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Anti-hydrate Surface Design for Utilization in CO₂ Sequestration Processes

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The undesired CO₂ hydrates formation in wellbores or pipelines often poses a significant risk to production safety. CO₂ hydrates can develop during numerous processes, such as CO₂ injection for geological or salt-water storage, production wells in CO₂ flooding for enhanced oil recovery, and CO₂ pipeline transportation. These hydrates form when gas-water two-phase conditions are met within the hydrate stability zone. Particularly during the transition of supercritical CO₂ into the gas phase, the decrease in temperature promotes the hydrate formation. Once these hydrates accumulate on a large scale and form blockages, the bulk hydrates significantly compromise the safety and efficacy of CO₂ storage or hydrocarbon production. To address the challenges posed by hydrates, an effective alternative solution is to develop a new generation of passive anti-hydrate surfaces that can prevent hydrates from accumulating over time. These new surfaces can incorporate smart properties such as anti-hydrate nucleation on the surface initially and possess low hydrate adhesion strength if hydrate deposition inevitably occurs. Therefore, it is necessary to understand the fundamental interactions between CO₂ hydrates and solid surfaces. To achieve this, the current study employs systematic atomistic modeling and large-scale molecular dynamics (MD) simulations to explore the underlying mechanisms and key factors influencing hydrate adhesion. The results indicate that the gas concentration in the vicinity of solid surfaces plays a crucial role in determining the structures of the hydrates intermediate layer formed on those surfaces. By increasing the gas content near solid surfaces, it becomes possible to weaken CO₂ hydrate adhesion, enabling the automatic detachment of hydrates under the influence of shear flow. With a better understanding of these mechanisms, it is conceivable to develop more effective anti-hydrate strategies and enhance the safety and efficiency of CO₂ utilization process.

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