Multiple scale (and multi-scale) reactive transport modeling of terrestrial systems

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An overview of some of the continuum approaches for modeling reactive transport across multiple scales in the Earth and Environmental sciences will be presented. Above the molecular scale, the pore scale is the first in which continuum methods are employed. Here fluid flow is described with the Navier-Stokes or Stokes equations, making possible the direct resolution of interfaces (reactive and non-reactive) and the flow field within individual pores. The potential for partial or complete diffusion control of reaction rates and the geometric reactive surface area are rigorously accounted for when the voxel resolution and numerical discretization are sufficiently fine. There is now an increased interest in Brinkman formulations to capture the transition from Stokes to Darcy flow, although reactive transport formulations that bridge the gap between the true pore scale and the micro-continuum scale are only now beginning to be developed. Micro-continuum modeling is another approach for the next scale up that neglects anything but the largest interfaces, relying instead on volume averaging of properties (permeability, diffusivity, porosity, and mineralogy) taken from high resolution microscopic and spectroscopic imaging. The next scale (1-1000m) is probably the most familiar to reactive transport modelers, with flow described by Darcy's Law and mineral reactivity represented with upscaled reactive surface area that may or may not have a rigorous geometric basis.

While the approaches mentioned above are typically applied to subsurface flow and transport, the presence of surface water flow and vegetation at the Earth's surface, as well as potentially complex topography, make modeling of reactive transport at the watershed scale a significant challenge. Particularly in this context, there is interest now in developing true multi-scale models that capture catchment scale behavior without loss of process fidelity or of spatial and temporal resolution of biogeochemical hotspots. While Reduced Order Models are a viable option for geochemical cycling at the catchment scale, we are pursuing high resolution approaches based on high performance computing. This is part of a larger effort to build "Virtual Ecosystems" based on community code.