Reactive Transport Benchmarks for Multicomponent Diffusion and Electrical Double Layer Transport

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The subsurface science and engineering community is being driven to provide accurate assessments of risk and engineering performance for important issues associated with groundwater flow and reactive transport As a result, the complexity and detail of subsurface processes, properties, and conditions that can be simulated has significantly expanded. With ever-increasing levels of sophistication (and opportunities for error), how does one establish the validity of a simulator formulation prior to application? In the absence of closed form solutions for realistically complex applications, benchmark problems with an accepted set of results will be indispensable to qualifying codes for various environmental and earth science applications. In this work, we present results from two benchmarks developed to represent 1) multicomponent diffusion and electrochemical migration based on the Nernst-Planck equation, and 2) transport and reactive processes with a discrete treatment of the electrical double layer (EDL).

The benchmark on multicomponent diffusion based on the Nernst-Planck equation considers three separate problems in which the unequal diffusion rate of charged species results in electrochemical migration, resulting in non-Fickian diffusion. The last of these sub-problems considers transverse dispersion in both 1D and 2D systems. Codes compared in the benchmark simulations include MIN3P, CrunchFlow, PHREEQC, and Flotran. A second benchmark takes a graded approach to problems of increasing complexity associated with transport and reaction in compacted bentonite, with the last sub-problem representing explicitly processes in a discrete electrical double layer in which anion exclusion occurs. The problem requires a calculation of double layer thickness as a function of ionic strength, with distinct transport properties assigned to ions in this second continuum. Codes used in the comparison include CrunchFlow, PHREEQC, and MIN3P.