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Modeling Dissolution and Precipitation Dynamics During Dedolomitization

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We simulate the processes of dedolomitization and calcium carbonate precipitation using particle tracking. The study is stimulated by the results of a laboratory experiment that examined reactive transport of injected $CaCl_2$/HCl, into a column of sucrosic dolomite particles, with a constant flow field. The injected fluid supplies Ca^{2+} and H^+. Dedolomitization is a protonation reaction yielding carbonic acid, which in a deprotonation reaction yields CO_3^{2-}; reaction with the abundant Ca^{2+} forms the precipitate $CaCO_3$. The novelty of the simulation is to treat the dynamics of the rate-limiting reactants with a particle tracking method; the dedolomitization and precipitation processes involve multi-step, multi-species chemical reactions, with both irreversible and reversible stages. At each time step the local concentration of H^+ determines the probability (assuming local carbonate equilibria) of precipitation and dissolution. The precipitation changes the porosity which in turn changes the local flow field. The particle tracking is governed by spatial and temporal distributions within a continuous time random walk framework. This includes the option of either advective-dispersive (Fickian) transport or the effects of disorder of heterogeneous media — non-Fickian behavior. The dynamics of dedolomitization are examined for different flow conditions. The fluctuations in the local velocity distributions, due to porosity changes, create conditions for positive feedbacks leading to preferential pathways, large-scale nonlinearity and precipitation banding. These features have been observed in the laboratory experiments and are now accounted for by the simulation results at similar time frames, velocities and pH levels.