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Molecular Dynamics Simulation on the Adsorption and Transport of Oil-Water Two-Phase in the Nanochannel

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Due to the size effect of nanochannels and the strong influence of nanochannel surfaces, these ultra-confined water and oil molecules behave extraordinary differently from their bulk counterpart. Therefore, it is of great necessary to study the adsorption and transport of water and oil molecules in the nanochannel.
In this paper, we investigate the adsorption and transport mechanism of oil-water in nanochannel by the molecular dynamic simulation with the established sandwich-like models, in which the water and oil molecules were confined. To quantitatively illustrate the mechanisms, several parameters were calculated including radial distribution functions, interaction energy, density distribution normal to the substrate, the diffusion coefficient and the center of mass displacement. More importantly, the influence of channel width and channel component on adsorption and transport of oil-water was studied, aiming at providing guidelines and support to microscopic flow mechanism in nanoscale.
Firstly, we can observe competitive adsorption of oil and water molecules on the calcite nanochannel surface under the influence of electrostatic force. According to the density distribution function and radial distribution function, water molecules firstly get to the surface and form water films, and the oil molecules are distributed over the water film. Because the electrostatic interaction between water molecules and channel surface is far larger than that between oil molecules and channel surface. The adsorption of water molecules increase the water wetness of the channel surface and indirectly accelerate the transport of oil molecules. As a result, the diffusion coefficient of oil molecules at the center of a 10-nm channel is almost 3 times more than water molecules near the channel surface. Secondly, the channel width play a important role in adsorption and transport of oil-water in nanochannel. The formation of water film compresses the effective flow space, the center of mass displacement of oil-water two-phase in a 10-nm channel is over 20 times larger than that in a 4-nm channel. Meanwhile, in a 1-nm channel, the water film almost occupies the whole flow space, and the oil-water two-phase are almost impossible to flow, forming an obviously “water lock effect”. Thirdly, channel component is found to play an important role in adsorption and transport of oil-water in nanochannel. The adsorption energy of oil and water on dolomite surface is greater than that on calcite surface, that is, the adsorption of oil and water on dolomite surface is more intensely.Naturally, the center of mass displacement and transport velocity of oil-water molecules in dolomite channel is smaller.
Our findings would contribute to revealing the transportation and adsorption mechanism of oil-water two-phsase in nanochannels and therefore are very important for design of oil extraction in nanochannels.

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