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Analysis of Surfactant and Polymer Behavior on Water/Oil Systems as Additives in Enhanced Oil Recovery (EOR) Technology through Molecular Dynamics Simulation: A Preliminary Study

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Abstract

The decline in oil production has led to the development of the Enhanced Oil Recovery (EOR) technology to increase oil production. Chemical injection is one of the methods in EOR by injecting surfactants or polymers into reservoir wells. To understand the properties and dynamics of surfactants and polymers at the nanoscale, computational studies using molecular dynamics simulation were carried out. In this study, surfactant Sodium Dodecyl Benzene Sulfonate (SDBS) and polymers such as Polyacrylamide (PAM) were used to investigate their effect on the oil-water interface system at the atomic level. Molecular dynamics simulation was carried out using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to calculate the diffusion coefficient and Interface Formation Energy (IFE) value for the addition of the surfactant and polymers. The simulation results show that the addition of the surfactant and polymers affects the water-oil interface system differently. The diffusion coefficient results indicates that there are strong interactions between SDBS and dodecane with D of 0.01358. While for PAM, the interactions with water are more significant with D of 0.059. The results of the IFE calculation value also show that the addition of SDBS and PAM makes the water-oil interface system more stable with the negative IFE value of -197.51 and -13.13 Kcal/mol respectively. The results of this study will be used as a reference and a basis for designing new surfactants or polymers that will led to more oil recovery.

INTRODUCTION

Fossil energy sources, especially petroleum, play an important role in fulfilling energy needs for the industrial and household sectors in Indonesia. The demand for petroleum will continue to increase until 2050, but oil production has inclined over the past decade due to the limited number of reservoir wells and new wells (Suharyati et al., 2019). To increase domestic oil and gas production, Enhanced Oil Recovery (EOR) method can be the answer. Chemical injection is one of the EOR technology that can increase oil production by 5-30% after the primary and secondary methods cannot produce oil anymore (Abidin et al., 2012).

Chemical injection is an EOR method by injecting water-soluble compounds such as surfactants, polymers, surfactant-polymers (SP), alkaline-polymer surfactants (ASP), and so on (Alvarado and Manrique, 2010). Surfactants were chosen as compounds in chemical injection because they have the ability to affect the water-oil interface and the properties of the rock surface (Zulkifli et al., 2020). As for polymers in chemical injection applications, they can change the viscosity of water due to their nature as thickening agents and change the mobility ratio, they also form a slug with oil, resulting in a better vertical and area sweep effect and the oil is pushed towards the production pump (Abidin et al., 2012).

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Various types of surfactants that are often used include anionic, cationic, non-ionic, and zwitterionic surfactants. The use of surfactants can increase the oil yield up to 9.11% in ionic surfactants (Massarweh and Abushaikha, 2020). Sodium Dodecyl Benzene Sulfonate (SDBS) is one of the anionic surfactants that is often used in EOR applications (Bera and Mandal, 2015). This surfactant has the capability to form microemulsions in oil and water systems which can reduce surface tension or interfacial tension (IFT) and also change the properties of rocks (Zulkifli et al., 2020; Bera and Mandal, 2015). Besides that, polymers commonly used in EOR applications include polyacrylamide (PAM), Partially hydrolyzed polyacrylamide (HPAM), and biopolymer Xanthan Gum (XG) [7]. Polyacrylamide (PAM) is the first polymer used as a thickening agent in EOR because of its relatively high molar mass [7]. PAM is generally used as a model for modification of polymer compounds in EOR applications by changing their structure or synthesising new acrylamide-based copolymers with improved properties such as shear resistance, brine compatibility, and temperature stability (Wever et al., 2011).

In addition to the great potential of surfactants and polymers in EOR applications, facts in the field show that there are still many results that are not optimal due to the unsuitability of the compounds used in the reservoir (Abidin et al., 2012). Things such as the partial charge of the molecule, the charge of the surfactant head, and the length of the surfactant tail can affect the interactions that occur in water-oil systems as well as rocks (Ahmadi et al., 2020). In addition, the rheological properties of polymers and problems of thermal, physical, chemical and bacterial degradation limit the application of polymers in EOR (Abidin et al., 2012). It is undeniable that there is still a need for better designs for surfactants and polymers to overcome the existing limitations and problems. For this reason, it is necessary to have a fundamental understanding of the properties, structure and dynamics of surfactants as well as polymers from the atomic level (Sun et al., 2020).

As technology develops, the computational method Molecular Dynamics (MD) is the right choice for studying the properties of liquid interfaces at the atomic level. In addition to providing information about atomic behaviour that cannot be obtained from experimental methods, this method also has the advantage of being able to visualise molecular dynamics at the molecular level (Wang et al., 2020). Several molecular dynamics studies conducted for surfactants and polymers include the properties of surfactants on oil and rocks (Tang et al., 2018; Tang et al., 2019; Zhou et al., 2021), the effect of surfactants on the water-oil interface system (Sun et al., 2020; Jang et al., 2004; Yang et al., 2020), studies polymer structure and dynamics (Ong et al., 2018; Nnyigide et al., 2021), and so on. Research with surfactant compounds studied the behavior of surfactants in water-oil interface systems with analyzes such as Interface Formation Energy (IFE), Interfacial Tension (IFT), Diffusion Coefficient values, and Radial Distribution Function (RDF) Jang et al., 2004; Xu et al., 2013; Meng et al., 2019). Research with polymer compounds tends to observe the properties of polymers by analysis such as the number of hydrogen bonds and RDF (Ong et al., 2018; Gurina et al., 2020).

Due to the lack of research comparing the properties of surfactants and polymers in water-oil interface systems, this research therefore analyses the effect of adding surfactants and polymers to the water-oil system through molecular dynamics simulations using the Large-scale Atomic/Molecular Massively application. Parallel Simulator (LAMMPS) with the selected surfactants and polymers are SDBS and PAM. The analysis carried out includes calculating the diffusion coefficient of oil and water molecules and calculating the IFE value for the oil-water system with and without the addition of SDBS and PAM.

MODELS AND METHODS

In this study, the size of the simulation box is 51x54x54 $Å^3$, which consists of a mixture of water molecules, oil molecules, and surfactant or polymer molecules. Here, dodecane is used to represent oil molecules while the surfactant and polymer is SDBS and PAM, as shown in Figure 1. A slab with 120 dodecane molecules and 2000 water molecules represents the water-oil system in the reservoir with variation %wt of SDBS and PAM in between, as shown in Table 1. The water model is from SPC/E, in which the bond lengths are constant through the use of the RATTLE algorithm. All the simulations were carried out under the GROMOS 54a7 force field (Schmid et al., 2011), and the cutoff distance is 12 Å. 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.

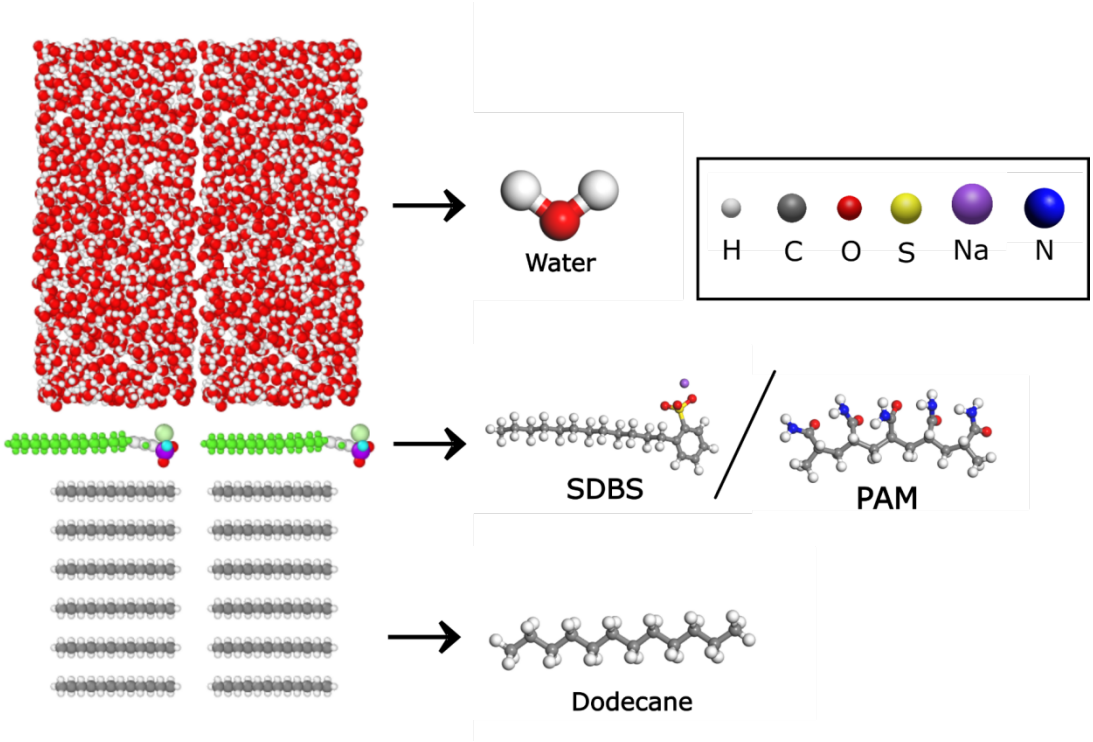

Figure 1. The simulation systems and the structures of water, dodecane, SDBS, and PAM.

Table 1. Simulation Model Variations

System	Dodecane		Water		Surfactant/Polymer	
	Total	%wt	Total	%wt	Total	%wt
Water-oil	120	36%	2000	64%	-	-
12-SDBS	120	34%	2000	59%	12	7%
12-PAM	120	34%	2000	59%	12	7%

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.

RESULTS AND DISCUSSION

Analysis of dynamics of oil-water interface systems with the addition of surfactants and polymers

Molecular dynamics simulations were carried out using the trajectory data generated during the simulation to observe the dynamics of the water-oil, water-oil surfactant, and water-oil polymer systems. Equilibration with the NPT ensemble was performed first to achieve a more normal volume and density of the system. The surfactant used is Sodium Dodecyl Benzene Sulfonate (SDBS) and the polymer used is polyacrylamide oligomer (PAM) with reference to research by Kendhale et al. (2006) with modification of the number of

monomers to 5 monomers and the end of the chain to one methyl. Figure 2 shows a simulated snapshot for 4 ns of a water-oil system.

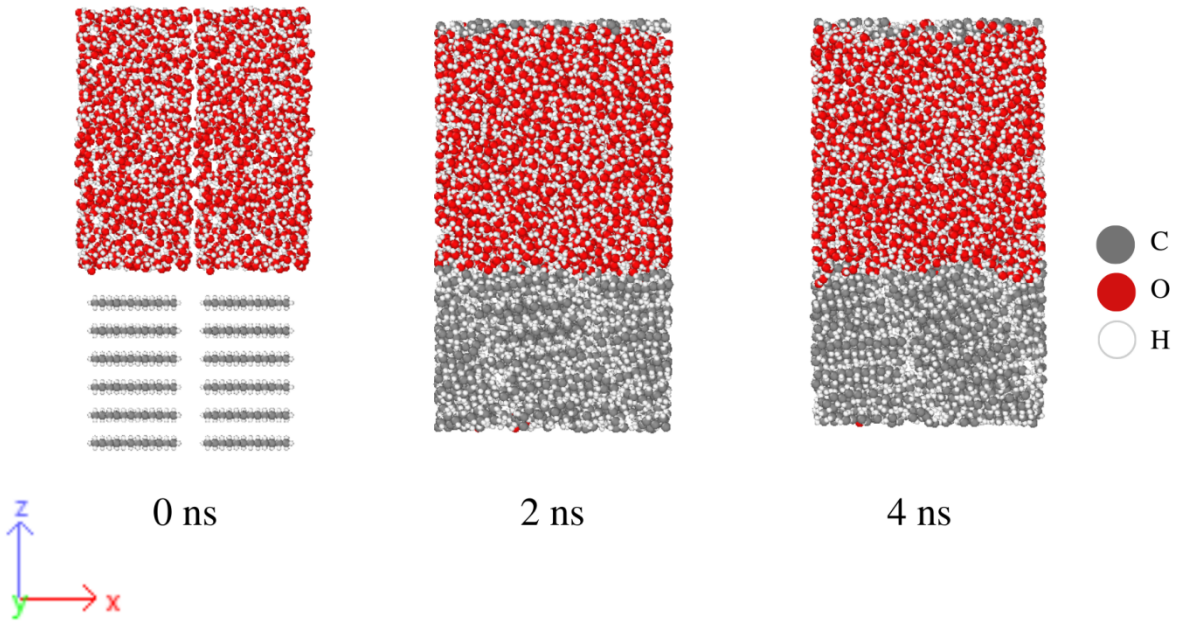

Figure 2. Visualization of simulated water-oil system for 4 ns. The red, white, and grey colours represent the O, H, and C atoms.

At the start of the simulation, the water and oil systems are spaced about 5 Angstroms in the z direction. Equilibration was performed in the NPT ensemble for 2 ns. During equilibration, the water and oil systems gradually combine to form a water-oil slab as the volume of the simulation box decreases. The volume of the simulation box at the end of the NPT equilibrium decreased from 47 x 54 x 83 Angstrom to 36.5 x 41.9 x 64.5 Angstrom. After the system was sufficiently equilibrated, NVT simulations were carried out for 2 ns to see the dynamics that occur in the water-oil system. As shown in Figure 2, not significant change was observed from the start of the NVT simulation at 2 ns to the end of the simulation at 4 ns at the oil-water interface system. Each system moves in its own region of the system and none of the molecules mix.

Molecular dynamics simulations were carried out for the water-oil-SDBS system shown in Figure 3. At the equilibrium stage, the water, oil and SDBS systems began to combine to form a water-oil-surfactant interface system as the volume of the simulation box decreased. The volume of the simulation box at the end of the NPT equilibrium decreased from 51 x 54 x 88 Angstrom to 38.6 x 40.9 x 66.7 Angstrom. Simulation time of 2 ns indicates an equilibrated system. NVT simulations over a continued 2 ns showed no significant change in the system except for small fluctuations of the positions of the water, oil and SDBS molecules. During the simulation, the water molecules tend to move and bind around the hydrophilic head groups of the surfactants while the dodecane molecules tend to move around the hydrophobic tails of the surfactants as shown in Figure 4. Those results represent the behaviour of hydrophilic molecules that love to interact with water and hydrophobic molecules that love to interact with oil.

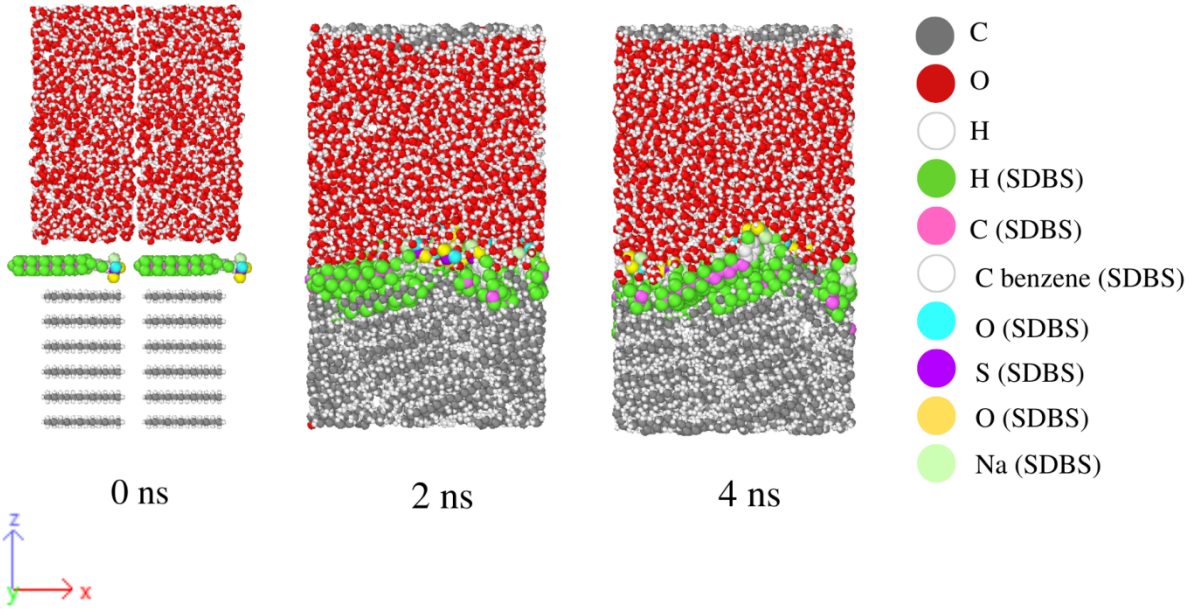

Figure 3. Visualization of molecular dynamics simulation on water-oil-SDBS system. The red, white, and gray colors represent O, H, and C atoms and the remaining colors represent SDBS.

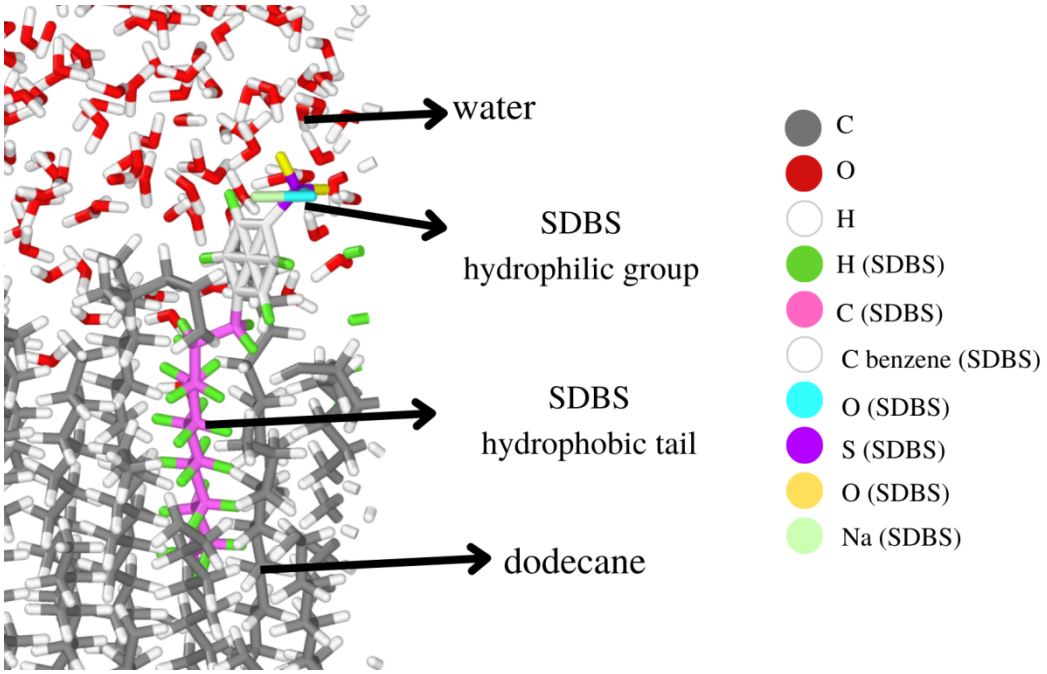

Figure 4. Visualization of the interactions between water, dodecane, and SDBS molecules.

The same simulation is carried out on the water-oil-PAM system shown in Figure 5. At the equilibrium stage, the water, oil, and PAM systems begin to combine to form an interface system from 0 ns to 2 ns simulation as the volume of the simulation box decreases. The volume of the simulation box at the end of the NPT equilibrium decreased from 47 x 58 x 93 Angstrom to 35.2 x 43.5 x 69.7 Angstrom. After the system was sufficiently equilibrated, further simulations were carried out with the NVT ensemble for 2 ns to see the dynamics that occur in the water-oil-PAM system. During the NVT simulation, no significant changes were seen in the water-oil-PAM system. Figure 6 shows the positions of the water, PAM, and dodecane molecules in the simulation. Water molecules tend to move and are attracted to the amide groups in PAM. This result

shows the hydrophilic properties of amide group of PAM, which tend to change the water properties rather than the oil properties.

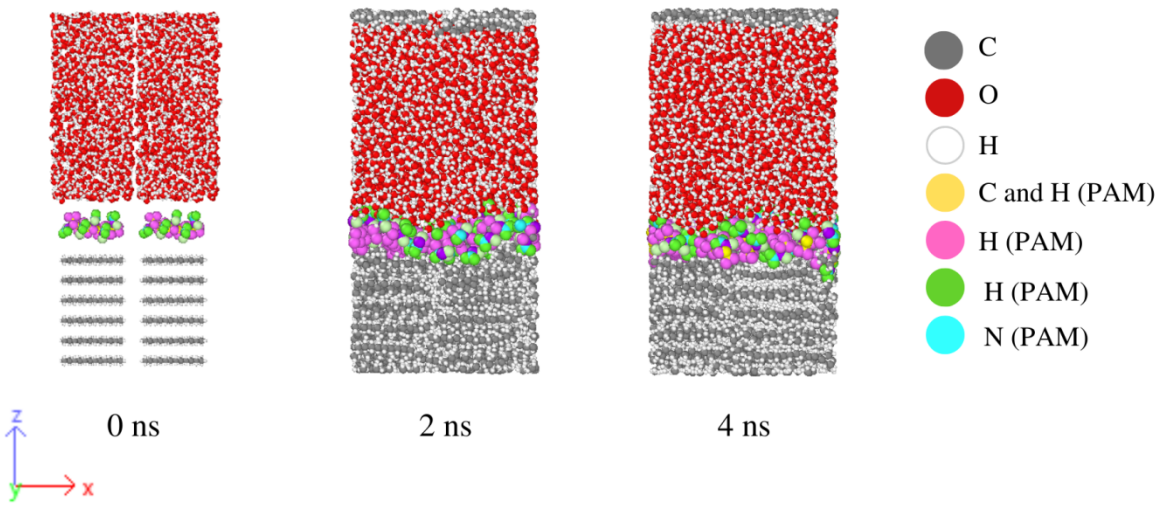

Figure 5. Visualization of molecular dynamics simulation on the water-oil-PAM system. The red, white and gray colors represent O, H and C atoms and the remaining colors represent PAM.

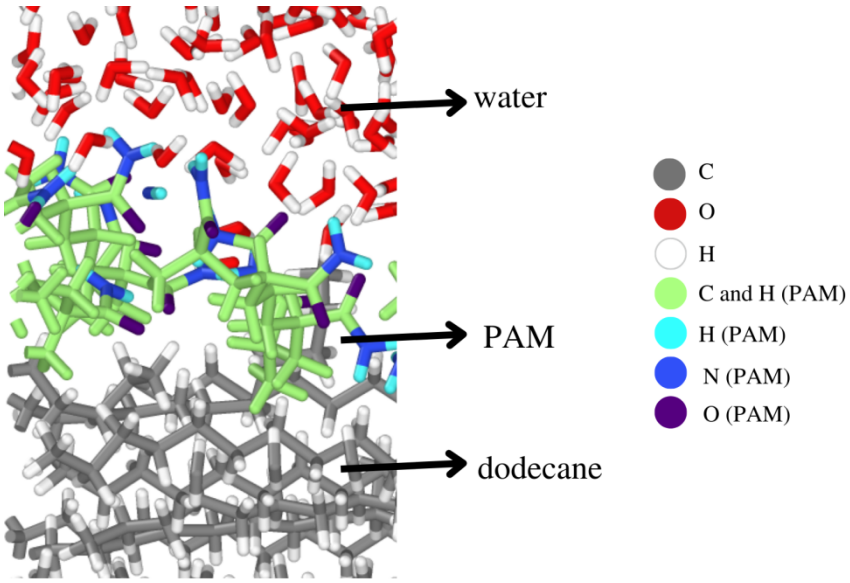

Figure 6. Visualization of the interactions between water, dodecane, and PAM molecules

As a comparison, Figure 7 shows the visualization of oil-water, SDBS-oil-water, and oil-water-PAM systems after the NVT simulation. The presence of SDBS molecules makes the position of dodecane even more random when compared to the water-oil system alone, as can be seen in Figure 7. This indicates that there are many interactions that occur between the hydrophobic tails of SDBS and dodecane molecules and shows a tendency to form the initial stage of microemulsions (Mahboob et al., 2022). As for the water-oil-PAM system, the presence of PAM molecules does not change the position of the dodecane molecules too much. This can be seen from the position of the dodecane molecules which are still arranged in a straight line as at the beginning of the simulation. The possibility that occurs is the presence of PAM molecules has more effect on water molecules due to their nature as thickening agents (Abidin et al., 2012).

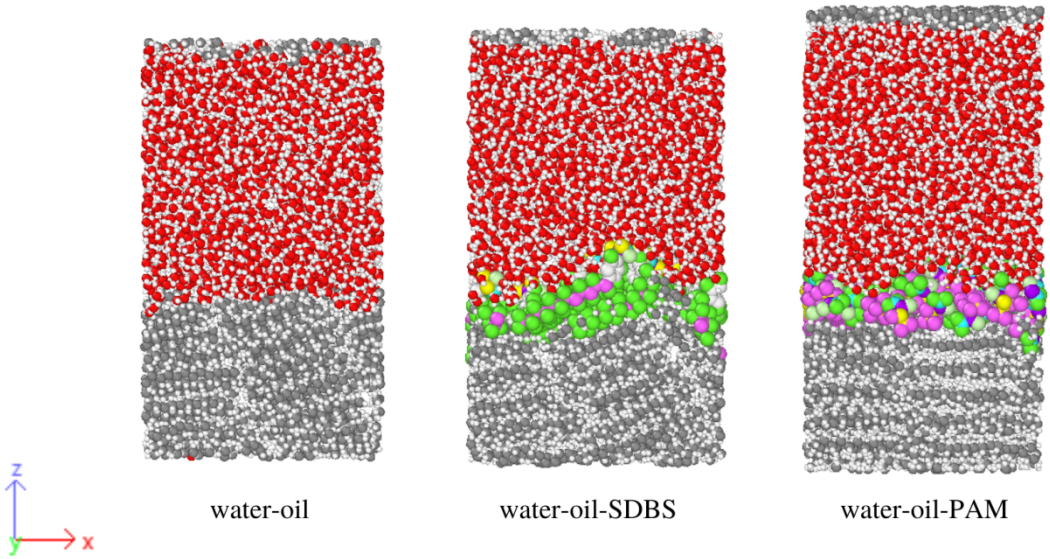

Figure 7. Visualization of all systems after NVT simulation

From the simulation results, the presence of surfactants and polymers affects the contours of the water-oil system, this indicates an interaction between the addition of surfactants and polymers to the water and oil. Qualitatively, surfactants and polymers can be designed so that they can interact a lot with the oil-water system which is indicated by the many changes in the visualization of the system during the simulation. But the visualization results are not enough to explain the phenomena that occur in more detail. For this reason, an analysis of the value of the diffusion coefficient through MSD calculations and IFE values of the three systems was carried out to support the visualization analysis of the simulation results in this study.

Diffusion coefficient value analysis

In this study, the data for calculating displacement magnitude values were obtained from the NVT simulated trajectory of 2 ns. The simulation data was obtained in the form of a LAMMPS Trajectory and then exported into a series of data containing the type of atom and its Displacement Magnitude value. The resulting data is then processed using the Matlab script with following equation.

$$Displacement(i+1) = \frac{\Sigma disp^2}{length(disp)} \quad (1)$$

where **i** is the name of the previously defined data file and **disp** is the previously obtained Displacement Magnitude value. Then a plot is made of resulting value from the equation against time and with the diffusion coefficient is one-sixth of the slope plot value (Wang and Hou, 2011). The value of the diffusion coefficient to be analyzed in this study is the value of the diffusion coefficient of dodecane and water to observe the behavior of dodecane and water upon the addition of SDBS surfactant and PAM polymer at the interface. The value of the diffusion coefficient can be used to describe how easily atoms or molecules move in a space per unit time. The values of the diffusion coefficients of dodecane (CH) and water (OH) for all systems are shown in Table 2.

Table 2. The value of the diffusion coefficient of dodecane (CH) and water (OH) in the simulation

System	Diffusion coefficient value (A^2/ps)	
	CH	OH
Water-oil	0.00945	0.055

Water-oil-SDBS	0.01358	0.056
Water-oil-PAM	0.00363	0.059

As shown in Table 2, there is an increase in the value of the diffusion coefficient of dodecane from 0.00945 to 0.01358 when surfactant SDBS was added to the water-oil system. This explains the phenomenon that occurs in Figure 7 where the presence of SDBS makes the position of dodecane even more random when compared to the water-oil system alone. This also indicates the tendency of dodecane molecules to move closer to the hydrophobic surfactant carbon chains. The presence of hydrophilic groups in surfactants also slightly increases the value of the water diffusion coefficient from 0.055 to 0.056 which indicates the tendency of water to move towards the hydrophilic groups.

In the water-oil-PAM system, the value of the diffusion coefficient for dodecane shows a decrease from 0.00945 to 0.00363 and the diffusion value for water shows an increase from 0.055 to 0.059 when compared to the water-oil system. This can explain the phenomenon in Figure 7 where the dodecane molecules do not seem to change their position much and indicate more interactions with water molecules.

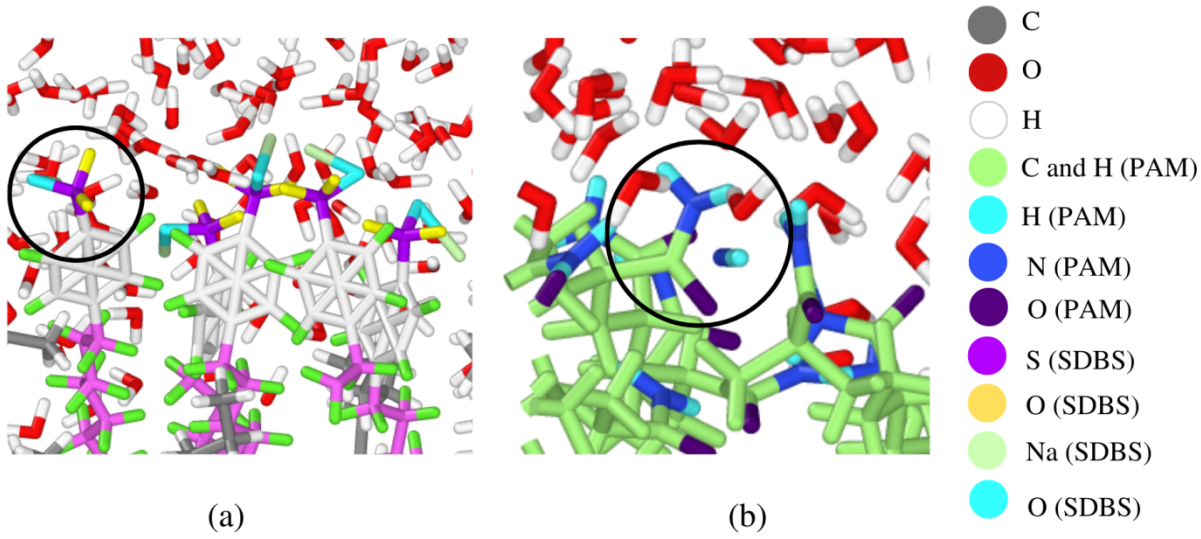

Figure 8. System visualization of (a) hydrophilic sulfonate groups in SDBS and (b) hydrophilic amide groups in PAM.

Figure 8 shows a comparison between the water-oil-SDBS and water-oil-PAM systems in a 15 Angstrom diameter slab to see the interactions with water and dodecane more clearly. In the water-oil-SDBS system, the difference in the separate surfactant structure between the hydrophilic and hydrophobic groups is clearly visible where the surfactant geometry were vertically aligned (Figure 8(a)). As for the PAM molecule, due to its structure which has amide groups on both sides, some of the amide groups are facing the dodecane molecule and some are facing the water molecule (Figure 8(b)). The sulfonate group in SDBS is shown with a black circle in Figure 8(a) while the amide group in PAM is shown with a black circle in Figure 8(b). The sulfonate group in SDBS and the amide group in PAM are groups that have hydrophilic or water-loving characteristics (Wang and Hou, 2011; Chusuei, 2018). This could explain the value of the diffusion coefficient of dodecane in PAM which is the smallest of all systems, namely because dodecane molecules do not interact much with the amide groups which are more hydrophilic so that the molecules do not move much. The presence of the amide group facing the water molecule can also explain why the value of the diffusion coefficient of water in the oil-PAM water system shows the largest number of all systems. In the same number of molecules, there are more amide groups in PAM than sulfonic groups in SDBS to bind with water. This is related to the properties of polymers in EOR applications, where polymers tend to change the properties of water as a thickening agent resulting in differences in the mobility ratio and oil will be more easily pushed (Abidin et al., 2012).

Analysis of the diffusion coefficient values of dodecane and water from the simulation results in this study can be used as a basis for designing surfactants and polymers with more appropriate interactions. From the simulation results, an increase in the value of the diffusion coefficient can be associated with a stronger

interaction that occurs between the surfactant or polymer and the observed molecule. In terms of surfactant interaction with oil, SDBS has advantages because it has a non-polar and hydrophobic benzene ring structure in its carbon chain, thereby increasing its interaction with dodecane when compared to other anionic surfactants such as SDS which only has aliphatic carbon chains. Because of this difference, the predicted value of the dodecane diffusion coefficient on SDS will have a smaller value than SDBS. To design a surfactant that interacts more strongly with oil, the surfactant can be modified to make it more hydrophobic with an indication of an increasing value of dodecane diffusion coefficient. In terms of surfactant interaction with water, because water is a polar compound, it will interact more with the polar surfactant head groups. SDBS itself has a higher polarity when compared to SDS (Meng et al., 2019), this can predict that the value of the water diffusion coefficient in SDS will not be as large as SDBS. To design a surfactant that wants to interact more strongly with water, the surfactant head group can be modified to have stronger polarity, such as replacing the metal atoms bonded in the SDBS head group with metal atoms that are more electropositive. The indication that will be seen is the increasing value of the water diffusion coefficient.

In terms of polymer interaction with the water-oil system, the analysis can be focused on looking at the value of the diffusion coefficient of water because the addition of polymer in EOR applications is aimed at changing the properties of water where the polymer functions as thickening agents which can increase the viscosity of water (Abidin et al., 2012). PAM has polar amide groups which will interact a lot with water. To design polymers that interact stronger with water, polar groups can be added to polymer compounds, for example by increasing the molar mass of PAM or changing PAM to HPAM. HPAM has an anionic group that has a higher polarity because there are ionic bonds in it so it is predicted that it will interact more strongly with water which causes an increase in the value of the diffusion coefficient in water.

Analysis of Interface Formation Energy (IFE) values

IFE value analysis was used to see the effect of adding one molecule of surfactant/polymer to the water-oil interface system. In principle, the more negative the IFE value, the more thermodynamically stable the system (Zulkifli et al., 2020; Jang et al., 2004). The formula for calculating the IFE value is following equation (2) with the energy value used is the energy value obtained during the simulation using the NVT ensemble. The energy value of each system is shown in Table 3 below.

$$IFE = \frac{E_{total} - (E_s + E_{am})}{n} \quad (2)$$

where **Etotal** is the energy of the system, **Es** is the energy of one surfactant or polymer, **Ewo** is the energy of a water-oil system, and **n** is the amount of surfactant or polymer in the system (Sun et al., 2020; Ong et al., 2018). The IFE value is used to calculate the average value of adsorption energy per surfactant molecule at the water-oil interface (Gurina et al., 2020). The IFE value is also used to see the stability energy at the interface system (Gurina et al., 2020; Schmid *et al.*, 2011; Kendhale et al., 2006). The energy value of each system is shown in Table 3 below.

Table 3. System energy value in NVT simulation

System	Energy (Kcal/mol)
1 molecule PAM	-49.38
1 molecule SDBS	-217.72
Water-oil	-10442.99
Water-oil-12SDBS	-13030.83
Water-oil-12PAM	-10818.26

From Table 3 we can see that the addition of SDBS molecules as well as PAM shows a tendency for the system energy to decrease to become increasingly negative. The difference in energy trends during the simulation is also shown in Figure 9. At the beginning of the simulation, the energy is still high, indicating that the system is still unstable and convergent. In the simulation time of 0-300 ps, the energy starts to decrease and reaches a convergent state at the simulation time of 500 ps and so on with the addition of SDBS and PAM to the system, the energy graph becomes stable faster than the water-oil system. The system with the lowest energy value is shown by the orange-colored line belonging to the water-oil-SDBS system, followed by the water-oil-PAM system and the water-only system which are depicted by the blue and gray lines, respectively. This indicates that the addition of surfactant makes the system energy more stable. To prove this, the IFE value is calculated to see the effect of one surfactant or polymer molecule on the interfacial stability shown in Table 4.

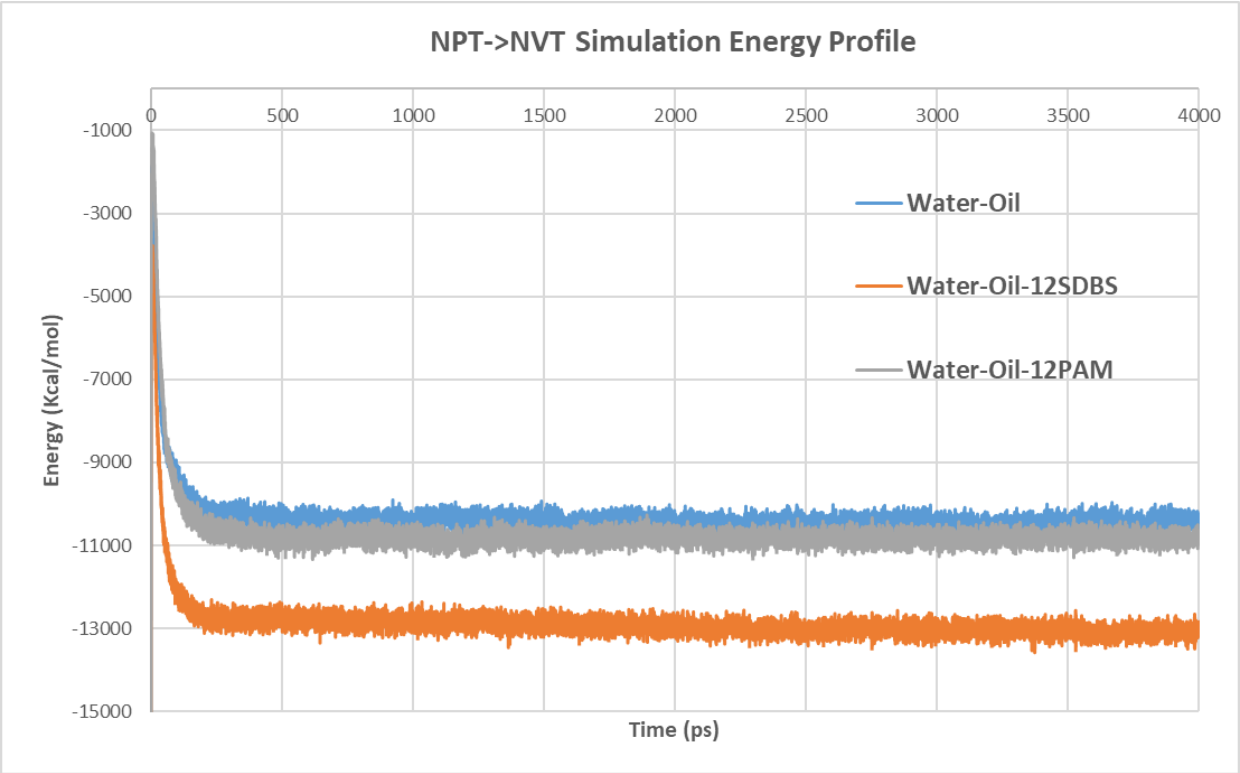

Figure 9. System energy profile on simulation

Table 4. IFE value from the addition of SDBS and PAM

System	IFE (Kcal/mol)
Water-oil-12SDBS	-197.51
Water-oil-12PAM	-13.13

The IFE value from the addition of SDBS shows the most negative value with value of -197.51 Kcal/mol indicating the most stable interface system. This is in accordance with one of the functions of surfactants, namely as a stabilizer in emulsions (Zembyla et al., 2020). The tendency of SDBS to form emulsions can also be seen from the system visualization in Figure 3 as well as from the results of the dodecane diffusion coefficient in the water-oil-SDBS system which is the highest. An increasingly negative IFE value indicates an easier interface system to form (Li et al., 2017). As for the IFE value of the water-oil-PAM system, it shows more positive value than the water-oil-SDBS system with -13.13 compare to -197.51 Kcal/mol respectively. This shows that PAM could form emulsions that are not too strong when compared to SDBS and the addition of PAM polymer is more intended to change the properties of water and push oil towards the production

pump, as indicated by the diffusion coefficient result in Table 2. The IFE value can also be used to explain the strength of the interaction between surfactants and polymers in water-oil systems, where the more negative the IFE value, the more interactions that occur (Xu et al., 2013). The most negative value for the water-oil-SDBS system indicates the higher number of interactions between SDBS with water and oil when compared to the more positive IFE value of PAM where PAM only interacts a lot with water.

Analysis of IFE values in this simulation are more suitable to be used as a basis for designing surfactants with better performances. This is because besides being able to describe the stability of the addition of a molecule, the IFE value can also be used to see the strength of the intermolecular interactions between molecules added with water and oil, where surfactants significantly interact with both. The strong interaction that occurs between surfactants and water and oil, which is indicated by the increasingly negative IFE value, can also be interpreted by the greater potential of surfactants in reducing the value of the interfacial tension of the water-oil system (Xu et al., 2013). Therefore, surfactants can be designed by strengthening the hydrophobic nature of the carbon tails and the hydrophilic nature of the head group so that an increasingly negative IFE value will be obtained.

CONCLUSION

Analysis of system dynamics through visualization of molecular dynamics simulation results shows the tendency of SDBS surfactants to interact and change the contours of the oil system due to the influence of the hydrophobic chains which also attract water molecules to the hydrophilic head groups forming the initial stage of microemulsion formation behaviour. The addition of the PAM polymer does not appear to have much effect on the contours of the oil system, but its amide group has the potential to change the property of water in an oil-water system. The value of the diffusion coefficient of dodecane for water-oil, water-oil-SDBS, and water-oil-PAM is 0.00945; 0.01358; and 0.00363 Å2/ps and the value of the water diffusion coefficient respectively is 0.055; 0.056, and 0.059 Å2/ps. The trend of increasing the value of the diffusion coefficient of dodecane in the water-oil-SDBS system shows the many interactions that occur between SDBS and dodecane molecules and the increasing value of the diffusion coefficient of water in the water-oil-PAM system shows the many interactions that occur between water and PAM. Analysis of the IFE value on the addition of SDBS and PAM molecules showed a tendency for negative values of -197.51 and -13.13 Kcal/mol respectively, indicating that their addition made the water-oil interface system more stable. In this case, SDBS with the most negative IFE value shows great potential to form a water-oil interface system which leads to the formation of microemulsions. The results of research on dynamics analysis, diffusion coefficient, and IFE values from the addition of SDBS surfactants and PAM polymers in changing the water-oil interface properties can be used as a reference as a basis for designing surfactants or polymers for future EOR applications.

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