A Fully Implicit Finite Volume Scheme For Flows With Reactive Transport In Porous Media

E. Ahusborde, B. Amaziane, M. Id Moulay
LMAP-IPRA, CNRS/UNIV PAU & PAYS ADOUR, UMR 5142,
Av. de l'Université, 64000 Pau, France

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Introduction

Reactive transport modeling is used in many energy and environmental applications related to subsurface flows. The model mainly describes the transport of solutes coupled with chemical reactions and leads to a system of advection-diffusion PDEs coupled with algebraic or ordinary differential equations. The latter is used to predict with enough accuracy pressure variations, phases displacement, and species distributions in porous media. This is widely exploited for instance, in the geological storage of CO_2 and nuclear waste to study the reliability of the storage on time scale of thousands years. Another thread is the treatment of reactive contaminant plume migration in groundwater and the possible remediation process [1].

Two families of approaches for the numerical solving of reactive transport problems are widely used in literature [2]. One is the sequential approach which consists in splitting the chemical and transport problems. These latter are solved sequentially at each time step. We distinguish two types of splitting schemes, the sequential non-iterative approach [3] and the sequential iterative approach [4]. The other approach type is the global implicit approach which is a fully coupled procedure that consists in solving the entire nonlinear system gathering all equations at each time step. The latter may be seen as greedy in computing requirements but larger time steps during some periods of simulation and using methods as in [5] with adaptive Jacobian updates can reduce the computational time. Following this approach, in order to reduce the size of the nonlinear system, unknowns can be eliminated by a substitution of the chemical problem in the transport equations. This is called the Direct Substitutional Approach (DSA) [6]. Another method has been proposed in [7] that enables to keep the software codes for transport and chemistry distinct. We also cite [8] where a reduction scheme reformulates the nonlinear system in such a way that the coupling and nonlinearities are concentrated in a rather small number of equations leading to the decoupling of some linear equations from the nonlinear system using a global implicit method.

Mathematical model and numerical scheme

The studied model in this work is an isothermal multicomponent flow process in a porous medium, with chemical reactions that involve solutes, sorbed species and minerals. A set of nonlinear PDEs describes the mass conservation law for each component. The chemical interactions between these latter are expressed through mass action and species conservation laws. The reactions rates depend on the reaction type, either at equilibrium (differential algebraic equations) or kinetic reactions (ODEs). A Morel formulation is applied to reduce the number of component transport equations and eliminate equilibrium reaction rates [2].

Our numerical method is based on the DSA. The mass action laws and species conservation laws are substituted in the transport equations. An implicit euler scheme is used for time discretization. The spatial discretization is performed by a vertex-centred or cell-centered finite volume method combining an upwind scheme for the convective terms and a conforming finite element method with piecewise linear elements for the diffusive terms. A new reactive transport module is implemented in DuMu^X (DUNE for Multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media) [9, 10], a free and open-source simulator for flow and transport processes in porous media, based on the Distributed and Unified Numerics Environment DUNE [11]. The nonlinear system is linearized using a Newton's method with variable time stepping. The control of the time-step is based on the number of iterations required by the Newton method to achieve convergence for the last time iteration. The time-step is reduced, if the number of iterations exceeds a specified threshold, whereas it is increased if the method converges within less iterations. The linear systems are solved by solvers provided by [11] (Bi-conjugate Gradient Stabilized (BiCG-STAB) with ILU preconditioner is used by default). The module is validated by solving a PHREEQC test case proposed in [12] and the MoMaS Benchmark [13] Easy, Medium and Hard test cases, in 1D and 2D, with advective and dispersive transport conditions. The adaptive time step allows to control both the accuracy of the approximation and the convergence of Newton's iterations. It allows choosing large time steps when possible and saves CPU time. For heavy simulations, a parallel version of DuMu^X using the capabilities of DUNE and the MPI communication protocol is used to greatly reduce the

computing time. As an example, figure 1 illustrates the concentration profile for a component at $t = 10\ s$ for the 2D advective MoMaS Easy test case in accordance with the results given in [14]. The extension of our methodology for a two-phase multicomponent flow is in progress. A new module will be implemented following the fully implicit scheme. The module will be validated for several test cases given in the literature including CO_2 geological sequestration. The extension of the present approach to 3D problems will be discussed.

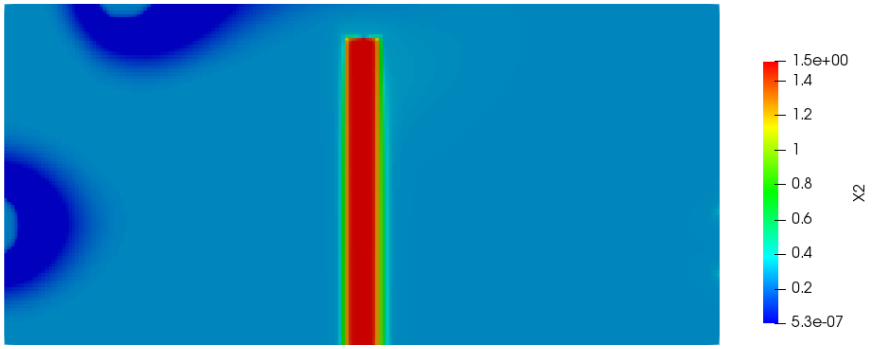

Figure 1: Concentration profile at $t = 10\ s$ for a component for the 2D advective MoMaS Easy test case

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