Operator Splitting Methods in Modelling of Multiphase Multicomponent Reactive Flow in Porous Media

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Abstract: One possible way of modelling subsurface flow and transport processes with (bio)chemical reactions is to discretize and solve the whole system of equations simultaneously. It is in general inefficient or infeasible to apply one and the same integration formula to the different parts of the system. Moreover, use of a single implicit integration formula for the whole problem readily leads to a very large nonlinear algebraic system, which is diffucult to solve.

Another possibility is to use an operator-splitting (OS) approach, breaking down a complicated problem into smaller subproblems, such that the different parts can be solved efficiently with suitable numerical schemes. Moreover, the OS approach offers room for massively parallel computing, where parallel simulation techniques are applied to the coupled problem. Unfortunately, OS approach introduces a splitting error.

Major difficulties with splitting methods occur for problems with inhomogeneous boundary conditions and with stiffness in reaction terms. The sources of OS errors for different flow and reaction rates in various situations will be discussed. Using a suitable time stepping and OS strategy, the errors could be decreased or completely avoided.

The goal in mathematical modelling is to solve given problems as accurate as possible keeping computational costs low. The code performance in the fully implicit approach and the OS approach will be compared and an error analysis will be presented. Furthermore, several test problems will be shown to provide guidance for optimal solution strategy in modelling of transport reactive processes in porous media.

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