisfied.

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