Efficient and Accurate Simulation of Large General Reactive Multicomponent Transport Processes in Porous Media by Model-Preserving a priori and a posteriori Decoupling Techniques

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Detailed modelling of reactive transport processes in the underground often requires the consideration of a wide range of reactive species. A prominent example is natural attenuation, that is the assessment and monitoring of microbially catalysed degradation processes of organic contaminants in the subsoil or aquifer. Similar to problems e.g. in combustion the reactions exhibit a wide range of reaction times, which advises to model those reactions being much faster than the time scale of the transport processes in a quasistationary manner, e.g. as (algebraicly described) equilibrium processes. Additionally not only mobile species (in solution) appear, but also immobile ones (attached to the porous skeleton). In summary, the resulting system is not semilinear and parabolic, but rather quasilinear and couples partial differential equations (pde), ordinary differential equations and algebraic equations. An often used approach is operator splitting, in which transport and reaction becomes (iteratively) decoupled. This procedure either introduces a further consistency error (in the non-interative version) which can only be controlled by the time stepping, or applies a fixed point type iteration of unclear convergence properties. We rather propose, after appropriate (mixed) finite element discretization, to deal with the full discrete nonlinear system (by a damped Newton's method). To make the problem still feasible we advise two means: The first is concerned with the continuous model and aims at a transformation of the dependent variables such that as many as possible are determined by decoupled linear pde's or by local algebraic relations, leading to a smaller coupled system. The problem lies here in the combined appearance of kinetics and equilibrium and mobile and immobile species. Alternatively to this exact a priori decoupling we use an a posteriori decoupling on the level of the linear system of equation in the Newton's method by ignoring weak couplings in the Jacobian matrix. The resulting benefit in the solution of the linear system should supersede a possible deterioration in the convergence of the iterative method, being now only an approximate Newtons's method.