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Molecular dynamics simulation of the influence of polyacrylamide on the stability of sodium dodecyl sulfate foam

Gang Wu, Qianqian Zhu, Congtai Yuan, Hongbing Wang, Chunling Li, Shuangqing Sun *, Songqing Hu *

College of Science, China University of Petroleum (East China), Qingdao 266580, China

HIGHLIGHTS

- The foam stability of SDS-PAM mixtures is investigated by MD simulations.
- The elasticity of foam liquid film increases with increasing of PAM concentration.
- The denser SDS monolayer is observed at HPAM 20% in the four foam systems.
- The foam stability of SDS-PAM systems is the best in the range of HPAM 20–30%.

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ABSTRACT

Molecular dynamics simulations were performed to investigate the effect of the concentration of polyacrylamide (PAM) and the hydrolysis degree of partially hydrolyzed polyacrylamide (HPAM) on the stability of sodium dodecyl sulfate (SDS) foams. The effect of polymer on the complex systems (PAM-SDS and HPAM-SDS) was investigated by analyzing the density distribution of SDS headgroups, the radial distribution function (RDF) of hydration of SDS headgroups, the mean square displacement (MSD) of hydrated water around the amide group. The results show that an increase of PAM concentration can enhance the interaction between PAM and SDS, increase the number of hydrated water molecules around SDS headgroups and weaken the mobility of the hydrated water molecules around PAM, which will be beneficial to improve the foam stability. It has been observed that the favorable structure of SDS monolayer for stable foam appears when the hydrolysis degree of HPAM is 20% in the four foam systems of our simulations. In all four foams, the numbers of water molecules around headgroups increase first with the increase of HPAM hydrolysis degree, reaching a maximum value at HPAM 20%, followed by a decrease with larger hydrolysis degrees. These observations indicate that the foam is the most stable when the hydrolysis degree of HPAM is within the range of 20–30%.

1. Introduction

Foam has been widely applied in many fields, such as mineral flotation (Evans et al., 1995), oil industry (Farajzadeh et al., 2010), paper industry (Vashisth et al., 2011), firefighting (Moe et al., 2012), food industry (Rodríguez Patino et al., 2008) and synthetic chemistry (Shankar et al., 2004). Foam flooding is a promising technology for tertiary oil recovery, which receives a wide attention from domestic and international. Foam flooding can increase the sweep efficiency and displacement efficiency, and improve the oil recovery. In addition, the operation is simple and the cost is low. However, there are certain restrictions on the application of foam flooding, such as poor stability and short validity period of foam. Foam stability can be improved obviously by adding polymer into the foam fluid.

In recent years, many experts and scholars have studied the effect of polymer on the stability of foam system (Kristen-Hochrein et al., 2011; Deng et al., 2015; Cheng et al., 2012; Yan et al., 2011; Yang and Yang, 2011; Fan et al., 2013; Liu et al., 2010; Kristen and von Klitzing, 2010). For instance, Fan and co-workers studied the effect of partially hydrolyzed polyacrylamide (HPAM), xanthan gum (XC) and other polymers on the stability of the α-olefin sulfonates (AOS) foam system. From their studies, they pointed out that HPAM improved the stability of the foam system by increasing the viscosity, and the surface tension of the system was slightly increased (Fan et al., 2013). Liu and co-workers studied the viscosity of PAM and HPAM by molecular dynamics simulation. They found that the viscosity of HPAM solutions

* Corresponding authors.
E-mail addresses: sunshuangqing@upc.edu.cn (S. Sun), songqinghu@upc.edu.cn (S. Hu).

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reduced with increasing NaCl mass fractions, and HPAM had a stronger thickening ability compared with PAM (Liu et al., 2010). The research on the stability of the foam system mainly focused on the experimental field. However, it is difficult to explain the interaction mechanism from a macroscopic view. Molecular dynamics (MD) simulation is a powerful method to investigate the relationship between the molecular structure and their properties at the atomistic level. Therefore, we used MD simulations to study the effect of PAM concentration and HPAM hydrolysis degree on the stability of the sodium dodecyl sulfate (SDS) foam system in this work.

2. Simulation details

To construct the initial configuration of SDS foam film, a sandwich model (Fig. 1) consisted of two surfactant monolayers and one water layer (Zhao et al., 2010; Li et al., 2013; Li et al., 2016), was built with periodic boundary conditions in all directions (Jang and Goddard, 2006; Bandyopadhyay et al., 1999). Then, two polymer chains with 20 degrees polymerization were symmetrically placed at the interface of the surfactant monolayers and water layer. For the surfactant monolayers in the sandwich model, 32 surfactants (8×4) were evenly arranged to be perpendicular to the *xy* plane and the dimension of SDS monolayer was 5.824×2.912 nm^2 (The occupied area of per SDS molecule was 0.53 nm^2). The thickness of water box was 3.3 nm and water molecule was described by simple point charge (SPC) model. In the water box for the foam system, the corresponding numbers of sodium ions (i.e. 32×2 Na^+) were added into the water phase randomly as counterions of surfactant molecules to guarantee an electrically neutral system. To avoid the interaction between periodic replicas, the *z* direction was kept large enough to be 14 nm through the constructing vacuum layer on both sides of the water box. The initial configuration of SDS foam system with a PAM chain is shown in Fig. 1.

In the SDS-PAM mixture systems, the number of polymer molecule chains was used to represent the concentration of the polymer. The four systems containing 0, 1, 2 and 3 PAM molecular chains were investigated. After hydrolysis of PAM, part of the amide (-CO-NH_2) groups were changed to a negatively charged carboxylate ion (-COO^-). To study the effect of the PAM hydrolysis, four ratios of -COO^- to -CO-NH_2 (1:9, 1:4, 3:7 and 2:3) were analyzed, and the corresponding hydrolysis degrees of HPAM were 10%, 20%, 30% and 40%, respectively.

All simulations were performed using the Materials Studio molecular dynamics program package. MD simulations were conducted with the COMPASS force field. For initial configurations, the energies were minimized with the Smart Minimizer method. After the minimization, all simulations were equilibrated at a constant volume and temperature (NVT) for approximately 4 ns with a time step of 1 fs (Li et al., 2016; Chen and Xu, 2013; Wang et al., 2016). The temperature of the system was kept at 298 K by Andersen thermostat. For the long-range electrostatic interactions, the Ewald method was used. The vdW interactions were calculated by the atom-based method and the interactions were cut off at 0.95 nm. The calculation results for the last 1 ns were used to analyze the foam properties.

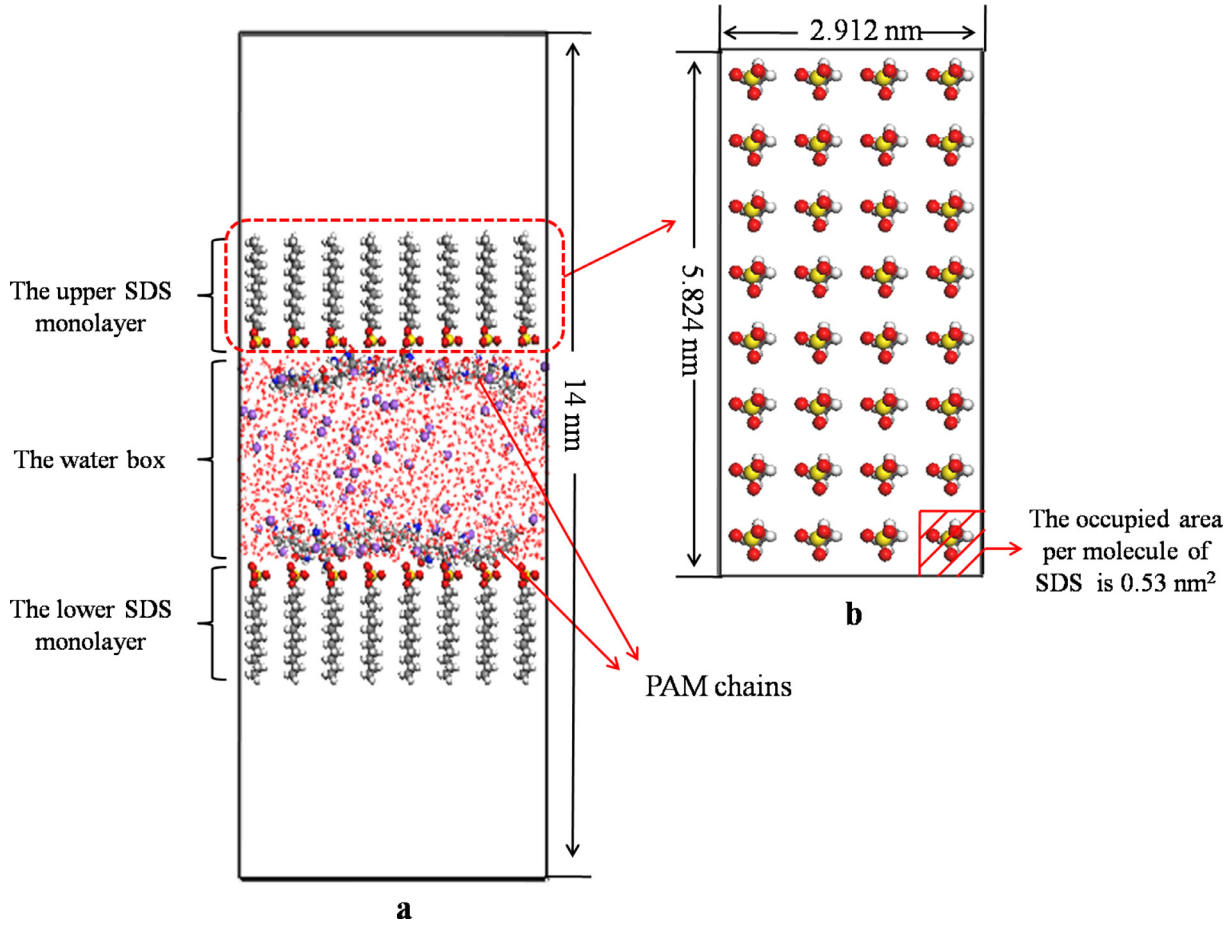

Fig. 1. (a) Front view of initial configuration of SDS foam system with one PAM. (b) Top view of the upper SDS monolayer.