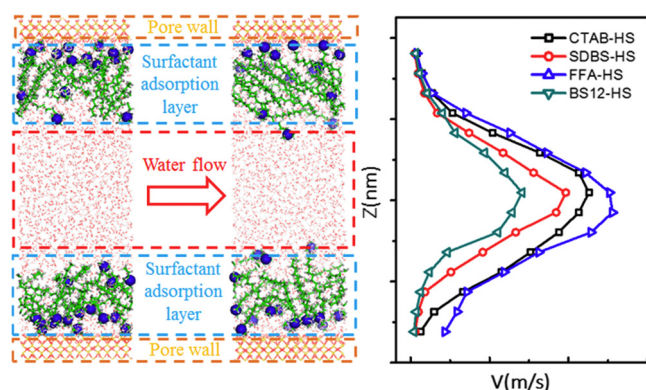


Regular Article

The effect of surfactant adsorption on surface wettability and flow resistance in slit nanopore: A molecular dynamics study

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GRAPHICAL ABSTRACT



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ABSTRACT

Hypothesis: Due to large surface/volume ratio, fluid flow resistance in nanopores is affected dramatically by surfactants adsorption, which dictates wettability and friction. Surfactants with different aggregated morphology and molecular alignment at solid/water interface are expected to affect friction and mobility of surfactant adsorption layer, both of which should be possible to contribute to surfactant drag reduction mechanism in nanopores.

Simulations: Molecular dynamics (MD) simulations were adopted to study the morphology of the adsorption layer of different types of surfactants on negatively charged hydrophilic silica surface and their effect on flow resistance in slit nanopores.

Findings: Flow resistance differs as surfactant adsorption morphologies vary. Adsorption layer composed of hemimicelles with “head on” orientation in low adsorption amount exhibits low flow resistance. As adsorption amount increases, adsorption layer evolves into the double layer in which less polar surfactant composition is found to be beneficial for improving hydrophobicity of pore wall and interfacial water diffusion. More ordered and tight intermolecular packing and high mobility of the adsorption layer are found to be propitious to reduce the flow friction.

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1. Introduction

The adsorption of surfactant at the solid/liquid interface can drastically change the hydrophobicity, surface charge, and the properties that govern interfacial processes such as wetting, imbibition, dispersion/flocculation, flotation, solubilization and detergency, which play important roles in many technological and industrial fields including micro fluid device, drug delivery, corrosion inhibition, chemical mechanical polishing and oil recovery, etc. [1,2].

Understanding the wettability and flow resistance of surfactant adsorbed mineral surfaces in nanoporous media is crucial for enhancing oil recovery, especially in low permeability reservoirs development. The flow of a fluid through a nanopore needs to overcome the flow resistance from the friction of solid/liquid interface and the inner interactions among the fluid molecules. In the media with well-developed pores and large surface/volume ratio, the interfacial interactions which are minor at the macroscale become important at the nanoscale [3,4]. Generally, the inorganic mineral surface is original water-wet (hydrophilic). During the formation of the oil reservoir, the adsorption of oil components alters the wettability of the reservoir rock to oil-wet (hydrophobic) [5,6]. In surfactant flooding, when the oil components are washed off, the reservoir rock becomes water-wet again. Therefore, the adsorption behavior of surfactant at hydrophilic mineral surface determines the eventual wettability property and flow resistance of the fluid in inorganic pores during the flooding process.

Surfactants tend to aggregate and form micellar structure both in the bulk fluid and at the solid/liquid interface [7]. Present experiments such as ellipsometry, UV absorption, atom force microscopy, specular neutron reflectivity, small angle neutron scattering, zeta potential are mainly focused on the studies about surfactant adsorption kinetics on solid/liquid interface and equilibrium adsorption of surfactant systems [1,8,9]. These studies could provide information and clues about the mechanism of surfactant adsorption at the surface/interface and evaluate its efficiency as a surface-active agent, but are still hard to access the structure of the aggregate surfactants at molecular level and the interaction between the fluid and the solid/liquid interface. Thus, in a microscopic scale, the characteristic features of the surfactant adsorption layer at the surface/interface are drawing more attention. It includes: (1) The coverage of surface/interface by the surfactants; (2) The orientation of the surfactant molecules at the surface/interfaces. These two aspects together determine the performance of surfactant and the properties of surface/interfaces affected by the adsorption (i.e. be more hydrophilic or hydrophobic) [1]. In some microchannel systems, it has been found that different types of surfactant have different drag reduction effect [10,11]. Since that with different types of surfactant and at different adsorption processes, the morphologies of surfactant aggregates vary [1,2,8,12], it requires systematic and molecular level study to establish the relationship among surfactant molecular alignment, macroscale adsorption morphologies and flow resistance in the microchannel.

The behavior of surfactants at the surface/interface is determined by various types of microscopic forces, including electrostatic attraction, hydrophobic contact and hydrogen bonding. On the benefit of microscopic observation, molecular dynamics (MD) simulations have been performed to study the surfactant adsorption and aggregate morphology at hydrophilic solid/liquid interface in molecular level [7,9,13–21]. The micelle formed by surfactant at the hydrophilic mineral surface is either spherical or elliptical in shape, whereas surfactants at the hydrophobic surface usually aggregate into hemimicelle [7,14,20]. The adsorption morphology of surfactant has been studied in detail in experiment and simulations, but there are few publications about the effect of

the surfactant adsorption on the flow behaviors of water in a slit pore. Some theoretical methods have been used to study the drag reduction effect of surfactant in nanoscale channels, but these studies were focused on the influence of surfactant aggregates on the bulk properties such as viscosity and rheology of the fluid rather than the surfactant adsorption layer [22]. Some research has reported the influence of the chemically modified surface on the friction of the fluid, but the chemical groups were bonded to the surface without movement, which is different from physical surfactant adsorption [23,24]. Although MD simulations have found some fundamental rules such that hydrophilic pore surface normally leads to larger flow resistance of water [23], the interfacial properties of surfactant adsorption layer are more than hydrophilicity: The aggregated morphology and the mobility of adsorption layer need to be considered.

In the present study, a series of surfactant molecules with different hydrophilic head groups were selected to investigate the morphologies and flow resistance of the adsorption layer in a hydrophilic slit pore. Using equilibrium molecular dynamics (EMD), surfactant adsorption models with different adsorption amounts and different molecular alignments were obtained. Then the density distribution, molecular headgroup orientation and orderness of molecular alignment were calculated to analyze the surfactant aggregated morphologies at different adsorption models. The velocity profile was monitored and the effect of the mobility of the adsorbent layer on the flow resistance was examined via nonequilibrium molecular dynamics (NEMD). The electric field strength near the solid surface, the hydrophobicity of the solvent accessible surface of the adsorption layer and the diffusion coefficient of interfacial water were further analyzed to explore the mechanism that determines the fluid friction. This study is expected to explore the answers to the following questions: (1) What is the difference in wettability of adsorption layer formed by different types of surfactant at the identical adsorption conditions? (2) Is the flow resistance in nanopores determined only by the hydrophilicity of the surfactant molecules or the individual aggregated morphology at constant adsorption conditions? (3) What is the role of the mobility of surfactant adsorption layer on the flow friction of fluid in nanopores?

2. Models and methods

2.1. Molecular models

The molecular models of a series of surfactant, including cationic surfactant cetyltrimethylammonium bromide (CTAB), anionic surfactant sodium dodecylbenzenesulfonate (SDBS), non-ionic surfactant *N,N*-dihydroxyethyl dodecyl amide (FFA) and zwitterionics surfactant dodecyl dimethyl betaine (BS12) were established and are shown in Fig. 1A. The pore model of sandstone was built based on silica (oxide quartz, α -SiO₂) which was hydroxylated. Some of the silanol groups on the quartz surface were deprotonated, leading to a surface charge density of -0.12 C m^{-2} [25]. The thickness of the silica substrate was 1.6 nm.

Two kinds of surfactant adsorption models with low and high amount of surfactants have been built. The low amount adsorption (LA) model consists 16 surfactant molecules which were placed 0.6 nm apart on the negatively charged, hydrophilic silica surface. Due to the symmetry of the pore model, there were 32 surfactant molecules in total in the LA simulation models. The high adsorption models consisted 32 surfactant molecules near each silica surface, including the high concentration in single layer (HS) and high concentration in double layer (HD) models (Fig. 1B).

In LA models, all the headgroups were initially facing towards the solid surface. The occupied surface area for each surfactant

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