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An REV-scale model for dissolution of porous rocks

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Modeling subsurface flow and reactant transport on large (km) scales necessarily involves statistical descriptions of the underlying pore space. Pore-scale models are one route to the constitutive models needed to close the macroscopic transport equations, but when the reaction rate is high, classical upscaling methods fail. Here we describe a different upscaling scheme based on concentration fluxes rather than concentration fields. The upscaling is based on two observations from finite-volume (OpenFOAM) simulations of dissolution in perioidic porous materials. First, that the concentration field in each unit cell of a periodic array can be mapped to a universal spatial distribution that depends only on the incoming concentration flux. Second, that the shape (and therefore the porosity) of a dissolving unit cell in one position can be mapped onto a different unit cell at a different
time. These two observations can be combined into an ansatz for the time-dependent
concentration field in a dissolving (initially periodic) array of grains. I will present numerical results in support of this ansatz over a range of Peclet and Damkohler numbers.

Based on the proposed ansatz, we have developed an REV-scale model for the dissolution of a porous matrix, which is valid for all Damkohler numbers. The predicted porosity evolution is compared with pore-scale simulations in the Figure, shows results for a square array of disks at Peclet numbers of 20 (left column) and 200 (right column); the rows have Damkohlet numbers of 0.02, 2, 200, and infinity. (transport limited kinetics). The symbols indicate the model predictions in different unit cells, and the solid lines are pore-scale simulations.

At low Damkohler numbers (Da < 1), the REV model can be approximated by a continuum
theory. In both cases (REV and continuum) a single constitutive model is all that is required. It accounts for the fraction of the incoming flux to the unit cell that is absorbed by the solid. It can be determined by pore-scale simulations of small samples.

Recently, we have extended the REV model to include a spatially varying macroscopic flow. The key idea is that the concentration fluxes leaving a unit cell (or REV) are distributed in proportion to the fluid volume flux. This approximation is valid whenever the REV-scale Peclet number is greater than 1, or when the reactant within the unit cell is well mixed. The fluid velocity can be derived from the porosity-dependent permeability of the unit cell, which can be determined along with the effective mass-transfer coefficient from pore-scale simulations on small samples.

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Participation

In-Person

References

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