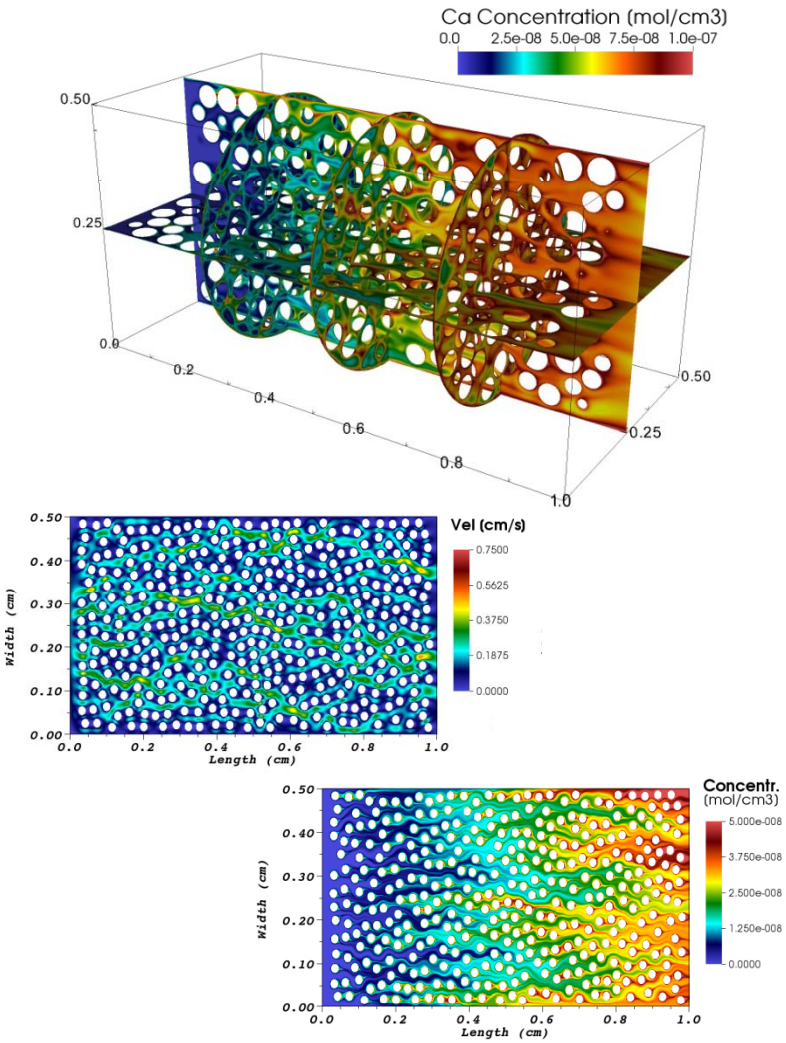
An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation



- The scale-dependence of geochemical reaction rates hinders their use in continuum scale models intended for the interpretation and prediction of chemical fate and transport in subsurface environments such as those considered for geologic sequestration of CO_2.
- Pore scale processes involving mass transport limitations to reactive surfaces may contribute to the discrepancy between laboratory-determined and continuum-scale or field rates.
- A pore scale model, composed of high-performance simulation tools and algorithms for incompressible flow and transport, is combined with a multicomponent geochemical reaction module to perform direct numerical simulation of reactive transport.
- Using the case of calcite dissolution as an example, the model is used to demonstrate that nonuniformity in the flow field at the pore scale has the effect of decreasing the overall reactivity of the system, even when systems with identical reactive surface area are considered.

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