Data-Intensive Models for Pore to Plume to Watershed Scales

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A new generation of reactive transport models is emerging that require intensive data inputs as initial/boundary conditions or as forcings. These models range from the pore scale, where the data typically involves physical and/or mineralogical data at high (micron) resolution, to plume scale where geophysical data may provide a detailed permeability structure, to watershed scale where forcings (e.g., precipitation) may vary in space and time over 10s of meter scales despite the kilometer scale of the domain. At the pore scale, the data includes a variety of sources ranging from X-ray synchrotron tomography, to FIB-SEM, to back-scattered electron microscopy that are used to describe the pore structure and it mineralogical (reactive) composition. Models, some at very high micron resolution, some using averaged values at the micro-continuum scale, are then used to simulate reactive transport processes. At the plume scale, the inclusion of high resolution heterogeneity (typically permeability) dates back more than 20 years, although the shift now is to the use of geophysics to provide these data inputs at the meter to 10s of meter scale. At the watershed scale the system forcings are much of the story, particularly in high elevation sites where the accumulation and subsequent melting of snow create a highly heterogeneous fabric within the spatial domain. These forcings are data-intensive because they involve high resolution data in both space and time. Additional heterogeneity is present in the initial conditions governing watershed function, including vegetation, soil types, and topography. Particularly at the watershed scale, these highly resolved data streams in time and space drive disparate processes like shallow subsurface biogeochemical processes in hillslopes and floodplains, soil production and chemical export, evapotranspiration regulated by plants, and exchange with the atmosphere. Taken together, these coupled processes result in a complex aggregated behavior at the watershed scale that may be difficult to unravel without the appropriate mechanistic models.