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Development of a Mesoscale Scale Simulator for Virtual Experiments on Complex Scaling Deposition Phenomena

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Summary

RO membranes are widely used in seawater desalination and water treatment. In such processes, sparingly soluble salts can exceed their solubility limit and precipitate on the membrane surface, forming scale that degrades membrane performance. Increasing water recovery and concentration ratio has made scale formation more complex. In brine treatment of groundwater and water purification process, organic substances from biological sources are often present along with inorganic salts. These organics can act as nucleation sites, while multivalent ions accelerate scaling. As a result, scale formation in practical RO processes involves complex interactions, making analytical modeling difficult. Additionally, some types of scale form over several years, requiring significant time to explore optimal treatment conditions. To address this, we developed a simulator that models scale formation on RO membrane surfaces at the mesoscale (micron size level). The simulator focuses on early-stage mechanisms such as supersaturation, nucleation, precipitation, and deposition. We employed the dynamic Monte Carlo (DyMC) method to simulate diffusion, reaction, and precipitation of scale components. Input parameters such as diffusion coefficients and surface attachment probabilities were derived theoretically by using computational chemistry methods. In this report, the simulation results were validated against experimental data on silica scaling. Good agreement was observed at low silica concentration conditions, while discrepancies at high silica concentration conditions suggested multilayer adsorption effects. Developed simulator can also incorporate factors such as pH and third-component effects, allowing application to more complex scaling systems. This tool is expected to contribute to the identification of optimal operating conditions that prevent scale formation in actual RO membrane processes.