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Benchmarking of numerical codes against analytical solutions for multidimensional multicomponent diffusive transport coupled with precipitation-dissolution reactions and porosity changes

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Numerical computer codes dealing with precipitation-dissolution reactions and porosity changes in multidimensional reactive transport problems are important tools in geoscience. Recent typical applications are related to CO_2 sequestration, shallow and deep geothermal energy, remediation of contaminated sites or the safe underground storage of chemotoxic and radioactive waste.

Although the agreement between codes using the same models and similar numerical algorithms is satisfactory, it is known that the numerical methods used in solving the transport equation, as well as different coupling schemes between transport and chemistry, may lead to systematic discrepancies. Moreover, due to their inability to describe subgrid pore space changes correctly, the numerical approaches predict discretization-dependent values of porosity changes and clogging times. In this context, analytical solutions become an essential tool to verify numerical simulations.

We present a benchmark study where we compare a two-dimensional analytical solution for diffusive transport of two solutes coupled with a precipitation-dissolution reaction causing porosity changes with numerical solutions obtained with the COMSOL Multiphysics code and with the reactive transport code OpenGeoSys-GEMS. The analytical solution describes the spatio-temporal evolution of solutes and solid concentrations and porosity. We show that both numerical codes reproduce the analytical solution very well, although distinct differences in accuracy can be traced back to specific numerical implementations.