

TWO MODEST IMPROVEMENTS FOR SEQUENTIAL ITERATIVE APPROACHES IN REACTIVE TRANSPORT

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Summary. We present here two different improvements for the SIA approach in reactive transport.

1. The SIA approach is very well-suited to reactive transport when the chemistry is at thermodynamic equilibrium. It allows to solve the non-linear chemical system locally instead of globally. However, when the chemistry is – if only partially – kinetically-controlled, this approach leads to treating kinetics as a displacement of equilibrium, which may cause convergence or precision problems, directly linked to the characteristic times of the kinetic laws.

For kinetically-controlled species, usually minerals, the chemical source terms of their equation of evolution may be explicitly written according to the associated kinetic laws. By separating the solving of the chemistry between the chemistry at equilibrium and the kinetically-controlled chemistry, we propose a modified operator-splitting approach, applied to a fixed-point algorithm. This methodology allows us to address and solve locally problems of convergence. Tested in the mainframe of the ALLIANCES code, this method has proven to be more precise and more robust in a series of test-cases. These test-cases were chosen close to real reactive transport cases in the context of nuclear waste storage simulations.

2. The fact that chemical concentrations come as a result of a local equilibrium makes impossible to write explicitly the chemical source term in the reactive-transport equation. It is fairly common to use an operator-splitting technique for sequential approaches and the direct substitution for a global approach. In both cases the jacobian is very often evaluated through a numerical approximation.

We propose here to evaluate the jacobian through an analytic calculation, using the mathematical properties of the chemical system (action mass laws), in the mainframe the Non Linear Conjugate Gradient method. This analytical calculation is possible although the analytical expression of the function whose jacobian is calculated is unavailable. Comparing it to the use of a numerical jacobian on a few test-cases, we see that the use of an exact jacobian improves the robustness of the algorithm and reduces the number of iterations to converge.