Optimal order convergence of a modified $\textit{BDM}_1$ mixed finite element scheme for reactive transport in porous media

by

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Optimal order convergence of a modified $BDM_1$ mixed finite element scheme for reactive transport in porous media

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Abstract

We present a higher order mass conservative finite element approach for the numerical approximation of reactive solute transport in porous media modeled by a coupled system of advection-diffusion-reaction equations. The lowest order Brezzi-Douglas-Marini ($BDM_1$) mixed finite element method is used. A modification based on the hybrid form of the approach is suggested for the discretization of the advective term. Thereby optimal second order convergence of the flux variable is obtained, as the performed numerical computations illustrate. This modification improves the convergence behavior of the classical $BDM_1$ scheme, which is known to be suboptimal of first order accuracy only for advection-diffusion problems; cf. [8]. Moreover, the new scheme shows more robustness for high Péclet numbers than the classical approach. A comparison with the Raviart-Thomas element ($RT_1$) of second order accuracy for the approximation of the flux variable is also presented. For the case of strongly advection-dominated problems we propose a full upwind scheme. Various numerical studies, including also a nonlinear test problem, are presented to illustrate the numerical performance properties of the considered numerical methods.

Keywords: reactive transport, mixed finite element methods, optimal order convergence

AMS subject classifications: 65M60, 76S05, 65M12

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1 Introduction

Multicomponent reactive transport phenomena in porous media are often studied in civil, environmental and technical engineering; cf., e.g., [1, 17]. The reliable and efficient numerical simulation of such processes is still a challenging task. Typically, the model equations are strongly coupled such that inaccuracies in one unknown directly affect all other unknowns. In large chemical systems with complex reaction mechanisms and interactions, numerical artifacts can then lead to completely wrong predictions; cf. [5, 12, 13, 16].

In this work we focus on the numerical approximation of transport systems that are modeled by the nonlinear set of partial differential equations

\[
\begin{align*}
\frac{\partial_t}{\partial t} (\Theta c_i) + \nabla \cdot (D_i \nabla c_i - Q c_i) &= R_i(c_1, \ldots, c_I) \quad \text{in } J \times \Omega, \\
c_i &= g_D, \quad \text{on } J \times \Gamma_D, \\
- D_i \nabla c_i \cdot n + Q c_i \cdot n &= g_F, \quad \text{on } J \times \Gamma_F, \\
c_i(0, \cdot) &= c_i^0(\cdot) \quad \text{in } [0] \times \Omega
\end{align*}
\]

for \( i = 1, \ldots, I \), with \( I \in \mathbb{N} \). Equation (1) includes the effects of advective, diffusive and reactive transport in a multicomponent system with the unknown vector \( c = (c_1, \ldots, c_I)^T \) of concentrations of mobile chemical species. In (1)–(4), we denote by \( J = (0, T] \) a finite time interval and \( \Omega \subset \mathbb{R}^2 \) is a domain with Lipschitz-continuous boundary \( \Gamma \) which is split into a flux boundary \( \Gamma_F \) and a Dirichlet boundary \( \Gamma_D \). The outer unit normal vector to \( \Omega \) is denoted by \( n \). To simplify the notation, Neumann boundary conditions are omitted in the sequel. They can be treated in a straightforward way.

The rates \( R_i(c_1, \ldots, c_I) \) model chemical reaction rates and sources and sinks. Further, \( \Theta \) denotes the volumetric water content, \( Q \) the Darcy flux and \( D_i \in \mathbb{R}^{2,2} \) is the diffusion-dispersion tensor of the \( i \)-th chemical species. If reactive transport in the subsurface is considered, the water flux \( Q \) and the volumetric water content \( \Theta \) are typically computed by solving the Richards equation, which (in its mixed pressure formulation) reads as

\[
\frac{\partial_t}{\partial t} (\Theta(\psi)) + \nabla \cdot Q = 0, \quad Q = -K(\Theta(\psi)) \nabla (\psi + z).
\]

Here, \( \psi \) is the hydraulic head pressure, \( \Theta(\cdot) \) is the given parametrization of the water content, \( K(\cdot) \) is the given hydraulic conductivity and \( z \) denotes the height against the gravity direction. For appropriate discretization techniques for solving (5) we refer to, e.g., [2] and the references therein.

Several numerical methods have been proposed and studied for solving the system of equations (1)–(4). Among these techniques the mixed finite element method has been applied successfully; cf. [4, 18, 19]. It is locally mass conservative and provides an accurate flux approximation as part of the formulation itself. Typically, the lowest order Raviart-Thomas element \( RT_0 \) is used for mixed finite element calculations; cf. [18, 19]. One argument for this is that the solution lacks the global regularity that is needed in optimal order error analysis to get an improvement by using higher order
techniques. A second argument might be the high algorithmic complexity of the mixed finite element approach that further increases for higher order elements; cf. Section 2. However, in our numerical calculations we have made the experience that higher order approximations of mixing processes lead to more accurate results even if the global regularity of the solution that is needed to get an improvement by using higher order approaches cannot be ensured globally; cf. [5, 4]. Our performed computer experiments have shown that higher order finite element methods are characterized by less inherent numerical diffusion than lower order ones; cf. [5, 4]. In lower order approaches an overrepresentation of the transverse mixing of the substances could be observed leading to an overprediction of chemical reaction mechanisms and degradation rates and, thereby, to wrong prognoses; cf. [5].

The simplest and computationally less expensive mixed approach to get a second order accurate approximation of the flux variable consists in using the lowest-order Brezzi-Douglas-Marini element $BDM_1$. For the Poisson equation or steady diffusion equations this result is well known; cf. [7]. By means of the Lagrange multiplier technique a second order accurate approximation of the scalar variable can also be ensured; cf. [7]. However, in [8] it was shown theoretically and numerically that the second order accurate approximation of the flux variable cannot be carried over to advection-diffusion equations. If advective terms are present, suboptimal first-order convergence of the flux approximation is obtained only, where the flux variable is defined as the total flux consisting of advective and diffusive transport.

In this work we will present a modification of the $BDM_1$ approach that ensures second order convergence of the flux variable also for advection-diffusion models with and without reaction. To solve our discrete systems we use a hybridization technique; cf. [7]. In this hybridization framework Lagrange multipliers are introduced that become the unknowns of the global system of discrete equations. They can be interpreted as approximations of the species concentrations on the interelement edges. The scalar and flux variables are then computed in a postprocessing step by solving local problems. Our observation and modification of the classical $BDM_1$ approach is simple but effective as our numerical calculations in Section 4 will show. It consists in using the Lagrange multipliers instead of the local concentrations for approximating the flux variable in the discrete system of equations. To be more precise, in the hybrid discrete form (cf. Eq. (10)) of the equation for the flux variable,

$$q_i = -D_i \nabla c_i + Qc_i,$$  

we use the Lagrange multiplier for approximating the scalar variable $c_i$ in the advective part of the right-hand side in (6). The same idea was used recently for the $RT_0$ mixed finite element method in [22, 20]. This modification results in the discrete Eq. (17). The standard $BDM_1$ approach is based on using the piecewise constant approximation of $c_i$ which, however, is not sufficient for getting second order convergence of the flux approximation for advection-diffusion problems. The difference in the presented realizations of the $BDM_1$ approach comes through the observation that in the modified
$BDM_1$ method the discrete advective part of the flux belongs to the space $H(\text{div}; \Omega)$ consisting of $L^2(\Omega)$ functions with their divergence belonging to $L^2(\Omega)$. This is not satisfied for the standard $BDM_1$ approach and seems to be the reason for the higher order convergence rate. Summarizing, if we denote by $q_{h,BDM_1}$ and $q_{h,BDM_1^{\text{new}}}$ the discrete approximations of the classical and the modified $BDM_1$ approximations, respectively, our numerical observation is that

$$\|q - q_{h,BDM_1}\| \leq Ch \quad \text{and} \quad \|q - q_{h,BDM_1^{\text{new}}}\| \leq Ch^2.$$  

Here, $\|\cdot\|$ denotes the $L^2$-norm and $h$ is the mesh diameter. This observation indicates optimal second order convergence of the modified $BDM_1$ approach also for advection-diffusion models. In this paper we show the convergence numerically, by considering several test problems, including a nonlinear one in Section 4. A rigorous proof of this numerical results is still an open problem and will be our work for the future.

In applications of practical interest, the size of diffusion in (1) is sometimes smaller by several orders of magnitude compared to the size of the flow field $Q$. Then the set of equations are advection-dominated. In such cases the system (1)–(4) admits solutions with sharp moving fronts, interior or boundary layers and complicated structures where important chemical phenomena take place. For problems with strong advection dominance the proposed modified $BDM_1$ approach has to be further modified to obtain stable approximations even though it is more robust than the standard $BDM_1$ approach. Without further modifications spurious non-physical oscillations may arise or the scheme may even diverge as it is usual for standard approximation schemes in the case of advection dominance. Therefore, we couple the modified $BDM_1$ approach with an additional upwind technique. This will lead to stable approximations also for strongly advection-dominated transport systems. However, since the upwind technique is known to be of first order accuracy only, the second order convergence rate of the flux approximation gets lost. In the case of moderate advection dominance, with Péclet number $\text{Pe} = 1000$, our numerical calculations will show that the modified $BDM_1$ method yields errors that are two orders of magnitude smaller than the errors of the standard $BDM_1$ approach. This shows that the scheme is more robust against advection dominance.

Finally, we note that for conforming non-mixed finite element approximations of advection-dominated problems, various classes of stabilization techniques were proposed in the literature. For a review and a discussion of these methods we refer to the recent work of John and Schmeyer [11]. Studies of stabilized higher order approaches are presented in [6].

The paper is organized as follows. In Section 2 we present the discretization of the equations (1)–(4) in time and space by using the backward Euler scheme and the $BDM_1$ mixed finite element method. Moreover, the hybridization of the set of discrete equations is sketched. In Section 3 our modification of the $BDM_1$ approach is introduced. In Section 4 the numerical performance properties of the schemes are studied for a variety of test problems with increasing complexity. The numerical results nicely illustrate the
improved second order convergence for the flux approximation in advection-diffusion models. The paper ends with a conclusion and an outlook.

2 Discretization

In this section we present the discretization of the system (1)–(4) by the \textit{BDM}_1 mixed finite element method in space and the backward Euler scheme in time. To simplify the notation, we assume in the following that the water content $\Theta$ and the water flux $Q$ are given functions. Moreover, $\Theta$ is considered to be constant in time. For simplicity, let $D_i \equiv D$, i.e. diffusion and dispersion are independent of the chemical species, and let $g_{F,i} = 0$ for all $i \in [1, \ldots, I]$, i.e. no-flow boundary conditions are assumed on $\Gamma_F$. Rewriting the equations (1)–(4) in their mixed form leads to the following system:

\[
\begin{align*}
\partial_t (\Theta c_i) + \nabla \cdot q_i &= R_i & \text{in } J \times \Omega, \\
q_i &= -D \nabla c_i + Q c_i & \text{in } J \times \Omega, \\
c_i &= g_{D,i} & \text{on } J \times \Gamma_D, \\
q_i \cdot n &= 0 & \text{on } J \times \Gamma_F, \\
c_i &= \Theta^n_i & \text{in } [0] \times \Omega.
\end{align*}
\]

Now, let $T_h$ be a decomposition of $\Omega$ into closed triangles $K \in T_h$ and let $E$ denote the set of all edges, whereas $E_D$ and $E_F$ are the edges on the Dirichlet and the flux boundary, respectively.

The discretization in time is done by the backward Euler method, where the time interval $J$ is divided in $N$ subintervals $(t_{n-1}, t_n)$, $n \in [1, \ldots, N]$, with $\tau_n = t_n - t_{n-1}$ denoting the time step size. For the spatial discretization with the \textit{BDM}_1 mixed finite element method we define the spaces

\[
\begin{align*}
V_h &= \{ q \in H(\text{div}; \Omega) : q|_K \in \text{BDM}_1(K) \forall K \in T_h \}, \\
W_h &= \{ w \in L^2(\Omega) : w|_K \in \mathcal{P}_0(K) \forall K \in T_h \},
\end{align*}
\]

where $\text{BDM}_1(K) = (\mathcal{P}_1(K))^2$ and $\mathcal{P}_k(K)$ is the space of polynomials of degree at most $k$ on $K$. Finally, we can define the fully discrete mixed weak formulation of the reactive transport equations at time level $n$:

**Problem 1** Let $c_{i,h}^{n-1}$ be given. For $i \in [1, \ldots, I]$ find $(q_{i,h}^n, c_{i,h}^n) \in V_h \times W_h$ satisfying

\[
\begin{align*}
\langle D^{-1} q_{i,h}^n, v_h \rangle_\Omega - \langle c_{i,h}^n, \nabla \cdot v_h \rangle_\Omega - \langle D^{-1} Q^n c_{i,h}^n, v_h \rangle_\Omega &= -\langle g_{D,i}, v_h \cdot n \rangle_{\Gamma_D}, \\
\frac{1}{\tau_n} \langle \Theta(c_{i,h}^n - c_{i,h}^{n-1}), w_h \rangle_\Omega + \langle \nabla \cdot q_{i,h}^n, w_h \rangle_\Omega &= \langle R_i, w_h \rangle_\Omega,
\end{align*}
\]

for all $v_h \in V_h$ and $w_h \in W_h$. 


The superscript \( n \) refers to the evaluation of a variable at time \( t = t_n \). Unfortunately, the linear system arising from this discretization leads to a high number of unknowns. Moreover, the system matrix that remains after a linearization is in general indefinite such that standard iterative linear solvers cannot be applied or might fail to converge.

To improve the properties of the linear systems and to reduce the global number of unknowns, a hybridization technique is used; cf. [7, 18]. This means that the condition \( V_h \subseteq V \) is relaxed and that the space \( V_h \) is replaced by the augmented space \( \tilde{V}_h = \{ q \in L^2(\Omega) : q|_K \in BDM_1(K) \ \forall K \in T_h \} \). Then, the continuity of the normal fluxes over interelement edges is no longer incorporated into the function space, but it is ensured by introducing Lagrange multipliers from the spaces

\[
\Lambda_h = \{ \lambda \in L^2(E) : \lambda|_E \in P_1(E) \ \forall E \in \mathcal{E} \},
\]

\[
\Lambda_{g,h} = \{ \lambda \in \Lambda_h : \langle \lambda - g, 1 \rangle_E = 0 \ \forall E \in \mathcal{E}_D \}
\]

and requiring an additional variational equation. The resulting mixed hybrid discrete formulation reads as:

**Problem 2** Let \( e^{n-1}_{i,h} \) be given. For \( i \in \{1, \ldots, I\} \) find \( (q^n_{i,h}, e^n_{i,h}, A^n_{i,h}) \in \tilde{V}_h \times W_h \times \Lambda_{g,h} \) satisfying

\[
\langle D^{-1} q^n_{i,h}, v_h \rangle_\Omega - \langle c^n_{i,h}, \nabla \cdot v_h \rangle_\Omega - \langle D^{-1} (q^n_{i,h} e^n_{i,h}), v_h \rangle_\Omega = - \sum_{k \in \mathcal{T}_h} \langle (\lambda^n_{i,h}, v_h \cdot n) \rangle_{\partial K}
\]

\[
\frac{1}{\tau^n} (\theta (c^n_{i,h} - c^{n-1}_{i,h}), w_h) + \langle \nabla \cdot q^n_{i,h}, v_h \rangle_\Omega = \langle R_i, w_h \rangle_\Omega,
\]

\[
\sum_{k \in \mathcal{T}_h} \langle (\mu_h, q^n_{i,h} \cdot n) \rangle_{\partial K} = 0
\]

for all \( v_h \in \tilde{V}_h, w_h \in W_h \) and \( \mu_h \in \Lambda_{0,h} \).

For an algebraic formulation of Problem 2, basis functions of the involved function spaces are needed. The linear basis functions \( \mu^{(1)}_E, \mu^{(2)}_E \) for the Lagrange multipliers on each edge \( E = \text{conv}(a_1, a_2) \) are defined by

\[
\mu^{(1)}_E(a_1) = 1, \quad \mu^{(1)}_E(a_2) = 0, \quad \mu^{(2)}_E(a_1) = 0, \quad \mu^{(2)}_E(a_2) = 1.
\]

The support of a basis function of \( \tilde{V}_h \) lies within one element \( K \in \mathcal{T}_h \) only. The basis functions can be defined by transforming the basis functions on the unit reference triangle \( \hat{K} \) to an arbitrary element by means of the the Piola transformation. Precisely, the basis functions on \( \hat{K} \) are defined as follows:

\[
\psi^{(1)}_{KE_1} (\hat{x}, \hat{y}) = (-2\hat{x}, 6\hat{x} + 4\hat{y} - 4)^T,
\]

\[
\psi^{(1)}_{KE_2} (\hat{x}, \hat{y}) = (4\hat{x}, -2\hat{y})^T,
\]

\[
\psi^{(1)}_{KE_3} (\hat{x}, \hat{y}) = (-2\hat{x} - 6\hat{y} + 2, 4\hat{y})^T,
\]

\[
\psi^{(2)}_{KE_1} (\hat{x}, \hat{y}) = (4\hat{x}, -6\hat{x} - 2\hat{y} + 2)^T,
\]

\[
\psi^{(2)}_{KE_2} (\hat{x}, \hat{y}) = (-2\hat{x}, 4\hat{y})^T,
\]

\[
\psi^{(2)}_{KE_3} (\hat{x}, \hat{y}) = (4\hat{x} + 6\hat{y} - 4, -2\hat{y})^T.
\]

The local numbering of the basis functions \( \psi^{(i)}_{KE} \) on \( K \) is done according to the global numbering of the Lagrange multipliers \( \mu^{(i)}_E, E \in \partial K, \ i = 1, 2, \) such that, due to the
properties of the Piola transformation and the definition of the basis functions, the following properties are satisfied:

\[ \langle \nabla \cdot v^{(i)}_{KE}, 1 \rangle_K = 1 \quad \text{for } E \subset \partial K, \ i = 1, 2, \quad (7) \]

\[ \langle v^{(i)}_{KE} \cdot n_E, 1 \rangle_E = \delta_{EE'} \quad \text{for } E, E' \subset \partial K, \ i = 1, 2, \quad (8) \]

\[ \langle \mu^{(j)}_{KE} v^{(i)}_{KE} \cdot n_{E'}, 1 \rangle_E = \delta_{EE'} \delta_{ij} \quad \text{for } E, E' \subset \partial K, \ i, j = 1, 2. \quad (9) \]

The basis functions for the scalar variables are given by respective characteristic functions \( \chi_K \) on the triangle \( K \). Recalling the properties (7)–(9), using the representation of the unknowns in terms of the basis functions,

\[
q^n_{i,h} = \sum_{K \in T_h} \sum_{E \subset \partial K} q^n_{i,KE} v^{(j)}_{KE},
\]

\[
A^n_{i,h} = \sum_{E \in E \subset \partial K} 2 \sum_{j=1}^{2} q^n_{i,KE} v^{(j)}_{KE},
\]

\[
c^n_{i,h} = \sum_{K \in T_h} c^n_{i,KE} \chi_K,
\]

and choosing the basis functions as test functions in the discrete mixed formulation leads to the following system of nonlinear equations:

**Equations for the fluxes:**

\[
\sum_{E \subset \partial K} \sum_{j=1}^{2} q^n_{i,KE} (D^{-1} v^{(j)}_{KE} v^{(l)}_{KE'}) K - c^n_{i,K} = \sum_{E \subset \partial K} 2 Q^n_{KE} c^n_{i,K} (D^{-1} v^{(j)}_{KE} v^{(l)}_{KE'}) K = -A^n_{i,E'} \quad \forall K \in T_h, \ E' \subset \partial K, \ l = 1, 2, \ i = 1, \ldots, I. \quad (10)
\]

**Mass conservation equations:**

\[
\frac{1}{\tau_n} \Theta_K (c^n_{i,K} - c^{n-1}_{i,K}) + \sum_{E \subset \partial K} 2 q^n_{i,KE} = |K| R_i \quad \forall K \in T_h, \ i = 1, \ldots, I, \quad (11)
\]

where \( \Theta_K := \int_K \Theta \, dx \).

**Equations for the Lagrange multipliers:**

\[
\sum_{K \in T_h, E_0 K} q^n_{i,KE} = 0 \quad \forall E \in E \setminus E_0, \ j = 1, 2, \ i = 1, \ldots, I. \quad (12)
\]

The coefficients \( Q^n_{KE} \) in (10) are associated to a representation of the water flux \( Q^n \) in the local \( BDM_1 \) basis. Defining the matrices \( (B^n_E)_{E,E'} := \langle D^{-1} v^{(j)}_{KE} v^{(l)}_{KE'} \rangle_K \) and insert-
ing them into the equations for the fluxes (10) yields that
\[
\sum_{E \in \partial K} \sum_{j=1}^{2} q_{i,E}^{n} B_{KE_j} E_i = c_{i,K}^{n} - A_{i,E_i}^{n} + \sum_{E \in \partial K} \sum_{j=1}^{2} B_{KE_j} E_i Q_{KE_j}^{n} c_{i,K}^{n} \quad \forall K \in \mathcal{T}_h, \ E' \subset \partial K, \ l = 1, 2.
\]

This set of equations represents a linear system of equations on each element from which the flux variable can be eliminated by means of
\[
q_{i,E}^{n} = \sum_{E' \in \partial K} \sum_{j=1}^{2} (B_{K}^{-1})_{E_j} E_{i} (c_{i,K}^{n} - A_{i,E_i}^{n}) + Q_{KE_j}^{n} c_{i,K}^{n},
\]
where \( B_{K}^{-1} \) is the inverse of the matrix \( B_{K} = (B_{E})_{E_j} E_{i} \). This relation is inserted into the mass conservation equation (11) to obtain that
\[
\frac{1}{\tau^n} \Theta_{K} (c_{i,K}^{n} - c_{i,K}^{n-1}) + \sum_{E,E' \in \partial K} \sum_{j=1}^{2} (B_{K}^{-1})_{E_j} E_{i} (c_{i,K}^{n} - A_{i,E_i}^{n}) = |K|R_{i}
\]
\( \forall K \in \mathcal{T}_h, \ i = 1, \ldots, I. \)

Finally, we introduce the variables
\[\]
in (15) and end up with the identity
\[
c_{i,K}^{n} \left( \Theta_{K} \frac{1}{\tau^n} + b_{K} \right) - c_{i,K}^{n-1} \Theta_{K} \frac{1}{\tau^n} - \sum_{E \in \partial K} \sum_{j=1}^{2} A_{i,E_i}^{n} b_{E_j} - |K|R_{i} = 0 \quad \forall K \in \mathcal{T}_h, \ i = 1, \ldots, I.
\]

Thus, on each element \( K \) a nonlinear system of equations is obtained which can be solved by a (local) Newton iteration for the unknowns \( c_{i,K}^{n}, \ i = 1, \ldots, I. \) Finally, the concentrations and fluxes are inserted into (12) to get the following overall global system of equations for the Lagrange multipliers:
\[
\sum_{K \in \mathcal{T}_h} \left\{ \sum_{E' \in \partial K} \sum_{j=1}^{2} (B_{K}^{-1})_{E_j} E_{i} (c_{i,K}^{n} - A_{i,E_i}^{n}) + Q_{KE_j}^{n} c_{i,K}^{n} \right\} = 0
\]
\( \forall E \in \mathcal{E} \setminus \mathcal{E}_D, \ j = 1, 2, \ i = 1, \ldots, I. \)

We note that according to (15) the local concentrations \( c_{i,K}^{n} \) in (16) depend on the Lagrange multipliers, i.e. \( c_{i,K}^{n} = c_{i,K}^{n} (\{l_{i,E_j}^{n}\}_{j=1, \ldots, I, E \in \partial K, \ l = 1, 2}) \). Hence, in each step of the global Newton iteration, the equations for the local concentrations need to be solved when the defect is calculated. For assembling the global Jacobian matrix, the derivatives of the concentrations with respect to the Lagrange multipliers are needed. We refer to [4, 18] where this is shown in detail for the case of the lowest order Brezzi-Douglas-Marini and Raviart-Thomas element, respectively. Once the global system for the Lagrange multipliers has been solved, the flux unknowns can be reconstructed efficiently on each element from equation (14).
Figure 1: Triangular element with degrees of freedom for the flux basis functions.

3 The new scheme

In [8] it has been shown theoretically as well as by a numerical experiment that for the linear elliptic advection-diffusion equation

\[ \nabla \cdot q = F, \quad q = -D \nabla c + Qc, \]

the classical \( BDM_1 \) scheme yields only a first order accurate approximation of the flux variable \( q \) in the \( L^2 \)-norm. Hence, the presence of the advective term \( Qc \) leads to a suboptimal convergence behavior of the flux. Therefore, using \( BDM_1 \) elements for such models becomes unattractive since the same approximation quality can also be obtained by lowest order Raviart-Thomas discretizations where the computational cost is lower. We will now introduce a modification of the scheme presented in the previous section to obtain optimal second order accuracy for the flux approximation. The idea is to discretize the advective term in (13) by using the Lagrange multipliers instead of the local concentration values. The same idea was previously used for the \( RT_0 \) approach in [22, 20]. It indeed is motivated by the well known observation that the Lagrange multipliers can be used to reconstruct a higher order piecewise linear approximation of the concentrations in the local Crouzeix-Raviart space [3]. The equations for the fluxes in the new scheme then read as:

\[
\sum_{E \in \partial K} \sum_{j=1}^{2} q_{n,K,E}^i B_{KE,E_j}^k = c_{n,K}^k - x_{i,E_j}^k + \sum_{E \in \partial K} \sum_{j=1}^{2} B_{KE,E_j}^k Q_{KE,A_{i,l}}^n(x_{E_j}^k) \quad (17)
\]

\[ \forall K \in \mathcal{T}_h, \ E' \subset \partial K, \ l = 1, 2. \]

Here, by \( x_{E}^k \) we denote the nodes of the triangle \( K \) corresponding to the degrees of freedom of the flux basis functions; cf. Fig. 1. The scheme is supplemented by equations (11) and (12). If an analogous modification is applied to a \( RT_0 \) discretization (cf. [20]), no increase in the order of convergence is observed, but the numerical results indicate that the scheme remains more robust for high Péclet numbers. In the following numerical examples, we will show that the new \( BDM_1 \) scheme, referred to as \( BDM_1^{\text{new}} \) from now on, is also more robust than the classical \( BDM_1 \) approach and, moreover, is of optimal order accuracy with respect to the flux approximation.
In the case of moderate advection dominance the $BDM_{1}^{new}$ scheme (11), (12) and (17) leads to stable approximations. Nevertheless, a further stabilization becomes necessary for strongly advection-dominated problems. In this case we now couple the modified $BDM_{1}$ approach with an additional upwind technique. The same technique has also been applied successfully in [22, 20] to the $RT_{0}$ mixed finite element approximation.

As our performed computations illustrate (cf. Section 4.4), the upwind scheme will lead to stable approximations also for strongly advection-dominated transport systems.

Nevertheless, the upwind scheme is of first order accuracy only.

The full upwind scheme $BDM_{1}^{upwind}$ is defined by equations (11), (12) along with

$$\sum_{E \in \partial K} \sum_{j=1}^{2} B_{l,KE,E}^{j} B_{KE,E}^{j} = c_{l,K}^{n} - \lambda_{l,K}^{n} + \sum_{E \in \partial K} \sum_{j=1}^{2} B_{KE,E}^{j} Q_{l,KE,J}^{n} \alpha_{l,E}^{n},$$

where

$$\alpha_{l,E}^{n} = \begin{cases} c_{l,K}^{n}, & \text{if } Q_{l,E}^{n} \geq 0, \\ 2 \lambda_{l,h}^{n} (x_{E}^{l}) - c_{l,K}^{n}, & \text{otherwise}. \end{cases}$$

4 Numerical studies

We shall now study the numerical performance properties of the $BDM_{1}^{new}$ scheme. This is done for test problems with a prescribed analytical solution, but also for more sophisticated scenarios including the simulation of the biodegradation of a contaminant and highly advection-dominated problems.

4.1 Elliptic transport equation

The first numerical test is devoted to a comparison with [8], where the suboptimal convergence for the classical $BDM_{1}$ scheme was shown. The simple elliptic model problem

$$\nabla \cdot q = F \quad \text{in } \Omega,$$

$$q = -D \nabla c + Q c \quad \text{in } \Omega,$$

$$c = 0 \quad \text{on } \partial \Omega$$

is considered on the unit square $\Omega = (0,1)^{2}$, where $Q = (0.9, 0.9)$, $D = I$ and $F$ is chosen such that $c(x,y) = x(1-x)y(1-y)$ is the analytical solution of problem (19). A uniform triangular mesh is used which is uniformly refined such that the mesh sizes are given by $h = (\sqrt{2}/2)^{k}$ for $k = 2,\ldots,7$. All integrals of the local stiffness matrices are evaluated exactly by using a quadrature formula of sufficiently high order. The linear system is solved by the BiCGStab method combined with an ILU preconditioner. The
Table 1: Computational results for $BDM_1$ and $BDM_{\text{new}}^1$ for the elliptic test problem

<table>
<thead>
<tr>
<th>$k$</th>
<th>$|q - q_{h,BDM}|$</th>
<th>$\alpha_h$</th>
<th>BiCGStab steps</th>
<th>$|q - q_{h,BDM_{\text{new}}^1}|$</th>
<th>$\alpha_h$</th>
<th>BiCGStab steps</th>
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<td>9.2751e-3</td>
<td>8</td>
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<td>1.5646e-4</td>
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<td>57</td>
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<td>7</td>
<td>2.2571e-4</td>
<td>1.00</td>
<td>131</td>
<td>9.8177e-6</td>
<td>2.00</td>
<td>109</td>
</tr>
</tbody>
</table>

The experimental order of convergence is calculated by means of

$$\alpha_h = \log_2 \left( \frac{\|q - q_h\|}{\|q - q_{h/2}\|} \right)$$

where $\| \cdot \|$ denotes the $L^2$-norm. Our numerical results for the classical approach are consistent to those obtained by Demlow; cf. [8]. The errors are of the same order of magnitude and the asymptotic convergence rate for the flux variable is $O(h)$. However, for our new scheme we clearly observe second order accuracy $O(h^2)$ for the flux, cf. Table 1. Obviously, we can overcome the suboptimal order of convergence without increasing the number unknowns. Additionally, the linear systems arising from the modified scheme seem to be better conditioned such that fewer iteration steps are required by the BiCGStab method for solving the system up to a given tolerance.

### 4.2 Comparison to the $RT_1$ element by using postprocessing of the concentrations

In the following, we compare our approach to the Raviart-Thomas element of second lowest order ($RT_1$ element). For this element type it has been shown that for problem (19), approximations of second order accuracy are obtained for both variables, the flux and the concentration; cf. [9]. Of course, the number of unknowns is higher for the $RT_1$ approach than for the $BDM_1$ based discretization. In particular, it holds that $\dim RT_1(K) = 8$, i.e. the local flux space is defined by eight degrees of freedom on each triangle compared to six degrees of freedom in the case of the $BDM_1$ element. The number of Lagrange multipliers, which corresponds to the size of the overall global system, remains the same for both discretizations since the two additional flux unknowns do not contribute to the normal fluxes across the interelement edges. However, the concentrations are approximated in the space of piecewise linear polynomials for the $RT_1$ method, which implies that the dimension of the local systems that need to be solved in each Newton step of the global iteration procedure is three times higher than in the case of the $BDM_1$ element. This leads to an increase of the cost for calculating the residual and assembling the Jacobian matrix in each Newton step. The CPU times that are summarized in Table 2 indicate that the $BDM_1$ approach is up to 30% faster than the $RT_1$ based method.
For the $BDM_{1}^{new}$ approach, we also reconstruct the concentration variable in the space of piecewise linear Crouzeix-Raviart elements by means of

$$\langle \tilde{c}_h - \lambda_h, 1 \rangle_E = 0 \quad \forall E \subset \partial K,$$

where $\lambda_h$ denotes the Lagrange multiplier associated with $c_h$. It is known for the RT approach as well as for the BDM method that this construction yields a higher order approximation of the scalar variable; cf. [7]. This can also be observed in our numerical studies; cf. Table 3. Therefore, as far as the discretization errors of the variables $c$ and $q$ with respect to the $L^2(\Omega)$ norm are concerned, the $BDM_{1}^{new}$ and $RT_1$ approach yield errors that are of the same order of magnitude. However, the $BDM_1$ method does not improve the order of convergence with respect to the norm in $H(div, \Omega)$, defined by $\|q\|_{div} = (\|q\|^2 + \|\nabla \cdot q\|^2)^{1/2}$. Here, the $RT_1$ approach provides an approximation of second order accuracy, whereas the $BDM_{1}^{new}$ and the $BDM_1$ approaches yield first order accuracy only; cf. Table 3. In this point $RT_1$ is superior to $BDM_{1}^{new}$ and $BDM_1$.

### 4.3 Transport of two mixing and reacting species

In the following test problem, the transport of two reacting and mixing substances (cf. [18]) is reconsidered in order to analyze if the second order accuracy of the flux variable is also preserved in the presence of nonlinear reaction terms. For this, let $\Omega = (0, 2) \times (0, 3)$ and $Q = (0, -1)^T$, $D_1 = D_2 = 0.1I$, $\Theta = 1.0$, and $\alpha_1 = 1$, $\alpha_2 = 2$. The governing equations are

$$\partial_t (\Theta c_i) - \nabla \cdot (D_i \nabla c_i - Q c_i) = -\Theta R_i + F_i, \quad R_i = \alpha_i c_i c_j^2, \quad i, j = 1, 2.$$
A constant time step size of $\tau = 0.001$ is chosen and the final time of simulation is $T = 1$. The coarsest grid with mesh size $h = \sqrt{2}$ on refinement level $k = 0$ is uniformly refined to compare the numerical errors. The source terms $F_i$ are prescribed such that the analytical solutions are given by

$$c_1(x,y,t) = x(2.0 - x)^3 \exp(-0.1t) / 27,$$
$$c_2(x,y,t) = (x - 1.0)^3 y^2 \exp(-0.1t) / 9.$$

Since the reaction rates $R_i$ are given by products of the involved chemical species, the chemical reaction only occurs if both species $c_1$ and $c_2$ are present. If, for instance, numerical diffusion leads to an artificial mixing of the species, an additional amount of mass may be degraded resulting in a loss of mass and, finally, a wrong prediction. However, Table 4 shows that this effect does not arise in the $BDM_{1}^{\text{new}}$ approach. Here, second order convergence is nicely observed for the flux and the reconstructed concentration variable. In the next section, we will analyze the effect of inherent numerical diffusion of the $BDM_{1}^{\text{new}}$ approach further for a more sophisticated model problem where advection dominates diffusion.

### 4.4 Advection-dominated problems

Many real world problems related to reactive subsurface transport of chemical species are dominated by advection. In this case, the commonly used numerical methods produce inaccurate and often completely wrong results. A remedy to overcome this shortcoming of standard approximation techniques are stabilization techniques. For an
overview over the most popular stabilization methods we refer to [11, 10]. In this section, we want to study the behavior of the proposed $BDM_{1}^{new}$ scheme for high Péclet numbers.

4.4.1 Contaminant biodegradation of two mixing species

In the case of an $RT_0$ based mixed approximation, it has already been observed in [20] that the discretization of the advective term in terms of the Lagrange multipliers leads to a more robust behavior for advection-dominated problems. To show that this holds analogously for the $BDM_{1}^{new}$ scheme, we recalculate a model problem for the simulation of contaminant biodegradation which has been widely used in the literature to compare different numerical schemes, cf., e.g., [5, 16]. In this model, a Monod degradation reaction between an electron donator $c_D$ (e.g. the contaminant) and an electron acceptor $c_A$ (e.g. oxygen) in the domain $\Omega = (0,0.5) \times (0,1)$ is considered. The process is governed by the set of equations

$$\partial_t (\Theta c_D) - \nabla \cdot (\Theta D_{\text{diff}} \nabla c_D - Q c_D) = -a_D \mu,$$

$$\partial_t (\Theta c_A) - \nabla \cdot (\Theta D_{\text{diff}} \nabla c_A - Q c_D) = -a_D \mu,$$

where the Monod term $\mu$ is defined by

$$\mu = c_{Bio} \frac{c_D}{K_D + c_D} \frac{c_A}{K_A + c_A}.$$

The reaction is catalyzed by the biomass $c_{Bio}$ which is kept constant in this simplified model. Furthermore, dispersion is neglected and only molecular diffusion $D_{\text{diff}}$ is considered. The initial and boundary conditions are shown in Fig. 3. Here, the same simulation parameters as in [5, 16] are chosen:

$$\Theta = 0.2, \quad Q = (0,-1)^T, \quad D_{\text{diff}} = 0.0001, \quad \alpha_D = 5.0, \quad \alpha_A = 0.5, \quad K_D = 0.1, \quad K_A = 0.1.$$

The simulation is done with a time step size of $\tau^n = 0.001$ on a preadapted grid with 32268 elements. The grid and the computational results are illustrated in Fig. 4. Our computational results show that almost all of the amount of contaminant is transported through the domain and reaches the outflow boundary. The predicted value of $c_D$ at the midpoint of the outflow boundary is 0.99987 at the final time $T = 3$, where an almost steady state has been reached. In [16], where an adaptive finite volume upwind method on a very fine adaptive grid with almost 250000 elements was used, a value of $c_D = 0.6$ was predicted only at the midpoint of the outflow boundary. Obviously, only a small amount of numerical diffusion is introduced by our scheme. Otherwise, an artificial mixing of the species and consequently an overprediction of the degradation would be observed. Inappropriate methods may even lead to a complete degradation of the contaminant within the domain which would have serious consequences in practice. However, we note that our scheme does not prevent the appearance of under- and
overshoots and negative values in the concentration profiles. This known drawback of mixed (hybrid) finite element methods for advection-diffusion problems can be solved by using mass lumping (with some special quadrature formula); cf. [14, 15, 21, 23]. In this way a discrete maximum principle can be guaranteed.

The computational results in Fig. 4 show that the use of full upwinding improves the monotonicity of the numerical method. Overshoots or undershoots can be prevented. Of course, more numerical diffusion is introduced leading to an overprediction of the degradation process as a consequence of an increased artificial mixing of the species. But the predicted outflow contaminant concentration is still approximately 50% of the injected amount which is almost the value obtained by the adaptive finite volume strategy in [16] with 250000 elements.

4.4.2 Elliptic model problem with varying Péclet numbers

In the last numerical example, the three variants of the $BDM_1$ based approximations that are presented in this paper are compared with respect to their convergence behavior in the case of high Péclet numbers. For this purpose, the elliptic model problem (19) which describes the stationary concentration distribution of a chemical species subject to an advection-diffusion process in a porous medium is reconsidered. The simulations are performed for different Péclet numbers, given by $\text{Pé} := L \sqrt{Q_x^2 + Q_y^2} / D$, where $L$ denotes the characteristic length of the domain. This is done by prescribing a variable magnitude for the flux vector $Q = (0, -Q_y)\top$ and choosing the right hand side $F$ accordingly such that the analytical solution is the same function as given in Section 4.1. The numerical results obtained for the three approaches $BDM_1$, $BDM^{new}_1$ and
Figure 4: Preadapted grid (left) and calculated concentration profiles for $c_D$ with $BDM_{1}^{new}$ (middle) and $BDM_{1}^{upwind}$ (right)

$BDM_{1}^{upwind}$ are summarized in Tables 5-7. As in the previous examples, for the $BDM_{1}$ and $BDM_{1}^{new}$ method a second order accurate approximation is observed for the reconstructed concentration profile. Moreover, for Péclet = 10, suboptimal first order accuracy is obtained for the flux variable for $BDM_{1}$. However, for very high Péclet numbers, it seems that also the classical $BDM_{1}$ scheme asymptotically reaches second order convergence for the flux approximation. However, the error is clearly larger than the error calculated with the modified approach $BDM_{1}^{new}$, where second order convergence for both variables is observed. The upwind method yields first order convergence in both variables which is also nicely preserved in the highly advection-dominated regime with Péclet = $10^5$, where the other methods fail to converge.
Table 6: Convergence results for $\text{P}e = 1000$

<table>
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<th>$|q - q_h|$</th>
<th>$|c - \tilde{c}_h|$</th>
<th>$|q - q_h|$</th>
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<td>2.697e-3</td>
<td>7.845e-4</td>
<td>8.183e-1</td>
</tr>
</tbody>
</table>

Table 7: Convergence results for $\text{BDM}_{1}^{\text{upwind}}$ for $\text{P}e = 10^5$

<table>
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<tr>
<th>$k$</th>
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</table>
5 Conclusion and outlook

In this paper we studied higher order mixed hybrid finite element discretizations of multicomponent reactive transport systems in porous media. It was shown numerically that the classical $BDM_1$ discretization scheme can be modified in a simple way to recover an optimal second order convergence rate for the flux variable also in the case that an advection term is present. For advection-diffusion problems, this second order accurate approximation of the flux variable is not provided by the $BDM_1$ scheme. The modification of the scheme does not increase the number of unknowns and leads to better conditioned linear systems resulting in fewer iteration steps for the linear solver. Using Lagrange multipliers, second order accurate reconstructions can also be calculated for the scalar variable. Therefore, with respect to the approximation in $L^2$, our modified scheme provides the same accuracy as the $RT_1$ element while saving up to 30% of the computational cost due to smaller local problems in the local elimination procedure.

Numerical tests in the context of contaminant biodegradation indicated that only a very small amount of numerical diffusion is introduced by the method. However, over- and undershoots were observed in our numerical study resulting in negative concentration values. For this reason, we also proposed a full upwind $BDM_1$ scheme to improve the monotonicity of the method. Using this technique, overshoots can be prevented. Regarding inherent numerical diffusion, the upwind scheme leads to numerical results that are comparable to those obtained by an adaptive finite volume discretization. Further numerical tests indicated that first order convergence in both variables can be guaranteed, even for problems with very high Péclet numbers.

So far, the results concerning the modified $BDM_1$ scheme are based on numerical studies only. Our work for the future is to analyze this method in a more rigorous and theoretical way. In particular, we aim to give a proof of convergence and to verify the convergence rates in terms of an a-priori error analysis.

Acknowledgments

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