Benchmark for reactive transport codes with application to concrete alteration

O. BILDSTEIN[1], F. CLARET[2], J. PERKO[3], D. JACQUES[3] AND C. I. STEEFEL[4]

[1]CEA, DEN, Cadarache, Saint Paul-lez-Durance, F-13108, France (olivier.bildstein@cea.fr)
[2]BRGM, Orléans, F-45060, France (f.claret@brgm.fr)
[3]SCK.CEN, Boeretang 200, Mol, B-2400, Belgium (jperko@sckcen.be, djacques@sckcen.be)
[4]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA (CISteefel@lbl.gov)

The subsurface science and engineering community is being driven to provide accurate assessments of risk and engineering performance for important issues with far-reaching consequences. The complexity and detail of subsurface processes, properties, and conditions that have to be addressed has significantly expanded. In the absence of closed form solutions for realistically complex applications, benchmark problems with an accepted set of simulation results will be indispensable to qualifying codes for various environmental and engineering applications.

We present a set of three benchmark problems pertaining to relevant processes of concrete alteration in the context of radioactive and hazardous waste immobilization and disposal: (1) atmospheric carbonation of concrete, (2) concrete-clay interactions in a geological repository environment, and (3) calcium leaching from fractured concrete. These problems can be used to demonstrate simulator conformance with norms established by the subsurface science and engineering community. In each case, the objective is to present a problem that tests the conceptual model capabilities, numerical implementation, process coupling, and accuracy.

Each benchmark contribution consists of several cases with gradually increasing complexity. This approach is used to isolate key attributes and the most sensitive parameters of the benchmark problem for higher scrutiny before addressing the full complement of interacting processes, properties, and conditions. Agreement between results obtained from a number of well-known reactive transport codes are used to establish confidence in the benchmarks. These benchmark exercices, involving the contribution of about ten international research teams, will be published in a special issue of Computational Geoscience.