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AI-aided high throughput experiments of calcium carbonate precipitation

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The precipitation of carbonate minerals influences the global carbon cycle and is a key process in carbon dioxide removal (CDR) technologies, such as geologic carbon storage and enhanced rock weathering. Calcium carbonate precipitation is highly complex, involving non-classical pathways and multiple polymorphs (e.g., vaterite, aragonite, and calcite), whose formation is strongly dictated by supersaturation, interfacial properties, and impurities. Transformations between different polymorphs may trigger more complex dynamics.

Traditional nanoscale characterization techniques (e.g., AFM) are limited by their field of view, making it difficult to quantify stochastic nucleation and growth events with statistical significance, while macroscopic batch experiments lack single-crystal scale resolution. Although current high-throughput microfluidic methods have expanded the sample size, they still face the trade-off between restricted solute availability in nanoliter droplets and optical resolution. Furthermore, existing automated data processing is primarily limited to categorical classification, incapable of precise size quantification for continuous crystal growth kinetics.

To address these limitations, we established an artificial intelligence (AI)-aided high-throughput experimental workflow capable of accurately identifying the polymorphs of thousands of crystals and precisely tracking their size evolution. Furthermore, we integrated reactive transport modeling (RTM) with a machine learning inversion strategy to train a neural network surrogate model, which was then used to derive reliable growth kinetic parameters from the experimental data. Through this framework, we directly observed the kinetic crossover point ($SI_{Cal} \approx 1.9$) between vaterite and calcite heterogeneous nucleation, and determined the growth kinetic parameters of vaterite under high supersaturation (n = 2.83, -lg k = 5.94), filling a critical data gap. The study further revealed a broad crystal size distribution jointly driven by asynchronous nucleation, spatial heterogeneity in supersaturation, and intrinsic growth rate difference. Our results emphasize that simply extrapolating low-saturation parameters would severely underestimate the growth rate of vaterite. The high-supersaturation data obtained in this study are crucial for accurately assessing underground pore structural evolution and heavy metal capture efficiencies. Overall, this versatile high-throughput framework provides a powerful tool for decoding fluid-mineral reactions across various complex environmental systems.