

A novel mechanistic model for mineral crystallization and inhibition

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Mineral crystallization is ubiquitous in various geological and industrial processes. The widely present natural biomolecules or artificial chemicals were observed to significantly impact the mineral crystallization kinetics (e.g., induction time). Despite such prevalence, the mechanism of mineral crystallization and inhibition have not been elucidated yet. In this study, a novel mechanistic model for mineral crystallization and inhibition has been developed and applied to gypsum, one of the most common and troublesome inorganic mineral scales in various industrial processes. Through this model, it is believed that gypsum nucleation may gradually transit from homogenous to heterogenous nucleation when gypsum saturation index (*SI*) decreases. Such transition is represented by a gradual decrease of surface tension at smaller *SI* values. This model assumes that the adsorption of inhibitors onto the gypsum nucleus can increase the nucleus superficial surface tension and prolong the induction time. Using the new model, this study accurately predicted the gypsum crystallization induction times with or without nine commonly used scale inhibitors over wide ranges of temperature (25–90 °C), *SI* (0.04–0.96), and background NaCl concentration (0–6 mol/L). The fitted affinity constants between scale inhibitors and gypsum show a good correlation with those between the same inhibitors and barite, indicating a similar inhibition mechanism via adsorption. Furthermore, by incorporating this model with the two-phase mineral deposition model our group developed previously, this study accurately predicts the gypsum deposition time on the membrane material surfaces reported in the literature. We believe that the model developed in this study can not only accurately predict the gypsum crystallization induction time with or without scale inhibitors, but also advance our understanding in mineral crystallization and inhibition.