http://journal.uir.ac.id/index.php/JGEET

E-ISSN : 2541-5794
P-ISSN : 2503-216X

Journal of Geoscience,
Engineering, Environment, and Technology
Vol 10 No 04-2/2025

RESEARCH ARTICLE

Analysis of the Effect of Cationic and Anionic Surfactants and Polymer Additives on the Water-Oil Interface in Enhanced Oil Recovery: A Molecular Dynamics

Frans Nicolas P. Naibaho[1], Muhammad Hasbi Ar-Raihan[1], Azis Adharis[1], Paramita Jaya Ratri[1], Tirta Rona Mayangsari[1,2,*]

[1] Department of Chemistry, Universitas Pertamina, Jalan Teuku Nyak Arief, Jakarta, 12220, Indonesia
[2] Collaboration Research Center for Advanced Energy Materials, National Research and Innovation Agency – Institut Teknologi Bandung, Jalan Ganesha 10, Bandung, 40132, Indonesia .

* Corresponding author : tirta.rm@universitaspertamina.ac.id
Tel.:+62-812-2291-6670

Received: Aug 18, 2025; Accepted: Dec 3, 2025.
DOI: 10.25299/jgeet.2025.10.1.1.24610

Abstract

The high demand for petroleum requires a more efficient production process. Enhanced Oil Recovery (EOR) technology with chemical injection methods can optimize oil production in reservoirs. To understand the properties of these chemicals, analysis at the atomic level is necessary. This research utilizes molecular dynamics simulations using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to analyze diffusion coefficients and Interface Formation Energy (IFE) values. Surfactants such as Dodecyl Trimethylammonium Bromide (DTAB), Sodium Dodecyl Sulfate (SDS), and Polyacrylic Acid (PAA) polymer are studied. Results indicate that DTAB, SDS, and PAA stabilize the water-oil system, shown by lower IFE values: -48.53, -178.33, and -231.78 kcal/mol, respectively. DTAB increases the diffusion coefficient of dodecane from 0.01 Å^2/ps to 0.039 Å^2/ps. SDS and PAA increase water diffusion coefficients from 0.0094 Å^2/ps to 0.0097 Å^2/ps (with SDS) and 0.0179 Å^2/ps (with PAA).

Keywords: EOR, DTAB, SDS, PAA, Molecular Dynamics

1. Introduction

Crude oil is a very important and strategic natural resource for Indonesia, especially as fuel to meet domestic needs. According to the Journal of Renewable Energy, Indonesia's oil reserves (proved reserves and probable reserves) in 2019 were 3.8 billion barrels, with a reserves-to-production (R/P) ratio of 9 years (Setyono & Kiono, 2021). One of the efforts to increase domestic oil production is using the Enhanced Oil Recovery (EOR) method. EOR is a tertiary oil production process carried out by injecting external energy sources and/or materials into reservoirs that can no longer be exploited through primary and secondary recovery (Putra & Kiono, 2021). One method used in EOR technology is chemical injection. In chemical injection, chemicals are added to reservoir wells to increase oil recovery, thereby enhancing the efficiency of a reservoir well that has passed its primary and secondary production phases.

Chemical injection has great potential for success when applied to reservoirs that have undergone water injection but still have significant amounts of unrecovered oil. There are three types of chemicals commonly used in chemical injection: polymers, surfactants, and alkalis (Ansyori, 2018). The surfactants used in chemical injection can be anionic, cationic, or non-ionic. To apply this chemical injection method in EOR, the appropriate surfactant or polymer must be selected to achieve optimal results. An efficient surfactant in this context is one that can reduce interfacial tension at a relatively low concentration to lower production costs (Bustamante-Rendón *et al.*, 2020). Other aspects are also influenced by the properties of the reservoir rock; if the injected surfactant does not match the rock properties, it will negatively impact oil production or other aspects. Therefore, a study on the properties and dynamics of specific surfactants is conducted to understand the transfer and interaction of ionic surfactants with the water/oil system at the molecular level.

One cationic surfactant commonly used in EOR applications is Dodecyl Trimethylammonium Bromide (DTAB), which performs well in forming interfaces with water and oil particles at relatively low concentrations (Schabes *et al.*, 2019). Sodium Dodecyl Sulfate (SDS) is an anionic surfactant frequently used in EOR to reduce surface tension between oil and water in oil reservoirs (Tavakkoli *et al.*, 2022). This reduction in surface tension helps oil separate more easily from the reservoir rock and move toward the production well, improving oil extraction efficiency.

In addition to surfactants, polymers also have the capability to be used as a medium in chemical injection. Polymers can increase water viscosity, thus reducing water mobility, allowing more water to interact with oil and push it toward the production well (Wang & Dong, 2009). The use of polymers in EOR can also help slow down reservoir pressure decline, extending the production life of the well. Polyacrylic Acid (PAA) is a polymer with carboxylic acid functional groups in its main chain that can form gels when interacting with water, enhancing oil recovery (Shamilov *et al.*, 2017).

From an experimental perspective, it remains a significant challenge to directly observe the microscopic details of the movement and interaction between surfactant molecules and the water-oil system (Tang *et al.*, 2019). With the rapid advancements in computer science and technology, computational simulation methods, including Molecular Dynamics (MD), have become a preferred approach to studying the properties and dynamics of surfactants or polymers in the water-oil system at the atomic level. Molecular dynamics simulations can provide information on the movement of interacting molecules by simulating how they attract, repel, and collide with each other. Using molecular dynamics simulations, properties such as interfacial tension, interface thickness, interface structure, and the interactions between surfactant, water, and oil molecules can be studied (Zhou *et al.*, 2021).

Numerous studies on surfactants in chemical injection have been conducted, including by Hou (2022), who examined the behavior of anionic, cationic, and non-ionic surfactants on carbonate rock surfaces (Hou *et al.*, 2022). This study used molecular dynamics simulations and analyzed the results through diffusion coefficients and IFE values obtained. Additionally, Tang (2018) conducted research comparing the efficiency of anionic and cationic surfactants in lifting heavy oil from reservoirs (Tang *et al.*, 2019). Both surfactants were simulated, and their efficiencies were compared through the analysis of diffusion coefficients and Interface Formation Energy (IFE).

To date, studies on the molecular dynamics mechanisms of the interaction between water/oil/surfactant or water/oil/polymer systems are still limited. Therefore, this research observes and compares the properties and dynamics of cationic surfactants, anionic surfactants, and polymers in the water/oil system. Dodecyl Trimethylammonium Bromide (DTAB) is used as a representative cationic surfactant, Sodium Dodecyl Sulfate (SDS) as an anionic surfactant, and Polyacrylic Acid (PAA) as a polymer.

2. Models and Methods

The simulation model used in this research consists of a water-oil system and a water-oil-surfactant system, with dodecane representing the oil, DTAB as the cationic surfactant, and SDS as the anionic surfactant (**Figure 1**). The force field used is GROMOS 54a7, obtained from the Automated Topology Builder (ATB) database and the cutoff distance is 12 Å. The water model used is the SPCE model. The size of simulation box is 51x54x87 Å^3, which consists of a mixture of water molecules, oil molecules, and surfactant or polymer molecules. The Particle–Particle Particle-Mesh (PPPM) method is used to calculate the long-range Coulombic interaction. Three-dimensional periodic boundary conditions were adopted in this simulation.

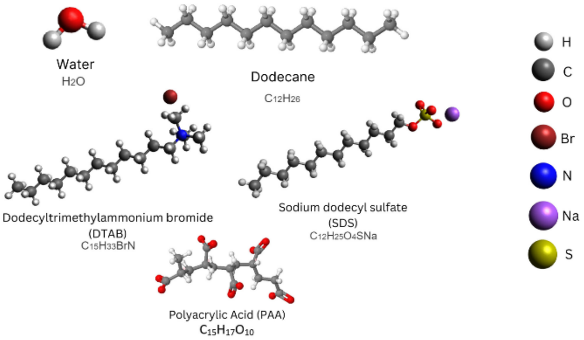

Fig 1. The molecular model used in the molecular dynamics simulation along with the atom colors.

In this study, all MD simulations were performed with the LAMMPS package. First, the system energy is minimized with the principle of optimizing the position of the atomic coordinates repeatedly until the lowest energy is reached. Then, an NPT simulation at 300 K and 1 atm was performed for 2 ns to reach equilibrium state and more normal density. Next, a 2 ns NVT simulation at 300 K was performed to collect atom trajectories for further analysis of MSD and IFE. Timestep of 1 fs used for all simulation and simulation trajectories captured every 2 ps.

3. Result and Discussion

3.1 Analysis of the Dynamics of the Water-Oil Interface System with the Addition of Surfactants and Polymers

The dynamics of the water-oil interface system were observed through trajectory data obtained from molecular dynamics simulations. There are three trajectory datasets collected: the water-oil system with the addition of the cationic surfactant DTAB, the water-oil system with the addition of the anionic surfactant SDS, and the water-oil system with the addition of the polymer PAA. The PAA model was constructed with 5 monomers, based on Quezada's study (Quezada *et al.*, 2021). Each system was first equilibrated for 2 ns to achieve more normal volume and density values, using an NPT ensemble where the pressure remained constant. Then, a subsequent simulation was performed for 2 ns to observe the dynamics occurring at the interface under constant volume and temperature, using an NVT ensemble. In total, the simulation time was 4 ns. **Figure 2** shows the visualization of the simulation of the water-oil system over 4 ns.

At the beginning of the simulation, water molecules were positioned at the top of the box and oil molecules at the bottom. The equilibration phase lasted until the simulation time reached 2 ns (nanoseconds). During equilibration, the water and oil molecules began to move closer to each other, but no water molecules entered the oil region or vice versa. Additionally, the initial box volume, which measured 47 x 54 x 83 Angstrom, decreased to 37 x 45.9 x 76.98 Angstrom. After the equilibration phase was completed, an NVT simulation was conducted for 2 ns to

Table 1. Simulation model variations

System	Dodecane		Water		Surfactant/Polymer		Type
	Total	%wt	Total	%wt	Total	%wt	
Water-Oil	120	36%	2000	64%			
12 DTAB	120	34%	2000	60%	12	6%	Cationic
12 SDS	120	34%	2000	60%	12	6%	Anionic
12 PAA	120	34%	2000	59%	12	7%	Polymer

observe the dynamics. As shown in **Figure 2**, no significant changes occurred after the system reached equilibrium. The water and oil molecules remained in their respective regions, with no mixing observed until the end of the simulation. Next, a molecular dynamics simulation was performed on the water-oil system with the addition of the cationic surfactant DTAB, as visualized in **Figure 3**.

At the beginning of the simulation, 12 DTAB molecules were added to the water-oil system and positioned between the water and oil molecules. During the equilibration phase, DTAB molecules began to interact with both water and oil, forming an interfacial system. Along with this, the box volume decreased from 51 x 54 x 87 Angstrom to 39 x 45.9 x 81.9 Angstrom. At 4 ns of simulation time, some surfactant molecules moved into the oil region, while others interacted with the water. This is due to the amphiphilic nature of the surfactant molecules, where the hydrophilic head of DTAB interacts with water, while the hydrophobic tail interacts with oil (Schabes *et al.*, 2019). In this case, the bromide ion at the DTAB head interacts with the positively charged hydrogen atoms of the water molecules, while the trimethylammonium group interacts with the negatively charged oxygen atoms of water. The hydrophobic alkyl dodecyl chain of the DTAB molecule interacts with oil molecules through van der Waals forces between the dodecyl alkyl chain and the oil molecules (Tang *et al.*, 2019). A clearer visualization of these interactions in the system is shown in **Figure 4**.

The next molecular dynamics simulation was performed on the water-oil system with the addition of the anionic surfactant SDS. In this simulation, 12 SDS molecules were added to the water-oil system and positioned between the water and oil molecules. At 2 ns of simulation time, during the equilibration phase, SDS molecules were already interacting with both water and oil. The box volume also decreased during equilibration from 51 x 54 x 87 Angstrom to 39 x 45.9 x 81.9 Angstrom. No significant changes occurred from 2 ns until the end of the simulation.

Regarding the interactions, the hydrophilic part of SDS, consisting of the sulfate group (SO_4^-), has strong interactions with water molecules through polar interactions such as hydrogen bonding, while the dodecyl chain of SDS tends to repel water and prefers to interact with oil molecules. However, as shown in **Figure 5**, SDS molecules tend to be closely packed together, unlike the behavior exhibited by DTAB in **Figure 4**, where the molecules are more spaced apart. This difference is because the anionic surfactant SDS tends to form micelles. Micelles are aggregates of surfactant molecules in solution that form clusters when the surfactant concentration in the solution reaches or exceeds the Critical Micelle Concentration (CMC), the concentration at which surfactant molecules start forming multilayered structures (Zendehboudi *et al.*, 2013). According to Massarweh's study (2023), the CMC value for SDS is 0.23 wt.%, while for DTAB, it is 0.46 wt.% (Massarweh & Abushaikha, 2023). Referring to this study, SDS has a lower CMC value compared to DTAB, making it easier for SDS to form micelles. When micelles are formed, the surfactant molecules initially located at the interface between the two phases move into the micelle structure (Cui *et al.*, 2008). As a result, the number of surfactant molecules at the interface decreases, reducing the interfacial thickness and, consequently, the surface tension between the two distinct phases. A clearer visualization of the interactions in this simulation is shown in **Figure 6**.

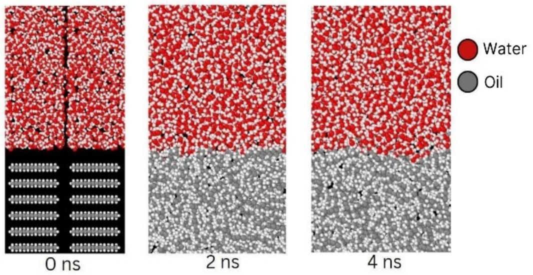

Fig 2. Visualization of the molecular dynamics simulation of the water-oil system using the NPT ensemble (2 ns) and NVT ensemble (4 ns).

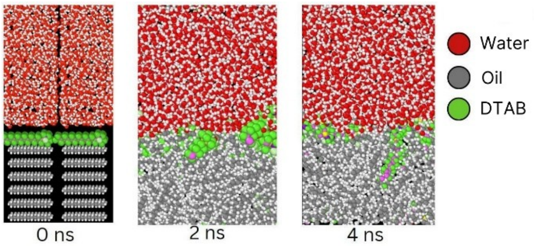

Fig 3. Visualization of the molecular dynamics simulation of the water-oil-DTAB system using the NPT ensemble (0-2 ns) and the NVT ensemble (2-4 ns).

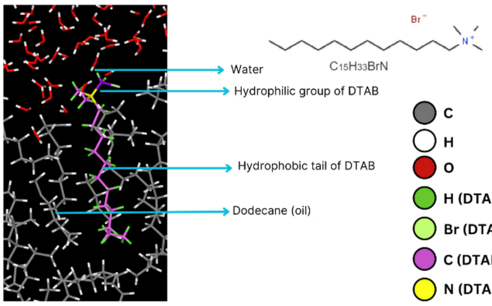

Fig 4. Visualization of the interactions and behavior of DTAB molecules with water and oil in the simulation of the water-oil-DTAB system.

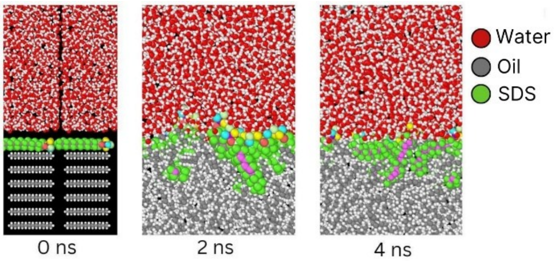

Fig 5. Visualization of the molecular dynamics simulation of the water-oil-SDS system using the NPT ensemble (0-2 ns) and the NVT ensemble (2-4 ns).

Next, a molecular dynamics simulation was conducted on the water-oil system with the addition of 12 PAA molecules. Similar to the previous two simulations, the PAA molecules were initially positioned between the water and oil molecules. During the equilibration phase, the box volume decreased from 47 x 58 x 93 Angstrom to 35 x 43.5 x 70 Angstrom, and it was observed that PAA molecules interacted with both water and oil. However, with the addition of PAA, the oil molecules appeared to move less. Structurally, PAA contains carboxyl groups (-COOH) on its polymer chain. These carboxyl groups form hydrogen bonds with water molecules because the oxygen in the carboxyl group has a hydrogen atom that can act as a donor in hydrogen bonding (Quezada *et al.*, 2021). Therefore, PAA

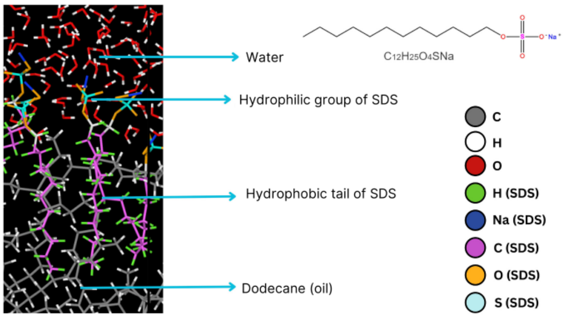

Fig 6. Visualization of the interactions and behavior of SDS molecules with water and oil in the simulation of the water-oil-SDS system.

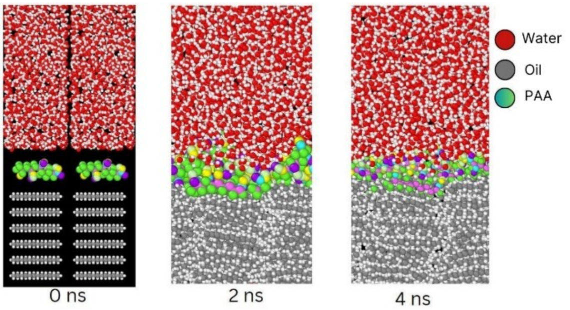

Fig 7. Visualization of the molecular dynamics simulation of the water-oil-PAA system using the NPT ensemble (0-2 ns) and the NVT ensemble (2-4 ns).

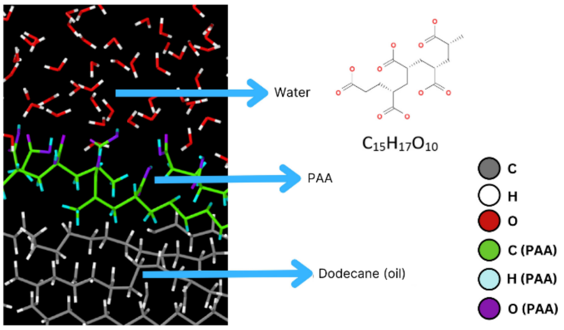

Fig 8. Visualization of the interactions and behavior of PAA molecules with water and oil in the simulation of the water-oil-PAA system.

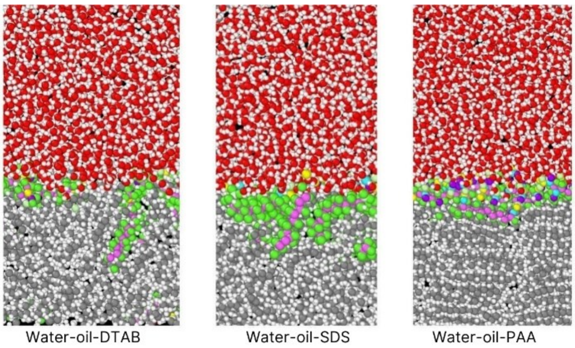

Fig 9. Comparison of the dynamics of the water-oil system with the addition of DTAB, SDS, and PAA at the end of the simulation.

tends to interact more with water, making the oil less mobile. This behavior aligns with the role of polymers in chemical injection, which is to increase water viscosity. With higher water viscosity, alterations in the reservoir are prevented, making it easier for oil to be pushed toward the production pipe (Wang & Dong, 2009). **Figure 7** shows that the water-oil-PAA system forms an interfacial thickness of about 6 Angstrom. This thickness affects the movement of molecules between the phases, as the PAA polymer layer hinders the diffusion of molecules from one phase to another, reducing the oil diffusion coefficient. A clearer visualization of these interactions in the system is shown in **Figure 8**.

Figure 9 shows the comparison of the dynamics of DTAB, SDS, and PAA in interacting with water and oil at the end of the simulation. DTAB and SDS exhibit similar behavior in interacting with oil, where the addition of both surfactants causes the oil molecules to become disordered. This is due to the alkyl chains of DTAB and SDS interacting with the oil, causing the oil molecules to move toward them (Tang *et al.*, 2019). In contrast, in the water-oil system with the addition of PAA, the oil molecules do not move significantly, as the carboxyl groups (-COOH) on the PAA molecules tend to interact more with water.

From the simulation results, it is evident that the addition of surfactants DTAB, SDS, and the polymer PAA to the water-oil system affects the conditions and dynamics within the system. Each molecule used in this study exhibits different behaviors, which consequently have varied effects and benefits. However, to fully understand these effects, visual results alone are insufficient. Therefore, an analysis of the Interface Formation Energy (IFE) values for each system, as well as an analysis of the water-oil diffusion coefficients, is conducted to support the visual findings from the simulations.

3.2 Analysis of IFE (Interface Formation Energy) Values

The calculation and analysis of IFE (Interface Formation Energy) values in this study were conducted to determine the effect of adding the surfactant DTAB, the surfactant SDS, and the polymer PAA on the water-oil interface system. The IFE value refers to the energy reduction when surfactant or polymer molecules interact with the water-oil interface. Therefore, the lower the IFE value of a system, the greater the stability of the interface (Cui *et al.*, 2008). The formula for calculating the IFE value is following equation (1) with the energy value used is the energy value obtained during the simulation using the NVT ensemble.

$$IFE = \frac{E_{total} - (E_s + E_{wo})}{n} \tag{1}$$

where $\boldsymbol{E_{total}}$ is the energy of the system, $\boldsymbol{E_s}$ is the energy of one surfactant or polymer, $\boldsymbol{E_{wo}}$ is the energy of a water-oil system, and n is the amount of surfactant or polymer in the system (Ong *et al.*, 2018). The energy value of each system is shown in Table 2 below.

Table 2. Total energy of each system after the NPT and NVT simulations

System	Energi (Kcal/mol)
1 molecule DTAB	-105,838
1 molecule SDS	-196,691
1 molecule PAA	-213,847
Water-oil	-9697,06
Water-oil-12DTAB	-10385,26
Water-oil-12SDS	-12033,67
Water-oil-12PAA	-12692,245

Each energy value was obtained after running molecular dynamics simulations with a total of 4,000,000 steps, equivalent to 4 ns. As shown in **Figure 10**, at the beginning of the simulation, each system still had high total energy, indicating instability. After about 0.3-0.4 ns, all systems experienced a decrease in total energy. In the water-oil system, after this decrease, the energy did not immediately converge but showed slight fluctuations until around 2.5 ns, after which it became stable. The total energy of the water-oil system after the simulation was -9,697.06 kcal/mol.

When surfactants DTAB, SDS, or the polymer PAA were added to the water-oil system, the total energy of the system decreased further. The total energy values for the water-oil system with DTAB, SDS, and PAA were -10,385.26 kcal/mol, -12,033.67 kcal/mol, and -12,692.25 kcal/mol, respectively. As observed in **Figure 10**, when the energy of the water-oil system with DTAB and SDS decreased, the graph did not immediately converge but continued to show slight fluctuations, indicating ongoing molecular movement until the end of the simulation. In contrast, for the water-oil system with PAA, the energy remained relatively unchanged from 0.3-0.4 ns, suggesting minimal molecular movement after equilibration. This behavior aligns with the visualization shown in **Figure 10**, where the positions of oil and PAA molecules remained stable throughout the simulation.

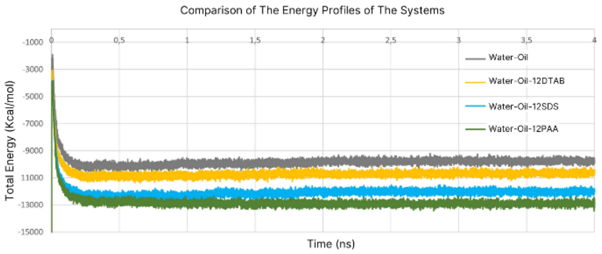

Fig 10. Comparison of the total energy profiles of all systems during the NPT and NVT simulations over a total duration of 4 ns.

Overall, the addition of surfactants and polymers successfully reduced the system's energy and increased stability. The water-oil system with PAA had the lowest total energy compared to the other systems. This is because PAA has carboxyl groups (-COOH) along its polymer chain that form hydrogen bonds with water. These hydrogen bonds make PAA highly soluble in water, creating a stable hydrophilic layer at the interface with the water phase (Shamilov *et al.*, 2017). Additionally, PAA contains a hydrophobic polymer chain consisting of carbon and hydrogen atoms, which tend to interact with oil. To further understand the effect of each surfactant or polymer molecule on the stability of the water-oil interface, the IFE values were calculated, as shown in **Table 3**.

Table 3. IFE values of the water-oil system with the addition of surfactants and polymer

System	IFE (Kcal/mol)
Water-oil-12DTAB	-48.53
Water-oil-12SDS	-178.33
Water-oil-12PAA	-231.78

3.3 Diffusion coefficient value analysis

The diffusion coefficient can explain how quickly a molecule moves or spreads within a medium (Wang & Hou, 2011). In this study, the diffusion coefficient value of oil is used as a reference to understand the effect of surfactants or polymers added to the water-oil system. To calculate the diffusion coefficient, displacement magnitude data obtained from LAMMPS trajectories of the NPT and NVT simulations were used. The trajectory data were then converted into a series of data with specific atom types and their displacement magnitudes using OVITO. Data for OH atoms from water molecules and CH atoms from oil molecules were extracted and processed using a Matlab script to generate a plot of displacement magnitude versus time. The slope of this plot represents the calculated diffusion coefficient value. The diffusion coefficient values for water and oil across all systems are shown in **Table 4**.

Table 4. Diffusion coefficient values for water (OH) and oil (CH) at the beginning and end of the simulation.

System	Diffusion Coefficient (Å^2/ps)	
	CH	OH
Water-oil	0.0100	0.0094
Water-oil-DTAB	0.0390	0.0107
Water-oil-SDS	0.0075	0.0097
Water-oil-PAA	0.0071	0.0179

To understand how the movement and position displacement of water and oil molecules change before and after adding surfactants or polymers, the oil diffusion coefficient is used as a reference. Thus, the effect of adding cationic surfactant DTAB, anionic surfactant SDS, and polymer PAA can be observed. As shown in **Table 4**, the diffusion coefficients of oil and water without the addition of surfactants or polymers were 0.01 and 0.0094.

When DTAB was added to the water-oil system, the oil and water diffusion coefficients increased. This was due to the interactions between DTAB, oil, and water, which caused oil and water molecules to move toward DTAB. **Figure 3** also shows this visually, with oil molecules appearing more disordered after adding DTAB. In contrast, when SDS was added, the water diffusion coefficient increased, but the oil diffusion coefficient tended to decrease. This was due to micelle formation, as shown in **Figure 5**, where SDS molecules were closely packed, forming clumps around hydrocarbon chains and reducing oil molecule diffusion.

Overall, both DTAB and SDS increased the water diffusion coefficient and contributed to emulsion formation. However, SDS did not improve the oil diffusion coefficient due to its tendency to form micelles. These results could vary under different simulation conditions, and reducing the number of SDS molecules may prevent micelle formation. Additionally, when PAA was added, the oil diffusion coefficient significantly decreased, while the water diffusion coefficient increased considerably compared to the surfactants. This is consistent with the high water affinity of PAA, which increases water viscosity, preventing reservoir alterations and maintaining a stable emulsion (Wang & Dong, 2009). The carboxyl groups on PAA are hydrophilic, explaining the significant reduction in oil diffusion when PAA is added.

Based on the analysis of the water and oil diffusion coefficients in this study, DTAB is more effective in increasing the oil diffusion coefficient compared to SDS. Although SDS lowers the IFE of the water-oil system and creates a more stable interface than DTAB, it does not enhance oil diffusion effectively. This is due to SDS's anionic nature, making it highly soluble in water (Tavakkoli *et al.*, 2022). Designing surfactants with better interactions with oil can be achieved by adding hydrocarbon chains to increase hydrophobicity. As a polymer, PAA enhances water diffusion more effectively than surfactants, indicating strong interactions with water molecules. Therefore, PAA is suitable for EOR applications requiring strong interactions with water.

4. Conclusion

The addition of cationic surfactant DTAB, anionic surfactant SDS, and polymer PAA to the water-oil system influenced the interface dynamics, as observed in molecular dynamics simulations. DTAB and SDS both increased disorder among oil molecules, but DTAB was more effective in altering the oil system's contour, while SDS formed micelles that restricted oil movement. PAA, with its hydrophilic carboxyl groups, primarily interacted with water, increasing water viscosity and stabilizing the interface. IFE analysis showed that DTAB, SDS, and PAA decreased system energy, enhancing stability, with IFE values of -48.53, -178.33, and -231.78 kcal/mol, respectively. PAA had the most significant energy reduction, indicating strong stabilization. Diffusion coefficients revealed that DTAB enhanced both water and oil diffusion, while SDS increased water diffusion but decreased oil diffusion due to micelle formation. PAA significantly reduced oil diffusion but increased water diffusion the most. Overall, DTAB promoted emulsion formation, SDS stabilized the interface without enhancing oil mobility, and PAA formed a thick, stable interface layer, demonstrating strong interactions with water.

Acknowledgements

This work was funded by the Directorate of Research, Technology, and Community Service, Ministry of Education, Culture, Research, and Technology

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