Mechanisms of RO Membrane Fouling by Surfactants: a Combination of Experiments and Simulation Studies

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Abstract:

Surfactants play an important role as cleaning, wetting, dispersing, emulsifying and foaming agents in many practical applications and products. The molecules of surfactants are composed of two different parts: a hydrophilic head and a hydrophobic tail. This kind of amphiphilic molecules are known to self-assemble into a variety of aggregate structures in aqueous solution, such as micelles, bilayers, vesicle, and lamellae[1]. Another fundamental property of surfactants is their tendency to adsorb at surfaces/interfaces from the bulk solution[2]. Because of their surface activity, surfactants are frequently used in industry and they are also one of the most discharged organic materials in wastewaters that are to be treated by membrane processes. However, it might be a huge obstacle for reverse osmosis (RO) membrane since the surfactant molecules will accumulate on the surface (considered as non-pores) and cause fouling to the membrane and adversely affect both the quantity (permeate flux) and quality (solute concentration) of the product water, resulting in loss of performance of the membrane[3,4]. Although RO membranes have received much attention from both academy and industry, the fouling mechanisms of solutes (especially surfactants) on RO membranes are still not fully understood.

Recently, Dissipative Particle Dynamics (DPD) simulation has been proved to be a valuable tool to study the dynamic and static structure of the assembly surfactants and can provide a detailed, mesoscopic level insight into the structure of the studied systems[5,6].

The objective of this work is to systematically deepen the understanding of fouling mechanism by modeling the behavior of surfactant molecules at the solution/membrane interface with DPD simulation and comparing with experimental data.

Firstly, DPD simulations were run to calculate the critical micelle concentration (CMC) of SDS (sodium dodecyl dulfate, an anionic surfactant) and other sodium alkyl sulfates with different chain lengths in aqueous solution. Following the top-down approach proposed by Groot and Warren[5], we used the model parameters for particle-particle interactions taken from Groot and Rabone[7]; in this approach, particle-particle interactions between solvent and surfactant are calculated from Flory-Huggins parameters χ. Our simulations show that the results are in good agreement with experimental data (for CMC), which indicates that the parameters can be used with confidence (see Fig.1).

Secondly, the membrane will be added to the simulation system for studying the interaction between membrane and surfactants and the choice of parameters involving the membrane will also be taken into account. The adsorption process depending on different factors such as surfactant concentration and membrane hydrophobicity will be discussed.

Finally, the structure of the adsorbed surfactant molecules/aggregates and the characteristic changes of the membrane will be investigated by atomic force microscopy (AFM) and sessile drop methods and further compared to the simulation study.

The extensions of our current work to a wider variety of systems, such as other membranes or other molecules (e.g. proteins), will permit more systematic classification of the adsorption mechanisms and adsorbed structures.

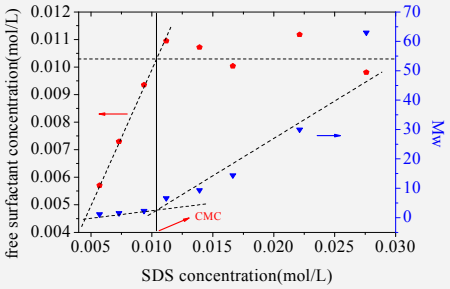

Fig.1 The concentration of free surfactants (containing unimers and small aggregates) and weight-average aggregation number (Mw) versus the total concentration of SDS. The vertical line corresponds to the CMC≈10.05×10^{-3}M which shows good agreement with the experimental values (≈8.3×10^{-3}M) [1,8].

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