

SeSBench – An initiative to benchmark reactive transport models for environmental subsurface processes

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As soil functions are governed by a multitude of interacting hydrological, geochemical and biological processes, simulation tools coupling mathematical models for interacting processes are needed. Coupled reactive transport models are a typical example of such coupled tools mainly focusing on hydrological and geochemical coupling (see e.g. Steefel et al., 2015). Mathematical and numerical complexity for both the tool itself or of the specific conceptual model can increase rapidly. Therefore, numerical verification of such type of models is a prerequisite for guaranteeing reliability and confidence and qualifying simulation tools and approaches for any further model application.

In 2011, a first SeSBench –Subsurface Environmental Simulation Benchmarking– workshop was held in Berkeley (USA) followed by four other ones. The objective is to benchmark subsurface environmental simulation models and methods with a current focus on reactive transport processes. The final outcome was a special issue in Computational Geosciences (2015, issue 3 – Reactive transport benchmarks for subsurface environmental simulation) with a collection of 11 benchmarks. Benchmarks, proposed by the participants of the workshops, should be relevant for environmental or geo-engineering applications; the latter were mostly related to radioactive waste disposal issues – excluding benchmarks defined for pure mathematical reasons. Another important feature is the tiered approach within a benchmark with the definition of a single principle problem and different sub problems. The latter typically benchmarked individual or simplified processes (e.g. inert solute transport, simplified geochemical conceptual model) or geometries (e.g. batch or one-dimensional, homogeneous). Finally, three codes should be involved into a benchmark.

The SeSBench initiative contributes to confidence building for applying reactive transport codes. Furthermore, it illustrates the use of those type of models for different environmental and geo-engineering applications. SeSBench will organize new workshops to add new benchmarks in a new special issue.

Steefel, C. I., et al. (2015). "Reactive transport codes for subsurface environmental simulation." Computational Geosciences 19: 445-478.