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# Newton method for reactive solute transport with equilibrium sorption in porous media

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ABSTRACT

We present a mass conservative numerical scheme for reactive solute transport in porous media. The transport is modeled by a convection–diffusion–reaction equation, including equilibrium sorption. The scheme is based on the mixed finite element method (MFEM), more precisely the lowest-order Raviart–Thomas elements and one-step Euler implicit. The underlying fluid flow is described by the Richards equation, a possibly degenerate parabolic equation, which is also discretized by MFEM. This work is a continuation of Radu et al. (2008) and Radu et al. (2009) [1,2] where the algorithmic aspects of the scheme and the analysis of the discretization method are presented, respectively. Here we consider the Newton method for solving the fully discrete nonlinear systems arising on each time step after discretization. The convergence of the scheme is analyzed. In the case when the solute undergoes equilibrium sorption (of Freundlich type), the problem becomes degenerate and a regularization step is necessary. We derive sufficient conditions for the quadratic convergence of the Newton scheme.



## 1. Introduction

The extensive use of chemical substances in industry in the last 100 years enhanced also considerably the number of possible contaminated sites. There are hundreds of thousands of such places only in the developed countries. Due to this an active remediation is practically impossible. To decide how dangerous such a site is or can become is a very difficult task. A reliable and efficient simulation tool for contaminant transport in saturated/unsaturated soil is needed. This includes a comprehensive mathematical model, mass conservative discretization tools, robust and fast convergent methods for solving the nonlinear discrete problems and finally efficient linear solvers.

The diffusive–advective–reactive transport with a delay caused by the sorption on the soil skeleton of a one-component solute can be mathematically modeled by the equation

$$\partial_t(\Theta(\psi)c) + \rho_b \partial_t \phi(c) - \nabla \cdot (D\nabla c - \mathbf{Q}c) = \Theta(\psi) r(c) \quad \text{in } J \times \Omega, \tag{1}$$

with $c(t, \mathbf{x})$ denoting the concentration of the solute, $D$ the diffusion–dispersion coefficient, $\rho_b$ the soil density, $\phi(\cdot)$ a sorption isotherm, $\psi(t, \mathbf{x})$ the pressure, $\Theta(\cdot)$ the water content, $\mathbf{Q}(t, \mathbf{x})$ the water flux and $r(\cdot)$ a reaction term. In this paper we assume $D$ to be a constant. For the ease of presentation we take $D = 1$. Further, $J = (0, T]$ $(0 < T < \infty)$ is the time interval, whereas $\Omega \subset \mathbb{R}^d (d \geq 1)$ is the computational domain having a Lipschitz continuous boundary $\Gamma$. Initial $c(t = 0) = c_I$ and homogeneous Dirichlet boundary conditions complete the model. We considered for the ease of

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presentation the case of one-component transport, but the present results can be extended to the case of a multi-component reactive transport, as long as the reactive term $r(\cdot)$ remains Lipschitz continuous. The same holds for more realistic boundary conditions (but regular enough) and a strictly positive non-constant diffusion coefficient.

For adsorption we consider two situations: Lipschitz continuous isotherms, as well as the commonly used Freundlich type isotherm

$$\phi(c) = c^{\alpha}, \quad \text{with } \alpha \in (0, 1]. \tag{2}$$

In the last case the derivative is singular at $c = 0$, so $\phi$ is not Lipschitz. To apply the Newton method for Freundlich type isotherms we employ a regularization step.

The water flux $\mathbf{Q}$ appearing in (1), as well as the water content $\Theta(\psi)$, are obtained by solving the mass balance equation for water, which is assumed incompressible

$$\partial_t \Theta(\psi) + \nabla \cdot \mathbf{Q} = 0 \tag{3}$$

and the Darcy's law

$$\mathbf{Q} = -K(\Theta(\psi))\nabla(\psi + z), \tag{4}$$

together with initial $\Psi(t = 0) = \Psi_I$ and homogeneous Dirichlet boundary conditions. Combining the Eqs. (3) and (4) one obtains the Richards equation, which is a typical mathematical model for water flow through saturated/unsaturated soil. For the coefficient functions $\Theta(\cdot)$ and $K(\cdot)$ functional dependencies of the pressure are assumed, so that the unknowns in (3)–(4) are reduced to two.

In [1,2] we have proposed and analyzed a mass conservative scheme for the Eq. (1) based on the MFEM for the spatial discretization and Euler implicit (EI) for the discretization in time. We have shown (see [2]) that the difference between the solution of the nonlinear fully discrete problems and the exact solution (which is called in the following the discretization error) vanishes as the time step and the mesh diameter are approaching zero. The order of convergence naturally depends on the accuracy of the scheme for the water flow. However, at each time step one has to solve the fully discrete nonlinear problems resulting after the mixed finite element (MFE) discretization, this being a challenging problem in itself. The objective of this work is to analyze the applicability of the Newton method for solving these nonlinear systems. Sufficient explicit conditions for the quadratic convergence of the method are derived.

Most of the papers dealing with numerical schemes for transport equations cope to estimate the discretization error and assume that the fully discrete nonlinear problems are solved exactly. We mention [3] for a conformal FEM discretization and [4] for finite volume schemes. Furthermore, a characteristic mixed method is studied in [5], upwind MFEM is considered in [6], whereas combined finite volume mixed hybrid finite elements are employed in [7,8]; see also [9] for a review. In [1, 2] we presented and analyzed an EI-MFE scheme that is based on the lowest-order Raviart–Thomas ($RT_0$) elements for the Eq. (1). The resulting fully discrete nonlinear problems are commonly solved by different methods: the Newton scheme (which is locally quadratic convergent), some robust first-order linearization schemes (see [10–12]), or the Jäger–Kačur scheme [13]. The convergence of the Newton method applied to the system provided by a MFE discretization of an elliptic problem is studied in [14]. Concerning the systems provided by the MFE discretization of degenerate parabolic equations we mention [10] for a robust linear scheme and [15] for the Newton method. There, the fast diffusion case is considered, whereas here we have slow diffusion. Furthermore, the nonlinear term in the cited papers depends only on the solution and not on time, whereas the convection vector is constant and there is no reaction term.

The paper is structured as follows. The next section provides the continuous problem, the assumptions and presents the discretization scheme. In the first part of Section 3 we define the Newton scheme and prove its convergence. This is done for the diffusive–convective–reactive solute transport without sorption. We also explain how to include equilibrium, Lipschitz continuous sorption isotherms. Next we consider equilibrium non-Lipschitz sorption and perform a regularization step. We show the consistence of the regularization scheme and present the Newton scheme for this case, proving its convergence. In Section 5 we give some concluding remarks.

## 2. Euler implicit mixed finite element discretization

Throughout this paper we use common notations in the functional analysis. By $\langle \cdot, \cdot \rangle$ we mean the inner product on $L^2(\Omega)$. Further, $\|\cdot\|$ and $\|\cdot\|_{L^4(\Omega)}$ stand for the norms in $L^2(\Omega)$ and $L^4(\Omega)$, respectively. The functions in $H(\text{div}; \Omega)$ are vector valued, having a $L^2$ divergence. By $C$ we mean a positive constant, not depending on the unknowns or the discretization parameters and by $L_f$ the Lipschitz constant of a function $f(\cdot)$. Furthermore, $\mathcal{T}_h$ is a regular decomposition of $\Omega \subset \mathbb{R}^d$ into closed $d$-simplices; $h$ stands for the mesh diameter. Here we assume $\overline{\Omega} = \cup_{T \in \mathcal{T}_h} T$, hence $\Omega$ is polygonal. Correspondingly, we define the discrete subspaces $W_h \subset L^2(\Omega)$ and $V_h \subset H(\text{div}; \Omega)$:

$$\begin{aligned} W_h &:= \{p \in L^2(\Omega) |\ p \text{ is constant on each element } T \in \mathcal{T}_h\}, \\ V_h &:= \{\mathbf{q} \in H(\text{div}; \Omega) | \mathbf{q}_{|T} = \mathbf{a} + b\mathbf{x} \text{ for all } T \in \mathcal{T}_h\}. \end{aligned} \tag{5}$$

In other words, $W_h$ denotes the space of piecewise constant functions, while $V_h$ is the $RT_0$ space (see [16]). For the discretization in time we let $N \in \mathbb{N}$ be strictly positive, and define the time step $\tau = T/N$, as well as $t_n = n\tau (n \in \{1, 2, \ldots, N\})$.