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Modelling and efficient Simulation of general Multicomponent Reaction and

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Modelling and efficient simulation of reactive transport in porous media plays a major role, in particular concerning the fate of contaminants in soils and aquifers. This is a formidable task, as one has to deal with a microscopically heterogeneous system consisting of the phases fluid-air-solid. Reactions to considered often are heterogeneous, i.e. they involve two phases. We present a comprehensive model taking saturated-unsaturated fluid flow and homogeneous and heterogeneous reactions for multiple components, both in quasi-static equilibrium and in kinetic non-equilibrium, into account. In this way ariving at a highly nonlinear time-dependent problem in 10 or more varables, at least in three spatial dimensions a reduction in complexity is desired. Therefore various transformation techniques are presentd with the aim to decouple the problem as far as possible. The remaining nonlinear system is approximated with Newton's method using the multigrid method for the arising linear subproblems. As spatial discretization hybridized mixed finite elements are chosen due to their advantageous qualitative properties. As we have to deal with global nonlinear problems, local nonlinear problems have to be solved in the process of static condensation. Large gradients and small reaction zones require grid adaptation based on a posteriori error indicators. In the time discretization the stiffness of the system has to be taken into account, e.g. by appropriate multistep methods.