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MOLECULAR DYNAMICS STUDY OF OLEIC ACID-BASED SURFACTANTS FOR ENHANCED OIL RECOVERY

STUDI MOLEKULAR DINAMIK SURFAKTAN BERBASIS ASAM OLEAT UNTUK PENINGKATAN PENGURASAN MINYAK

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ABSTRAK

Surfaktan telah secara luas digunakan dalam teknologi Enhanced Oil Recovery (EOR). Hanya dengan adanya isu tentang lingkungan menjadikan surfaktan kurang disukai, sehingga surfaktan yang mudah terdegradasi di dalam lingkungan menjadi pilihan yang tepat untuk menjadikan lingkungan lebih aman. Bagaimanapun pemilihan surfaktan yang mempunyai kinerja bagus memakan waktu yang cukup lama dan biaya yang tidak sedikit. Simulasi Molekular Dinamik (MD) adalah salah satu alternatif untuk menurunkan biaya dan waktu seleksi surfaktan. Dalam studi ini, surfaktan berbasis asam oleat yang dikombinasi dengan variasi panjang rantai polietilen glikol dievaluasi. Surfaktan yang potensial dipilih menggunakan simulasi MD untuk mengevaluasi kemampuan surfaktan dalam menurunkan tegangan antarmuka (IFT) antara minyak dan air, yang merupakan salah satu parameter yang penting untuk EOR untuk mengemulsi minyak. Simulasi MD dilakukan menggunakan software GROMACS dengan Gromos force field dan model air SPC. Ujung karboksil asam oleat digantikan dengan panjang rantai polietilen glikol yang berbeda. Keseluruhan simulasi MD disiapkan dalam campuran oktadekana-air pada rentang suhu 303 – 363 K. Hasil simulasi menunjukkan bahwa peningkatan jumlah polietilen glikol tidak selalu diiringi dengan penurunan IFT antara air dan oktadekana. Hasil tersebut divalidasi dengan data pengujian di laboratorium dan menunjukkan profil yang sama. Simulasi emulsi minyak menunjukkan bahwa semua sampel surfaktan mempunyai kinerja dan kestabilan yang baik seperti ditunjukkan pada kecepatan emulsi dan kestabilan emulsi pada berbagai suhu. Pengujian terakhir yang dilakukan adalah uji wettability. Hasil simulasi menunjukkan bahwa kedua surfaktan, Oleat-PEG100 dan Oleat-PEG400 dapat mengubah kebasahan batuan dari oil-wet menjadi water-wet. Dari seluruh hasil studi didapatkan bahwa Oleat-PEG400 merupakan kandidat surfaktan terbaik dengan kinerja terbaik.

Kata Kunci: *surfaktan, asam oleat, etilen glikol, interfacial tension, emulsifikasi, oktadekana, simulasi molekular dinamik.*

ABSTRACT

Surfactants have been intensively used for Enhanced Oil Recovery (EOR). Nevertheless, environmental issues cause some surfactants to become unfavored in EOR application. Biodegradable surfactants are the suitable choice to make the environment safer. However, screening surfactants that have a good performance for EOR are time-consuming and costly. Molecular Dynamics (MD) simulation is an alternative solution to reduce cost and time. In the present study, oleic acid-based surfactants that combined with the various length of polyethylene glycol were studied. The potential surfactants were screened by MD simulation to evaluate their ability to reduce the Interfacial Tension (IFT) between oil and water layers, which is the critical parameters for EOR, and their ability to emulsify oil molecules. MD simulations were performed by GROMACS software with Gromos force field and SPC water model. Carboxyl-terminal of the oleic acid was substituted by a different length of polyethylene glycol. All MD simulations were prepared in octadecane–water mixture with temperature ranges of 303-363 K. Our simulations found that the increasing number of polyethylene glycol was not always followed by the decreasing of IFT value between octadecane and water layers. These results were validated with the experimental data and found the similar IFT profile. The simulation of oil emulsification showed that all surfactant samples have good performance and stability as exhibited by their emulsification rate and emulsion stability in different temperatures. The last test to get the best surfactant was the wetability test. The simulation gave the result that both PEG_{100}-oleic and PEG_{400}-oleic were able to change wetability of rocks from oil-wet to water-wet. Accordingly, PEG_{400}-oleic is the best nonionic surfactant candidate due to its performance in each simulation test.

Keywords: surfactant, oleic acid, ethylene glycol, interfacial tension, emulsification, octadecane, molecular dynamics simulation

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I. INTRODUCTION

EOR process is done through several extraction stages, namely primary, secondary and tertiary extraction (Yela et al. 2016). At primary extraction, the oil is lifted from the well to the surface using energy in the reservoir. However, the energy is not always enough to lift the oil. At this point the mechanical method is still needed by pumping or by gas injection. This method of extraction is able to provide as much oil gain 12–15% from *Original Oil in Place* (OOIP).

The second extraction stage is performed by injecting water or gas in order to increase crude oil mobility. Water helps oil move, then gas injection provides additional thrust force so as to add 10-15% oil removed. Bachman, et al. (2014) mentioned that this second extraction can increase oil yield up to 40-50%. This condition shows that about half of the total crude oil is still trapped in the pores of rocks in the reservoir. Therefore, after the second extraction process it is still necessary to perform further extraction steps to increase oil recovery.

The third extraction step is also called the EOR method carried out through thermal processing, gas injection, and flooding with chemical compounds. The thermal process may involve water vapor or flammable gas to increase the temperature in the reservoir. Thermal processing and gas injection aimed like cracking so that the oil is easier to flow. The addition of chemicals aims to reduce surface tension in the reservoir. The chemical used in the EOR may be a hydrocarbon solvent, a synthetic surfactant, a polymer, a gas or a combination of such substances. This third stage of extraction can increase the amount of oil raised by 5-25%. However, this third stage of extraction is considered uneconomical and even harmful to the environment, so it is necessary to find a more economical and environmentally friendly alternative to chemicals (Perfumo et al. 2010).

The surfactant criteria for EOR and how the election is described in the review (Negin et al. 2017). The stability and effectiveness of a surfactant should be able to withstand temperature, pressure, divalent metal content, and high salinity. This can be achieved by choosing the appropriate chemicals in terms of both types and quantities. The type and quantity of chemicals in the surfactant formula can also affect the stability of emulsion and viscosity, the change of wetness of the rock and the ability to reduce IFT.

In many literatures it is mentioned that the IFT is one of the important factors in the selection of EOR surfactant candidates. This has been suggested by Cayias et al. (1977) and Touhami et al. (1998). IFT is a quantitative index of the behavior of molecules at a two-fluid interface that determines the stability and performance of the interface. If IFT increases then the two-fluid interface becomes stronger and vice versa until nothing can dissolve between the two fluids. Typically, IFTs have mN/m or dyne/cm units (Meybodi et al. 2016).

Of all surfactant groups, nonionic and cationic surfactants are the most influential surfactants in reducing the interface voltage values (Mosayebi, et al. 2016). The widely used commercial EOR surfactants such as sulfonic acid and its (anionic) salts, alpha-olefin sulfonates (anionic), ethoxylated ethoxylates (nonionic) and ethoxylated ethylenzenes are IFT-derived surfactant surfactants. The PEGn-oleate surfactant used in the present study belongs to an ethoxylated alkyl alcohol type.

In addition to reducing IFT values, surfactants should also be able to form microemulsions at the water-oil interface. The formation of this microemulsion which contributes to the reduction of IFT value from oil-water. With so many criteria to be met by surfactant candidates, the cost to be incurred will be very expensive and the experiment time becomes very long. Therefore, it needs an approach that can reduce the cost and time that is through the molecular dynamics simulation approach.

Molecular dynamics (MD) simulation is a computational approach used to simulate complex systems with modeling at the atomic level. MD simulation is one method that is done to model the real state of the system by taking into account the interactions between atoms. By using the MD simulation, phenomena occurring at the atomic level are used to explain real phenomena in various fields. The energy in the MD simulation is calculated using an atomic force field model containing information on antagonic interaction calculations in complex systems (Meller 2001). The use of MD simulations has been very extensive including physics, chemistry, biology, and pharmacy (Berendsen et al. 1995). In addition, MD simulations have also been used in the fields of petroleum and natural gas (Pal et al. 2018). The MD simulation in the oil field has been used to calculate the IFT value (Liu et al. 2017; Wang et al. 2018), emulsion formation (Lowry et al. 2016) and changes in wetness of the rocks (Zhang et al. 2017; Zhou et al. 2018).

The aim of this research is to get candidate of oleic acid based nonionic surfactant through simulation approach of molecular dynamics. The selected surfactants are combination of oleic acid with various length of polyethylene glycol.

II. METHODOLOGY

A. Structures Preparation

Structure of octadecane as oil model and all the surfactants was sketched by Marvin Sketch 18.10 and saved in MDL molfile format. All those structures then convert using PRODRG server (Schuttelkopf, A.W and van Aalten, D.M.F. 2004) and generating three files with .pdb, .gro and .itp format. We have choosen polar/aromatic's H option in PRODRG converted structure result.

In order to calculate IFT value, the molecules of water, oil, and surfactants were packed in a simulation box using PACKMOL (Matinez et al. 2009). The surfactants molecules were put at the water/oil interface. Meanwhile, in the emulsifying simulation, all the structures were packed using GROMACS. Diagram of the box simulation show in Figure 1.

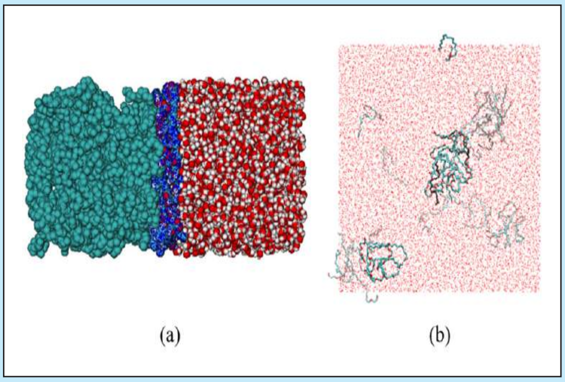

Figure 1
Simulation box for (a) IFT calculation and (b) Emulsifying ability test.

B. Simulations Details

All simulations were carried out using GROMACS 2016 (Berendsen et al. 1995 and Abraham et al. 2015). Energy minimization proccesses were performed twice using steepest descent algorithm with and without define the position restraint respectively. Electrostatic interaction were treated with Particle Mass Ewald with a cut-off 1.0 nm. All bond were constraint with LINCS algorithm to make the 2 fs time step can be used. The force field for all simulations were GROMOS 54A7 FF (Schmid et al. 2011). Visualization of trajectory is using VMD (Humprey et al. 1996).

C. IFT Measurement

To validate the simulation results, IFT measurement in the laboratory was performed by using Spinning Drop Tensiometer TX-500 C/D at reservoir temperature, 60^{o}C. IFT tube was filled with surfactant solution and injected with crude oil as much as 2 μL. The tube was put and run at rate 6000 rpm. Density difference between oil and surfactant was required to calculate the IFT value.

D. Wettability Analysis

One of the role of surfactant to alter the core wettability was evaluated by conducting wettability analysis through contact angle measurement. Preparate core on glass was soaked with formation water for two weeks followed by soaking core with surfactant solution. Contact angle of target core soaked with surfactant and without surfactant were compared to observe the effect of surfactant on wettability changes. Contact angle was measured by using THETA Optical Tensiometer basic system. Preparate core was put on the sample bench and crude oil was pull in. Crude oil was then dispense at one drop on the core surface. The contact angle between core and oil was measured and recorded.

III. RESULTS AND DISCUSSION

The first screening of surfactant candidate to be performed is the surfactant's ability to reduce the IFT value of the oil-water. This filtering is carried out at 90°C in the hope that at high temperatures there can be a noticeable difference in the decrease in IFT values between one surfactant candidate and another surfactant candidate. IFT values for the PEG-oleate group can be seen in Figure 2. From the figure, there are two best surfactant candidates because they have a similar IFT value of PEG_{100}-Oleate and PEG_{400}-Oleate. Both lowered IFT values by 3.99 and 4.08 dyne / cm respectively. This IFT decline, in experiments for PEG_{400}-Oleate can reach 10^{-3} dyne / cm. The decrease in IFT values in the simulation looks small because in a MD simulation there are some parameters that are not calculated or an approximation. In addition, the number of particles used in the simulation can not match the number of particles under experimental conditions that are surely far more numerous. However, qualitatively the MD simulation can confirm the experimental results and is expected to predict the experimental results that have not been done. Of the two best PEG-oleate surfactant candidates, only PEG_{400}-Oleate has been experimentally performed while PEG_{100}-Oleate has not been performed because PEG_{100} is not sold in the market.

EOR surfactant candidates must have high temperature resistance. The best candidates of the first stage of PEG_{100}-Oleate and PEG_{400}-oleate were tested for their stability in the 30 to 90°C temperature range. IFT drop-off data on the temperature range can be seen in Figure 3.

As IFT values decrease at various temperatures as shown in Figure 3, these two surfactant candidates

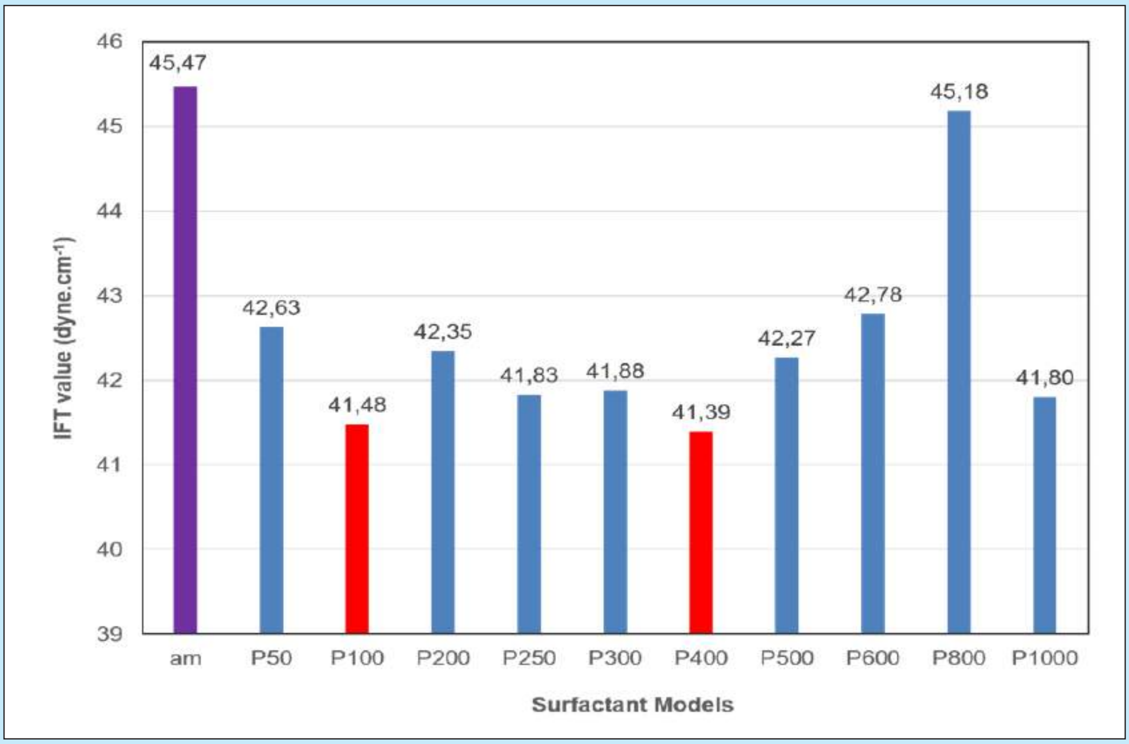

Figure 2
IFT value of PEG-oleate at temperature 90°C.

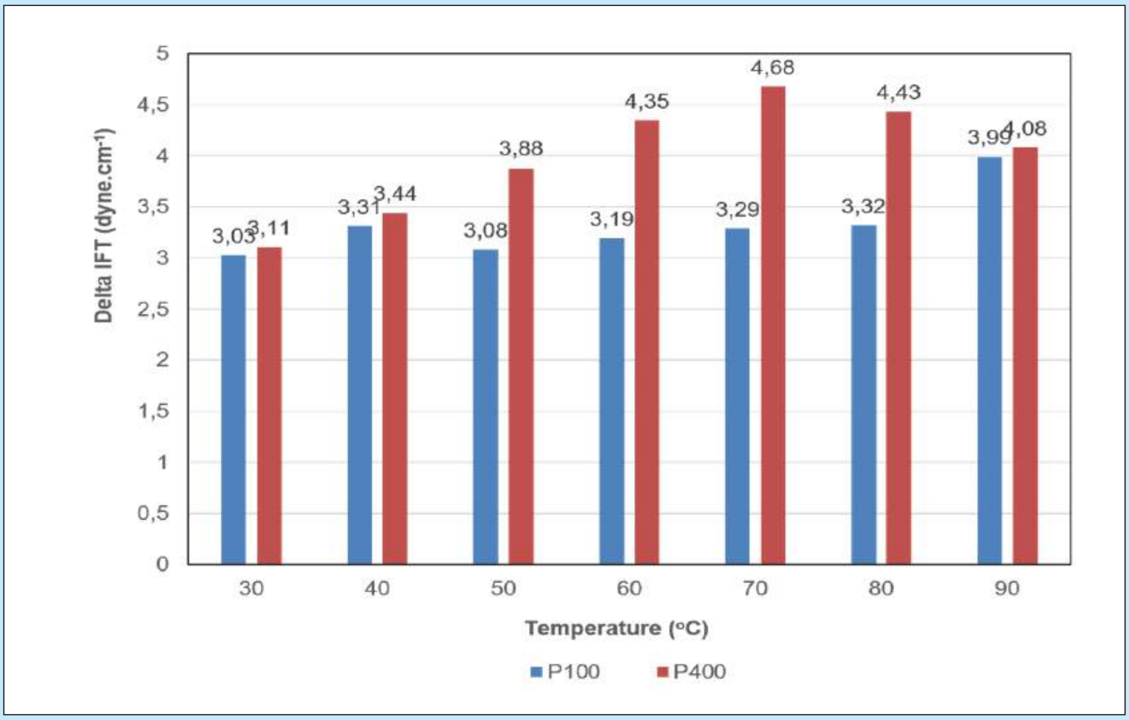

Figure 3
IFT drop data at various temperatures.

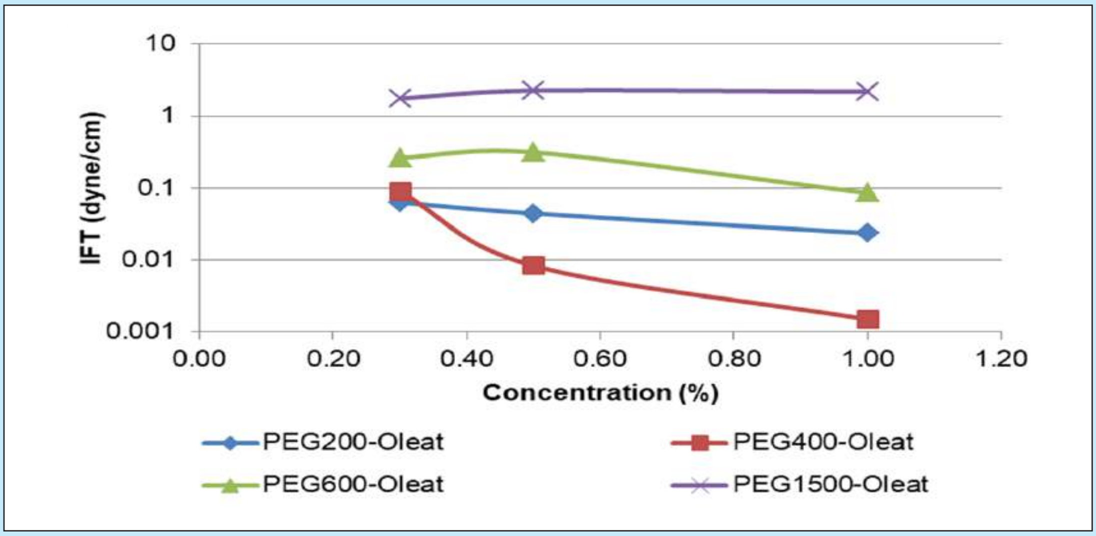

Figure 4
Laboratory results of IFT measurement of PEG-based surfactants

have sufficient stability within the temperature range. However, the best performance was demonstrated by PEG_{400}-Oleate at 70°C with an IFT reduction of 4.68 dyne / cm.

In order to validate the results of IFT simulation of nonionic surfactants at different hydrophilic group, the IFT measurement in the laboratory using Spinning Drop Tensiometer TX-500 C/D at 60^{o}C were conducted. Various surfactant from PEG_{200}-Oleate until PEG_{1500}-Oleate at various concentration in salinity 17000 ppm were measured and displayed on Figure 4. As can be seen from the Figure 4, the

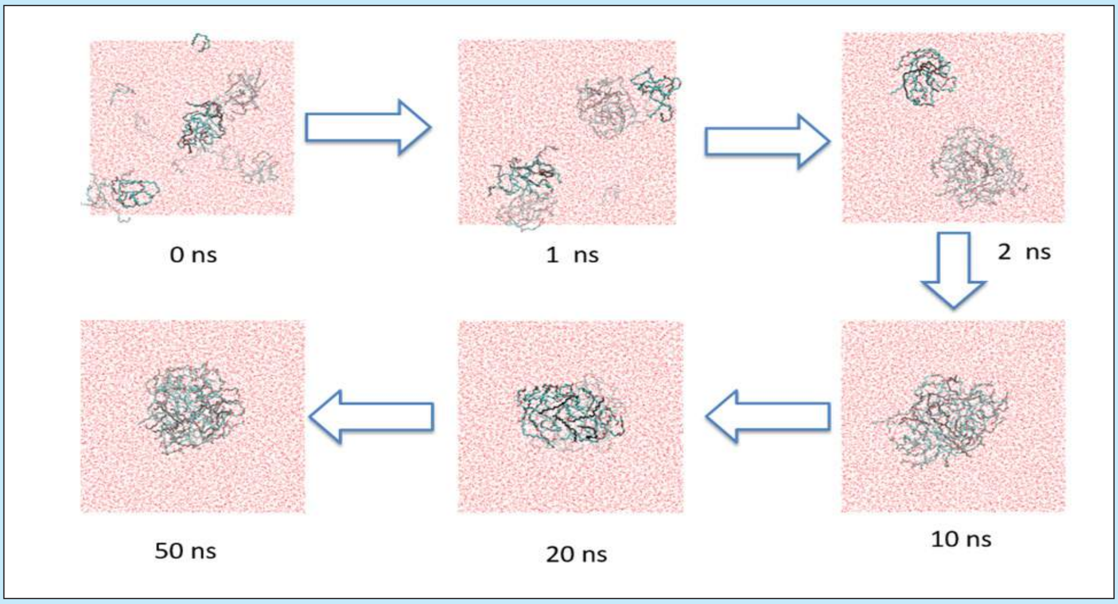

Figure 5
Emulsification process of PEG$_{100}$–oleat.

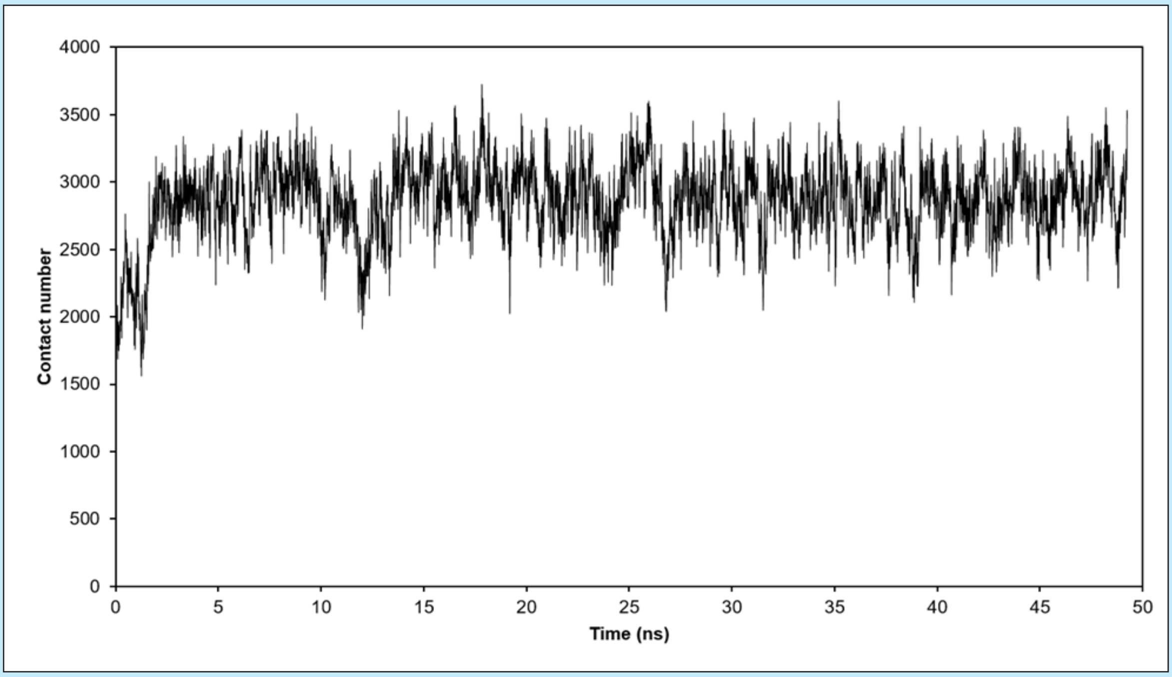

Figure 6
Contact number between PEG$_{100}$–oleat and octadecane.

IFT of PEG$_{400}$-Oleate has the lowest IFT between all PEG-based nonionic surfactans. This IFT result confirming the simulation study that the best candidate for lowering IFT of oil and water was PEG$_{400}$-Oleate.

The next test process conducted on surfactant candidate is a test of oil emulsifying ability. Visual analysis using VMD 1.9.3 software. From the simulation results of molecular dynamics it is known that both PEG$_{100}$-oleate and PEG$_{400}$-oleate can form emulsions with oil. The visualization of the emulsion formation process by PEG_{100}-oleate can be seen in Figure 5. The red color in the image represents the water molecule, the black color representing the oil and the color of cyan representing the surfactant.

The emulsion formation process occurring on a system containing PEG_{100}-oleate begins with the formation of several separate emulsions as shown in Figure 5 with a simulation time of 1 ns and 2 ns. After passing 2 ns, the emulsion formed merges to form one emulsion and stable until the end of the simulation. The number of contacts between the PEG_{100}-oleate molecule and the oil is shown in Figure-6. Considering the amount of contact formed between PEG_{100}-oleate and the oil molecule, it is known that the emulsion has stabilized since before 3 ns. The average number of contacts between PEG_{100}-oleate and oil is about 3000 contacts. The presence of fluctuations occurring at the number of contacts indicates that the emulsion is dynamic.

Emulsion formation that occurs on systems containing PEG_{400}-oleate has a faster rate than PEG_{100}-oleate. When viewed from the snippet in Figure 7, the emulsion has been formed since the simulation time of 1 ns. This emulsion lasts until the end of the simulation (50 ns). By looking at the shape and position of the emulsion at 3, 8, 36, and 50 ns it can be seen that the emulsion is dynamic so that the shape and position change in the simulation box. This is because the surfactant not only interacts with oil but also with water molecules present in all parts of the simulation box.

The average number of contacts formed by PEG_{400}-oleate with more oil than PEG_{100}-oleate is 3500 contacts. Figure 8 shows the number of contacts. Through the data the number of contacts in Figure 8 can strengthen the visualization data that the emulsion formation process has occurred since about 1 ns simulation time. Thus, PEG_{400}-oleate can be said to be a better surfactant candidate because it has a faster emulsion-forming rate and has more contacts than PEG_{100}-oleate.

The last test done to get the best surfactant candidate is the ability of surfactants to change the wetness of rocks. Analysis of this test uses VMD software. Figure 9 shows the process that occurs in a simulation box containing PEG_{100}-oleate over a span of 1 ns. The red yellow color shows an image

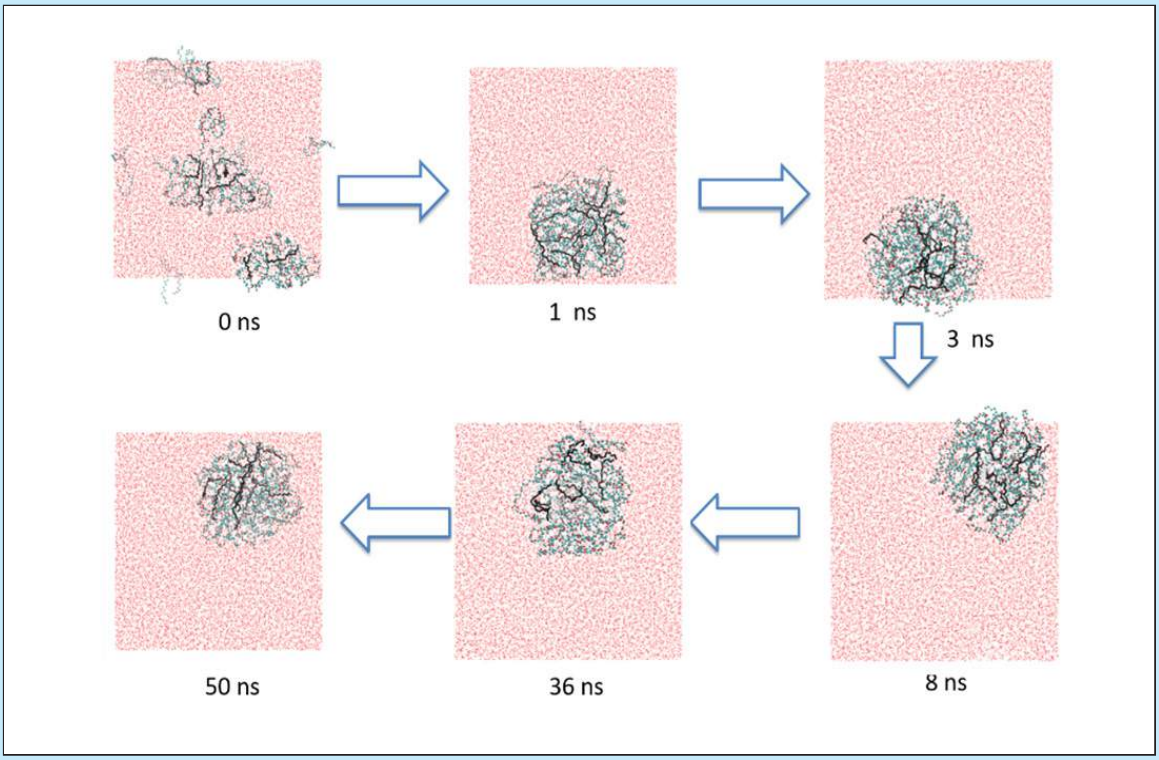

Figure 7
Emulsification process of PEG_{400}–oleat.

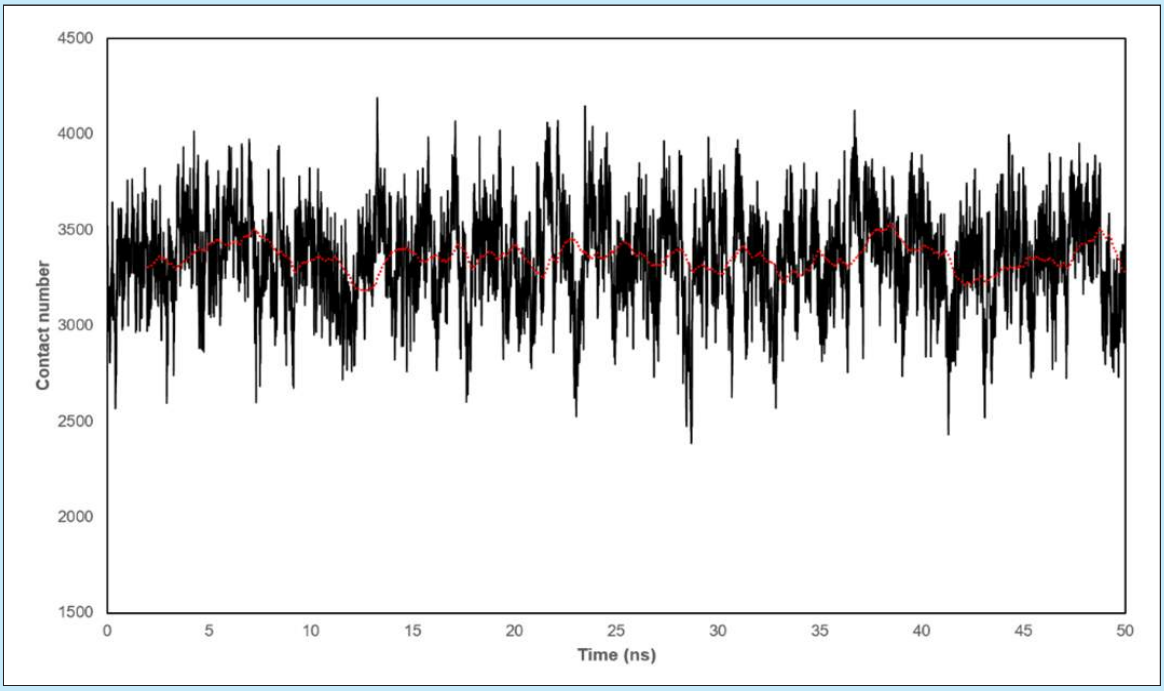

Figure 8
Contact number between PEG_{400}–oleat and octadecane.

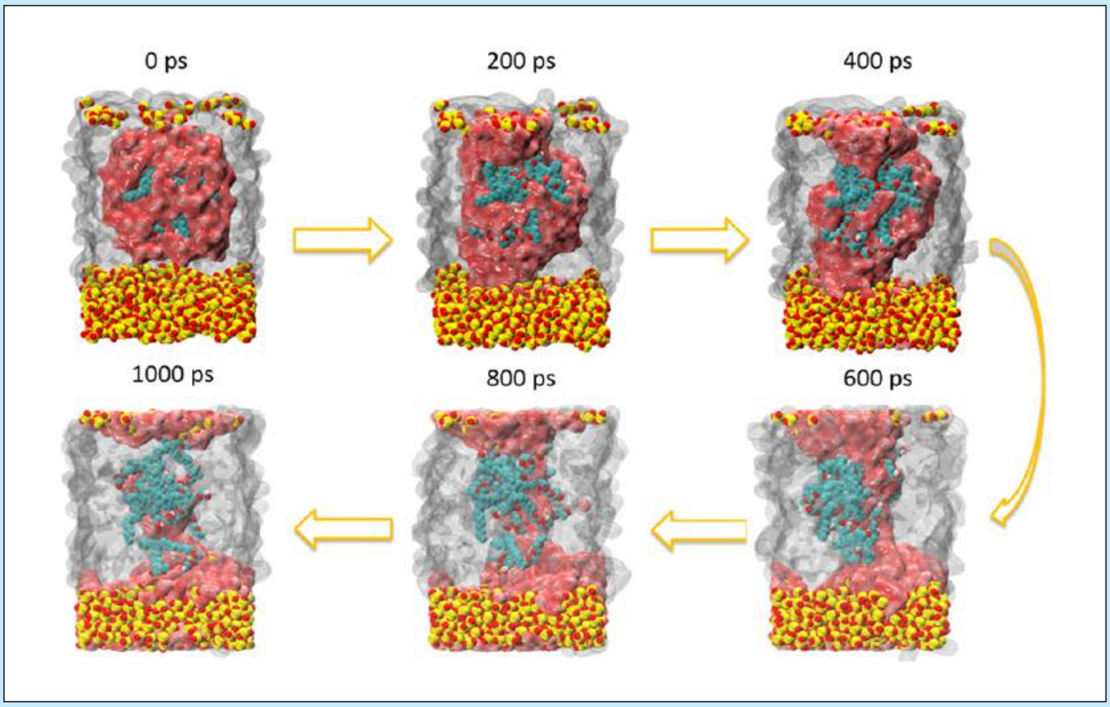

Figure 9
Wettability changes in systems containing PEG100-oleate. Silicate was depicted by van der waals representation, in which sulfur and oxigen atoms was shown in yellow and red, respectively. Surfactant molecules was represented with cyan van der Waals balls, while oil and water were resepectively displayed as grey and magenta surface representations.

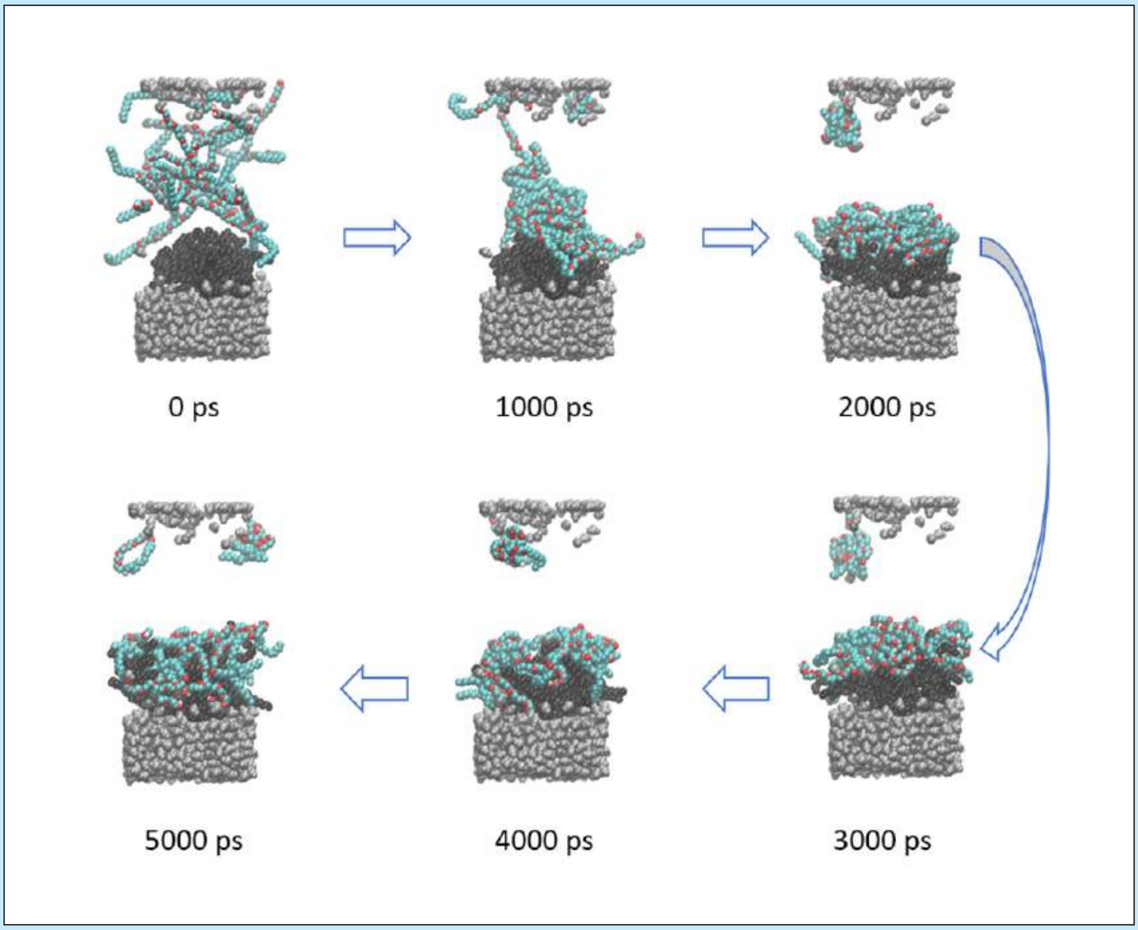

Figure 10
Changes in wetability on systems containing PEG400-oleate. Oil and surfactant were respectively represented by dark grey and cyan van der Waals representations, while silica was displayed as grey surface representation.

of rock represented by silicate (SiO_2). The red color represents the water molecule, the blue color represents surfactant while the gray color represents oil.

From Figure-10 it can be seen that at the start of the simulation time (0 ps), the rock surface interacts with oil. With increasing simulation time, water replaces the oil position to interact with the rock surface. At the end of the simulation time (1000 ps) almost the entire surface of the rock which is initially moistened with oil turns into moistened with water.

Figure 10 shows the wetability change process on a system containing PEG_{400}-oleate surfactant candidates. Water molecules are not shown to increase clarity of oil position (black) and surfactant (cyan, red, white). From the picture, it can be seen that the presence of surfactants seems to lift oil which was initially strongly bound to the rock. The process of changing the position of the oil will then be replaced by water. So that the part of the rock that was initially moistened with oil turns into moistened with water. This shows that both PEG100-oleate and PEG400-oleate have the ability to change the wetability of rocks from those initially moistened by oil to become moistened with water.

In addition, laboratory test of wettability alteration was also showing the same tendency. The design of soaking and dropping fluid on wettability analysis are presented in Table 1. Core-1 was soaked with formation water for four weeks, as well as Core-3 which soaked by oil. Fluid saturated-core was dropped by oil whereas oil saturated-core was dropped by formation water or surfactant. In the other hand, Core-2 was soaked by formation water for the

Table 1
Soaking design of wettability core,

Soaking	C1	C2	C3
Week-1	FW	FW	Oil
Week-2	FW	FW	Oil
Week-3	FW	PEG400-Oleate	Oil
Week-4	FW	PEG400-Oleate	Oil

Table 2
Wettability changes analysis of targeted core.

Dropping Fluid	C1	C2	C3
Oil	14.34	19.78	N/A
FW	N/A	N/A	89.47
PEG400-Oleate	N/A	N/A	49.87l

first two weeks, followed by soaking with surfactant PEG$_{400}$-Oleate for the next two weeks.

The results of contact angle measurement are displayed in Table 2. Comparation between core that soaked with formation water (C1) and surfactant PEG400-Oleate (C2) shows that the core was originally strong oil wet with the value of contact angle 14.34 when dropping with oil, whereas the core that soaked with surfactant PEG$_{400}$-Oleate shows a higher contact angle at 19.78, indicating wettability changes of the rock to become more water wet. The same tendency was found for the oil-saturated core (C3). As can be seen from Table-2, the core with dropping fluid formation water was higher than surfactant PEG$_{400}$-Oleate, 89.47 and 49.87 consecutively. It shows that alteration of core wettability was occured from oil wet to the less oil wet.

IV. CONCLUSIONS

In this research, design and screening of oleic acid-based surfactant candidates has been performed. Based on the interfacial tension values, the best nonionic surfactant candidates are PEG$_{100}$-oleate and PEG$_{400}$-oleate with IFT decrease of 3.99 and 4.08 dyne/cm, respectively. The emulsification test results of PEG$_{400}$-oleate and PEG$_{100}$-oleate showed that both of the surfactant candidates were capable of emulsifying the oil model starting at the time of simulation respectively before 1 ns and about 3 ns. The amount of oil-surfactant contact formed by PEG$_{400}$-oleate is greater than that of PEG$_{100}$-oleate at 3500 by 3000. From wetability test, both of then can chane the wetability. Thus, the best nonionic surfactant candidate is owned by PEG$_{400}$-oleate. Laboratory studies also verified the simulation results, that the best surfactant which have the lowest IFT and ability to alter wettability of the core was PEG$_{400}$-Oleate.

CONFLICT OF INTEREST

The authors states there is no conflict of interest with any party.

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REFERENCES

Abraham, M.J., Hess, B., Lindahl, E., 2015, 'GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers', *SoftwareX*, 1–2, 19–25**.**

Bachman, R.T., Johnson, A.C., and **Edyvean, R.G.J.,** 2014, 'Biotechnology in the petroleum industry: an overview', *International Biodeteriation & Biodegradation*, 86, 255–237.

Berendsen, H.J.C, van der Spoel, D., dan **van Drunen, R.,** 1995, 'A message-passing parallel molecular dynamics implementation', *Computer Physics Communications*, 91, 41–56.

Cayias, J.L., Schechter, R.S., and **Wade, W.H.,** 1977, 'The utilization of petroleum sulfonat for producting of low interfacial tension between hydrocarbons and water', *Journal of Colloids Interface Science*, 59, 31–41.

Humprey, W., Dalke, A. and **Schulten, K.** 1996. VMD: 'Visual Molecular Dynamics', *Journal of Molecular Dynamics*, **14.1**, 33–38.

Liu, Z., Xu, Z., Zhou, H., Wang, Y., Liao, Q., Zhang, L., and **Zhao, S**., 2017, 'Interfacial behaviors of betaine and binary betaine/carboxylic acid mixures in molecular dynamics simulation', *Journal of Molecular Liquids*, 240, 412–419.

Lowry, E., Sedghi, M., Goual, L., 2016, 'Molecular simulaitons of NAPL removal from mineral surfaces using microemulsions and surfactants', *Colloids and Surfaces A: Physicochemcal and Engineering Aspects*, 506, 485–494.

Martinez, L., Andrade, R., Birgin, E.G., and **Martinez, J.M.,** 2009, 'PACKMOL: A Package for Building Initial Configurations for Molecular Dynamics Simulations', *Journal of Computational Chemistry*, 30, 2157–2164.

Meller, J., 2001, 'Molecular Diynamics', *Encyclopedia of Life Sciences*, 1–8.

Meybodi, M.K., Daryasafar, A., and **Karimi, M.** 2016. 'Determination of hydrocarbon–water intefacial tension using a new empirical correlation', *Fluid Phase Equilibria*, 415, 42–50.

Mosayebi, A., Angaji, M.T., Khadiv-Parsi, P., 2016, 'The effect of temperature on the interfacial tension between crude oil and ethoxylated nonylphenols', *Petroleum Science and Technology*, 34, 1315–1322.

Negin, C., Ali, S. and **Xie, Q.,** 2017, 'Most common surfactants employed in chemical enhanced oil recovery', *Petroleum 3*, 197–211.

Pal, N., Saxena, N., Laxmi, K.V.D., and **Mandal A**., 2018, 'Interfacial behaviour, wettability alteration and emulsification characteristics of a novel surfactant: Implications for enhanced oil recovery', *Chemical Engineering Scienc*e, 187, 200–212.

Perfumo, A., Rancich, I., and **Banat, I.M.,** 2010, '*Possibilities and challenges for biosurfactants use in petroleum industry'*, Biosurfactant Advances in Experimental Medicine and Biology, ed Sen R, New York Springer, 135–145.

Schmid, N., Eichenberger, A.P., Choutko, A., Riniker, S., Winger, M., Mark, A.E., and **van gunsteren, W.F.** 2011. 'Definition and testing of the GROMOS force-field versions 54A7 and 54B7', *European Biophys Journal*, 40, 843–856.

Schuttelkopf, A.W and **van Aalten, D.M.F.,** 2004, PRODRG: 'a tool for high-throughput crystallography of protein-ligand complexes', *Acta Crystallographica*, D60, 1355–1363.

Touhami, T., Hornof, V., and **Neale, G.H.,** 1998, 'Dynamic interfacial tension behavior of acidified oil/surfactant enhanced system', *Journal of Colloids Surfaces A: Physicochemistry Engineering Aspects*, 277, 4 – 11.

Wang, R., Peng, F., Song, K., Feng, G., and **Guo, Z.,** 2018, 'Molecular dynamics study of interfacial properties in CO_2 enhanced oil recovery', *Fluid Phase Equilibria*, 22, 18–37.

Yela, A.C.A, Martinez, M.A.T., Pineros, G.A.R., Lopez, V.C., Villamizar, S.H., Velez, V.L.N., Abraham, W., Florez, M.J.V., Barrios, A.F.G., 2016, 'A comparison between conventional Pseudomonas aeruginosa rhamnolipids and Escherichia coli transmembrane proteins for oil recovery enhancing', *International Biodeterioration & Biodegradation*, 112, 59–65**.**

Zhang, L., Li, B., Xia, Y., and **Liu, S.,** 2017, 'Wettability modification of Wender lignite by adsorption of dodecyl poly ethoxylated surfactants with different degree of ethoxylation: A molecular dynamics simulation study', *Journal of Molecular Graphics and Modelling*, 76, 106–117.

Zhou, P., Hou, J., Yan, Y., and **Wang, J.,** 2018, 'The effect of surfactant adsorption on surface wettability and flow resistance is slit nanopore; A molecular dynamics study', *Journal of Colloids and Interface Science*, 513, 379–388.