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NON-FICKIAN COUPLED DIFFUSION MODELS IN POROUS MEDIA

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Abstract: In this paper we propose a numerical scheme to approximate the solution of a non-Fickian coupled model that describes diffusion in porous media. The model is defined by a system of a quasilinear elliptic equation, which governs the fluid pressure, and a quasilinear integro-differential equation, which models the convection-diffusion transport process. The numerical scheme is based on a conforming piecewise linear finite element method for the discretization in space. The fully discrete approximation is obtained with an implicit-explicit method. Estimates for the continuous in time and the fully discrete methods are derived, showing that the numerical approximation for the concentration and the pressure are second order convergent in a discrete L^2-norm and in a discrete H^1-norm, respectively.

keywords: non-Fickian diffusion, porous media, integro-differential equation, finite element method, finite difference method, supraconvergence.

1. Introduction

Transport processes in porous media are usually modeled by the classical convection-diffusion equation

$$\phi\frac{\partial c}{\partial t} + \nabla\cdot(vc) + \nabla\cdot J = q_1 \text{ in } \Omega\times(0,T], \tag{1}$$

where Ω represents the spatial domain, ϕ is the porosity of the medium, c is the concentration of the diffusion specie, being v its velocity, and J designates the mass flux defined by Fick' law

$$J = -D\nabla c. \tag{2}$$

In (2), D denotes the diffusion tensor that depends on the velocity v and is given by

$$D(v) = d_m\phi I + \alpha_t\|v\|I + (\alpha_\ell - \alpha_t)\frac{1}{\|v\|}vv^T,$$

where $\|.\|$ denotes the euclidian norm, I is the two dimensional identity matrix, d_m is the molecular diffusion coefficient, and α_ℓ and α_t are the transversal and the longitudinal dispersivities, respectively. The parabolic equation

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defined by (1), (2) is usually coupled with the elliptic pressure equation

$$-\nabla\cdot\left(\frac{K}{\mu}\nabla p\right)=q_2 \text{ in } \Omega, \tag{3}$$

where the permeability tensor K and/or the viscosity μ can depend on the concentration. The velocity v in equation (1) depends on the pressure p through Darcy's law

$$v=-\frac{K}{\mu}\nabla p \text{ in } \Omega.$$

In (1) and (3), q_1 and q_2 represent source and sink terms.

Despite the popularity of this model, gaps between experimental data and simulation results were observed in several scenarios. Without being exhaustive we mention [5], [6], [7], [8], [9], [10], [19], [22], and [30]. To overcome the limitations of traditional diffusion models, several non-Fickian models were proposed in the literature. For instance, in [26], [32], and [33], hyperbolic equations were introduced to replace the classical diffusion equations. Continuous time random walks models were tested, e.g., in [5], [6], [7] and [10]. In the present paper, we consider an integro-differential model identical to those proposed in [8], [9], and [23], and that have been extensively studied in the literature. We refer [27] for an overview on non-Fickian models for diffusion in porous media. It should be noted that integro-differential models have been also used to describe diffusion in viscoelastic materials ([11], [12], [17], [21]).

In what follows the diffusion equation (1), (2) is replaced by the following integro-differential equation

$$\frac{\partial c}{\partial t}-\nabla\cdot(D\nabla c)+\nabla\cdot(Bc)=\int_0^t K_{er}(t-s)\nabla\cdot(E\nabla c)(s)\,ds+q_1 \text{ in } \Omega\times(0,T], \tag{4}$$

where $K_{er}(s)$ denotes a memory kernel. In this work we use the following notation: if $w:\overline{\Omega}\times[0,T]\to\mathbb{R}$ then by $w(t)$ we denote the function $w(t):\overline{\Omega}\to\mathbb{R}$ such that $w(t)(x)=w(x,t)$. Equation (4) is established using the mass conservation law (1) with the mass flux J given by

$$J=J_F+J_{nF}+J_{ad}, \tag{5}$$

where J_{ad} stands for the advective mass flux, while J_F and J_{nF} represent the Fickian and non-Fickian dispersive mass fluxes, respectively. In (5), J_F is defined by (2), $J_{ad} = Bc$, and J_{nF} is the nonlocal in time operator

$$J_{nF}(t) = \int_0^t K_{er}(t-s)(E\nabla c)(s)\, ds,$$

where E depends on the velocity v and eventually on the concentration c. Equation (4) for the concentration is coupled with the elliptic equation

$$-\nabla \cdot (A\nabla p) = q_2 \text{ in } \Omega \times (0, T], \tag{6}$$

which is a natural extension of the pressure equation (3).

As already mentioned, the classical convection-diffusion equation is not able to capture the behavior of diffusion processes in porous media. For illustration, we reproduce in Figure 1 some of the results presented in [19]. In that figure, the results of two laboratory tracer experiments described in [30] (left image) and [5] (right image) are compared with the best-fit curves obtained with the classical diffusion equation (1), (2), and the integro-differential equation (4) with $K_{er}(s) = \dfrac{1}{\tau}e^{-\frac{s}{\tau}}$. The measured concentration values are represented by dots, and we observe that the integro-differential model (green line), unlike the classical model (blue line), accurately describes the experimental data in particular the late-time tails. More details about Figure 1 can be found in [19].

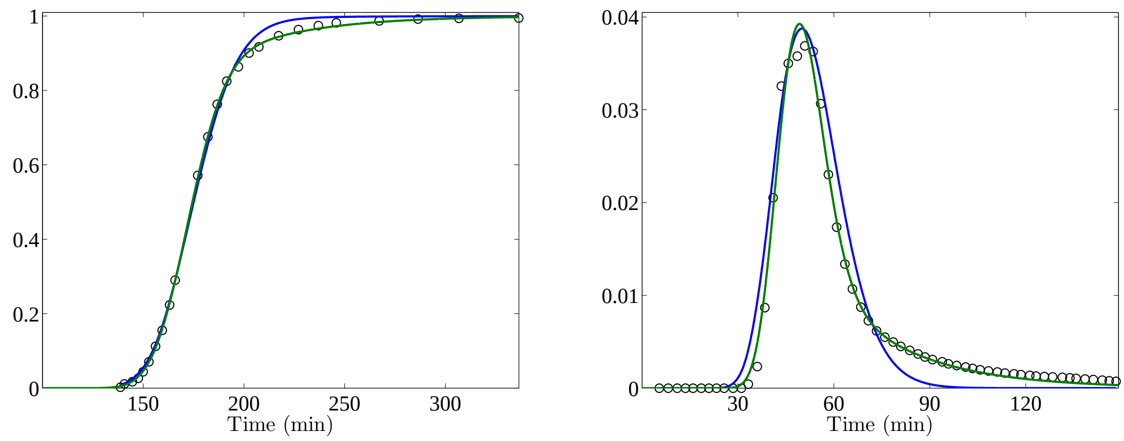

FIGURE 1. Time evolution of the concentration at a specific point of the domain, as given by (4) (green line) and by (1), (2) (blue line). The experimental data are represented by dots.

The development of efficient and accurate numerical methods to solve the integro-differential equation (4) has attracted the attention of several researchers during the last decades. A significative number of contributions can be found in the literature. Without being exhaustive we mention [24], [25], [29], and [35], for the study of semi-discrete finite element approximations, [28] for the analysis of semi-discrete lumped mass approximations, [13], [14], and [31], for the construction of semi-discrete finite volume approximations, and [1], [3], [4], and [20], for finite difference methods presenting the same qualitative behavior as the continuous integro-differential initial boundary value problems. We note that the finite difference methods studied in this last group of papers can be seen as piecewise linear finite element methods with convenient quadrature rules.

To the best of our knowledge the numerical discretization of the non-Fickian coupled problem (4), (6) was not yet analysed. In this paper we introduce finite difference methods for the approximation of the pressure and the concentration whose errors are second order convergent in discrete H^1 and L^2 norms, respectively. From these result we conclude that the numerical velocity is also a second order approximation. In this way, we extend to non-Fickian coupled problems, the results presented in [18] and [15] for piecewise linear finite element methods. We point out that these results are somehow unexpected in the context of finite difference methods as well as finite element methods. In fact, the truncation errors induced by the spatial discretizations that we consider are only of first order when non-uniform grids are used and it is also well known that piecewise linear finite element methods are first order convergent with respect to the H^1-norm. Moreover we note that the analysis in this paper differs from the one used in [18] and [15], which is based on the definition of a convenient auxiliary problem and was introduced by Wheeler in [34]. Here, we apply the approach of [20].

The remaining of the paper is organized as follows. Section 2 is devoted to the construction of the semi-discrete approximation for the solution of the coupled system (4), (6). In this section we also introduce the variational formulation and the finite difference scheme. The convergence analysis of the semi-discrete approximation for the pressure and the concentration is presented in Section 3. The main result of this section is Theorem 1 which establishes the second order convergence rate of the numerical scheme for the pressure and the concentration with respect to discrete versions of the H^1-norm and L^2-norm, respectively. An implicit-explicit (IMEX) method to compute the fully discrete approximations (in time and space) for the pressure and concentration is studied in Section 4. In Section 5, some numerical experiments are included and in Section 6 we present some conclusions.

2. Space discretization

Let $\Omega = (0,1)\times(0,1)$. We consider the coupled system (4), (6) with Dirichlet boundary conditions

$$p = p_b \text{ on } \partial\Omega \times (0,T]\,, c = 0 \text{ on } \partial\Omega \times (0,T], \tag{7}$$

and known initial concentration and pressure

$$c(0) = c_0 \text{ in } \Omega,\ p(0) = p_0 \text{ in } \Omega. \tag{8}$$

In (4), (6) the coefficient functions A, D, and E are second order diagonal square matrices with entries a_i, d_i, and e_i, $i = 1, 2$, respectively, where a_i depends on c, d_i and e_i depend on c, $\dfrac{\partial p}{\partial x}$ and eventually on the time and space variables. The two dimensional vector B has entries b_1 and b_2 which depend on $\dfrac{\partial p}{\partial x}$ and $\dfrac{\partial p}{\partial y}$, respectively, and both depend also on c.

By $L^2(\Omega)$, $L^2(\partial\Omega)$, $H^1(\Omega)$, and $H^1_0(\Omega)$ we denote the usual Hilbert spaces. In $L^2(\Omega)$ we consider the usual inner product $(.,.)$ being the induced norm represented by $\|\cdot\|$. By $[V]^2$ we represent the usual cartesian product of the vector space V.

Assuming that q_1, q_2, c_0, $p_0 \in L^2(\Omega)$, and $p_b \in L^2(\partial\Omega)$, the weak solution of the system (4)-(8) can be obtained by solving the following variational problem: find $p(t) \in H^1(\Omega)$ and $c(t) \in H^1_0(\Omega)$, with $p(t) = p_b(t)$ on $\partial\Omega$ and $\dfrac{dc}{dt}(t) \in L^2(\Omega)$, such that

$$(A(c(t))\nabla p(t), \nabla w) = (q_2(t), w),\ \forall w \in H^1_0(\Omega), \tag{9}$$

$$\begin{aligned}(\frac{dc}{dt}(t), w) &+ (D(c(t), \nabla p(t))\nabla c(t), \nabla w) - (B(c(t), \nabla p(t))c(t), \nabla w)\\ &+ \int_0^t K_{er}(t-s)(E(c(s), \nabla p(s))\nabla c(s), \nabla w)ds = (q_1(t), w),\ \forall w \in H^1_0(\Omega),\end{aligned} \tag{10}$$

for $t \in (0, T]$. In the above formulation the kernel function can be defined by $K_{er}(s) = \dfrac{1}{\tau} e^{-\frac{s}{\tau}}$, but it is not limited to that case. We remark that the inner product in $[L^2(\Omega)]^2$ is also denoted by $(.,.)$.

In what follows we derive the semi-discrete approximation for the pressure and concentration defined by the coupled variational problem (9), (10). We start by introducing some basic definitions and notations.

In $\overline{\Omega}$ we introduce a non-uniform rectangular grid which is the cartesian product of two 1D non-uniform grids $\{x_i, i = 0, \ldots, N_x\}$, $\{y_j, j = 0, \ldots, M_y\}$. Let $h = (h_1, \ldots, h_{N_x})$ and $k = (k_1, \ldots, k_{N_y})$ be vectors of positive entries such that $\displaystyle\sum_{i=1}^{N_x} h_i = \sum_{j=1}^{N_y} k_j = 1$. Let $x_i = x_{i-1} + h_i, i = 1, \ldots, N_x$, with $x_0 = 0$ and let $\{y_j, j = 0, \ldots, N_y\}$ be defined analogously with h replaced by k. By H we represent the step size vector (h, k). In $\overline{\Omega}$ we define the grid

$$\overline{\Omega}_H = \{(x_i, y_j),\, i = 0, \ldots, N_x;\, j = 0, \ldots, N_y\}.$$

We also introduce the set of grid points $\Omega_H = \overline{\Omega}_H \cap \Omega$, $\partial\Omega_H = \overline{\Omega}_H \cap \partial\Omega$.

We consider a sequence of grids Ω_H such that the maximal mesh-size $H_{max} = \max\{h_i, k_j,\, i = 1, \ldots, N_x;\, j = 1, \ldots, N_y\}$ tends to zero. We use the symbol "Λ" for the sequence of mesh-size vectors and write "$H \in \Lambda$" for the convergence when $H_{max} \to 0$ and with respect to H running through this sequence. By W_H we represent the space of grid functions defined in $\overline{\Omega}_H$ and by $W_{H,0}$ the subspace of W_H of grid functions vanishing on $\partial\Omega_H$. By R_H we denote the operator of pointwise restriction to the grid $\overline{\Omega}_H$. Let $\mathcal{T}_H$ be a triangulation of $\overline{\Omega}$ using the set $\overline{\Omega}_H$ as vertices. We denote by $\operatorname{diam}\Delta$ the diameter of the triangle $\Delta \in \mathcal{T}_H$. By $P_H v_H$ we denote the continuous piecewise linear interpolant of v_H with respect to $\mathcal{T}_H$.

In $W_{H,0}$ we introduce the inner product

$$(v_H, w_H)_H = \sum_{(x_i,y_j)\in\overline{\Omega}_H} |\square_{i,j}| v_H(x_i, y_j) w_H(x_i, y_j),\ w_H, v_H \in W_{H,0},$$

where $|\square_{i,j}|$ denotes the area of $\square_{i,j}$ with $\square_{i,j} = (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2}) \cap \Omega$ and $x_{i\pm 1/2} = x_i \pm \dfrac{h_i}{2}$, being $y_{j\pm 1/2}$ defined analogously. By $\|\cdot\|_H$ we denote the norm induced by this inner product.

For $v_H = (v_{1,H}, v_{2,H})$, $w_H = (w_{1,H}, w_{2,H}) \in [W_H]^2$, we use the notation

$$(v_H, w_H)_{H,+} = (v_{1,H}, w_{1,H})_{H,x} + (v_{2,H}, w_{2,H})_{H,y},$$

where

$$(v_H, w_H)_{H,x} = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y-1} h_i k_{j+1/2} v_H(x_i, y_j) w_H(x_i, y_j),\ w_H, v_H \in W_H,$$

$$(v_H, w_H)_{H,y} = \sum_{i=1}^{N_x-1} \sum_{j=1}^{N_y} h_{i+1/2} k_j v_H(x_i, y_j) w_H(x_i, y_j),\ w_H, v_H \in W_H.$$

We define $\|w_H\|_{H,x} = \sqrt{(w_H, w_H)_{H,x}}$ and $\|w_H\|_{H,y} = \sqrt{(w_H, w_H)_{H,y}}$.

Let D_{-x} and D_{-y} be the usual backward finite difference operators with respect to the variables x and y, respectively,

$$D_{-x} w_H(x_i, y_j) = \frac{w_H(x_i, y_j) - w_H(x_{i-1}, y_j)}{h_i},$$

$$D_{-y} w_H(x_i, y_j) = \frac{w_H(x_i, y_j) - w_H(x_i, y_{j-1})}{k_j},$$

and let ∇_H be the discrete version of the gradient operator ∇ defined by $\nabla_H w_H = (D_{-x} w_H, D_{-y} w_H)$. We introduce the following discrete version of the H^1-norm

$$\|w_H\|_{1,H} = \left(\|w_H\|_H^2 + \|\nabla_H w_H\|_{H,+}^2\right)^{1/2},$$

where

$$\|\nabla_H w_H\|_{H,+}^2 = \|D_{-x} w_H\|_{H,x}^2 + \|D_{-y} w_H\|_{H,y}^2.$$

With these definitions holds the following discrete Poincaré-Friedrichs inequality

$$\|w_H\|_H^2 \leq \frac{1}{2} \|\nabla_H w_H\|_{H,+}^2,\ \forall w_H \in W_{H,0}.$$

In order to define the discrete approximations in space $c_H(t)$ and $p_H(t)$ we introduce the following notation:

$$M_h(w_H)(x_i, y_j) = \frac{w_H(x_i, y_j) + w_H(x_{i-1}, y_j)}{2},$$

$$M_k(w_H)(x_i, y_j) = \frac{w_H(x_i, y_j) + w_H(x_i, y_{j-1})}{2},$$

$$(M_H w_H, \nabla_H v_H)_{H,+} = (M_h(w_H), D_{-x} w_H)_{x,+} + (M_k(w_H), D_{-y} w_H)_{y,+}$$

and

$$D_h w_H(x_i,y_j) = \frac{h_i D_{-x} w_H(x_{i+1},y_j) + h_{i+1} D_{-x} w_H(x_i,y_j)}{h_i + h_{i+1}},$$

being the finite difference operator D_k defined analogously with respect to the variable y. To approximate the coefficient functions, we introduce the diagonal matrices $A_H(t), D_H(t)$ and $E_H(t)$ whose entries $a_{\ell,H}(t)$, $d_{\ell,H}(t)$ and $e_{\ell,H}(t)$, $\ell = 1,2$, respectively, depend on the numerical concentration $c_H(t)$ and pressure $p_H(t)$, that are given by

$$a_{1,H}(t) = a_1(M_h(c_H(t))), \quad d_{1,H}(t) = d_1(M_h(c_H(t)), D_{-x}p_H(t)),$$

and

$$e_{1,H}(t) = e_1(M_h(c_H(t)), D_{-x}p_H(t)).$$

The vector $B_H(t)$ depends on $c_H(t)$ and $p_H(t)$

$$b_{1,H}(t) = b_1(c_H(t), D_h p_H(t)).$$

The entries $a_{2,H}(t)$, $d_{2,H}(t)$, $e_{2,H}(t)$ and $b_{2,H}(t)$ are defined analogously.

We now define the semi-discrete approximations $c_H(t)$ and $p_H(t)$ for the solution of (9), (10): find $p_H(t) \in W_H$ and $c_H(t) \in W_{H,0}$, with $p_H(t) = R_H p_{b_H}(t)$ on $\partial\Omega_H$ and $\frac{dc_H}{dt}(t) \in W_{H,0}$, such that

$$(A_H(t)\nabla_H p_H(t), \nabla_H w_H)_{H,+} = (q_{2,H}(t), w_H)_H, \tag{11}$$

for all $w_H \in W_{H,0}$,

$$(\frac{dc_H}{dt}(t), w_H)_H + a_H(c_H(t), w_H) + \int_0^t b_H(s,t,c_H(s),w_H)\,ds = (q_{1,H}(t), w_H)_H, \tag{12}$$

for all $w_H \in W_{H,0}$, and

$$p_H(0) = p_{0,H} \text{ in } \Omega_H, \; c_H(0) = c_{0,H} \text{ in } \Omega_H, \tag{13}$$

for $t \in (0,T]$, where $p_{0,H}$ and $c_{0,H}$ are approximations for p_0 and c_0 in W_H, respectively. In (11) and (12), $a_H(c_H(t), w_H)$ and $b_H(s,t,c_H(s),w_H)$ are given by

$$a_H(c_H(t), w_H) = (D_H(t)\nabla_H c_H(t), \nabla_H w_H)_{H,+} - (M_H(B_H(t)c_H(t)), \nabla_H w_H)_{H,+},$$

$$b_H(s,t,c_H(s),w_H) = K_{er}(t-s)(E_H(s)\nabla_H c_H(s), \nabla_H w_H)_{H,+}$$

and

$$q_{\ell,H}(x_i,y_j,t) = \frac{1}{|\square_{i,j}|}\int_{\square_{i,j}} q_\ell(x,y,t)dxdy, \; (x_i,y_j) \in \Omega_H, \ell = 1,2.$$

We observe that (11) and (12) can also be obtained from the finite element coupled variational equations

$$(A(P_Hc_H(t))\nabla P_Hp_H(t), \nabla P_Hw_H) = (q_2(t), P_Hw_H),\ \forall w_H \in W_{H,0}, \tag{14}$$

$$\begin{aligned}(\frac{d}{dt}P_Hc_H(t), P_Hw_H) &+ (D(P_Hc_H(t), \nabla P_Hp_H(t))\nabla P_Hc_H(t), \nabla P_Hw_H)\\ &-(B(P_Hc_H(t), \nabla P_Hp_H(t))P_Hc_H(t), \nabla P_Hw_H)\\ &+\int_0^t K_{er}(t-s)(E(P_Hc_H(s), \nabla P_Hp_H(s))\nabla P_Hc_H(s), \nabla P_Hw_H)\,ds\\ &= (q_1(t), P_Hw_H),\ \forall w_H \in W_{H,0}\end{aligned} \tag{15}$$

using suitable quadrature rules (see [16]).

Remark 1. *The discrete in space coupled variational problem (11), (12) is equivalent to the following finite difference method*

$$-\nabla_H^* \cdot (A_H(t)\nabla_Hp_H(t)) = q_{2,H}(t), \tag{16}$$

$$\begin{aligned}\frac{dc_H}{dt}(t) - \nabla_H^*.(D_H(t)\nabla_Hc_H(t)) &+ \nabla_{c,H}^* \cdot (B_H(t)c_H(t))\\ &= \int_0^t K_{er}(t-s)\nabla_H^* \cdot (E_H(s)\nabla_Hc_H(s))ds + q_{1,H}(t),\end{aligned} \tag{17}$$

complemented by the initial conditions (13) and the boundary conditions $c_H(t) = 0$ *and* $p_H(t) = R_Hp_b(t)$ *on* $\partial\Omega$*. Here,* $\nabla_H^*w_H = (D_xw_H, D_yw_H)$ *and* $\nabla_{c,H}^*w_H = (D_{c,x}w_H, D_{c,y}w_H)$*, where*

$$D_xw_H(x_i, y_j) = \frac{w_H(x_{i+1}, y_j) - w_H(x_i, y_j)}{h_{i+1/2}},$$

$$D_{c,x}w_H(x_i, y_j) = \frac{w_H(x_{i+1}, y_j) - w_H(x_{i-1}, y_j)}{h_i + h_{i+1}},$$

with $h_{i+1/2} = \dfrac{h_i + h_{i+1}}{2}$ *and the corresponding operators in y-dimension,* D_y *and* $D_{c,y}$*, are defined analogously.*

In the following section we show that the solutions $p_H(t)$ and $c_H(t)$ of the finite difference problem (16), (17), or equivalently, the fully discrete in space piecewise linear finite element solutions of the variational problem (14), (15), are second order convergent approximations for the pressure $p(t)$ and concentration $c(t)$.

3. Convergence analysis

This section is dedicated to derive error estimates for the numerical solutions of our finite difference scheme, namely,

$$e_{H,p}(t) = R_H p(t) - p_H(t) \quad \text{and} \quad e_{H,c}(t) = R_H c(t) - c_H(t).$$

A possible approach could be to follow the procedure introduced by Wheeler in [34] and used, e.g., in [18]. However, this technique requires that the sequence of spatial grids is quasi-uniform in the sense that

$$\frac{H_{max}}{H_{min}} \le C, \text{ for } H \in \Lambda.$$

Here we propose a type of analysis that avoids the above smoothness assumption on the spatial grids. In addition, our approach is less restrictive regarding the regularity of the solutions p and c.

Nevertheless, the convergence analysis that we present still requires some regularity conditions on p and c as well as in the coefficient functions of the model. For the coefficients functions we assume the following:

$$\begin{aligned} &A \in C^1_B(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R}), \quad d_\ell,\, b_\ell,\, e_\ell \in C^1_B(\mathbb{R}^2) \cap W^{2,\infty}(\mathbb{R}^2),\\ &0 < A_{min} \le A \text{ in } \mathbb{R}, \quad \text{and} \quad 0 < D_{min} \le d_\ell \text{ in } \mathbb{R}^2,\ \ell = 1, 2. \end{aligned}$$

Here, $C^1_B(\mathbb{R})$ and $C^1_B(\mathbb{R}^2)$ represent the space of functions defined in $\mathbb{R}$ and $\mathbb{R}^2$, respectively, with bounded first order partial derivatives. By $W^{2,\infty}(\mathbb{R})$ and $W^{2,\infty}(\mathbb{R}^2)$ we denote the usual Sobolev spaces. To simplify the proofs of the convergence results, we start by introducing some notation. Let $\tilde{A}_H$ and A^*_H be defined as A, replacing a_1, a_2 by $\tilde{a}_1$, $\tilde{a}_2$ and a^*_1, a^*_2, respectively, with

$$\begin{aligned} \tilde{a}_1(x_i, y_j, t) &= a_1(c(x_{i-1/2}, y_j, t)),\\ \tilde{a}_2(x_i, y_j, t) &= a_2(c(x_i, y_{j-1/2}, t)),\\ a^*_1(x_i, y_j, t) &= a_1(\frac{1}{2}(c(x_{i-1}, y_j, t) + c(x_i, y_j, t))),\\ a^*_2(x_i, y_j, t) &= a_2(\frac{1}{2}(c(x_i, y_{j-1}, t) + c(x_i, y_j, t))). \end{aligned}$$

$\tilde{D}_H$ and D^*_H are defined in a corresponding way.

In the following, $\|.\|_{C^q}$ denotes the usual norm in $C^q(\overline{\Omega})$, $q \in \mathbb{N}_0$.

Proposition 1. *If $p(t) \in H^3(\Omega)$, $c(t) \in H^2(\Omega)$, then there exists a positive constant C such that*

$$\|\nabla_H e_{H,p}(t)\|_{H,+} \leq C\Big(\|p(t)\|_{C^1}\|e_{H,c}(t)\|_H + \tau_p(t)\Big), \tag{18}$$

where

$$\tau_p(t) = \Big(\sum_{\Delta\in\mathfrak{T}_H} (\operatorname{diam}\Delta)^4\big(\|c(t)\|^2_{H^2(\Delta)} + \|c(t)\|^4_{H^1(\Delta)}\big)\Big)^{1/2} + \big(\|p(t)\|_{C^1}+1\big)\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|p(t)\|^2_{H^3(\Delta)}\Big)^{1/2}\Big). \tag{19}$$

Proof: We start with the following decomposition

$$(A_H(t)\nabla_H e_{H,p}(t), \nabla_H e_{H,p}(t))_{H,+} = \sum_{i=1}^{3}\tau_A^{(i)}(e_{H,p}(t)),$$

where

$$\tau_A^{(1)}(e_{H,p}(t)) = ((A_H(t) - A_H^*(t))\nabla_H R_H p, \nabla_H e_{H,p}(t))_{H,+},$$

$$\tau_A^{(2)}(e_{H,p}(t)) = ((A_H^*(t) - \tilde{A}_H(t))\nabla_H R_H p, \nabla_H e_{H,p}(t))_{H,+},$$

and

$$\begin{aligned}\tau_A^{(3)}(e_{H,p}(t)) &= (\tilde{A}_H(t)\nabla_H R_H p, \nabla_H e_{H,p}(t))_{H,+}\\ &-\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i\int_{y_{j-1/2}}^{y_{j+1/2}} a_1(x_{i-1/2},y,t)\frac{\partial p}{\partial x}(x_{i-1/2},y,t)\,dy D_{-x}e_{H,p}(x_i,y_j,t)\\ &-\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j\int_{x_{i-1/2}}^{x_{i+1/2}} a_2(x,y_{j-1/2},t)\frac{\partial p}{\partial y}(x,y_{j-1/2},t)\,dx D_{-y}e_{H,p}(x_i,y_j,t),\end{aligned}$$

with $a_1(x_{i-1/2},y,t) = a_1(c(x_{i-1/2},y,t))$, $a_2(x,y_{j-1/2},t) = a_2(c(x,y_{j-1/2}))$ to shorten notation. Since $p(t) \in H^3(\Omega)$ and $H^3(\Omega)$ is continuously embedded in $C^1(\overline{\Omega})$, holds $\|\nabla_H R_H p(t)\|_{H,+} \leq \|\nabla p(t)\|_{C^0}$, and then

$$|\tau_A^{(1)}(e_{H,p}(t))| \leq C\|p(t)\|_{C^1}\|e_{H,c}(t)\|_H\|\nabla_H e_{H,p}(t)\|_{H,+}.$$

To obtain an estimate for $\tau_A^{(2)}(e_{H,p}(t))$ we observe that, for $g(c(x_i, y_j)) = M_h c(x_i, y_j) - c(x_{i-1/2}, y_j)$, one gets

$$\begin{aligned} k_{j+1/2}|g(c(x_i, y_j))| &\leq k_{j+1/2} \int_{y_{j-1/2}}^{y_{j+1/2}} |g(\frac{\partial c}{\partial y}(x_i, y))| \, dy \\ &+ \int_{y_{j-1/2}}^{y_{j+1/2}} |g(c(x_i, y))| \, dy \\ &\leq k_{j+1/2} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1}}^{x_i} |\frac{\partial^2 c}{\partial x \partial y}| \, dxdy \\ &+ h_i \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1}}^{x_i} |\frac{\partial^2 c}{\partial x^2}| \, dxdy, \end{aligned}$$

being the last inequality derived using the Bramble-Hilbert Lemma. We note that

$$h_{i+1/2} M_k c(x_i, y_j) - c(x_i, y_{j-1/2})$$

can be estimated in a similar way,

$$|\tau_A^{(2)}(e_{H,p}(t))| \leq C\|p(t)\|_{C^1} \Big(\sum_{\Delta \in \mathfrak{T}_H} (\text{diam}\, \Delta)^4 \|c(t)\|^2_{H^2(\Delta)} \Big)^{1/2} \|\nabla_H e_{H,p}(t)\|_{H,+}.$$

To conclude the proof we observe that Lemma 5.1 of [16] can be applied to establish the estimate,

$$\begin{aligned} |\tau_A^{(3)} e_{H,p}(t))| \leq C\Big(\sum_{\Delta \in \mathfrak{T}_H} (\text{diam}\, \Delta)^4 \big(\|p(t)\|^2_{C^1} \big(\|c(t)\|^4_{H^1(\Delta)} + \|c(t)\|^2_{H^2(\Delta)} \big) \\ + \|c(t)\|^2_{H^1(\Delta)} \|p(t)\|^2_{H^2(\Delta)} + \|p(t)\|^2_{H^3(\Delta)} \big) \Big)^{1/2} \|\nabla_H e_{H,p}(t)\|_{H,+}. \end{aligned}$$

■

To simplify notation in the next proposition, we write

$$\begin{aligned} d_1(x_{i-1/2}, y, t) &= d_1(c(x_{i-1/2}, y, t), \frac{\partial p}{\partial x}(x_{i-1/2}, y, t)), \\ d_2(x, y_{j-1/2}, t) &= d_2(c(x, y_{j-1/2}, t), \frac{\partial p}{\partial y}(x, y_{j-1/2}, t)). \end{aligned} \tag{20}$$

Proposition 2. *Assume that* $p(t)$, $c(t) \in H^3(\Omega)$ *and* $\dfrac{\partial^2 p}{\partial x \partial y}(t) = \dfrac{\partial^2 p}{\partial y \partial x}(t)$ *in* Ω. *For the functional*

$$\begin{aligned}\tau_D(w_H) &= (D_H(t)\nabla_H c_H(t), \nabla_H w_H)_{H,+}\\ &-\sum_{i=1}^{N_x}\sum_{j=1}^{M_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} d_1(x_{i-1/2}, y, t)\frac{\partial c}{\partial x}(x_{i-1/2}, y, t)dy D_{-x} w_H(x_i, y_j)\\ &-\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} d_2(x, y_{j-1/2}, t)\frac{\partial c}{\partial y}(x, y_{j-1/2}, t)dx D_{-y} w_H(x_i, y_j),\end{aligned}$$

for $w_H \in W_{H,0}$, *holds*

$$\tau_D(w_H) = -(D_H(t)\nabla_H e_{H,c}(t), \nabla_H w_H)_{H,+} + \tau_{D,e}(w_H),$$

where

$$\begin{aligned}\tau_{D,e}(w_H) &\leq C\Big(\|c(t)\|_{C^1}\big(1 + \|p(t)\|_{C^1}\big)\Big(\|e_{H,c}(t)\|_H\\ &+ \Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|p(t)\|^2_{H^3(\Delta)}\Big)^{1/2}\Big)\\ &+ (1 + \|c(t)\|_{C^1})^3\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\Big(\|c(t)\|^2_{H^3(\Delta)} + \|c(t)\|^4_{H^2(\Delta)}\\ &+ \|p(t)\|^2_{H^3(\Delta)} + \|p(t)\|^4_{H^2(\Delta)}\Big)\Big)^{1/2}\Big)\|\nabla_H w_H\|_{H,+}.\end{aligned}$$

Proof: For $\tau_D(w_H)$ holds the decomposition

$$\tau_D(w_H) = -(D_H(t)\nabla_H e_{H,c}(t), \nabla_H w_H)_{H,+} + \sum_{i=1}^{3}\tau_D^{(i)}(w_H), \qquad (21)$$

with $\tau_D^{(1)}(w_H)$, $\tau_D^{(2)}(w_H)$, and $\tau_D^{(3)}(w_H)$ defined by

$$\begin{aligned}\tau_D^{(1)}(w_H) &= (\big(D_H(t) - D_H^*(t)\big)\nabla_H R_H c(t), \nabla_H w_H)_{H,+},\\ \tau_D^{(2)}(w_H) &= (\big(D_H^*(t) - \tilde{D}_H(t)\big)\nabla_H R_H c(t), \nabla_H w_H)_{H,+},\end{aligned}$$

and

$$\tau_D^{(3)}(w_H) = (\tilde{D}_H(t)\nabla_H R_H c, \nabla_H w_H)_{H,+}$$
$$-\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} d_1(x_{i-1/2}, y, t)\frac{\partial c}{\partial x}(x_{i-1/2}, y)dy D_{-x}w_H(x_i, y_j)$$
$$-\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} d_2(x, y_{j-1/2}, t)\frac{\partial c}{\partial y}(x, y_{j-1/2}, t)dx D_{-y}w_H(x_i, y_j).$$

For $\tau_D^{(1)}(w_H)$ we can easily establish the estimate

$$|\tau_D^{(1)}(w_H)| \leq C\|c(t)\|_{C^1}\Big(\|e_{H,c}(t)\|_H + \|e_{H,p}(t)\|_{1,H}\Big)\|\nabla_H w_H\|_{H,+}.$$

For $\tau_D^{(2)}(w_H)$ we have $\tau_D^{(2)}(w_H) = \tau_D^{(2,1)}(w_H) + \tau_D^{(2,2)}(w_H)$ with

$$\tau_D^{(2,1)}(w_H) = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i k_{j+1/2}\frac{\partial d_1}{\partial x} g_1(c(x_i, y_j, t)) D_{-x}c(x_i, y_j, t) D_{-x}w_H(x_i, y_j)$$
$$+\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} h_{i+1/2}k_j\frac{\partial d_2}{\partial x} g_2(c(x_i, y_j, t)) D_{-y}c(x_i, y_j, t) D_{-y}w_H(x_i, y_j),$$

where $g_1(c(x_i, y_j, t) = M_h c(x_i, y_j, t) - c(x_{i-1/2}, y_j, t)$, $g_2(c(x_i, y_j, t) = M_k c(x_i, y_j, t) - c(x_i, y_{j-1/2}, t)$, and

$$\tau_D^{(2,2)}(w_H) = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i k_{j+1/2}\frac{\partial d_1}{\partial y} g_1(p(x_i, y_j, t)) D_{-x}c(x_i, y_j, t) D_{-x}w_H(x_i, y_j)$$
$$+\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_{i+1/2}k_j\frac{\partial d_2}{\partial y} g_2(p(x_i, y_j, t)) D_{-y}c(x_i, y_j, t) D_{-y}w_H(x_i, y_j),$$

with $g_1(p(x_i, y_j, t)) = D_{-x}p(x_i, y_j, t) - \frac{\partial p}{\partial x}(x_{i-1/2}, y_j, t)$ and $g_2(p(x_i, y_j, t)) = D_{-y}p(x_i, y_j, t) - \frac{\partial p}{\partial y}(x_i, y_{j-1/2}, t)$. In $\tau_D^{(2,\ell)}(w_H)$, $\ell = 1, 2$, the partial derivatives of d_1 and d_2 are evaluated at convenient points.

Following the steps used to estimate $\tau_A^{(2)}(e_{H,p}(t))$ on the proof of Proposition 1, it can be shown that

$$|\tau_D^{(2,1)}(w_H)| \leq C\|c(t)\|_{C^1}\Big(\sum_{\Delta\in\mathfrak{T}_H}(\mathrm{diam}\,\Delta)^4\|c(t)\|^2_{H^2(\Delta)}\Big)^{1/2}\|\nabla_H w_H\|_{H,+}.$$

To estimate $\tau_D^{(2,2)}(w_H)$ we observe that if $p(t)\in H^3(\Omega)$ then $\dfrac{\partial p}{\partial x}\in H^2(\Omega)$. Under the previous assumptions for g_1, we get

$$\begin{aligned}
k_{j+1/2}|g_1(p(x_i,y_j,t))| &\leq k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(\frac{\partial p}{\partial y}(x_i,y,t))|dy\\
&+\int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(p(x_i,y,t))|dy\\
&\leq k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i-1}}^{x_i}|\frac{\partial^3 p}{\partial x^2\partial y}(t))|dxdy\\
&+h_i\int_{y_{j-1/2}}^{y_{j+1/2}}|\frac{\partial^3 p}{\partial x^3}(t)|dxdy,
\end{aligned}$$

being the last upper bound obtained using the Bramble-Hilbert Lemma. For g_2 holds a similar result, and we obtain

$$|\tau_D^{(2,2)}(w_H)| \leq C\|c(t)\|_{C^1}\Big(\sum_{\Delta\in\mathfrak{T}_H}(\mathrm{diam}\,\Delta)^4\|p(t)\|^2_{H^3(\Delta)}\Big)^{1/2}\|\nabla_H w_H\|_{H,+}.$$

Lemma 5.1 of [16] allows us to deduce the upper bound for $\tau_D^{(3)}(w_H)$,

$$\begin{aligned}
|\tau_D^{(3)}(w_H)| \leq C(1+\|c(t)\|_{C^1})^3\Big(\sum_{\Delta\in\mathfrak{T}_H}(\mathrm{diam}\,\Delta)^4\Big(\|c(t)\|^2_{H^3(\Delta)}+\|c(t)\|^4_{H^2(\Delta)}\\
+\|p(t)\|^2_{H^3(\Delta)}+\|p(t)\|^4_{H^2(\Delta)}\Big)\Big)^{1/2}\|\nabla_H w_H\|_{H,+}.
\end{aligned}$$

Finally, taking into account (18) we conclude the proof.

■

Under the assumptions of Proposition 2 and following its proof we can derive the next result.

Proposition 3. *For $w_H \in W_{H,0}$, the functional*

$$\tau_E(w_H) = \int_0^t K_{er}(t-s)(E_H(s)\nabla_H c_H(s), \nabla_H w_H)_{H,+} ds$$
$$- \int_0^t K_{er}(t-s) \sum_{i=1}^{N_x} \sum_{j=1}^{N_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} e_1(x_{i-1/2}, y, s) \frac{\partial c}{\partial x}(x_{i-1/2}, y, s)\, dyds$$
$$D_{-x} w_H(x_i, y_j)$$
$$- \int_0^t K_{er}(t-s) \sum_{i=1}^{N_x-1} \sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} e_2(x, y_{j-1/2}, s) \frac{\partial c}{\partial y}(x, y_{j-1/2}, s)\, dxds$$
$$D_{-y} w_H(x_i, y_j),$$

with e_ℓ, $\ell = 1, 2$, defined by (20) with d_ℓ replaced by e_ℓ, admits the representation

$$\tau_E(w_H) = -\int_0^t K_{er}(t-s)(E_H(t)\nabla_H e_{H,c}(s), \nabla_H w_H)_{H,+} ds$$
$$+ \int_0^t K_{er}(t-s) \tau_{E,e}(w_H) ds,$$

where

$$\tau_{E,e}(w_H) \leq C\Big(\|c(s)\|_{C^1}\big(1 + \|p(s)\|_{C^1}\big)\Big(\|e_{H,c}(s)\|_H$$
$$+\Big(\sum_{\Delta \in \mathfrak{T}_H} (\operatorname{diam}\Delta)^4 \|p(s)\|^2_{H^3(\Delta)}\Big)^{1/2}\Big)$$
$$+(1 + \|c(s)\|_{C^1})^3 \Big(\sum_{\Delta \in \mathfrak{T}_H} (\operatorname{diam}\Delta)^4 \Big(\|c(s)\|^2_{H^3(\Delta)} + \|c(s)\|^4_{H^2(\Delta)}$$
$$+\|p(s)\|^2_{H^3(\Delta)} + \|p(s)\|^4_{H^2(\Delta)}\Big)\Big)^{1/2}\Big) \|\nabla_H w_H\|_{H,+}.$$

In the following result we use the abbreviation

$$b_1(x_{i-1/2}, y, t) = b_1(c(x_{i-1/2}, y, t), \frac{\partial p}{\partial x}(x_{i-1/2}, y, t)),$$
$$b_2(x, y_{j-1/2}, t) = b_2(c(x, y_{j-1/2}, t), \frac{\partial p}{\partial y}(x, y_{j-1/2}, t)). \qquad (22)$$

Proposition 4. *Let $w_H \in W_{H,0}$ and τ_B be the functional given by*

$$\begin{aligned}
&\tau_B(w_H) = -(M_H(B_H(t)c_H(t)), \nabla_H w_H)_{H,+} \\
&+\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} b_1(x_{i-1/2}, y, t)c(x_{i-1/2}, y, t)dyD_{-x}w_H(x_i, y_j) \\
&+\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} b_2(x, y_{j-1/2}, t)c(x, y_{j-1/2}, t)dxD_{-y}w_H(x_i, y_j).
\end{aligned}$$

If $p(t) \in H^3(\Omega)$, $\dfrac{\partial^2 p}{\partial x\partial y}(t) = \dfrac{\partial^2 p}{\partial y\partial x}(t)$ in Ω, $c(t) \in H^2(\Omega)$, and the spatial grid satisfies

$$\frac{k_j}{k_{j+1}} \leq C, \quad \frac{h_i}{h_{i+1}} \leq C, \tag{23}$$

then for $\tau_B(w_H)$ we have

$$\tau_B(w_H) = (M_H(B_H(t)e_{H,c}(t)), \nabla_H w_H)_{H,+} + \tau_{B,e}(w_H),$$

where

$$\begin{aligned}
\tau_{B,e}(w_H) \leq C\Big(&\|c(t)\|_{C^0}\big(1 + \|p(t)\|_{C^1}\big)\|e_{H,c}(t)\|_H \\
&+ \big(\|c(t)\|_{C^0}\big(1 + \|p(t)\|_{C^1}) + 1\big) \\
&\Big(\sum_{\Delta\in\mathfrak{T}_H} (\operatorname{diam}\Delta)^4\big(\|c(t)\|^4_{H^1(\Delta)} + \|c(t)\|^2_{H^2(\Delta)} \\
&+ \|p(t)\|^4_{H^2(\Delta)} + \|p(t)\|^2_{H^3(\Delta)}\big)\Big)^{1/2}\Big)\|\nabla_H w_H\|_{H,+}.
\end{aligned}$$

Proof: For $\tau_B(w_H)$ holds the representation

$$\tau_B(w_H) = (M_H(B_H(t)e_{H,c}(t)), \nabla_H w_H)_{H,+} + \sum_{i=1}^{3} \tau_B^{(i)}(w_H),$$

where

$$\begin{aligned}
\tau_B^{(1)}(w_H) &= (M_H((B^*_H(t) - B_H(t))R_Hc(t)), \nabla_H w_H)_{H,+}, \\
\tau_B^{(2)}(w_H) &= (M_H((\tilde{B}_H(t) - B^*_H(t))R_Hc(t)), \nabla_H w_H)_{H,+},
\end{aligned}$$

and

$$\begin{aligned}\tau_B^{(3)}(w_H) &= (M_H(\tilde{B}_H(t)R_Hc), \nabla_H w_H)_{H,+}\\ &- \sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} b_1(x_{i-1/2}, y, t)c(x_{i-1/2}, y, t)dy D_{-x}w_H(x_i, y_j)\\ &- \sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} b_2(x, y_{j-1/2}, t)c(x, y_{j-1/2}, t)dx D_{-y}w_H(x_i, y_j).\end{aligned}$$

For $\tau_B^{(1)}(w_H)$, we can easily establish the following estimate

$$|\tau_B^{(1)}(w_H)| \le C\|c(t)\|_{C^0}\Big(\|e_{H,c}(t)\|_H + \|\nabla_H e_{H,p}(t)\|_{H,+}\Big)\|\nabla_H w_H\|_{H,+}.$$

An estimate for $\tau_D^{(2)}(w_H)$ can be obtained following the approach used to estimate $\tau_D^{(2)}(w_H)$ in the proof of Proposition 2. For this, we must replace g_i, $i = 1, 2$, (introduced in the construction of the upper bound for $\tau_D^{(2,2)}(w_H)$) by $g_1(x_i, y, t) = D_h p(x_i, y_j, t) - \dfrac{\partial p}{\partial x}(x_i, y_j, t)$ and $g_2(x_i, y, t) = D_k p(x_i, y_j, t) - \dfrac{\partial p}{\partial y}(x_i, y_j, t)$, respectively. In this case we obtain

$$\begin{aligned}|\tau_B^{(2)}(w_H)| &\le C\|c(t)\|_{C^0}\Big(\Big(\sum_{\Delta\in\mathfrak{T}_H} (\mathrm{diam}\,\Delta)^4 \|c(t)\|^2_{H^2(\Delta)}\Big)^{1/2}\\ &\quad + \Big(\sum_{\Delta\in\mathfrak{T}_H} (\mathrm{diam}\,\Delta)^4 \|p(t)\|^2_{H^3(\Delta)}\Big)^{1/2}\Big)\|\nabla_H w_H\|_{H,+}.\end{aligned}$$

Considering now Lemma 5.5 of [16] we obtain for $\tau_B^{(3)}(w_H)$ the estimate

$$\begin{aligned}|\tau_B^{(3)}(w_H)| \le C\big(\|c(t)\|_{C^0} + 1\big)\Big(\sum_{\Delta\in\mathfrak{T}_H} (\mathrm{diam}\,\Delta)^4\big(\|c(t)\|^4_{H^1(\Delta)} + \|c(t)\|^2_{H^2(\Delta)}\\ + \|p(t)\|^4_{H^2(\Delta)} + \|p(t)\|^2_{H^3(\Delta)}\big)\Big)^{1/2}\|\nabla_H w_H\|_{H,+}.\end{aligned}$$

Finally, combining the upper bound for $|\tau_B^{(1)}(w_H)|$ with Proposition 1 we conclude the proof.

■

Lemma 5.7 of [16] allows us to derive the next proposition.

Proposition 5. *If* $\frac{dc}{dt}(t) \in H^2(\Omega)$*, then there exists a positive constant* C *such that*

$$|\big((\frac{dc}{dt}(t)\big)_H, w_H\big)_H - \big(R_H\frac{dc}{dt}(t), w_H\big)_H| \leq C\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|\frac{dc}{dt}(t)\|^2_{H^2(\Delta)}\Big)^{1/2} \|\nabla_H w_H\|_{H,+}$$

for all $w_H \in W_{H,0}$.

From Propositions 1-5, with the aid of Gronwall's Lemma, we conclude the next convergence result.

Theorem 1. *If* p, $c \in L^\infty(0,T,H^3(\Omega))$, $p(t)$ *is such that* $\frac{\partial^2 p}{\partial x\partial y}(t) = \frac{\partial^2 p}{\partial y\partial x}(t)$ *in* Ω*, the spatial grids* $\overline{\Omega}_H$*,* $H \in \Lambda$*, satisfy (23), then there exists a positive constant* C *such that*

$$\|e_{H,c}(t)\|^2_H + \int_0^t \|\nabla_H e_{H,c}(s)\|^2_{H,+}ds \leq CH^4_{max},\ t\in[0,T], \tag{24}$$

and

$$\|e_{H,p}(t)\|_{1,H} \leq CH^2_{max},\ t\in[0,T], \tag{25}$$

■

Proof: For the error $e_{H,c}(t)$ we have

$$(\frac{de_{H,c}}{dt}, e_{H,c}(t))_H = (\frac{dc}{dt}(t) - (\frac{dc}{dt}(t))_H, e_{H,c}(t))_H + ((\frac{dc}{dt}(t))_H - \frac{dc_H}{dt}(t), e_{H,c}(t))_H, \tag{26}$$

where

$$\begin{aligned}|(\frac{dc}{dt}(t) - (\frac{dc}{dt}(t))_H, e_{H,c}(t))_H| &\leq C\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|\frac{dc}{dt}(t)\|^2_{H^2(\Delta)}\Big)^{1/2} \|\nabla_H e_{H,c}(t)\|_{H,+}\\ &\leq C\frac{1}{4\epsilon^2}\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|\frac{dc}{dt}(t)\|^2_{H^2(\Delta)} + \epsilon^2\|\nabla_H e_{H,c}(t)\|^2_{H,+},\end{aligned} \tag{27}$$

being $\epsilon \neq 0$ an arbitrary constant.

It can be shown that for $((\frac{dc}{dt}(t))_H - \frac{dc_H}{dt}(t), e_{H,c}(t))_H$ we have

$$((\frac{dc}{dt}(t))_H - \frac{dc_H}{dt}(t), e_{H,c}(t))_H = \tau_D(e_{H,c}(t)) + \tau_E(e_{H,c}(t)) + \tau_B(e_{H,c}(t)),$$

where $\tau_D(e_{H,c}(t)), \tau_E(e_{H,c}(t))$, and $\tau_B(e_{H,c}(t))$ are defined in Proposition 2, Proposition 3, and Proposition 4, respectively. We obtain

$$
\begin{aligned}
((\frac{dc}{dt}(t))_H - \frac{dc_H}{dt}(t), e_{H,c}(t))_H \leq &-(D_H(t)\nabla_H e_{H,c}(t), \nabla_H e_{H,c}(t))_{H,+} \\
&- \int_0^t K_{er}(t-s)(E_H(s)\nabla_H e_{H,c}(s), \nabla_H e_{H,c}(t))_{H,+} ds \\
&+ (M_H(B_H(t)e_{H,c}(t)), \nabla_H e_{H,c}(t))_{H,+} \\
&+ C\frac{1}{2\epsilon^2}\Big(\|c(t)\|^2_{C^1}\big(1+\|p(t)\|^2_{C^1}\big)\Big)\|e_{H,c}(t)\|^2_H \\
&+ C\frac{1}{4\epsilon^2}\int_0^t K_{er}(t-s)^2\Big(\|c(s)\|^2_{C^1}\big(1+\|p(s)\|^2_{C^1}\big)\Big)ds \int_0^t \|e_{H,c}(s)\|^2_H ds \\
&+ 6\epsilon^2\|\nabla_H e_{H,c}(t)\|^2_{H,+} + \tau_{e,c}(t),
\end{aligned} \tag{28}
$$

where

$$
\tau_{e,c}(t) = C\frac{1}{4\epsilon^2}\Big(\tau^{(1)}_{e,c}(t) + \int_0^t K_{er}(t-s)^2\tau^{(2)}_{e,c}(s)ds\Big),
$$

with

$$
\begin{aligned}
\tau^{(1)}_{e,c}(t) = &\big(1+\|c(t)\|^2_{C^1}\big(1+\|p(t)\|^2_{C^1}\big)\big)\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|c(t)\|^2_{H^3(\Delta)} \\
&+ \|c(t)\|^2_{C^1}\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|p(t)\|^2_{H^3(\Delta)} \\
&+ \|c(t)\|^2_{C^0}\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\big(1+\|c(t)\|^2_{H^1(\Delta)}+\|p(t)\|^2_{H^2(\Delta)}\big)^2,
\end{aligned}
$$

and

$$
\begin{aligned}
\tau^{(2)}_{e,c}(s) = &\big(1+\|c(s)\|^2_{C^1}\big(1+\|p(s)\|^2_{C^1}\big)\big)\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|c(s)\|^2_{H^3(\Delta)} \\
&+ \|c(s)\|^2_{C^1}\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|p(s)\|^2_{H^3(\Delta)}.
\end{aligned}
$$

From (26)-(28) we conclude the following

$$\frac{d}{dt}\|e_{H,c}(t)\|_H^2 \leq (-D_{min} + 9\epsilon^2)\|\nabla_H e_{H,c}(t)\|_{H,+}^2 \tag{29}$$

$$+ \frac{1}{2\epsilon^2}\|K_{er}\|_{L^2(0,T)}^2 \int_0^t \|\nabla_H e_{H,c}(s)\|_{H,+}^2 ds$$

$$+ C\frac{1}{\epsilon^2}\Big(\frac{1}{2} + \|c(t)\|_{C^1}^2\big(1 + \|p(t)\|_{C^1}^2\big)\Big)\|e_{H,c}(t)\|_H^2$$

$$+ \frac{1}{2\epsilon^2}\|K_{er}\|_{L^2(0,T)}^2\|c\|_{L^\infty(C^1)}^2\big(1 + \|p\|_{L^\infty(C^1)}^2\big)\int_0^t \|e_{H,c}(s)\|_H^2 ds$$

$$+ 2\tau_{e,c}(t), \tag{30}$$

where $\|.\|_{L^\infty(C^1)}$ represents the usual norm in the space $L^\infty(0,T,C^1(\Omega))$. Inequality (29) leads to

$$\|e_{H,c}(t)\|_H^2 + 2(D_{min} - 9\epsilon^2)\int_0^t \|\nabla_H e_{H,c}(s)\|_{H,+}^2 ds$$

$$\leq \|e_{H,c}(0)\|_{H,+}^2 + \frac{1}{2\epsilon^2}\|K_{er}\|_{L^2(0,T)}^2 \int_0^t\int_0^s \|\nabla_H e_{H,c}(\mu)\|_{H,+}^2 d\mu ds$$

$$+ C\frac{1}{\epsilon^2}\Big(\frac{1}{2} + \|c\|_{L^\infty(C^1)}^2\big(1 + \|p\|_{L^\infty(C^1)}^2\big)\Big)\int_0^t \|e_{H,c}(s)\|_H^2 ds$$

$$+ C\frac{1}{2\epsilon^2}\|K_{er}\|_{L^2(0,T)}^2\|c\|_{L^\infty(C^1)}^2\big(1 + \|p\|_{L^\infty(C^1)}^2\big)\int_0^t\int_0^s \|e_{H,c}(\mu)\|_H^2 d\mu ds$$

$$+ 2\int_0^t \tau_{e,c}(s) ds.$$

Let ϵ be such that $D_{min} - 9\epsilon^2 > 0$. Under the smoothness assumptions on c and p it can be shown that $2\displaystyle\int_0^t \tau_{e,c}(s)\, ds \leq CH_{max}^4$. As $e_{H,c}(0) = 0$, applying Gronwall's Lemma we conclude (24).

From Proposition 1 we conclude the error estimate (25) for the pressure $p_H(t)$.

■

Theorem 1 is the main result of this paper and it establishes the second order convergence rate of the finite difference scheme (16), (17), or equivalently, of the piecewise linear finite element method (14), (15).

4. Time discretization

Our goal in this section is to propose an IMEX method for the coupled non-Fickian problem (4), (6). The method is obtained by integrating in time the ordinary differential equation (17) or equivalently the discrete variational equation (12).

In the temporal domain $[0, T]$, let us introduce the uniform time grid $\{t_m = m\Delta t,\, m = 0, \ldots, M\}$, with $t_M = T$, and where Δt is a fixed time step. By p_H^m and c_H^m we represent the numerical approximations for $p(t_m)$ and $c(t_m)$, respectively, defined by the IMEX method

$$-\nabla_H^* \cdot (A_H^m \nabla_H p_H^{m+1}) = (q_2)_H^{m+1},\ \text{in } \Omega_H, \tag{31}$$

$$\begin{aligned} c_H^{m+1} = c_H^m + \Delta t \nabla_H^* \cdot (D_H^{m,m+1} \nabla_H c_H^{m+1}) - \Delta t \nabla_{c,H} \cdot (B_H^{m,m+1} c_H^m) \\ + \Delta t^2 \sum_{\ell=0}^{m} K_{er}(t_{m+1} - t_\ell) \nabla_H^* \cdot (E_H^{\ell,\ell+1} \nabla_H c_H^\ell) + \Delta t (q_1)_H^{m+1},\ \text{in } \Omega_H, \end{aligned} \tag{32}$$

for $m = 0, \ldots, M-1$, and with the initial conditions

$$c_H^0 = c_{0,H},\, p_H^0 = p_{0,H} \text{ in } \Omega_H, \tag{33}$$

and boundary conditions

$$c_H^\ell = 0,\, p_H^\ell = R_H p_b(t_\ell) \text{ on } \partial\Omega_H,\, \ell = 1, \ldots, M. \tag{34}$$

Here we used the following notation: the non-null entries of A_H^m are given by $a_1(M_h c_H^m)$, $a_2(M_k c_H^m)$, the non-null entries of $D_H^{m,m+1}$ are given by $d_1(M_h c_H^m,$ $D_{-x} p_H^{m+1})$, $d_2(M_k c_H^m,\, D_{-y} p_H^{m+1})$, being $B_H^{m,m+1}$ and $E_H^{\ell,\ell+1}$, $\ell = 0, \ldots, m$, defined analogously. By D_{-t} we denote the first order backward finite difference operator with respect to the time variable. We observe that (31), (32) is equivalent to the coupled discrete variational problem

$$(A_H^m \nabla_H p_H^{m+1}, \nabla_H w_H)_{H,+} = ((q_2)_H^{m+1}, w_H)_H,\ \text{for all } w_H \in W_{H,0}, \tag{35}$$

$$\begin{aligned} (D_{-t} c_H^{m+1}, w_H)_H = -(D_H^{m,m+1} \nabla_H c_H^{m+1}, \nabla_H w_H)_{H,+} + (M_H(B_H^{m,m+1} c_H^m), \nabla_H w_H)_{H,+} \\ + \Delta t \sum_{\ell=0}^{m} K_{er}(t_{m+1} - t_\ell)(E_H^{\ell,\ell+1} \nabla_H c_H^\ell, \nabla_H w_H)_{H,+} \\ + ((q_1)_H^{m+1}, w_H)_H,\ \text{for all } w_H \in W_{H,0}. \end{aligned} \tag{36}$$

In what follows we establish bounds for the errors

$$e^m_{H,p} = R_H p(t_m) - p^m_H \quad \text{and} \quad e^m_{H,c} = R_H c(t_m) - c^m_H.$$

Following the proof of Proposition 1, it can be shown that

$$\|\nabla_H e^{m+1}_{H,p}\|_{H,+} \le C\Big(\|p(t_{m+1})\|_{C^1}\|e^m_{H,c}\|_H + \tau_p(t_{m+1}) + \|p(t_{m+1})\|_{C^1}\int_{t_m}^{t_{m+1}} \|R_H \frac{dc}{dt}(s)\|_H\, ds\Big), \tag{37}$$

where $\tau_p(t_{m+1})$ is given by (19) with $t = t_{m+1}$.

We deduce in what follows several estimates needed to compute an upper bound for $\|e^{m+1}_{H,c}\|_H$. We observe that

$$(D_{-t}c^{m+1}_H - (\frac{dc}{dt})_H(t_{m+1}), e^{m+1}_{H,c})_H = -(D_{-t}e^{m+1}_{H,c}, e^{m+1}_{H,c})_H + \tau_{d,IE}(e^{m+1}_{H,c}), \tag{38}$$

where

$$|\tau_{d,IE}(e^{m+1}_{H,c})| \le C\Big(\int_{t_m}^{t_{m+1}} \|R_H \frac{d^2c}{dt^2}(s)\|_H\, ds \|e^{m+1}_{H,c}\|_H + \Big(\sum_{\Delta\in\mathfrak{T}_H}(\mathrm{diam}\,\Delta)^4\|\frac{dc}{dt}(t_{m+1})\|^2_{H^2(\Delta)}\Big)^{1/2}\|\nabla_H e^{m+1}_{H,c}\|_{H,+}\Big).$$

For

$$\begin{aligned}\tau_{D,d}(e^{m+1}_{H,c}) &= (D_H^{m,m+1}\nabla_H c^{m+1}_H, \nabla_H e^{m+1}_{H,c})_{H,+}\\ &-\sum_{i=1}^{N_x}\sum_{j=1}^{M_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} d_1(x_i, y, t_{m+1})\frac{\partial c}{\partial x}(x_{i-1/2}, y, t_{m+1})\, dy D_{-x}e^{m+1}_{H,c}(x_i, y_j)\\ &-\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} d_2(x, y_j, t_{m+1})\frac{\partial c}{\partial y}(x, y_{j-1/2}, t_{m+1})\, dx D_{-y}e^{m+1}_{H,c}(x_i, y_j),\end{aligned} \tag{39}$$

with $d_\ell(x_i, y, t_{m+1})$, $\ell = 1, 2$, defined by (20) with $t = t_{m+1}$, we have

$$\tau_{D,d}(e^{m+1}_{H,c}) = -(D_H^{m,m+1}\nabla_H e^{m+1}_{H,c}, \nabla_H e^{m+1}_{H,c})_{H,+} + \tau_{D,IE}(e^{m+1}_{H,c}), \tag{40}$$

where

$$|\tau_{D,IE}(e_{H,c}^{m+1})| \leq \tau_{D,e}(e_{H,c}^{m+1}) + C\|c(t_{m+1})\|_{C^1}\big(1+\|p(t_{m+1})\|_{C^1}\big)$$
$$\int_{t_m}^{t_{m+1}} \|R_H \frac{dc}{dt}(s)\|_H ds \|\nabla_H e_{H,c}^{m+1}\|_{H,+},$$

being $\tau_{D,e}(e_{H,c}^{m+1})$ given by

$$\tau_{D,e}(e_{H,c}^{m+1}) = C\Big(\|c(t_{m+1})\|_{C^1}\big(1+\|p(t_{m+1})\|_{C^1}\big)\Big(\|e_{H,c}^{m}\|_H$$
$$+\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\|p(t_{m+1})\|^2_{H^3(\Delta)}\Big)^{1/2}\Big)$$
$$+(1+\|c(t_{m+1})\|_{C^1})^3\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\sum_{f\in\{c,p\}}\Big(\|f(t_{m+1})\|^2_{H^3(\Delta)}$$
$$+\|f(t_{m+1})\|^4_{H^2(\Delta)}\Big)\Big)^{1/2}\Big)\|\nabla_H e_{H,c}^{m+1}\|_{H,+}.$$

For

$$\tau_{B,d}(e_{H,c}^{m+1}) = -(M_H(B_H^{m,m+1}c_H^m), \nabla_H e_{H,c}^{m+1})_{H,+}$$
$$+\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i\int_{y_{j-1/2}}^{y_{j+1/2}} b_1(x_i,y,t_{m+1})c(x_{i-1/2},y,t_{m+1})\,dy D_{-x}e_{H,c}^{m+1}(x_i,y_j)$$
$$+\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j\int_{x_{i-1/2}}^{x_{i+1/2}} b_2(x,y_j,t_{m+1})c(x,y_{j-1/2},t)\,dx D_{-y}e_{H,c}^{m+1}(x_i,y_j), \tag{41}$$

with b_ℓ, $\ell=1,2$, given by (22) and $t=t_{m+1}$, assuming (23), we can prove that,

$$\tau_{B,d}(e_{H,c}^{m+1}) \leq (M_H(B_H^{m,m+1}e_H^m), \nabla_H e_{H,c}^{m+1})_{H,+} + \tau_{B,IE}(e_{H,c}^{m+1}), \tag{42}$$

where

$$|\tau_{B,IE}(e_{H,c}^{m+1})| \leq \tau_{B,e}(e_{H,c}^{m+1}) + C\|c(t_{m+1})\|_{C^1}\big(1+\|p(t_{m+1})\|_{C^1}\big)$$
$$\int_{t_m}^{t_{m+1}} \|R_H \frac{dc}{dt}(s)\|_H ds \|\nabla_H e_{H,c}^{m+1}\|_{H,+}$$

being $\tau_{B,e}(e_{H,c}^{m+1})$ equal to

$$\tau_{B,e}(e_{H,c}^{m+1}) = C\Big(\|c(t_{m+1})\|_{C^0}\big(1+\|p(t_{m+1})\|_{C^1}\big)\|e_{H,c}^m\|_H$$
$$+\big(\|c(t_{m+1})\|_{C^0}\big(1+\|p(t_{m+1})\|_{C^1}\big)+1\big)\Big(\sum_{\Delta\in\mathfrak{T}_H}(\mathrm{diam}\,\Delta)^4\big(\|c(t_{m+1})\|_{H^1(\Delta)}^4$$
$$+\|c(t_{m+1})\|_{H^2(\Delta)}^2+\|p(t_{m+1})\|_{H^2(\Delta)}^4+\|p(t_{m+1})\|_{H^3(\Delta)}^2\big)\Big)^{1/2}\Big)\|\nabla_H e_{H,c}^{m+1}\|_{H,+}.$$

Finally, we establish an estimate for

$$\tau_{E,d}(e_{H,c}^{m+1}) = -\Delta t\sum_{\ell=0}^m K_{er}^{m+1,\ell}(E_H^{\ell,\ell+1}\nabla_H c_H^\ell, \nabla_H e_{H,c}^{m+1})_{H,+}$$
$$+\int_0^{t_{m+1}} K_{er}(t_{m+1}-s)\sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_i\int_{y_{j-1/2}}^{y_{j+1/2}} e_1(x_i,y,s)\frac{\partial c}{\partial x}(x_{i-1/2},y,s)dyds \tag{43}$$
$$D_{-x}e_{H,c}^{m+1}(x_i,y_j)$$
$$+\int_0^{t_{m+1}} K_{er}(t_{m+1}-s)\sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} k_j\int_{x_{i-1/2}}^{x_{i+1/2}} e_2(x,y_j,s)\frac{\partial c}{\partial y}(x,y_{j-1/2},s)dxds \tag{44}$$
$$D_{-y}e_{H,c}^{m+1}(x_i,y_j), \tag{45}$$

where $K_{er}^{m+1,\ell} = K_{er}(t_{m+1}-t_\ell)$. Using the decomposition

$$\tau_{E,d}(e_{H,c}^{m+1}) = \sum_{\ell=1}^6 \tau_{E,i}, \tag{46}$$

with

$$\tau_{E,1} = \Delta t\sum_{\ell=0}^m K_{er}^{m+1,\ell}(E_H^{\ell,\ell+1}\nabla_H e_{H,c}^\ell, \nabla_H e_{H,c}^{m+1})_{H,+}, \tag{47}$$

$$\tau_{E,2} = \Delta t\sum_{\ell=0}^m K_{er}^{m+1,\ell}((E_H^*(t_\ell,t_{\ell+1})-E_H^{\ell,\ell+1})\nabla_H R_H c(t_\ell), \nabla_H e_{H,c}^{m+1})_{H,+}, \tag{48}$$

with $E^*_H(t_\ell, t_{\ell+1})$ defined as $E^*_H(t_\ell)$ but considering the concentration and the pressure at time levels t_ℓ and $t_{\ell+1}$, respectively,

$$\tau_{E,3} = \Delta t \sum_{\ell=0}^{m} K_{er}^{m+1,\ell}((\tilde{E}_H(t_\ell, t_{\ell+1}) - E^*_H(t_\ell, t_{\ell+1}))\nabla_H R_H c(t_\ell), \nabla_H e_{H,c}^{m+1})_{H,+}, \tag{49}$$

with $\tilde{E}_H(t_\ell, t_{\ell+1})$ defined as $\tilde{E}_H(t_\ell)$ but considering the concentration and the pressure at time levels t_ℓ and $t_{\ell+1}$, respectively,

$$\tau_{E,4} = \Delta t \sum_{\ell=0}^{m} K_{er}^{m+1,\ell}((\tilde{E}_H(t_\ell, t_\ell) - \tilde{E}_H(t_\ell, t_{\ell+1}))\nabla_H R_H c(t_\ell), \nabla_H e_{H,c}^{m+1})_{H,+}, \tag{50}$$

$$\begin{aligned}\tau_{E,5} = &\int_0^{t_{m+1}} K_{er}(t_{m+1} - s)(E_H(s)\nabla_H R_H c(s) ds, \nabla_H e_{H,c}^{m+1})_{H,+} \\ &- \Delta t \sum_{\ell=0}^{m} K_{er}^{m+1,\ell}(\tilde{E}_H(t_\ell, t_\ell)\nabla_H R_H c(t_\ell), \nabla_H e_{H,c}^{m+1})_{H,+}, \end{aligned} \tag{51}$$

and

$$\tau_{E,6} = -\int_0^{t_{m+1}} K_{er}(t_{m+1} - s)(E_H(s)\nabla_H R_H c(s) ds, \nabla_H e_{H,c}^{m+1})_{H,+}$$

$$+\int_0^{t_{m+1}} K_{er}(t_{m+1} - s) \sum_{i=1}^{N_x} \sum_{j=1}^{N_y-1} h_i \int_{y_{j-1/2}}^{y_{j+1/2}} e_1(x_i, y, s) \frac{\partial c}{\partial x}(x_{i-1/2}, y, s) dy ds \tag{52}$$

$$D_{-x} e_{H,c}^{m+1}(x_i, y_j)$$

$$+\int_0^{t_{m+1}} K_{er}(t_{m+1} - s) \sum_{i=1}^{N_x-1} \sum_{j=1}^{N_y} k_j \int_{x_{i-1/2}}^{x_{i+1/2}} e_2(x, y_j, s) \frac{\partial c}{\partial y}(x, y_{j-1/2}, s) dx ds \tag{53}$$

$$D_{-y} e_{H,c}^{m+1}(x_i, y_j). \tag{54}$$

For $\tau_{E,1}$ we easily establish the upper bounds

$$
\begin{aligned}
|\tau_{E,1}| &\leq C\Big(\Delta t\sum_{\ell=0}^{m}(K_{er}^{m+1,\ell})^2\Big)^{1/2}\Big(\Delta t\sum_{\ell=0}^{m}\|\nabla_H e_{H,c}^{\ell}\|_H^2\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}\\
&\leq C\Big(\|K_{er}\|^2_{L^2(0,T)}+T\Delta t\|K'_{er}\|^2_{L^2(0,T)}\Big)^{1/2}\Big(\Delta t\sum_{\ell=0}^{m}\|\nabla_H e_{H,c}^{\ell}\|_H^2\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}\\
&\leq C\sqrt{1+\Delta t}\|K_{er}\|_{H^1(0,T)}\Big(\Delta t\sum_{\ell=0}^{m}\|\nabla_H e_{H,c}^{\ell}\|_H^2\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}. \qquad (55)
\end{aligned}
$$

Using (37), it can be shown that

$$
\begin{aligned}
|\tau_{E,2}| &\leq C\Big(\Delta t\sum_{\ell=0}^{m}(K_{er}^{m+1,\ell})^2\Big)^{1/2}\Big(\Delta t\sum_{\ell=0}^{m}\|c(t_\ell)\|^2_{C^1}\big(1+\|p(t_{\ell+1})\|_{C^1}\big)^2\|e_{H,c}^{\ell}\|_H^2\\
&+\Delta t\sum_{\ell=0}^{m}\|c(t_\ell)\|^2_{C^1}\big(\tau_p(t_{\ell+1})^2+\Delta t\int_{t_\ell}^{t_{\ell+1}}\|R_H\frac{dc}{dt}(s)\|_H^2\,ds\big)\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}\\
&\leq C\Big(\sqrt{1+\Delta t}\|K_{er}\|_{H^1(0,T)}\Big(\|c\|^2_{C^0(C^1)}(1+\|p\|_{C^0(C^1)})^2\Delta t\sum_{\ell=0}^{m}\|e_{H,c}^{\ell}\|_H^2\\
&+\|c\|^2_{C^0(C^1)}\Delta t\sum_{\ell=0}^{m}\tau_p(t_{\ell+1})^2+\Delta t\int_{t_\ell}^{t_{\ell+1}}\|R_H\frac{dc}{dt}(s)\|_H^2\,ds\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+},
\end{aligned}
\qquad (56)
$$

where $\|.\|_{C^q(C^r)}$ denotes the usual norm in $C^q(0,T,C^r(\overline{\Omega}))$, $q,r\in\mathbb{N}_0$.

Following the steps used in the proof of Proposition 2 to estimate $\tau_D^{(2)}(w_H)$, we obtain

$$
\begin{aligned}
|\tau_{E,3}| &\leq C\Big(\Delta t\sum_{\ell=0}^{m}(K_{er}^{m+1,\ell})^2\Big)^{1/2}\Big(\Delta t\sum_{\ell=0}^{m}\|c(t_\ell)\|_{C^1}\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\big(\|c(t_\ell)\|^2_{H^2(\Delta)}\\
&\qquad + \|p(t_{\ell+1})\|^2_{H^2(\Delta)}\big)\Big)\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}\\
&\leq C\sqrt{1+\Delta t}\|K_{er}\|_{H^1(0,T)}\|c\|_{C^0(C^1)}\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\big(\|c\|^2_{C^0(H^2)}\\
&\qquad + \|p\|^2_{C^0(H^3)}\Big)^{1/2}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}. \qquad (57)
\end{aligned}
$$

For $\tau_{E,4}$ we easily get

$$|\tau_{E,4}| \leq C\Big(\Delta t\sum_{\ell=0}^{m}(K_{er}^{m+1,\ell})^2\Big)^{1/2}\Big(\Delta t^2\sum_{\ell=0}^{m}\|c(t_\ell)\|_{C^1}^2\int_{t_\ell}^{t_{\ell+1}}\|R_H\frac{\partial^2 c}{\partial t\partial x}(s)\|_H^2\,ds\Big)^{1/2} \tag{58}$$

$$\|\nabla_H e_{H,c}^{m+1}\|_{H,+}$$

$$\leq C\Delta t\sqrt{1+\Delta t}\|K_{er}\|_{H^1(0,T)}\|c\|_{C^0(C^1)}\|c\|_{H^1(C^1)}\|\nabla_H e_{H,c}^{m+1}\|_{H,+}, \tag{59}$$

where $\|.\|_{H^q(C^r)}$ denotes the usual norm in $H^q(0,T,C^r(\overline{\Omega}))$, q, $r\in\mathbb{N}_0$.

As $\tau_{E,5}$ represents the error of the left-rectangular rule, we deduce that

$$|\tau_{E,5}| \leq C\Delta t\Big(\|K_{er}'\|_{L^2(0,T)}\|c\|_{L^2(C^1)} \tag{60}$$

$$+\|K_{er}\|_{L^2(0,T)}\big(\|c\|_{C^0(C^1)}\big(\|c\|_{H^1(C^0)}+\|p\|_{H^1(C^1)}\big)$$

$$+\|c\|_{H^1(C^1)}\big)\Big)\|\nabla_H e_{H,c}^{m+1}\|_{H,+}$$

$$\leq C\Delta t\|K_{er}\|_{H^1(0,T)}\Big(\|c\|_{C^0(C^1)}\big(1+\|c\|_{H^1(C^0)}+\|p\|_{H^1(C^1)}\big) \tag{61}$$

$$+\|c\|_{H^1(C^1)}\Big)\|\nabla_H e_{H,c}^{m+1}\|_{H,+}. \tag{62}$$

At last, for $\tau_{E,6}$ holds the following

$$|\tau_{E,6}| \leq C\int_0^{t_{m+1}}K_{er}(t_{m+1}-s)(1+\|c(s)\|_{C^1})^3$$

$$\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\Big(\sum_{f\in\{c,p\}}\Big(\|f(s)\|_{H^2(\Delta)}^4+\|f(s)\|_{H^3(\Delta)}^2\Big)+1\Big)\Big)^{1/2}ds \tag{63}$$

$$\|\nabla_H e_{H,c}^{m+1}\|_{H,+}$$

$$\leq C\|K_{er}\|_{L^2(0,T)}(1+\|c\|_{C^0(C^1)})^3$$

$$\Big(\sum_{\Delta\in\mathfrak{T}_H}(\operatorname{diam}\Delta)^4\Big(\sum_{f\in\{c,p\}}\Big(\|f\|_{L^4(H^2)}^4+\|f\|_{L^2(H^3)}^2\Big)+1\Big)\Big)^{1/2}ds \tag{64}$$

$$\|\nabla_H e_{H,c}^{m+1}\|_{H,+} \tag{65}$$

Now we assume the following smoothness conditions: $c\in C^2(0,T,C^0(\overline{\Omega}))\cap H^1(0,T,H^3(\Omega))$, $p\in H^1(0,T,H^3(\Omega))$, and $K_{er}\in H^1(0,T)$.

From (36)-(63) it is a straightforward task to prove the existence of positive constants C_i, $i = 1, 2, 3$, such that, for $m = 0, \ldots, M-1$, the following holds

$$\|e_{H,c}^{m+1}\|_H^2 + D_{min}\Delta t \|\nabla_H e_{H,c}^{m+1}\|_{H,+}^2 \leq \|e_{H,c}^m\|_H^2 + C_1\Delta t\Big(\|e_{H,c}^m\|_H^2 + \|e_{H,c}^{m+1}\|_H^2 + \Delta t \sum_{\ell=0}^{m} \|\nabla_H e_{H,c}^\ell\|_{H,+}^2\Big) + \tau_{e,d}^{m+1}, \tag{66}$$

where

$$|\tau_{d,e}^{m+1}| \leq C_2\Delta t\Big(\Delta t \int_{t_m}^{t_{m+1}} \big(\|R_H \frac{d^2c}{dt^2}(s)\|_H^2 + \|R_H \frac{dc}{dt}(s)\|_H^2\big) ds + \Delta t^2\Big) + C_3\Delta t \sum_{\Delta\in\mathfrak{T}_H} (\operatorname{diam}\Delta)^4 \Big(\|\frac{dc}{dt}(t_{m+1})\|_{H^2(\Delta)}^2 + \sum_{f\in\{c,p\}} \big(\|f(t_{m+1})\|_{H^2(\Delta)}^4 + \|f(t_{m+1})\|_{H^3(\Delta)}^2\big) + 1\Big).$$

Inequality (66) leads to

$$(1 - C_1\Delta t)\|e_{H,c}^{m+1}\|_H^2 + D_{min}\Delta t \sum_{\ell=0}^{m+1} \|\nabla_H e_{H,c}^\ell\|_{H,+}^2 \leq \|e_{H,c}^0\|_H^2 \tag{67}$$

$$+ D_{min}\Delta t \|\nabla_H e_{H,c}^0\|_{H,+} + C_1\Delta t\Big(\sum_{\ell=0}^{m} \|e_{H,c}^\ell\|_H^2 + \Delta t \sum_{\ell=0}^{m}\sum_{j=0}^{\ell} \|\nabla_H e_{H,c}^j\|_{H,+}^2\Big) + \sum_{\ell=1}^{m+1} \tau_{e,d}^\ell. \tag{68}$$

Considering now the discrete Gronwall's Lemma we conclude that, for Δt such that $1 - C_1\Delta t > 0$,

$$\|e_{H,c}^{m+1}\|_H^2 + \Delta t \sum_{\ell=0}^{m+1} \|\nabla_H e_{H,c}^\ell\|_{H,+}^2 \leq \frac{1}{\min\{1 - C_1\Delta t, D_{min}\}}\Big(\sum_{\ell=1}^{m+1} \tau_{e,d}^\ell + C_2\Delta t \sum_{\ell=0}^{m}\sum_{j=1}^{\ell+1} \tau_{e,d}^j e^{C_2 t(m-\ell+1)\Delta t}\Big), \tag{69}$$

with $C_2 = \dfrac{C_1}{\min\{1 - C_1\Delta t, D_{min}\}}$ for $m = 0, \dots, M-1$. Finally, we remark that the error estimate (69) leads to

$$\|e^{m+1}_{H,c}\|^2_H + \Delta t \sum_{\ell=0}^{m+1} \|\nabla_H e^{\ell}_{H,c}\|^2_{H,+} \leq C\Big(H^4_{max} + \Delta t^2\Big),\ m = 0, \dots, M-1, \quad (70)$$

while from (37) we get

$$\|\nabla_H e^{m+1}_{H,p}\|_{H,+} \leq C\Big(H^4_{max} + \Delta t^2\Big),\ m = 0, \dots, M-1. \quad (71)$$

5. Numerical results

This section is dedicated to some numerical experiments. We start by presenting two examples that illustrate the convergence result established in the previous section.

For $e^m_{H,p} = R_H p(t_m) - p^m_H$ and $e^m_{H,c} = R_H c(t_m) - c^m_H$ we compute the error indicators

$$\text{Error}_p = \max_{m=1,\dots,M} \|e^m_{H,p}\|_{1,H},$$

and

$$\text{Error}_c = \max_{m=1,\dots,M} \Big(\|e^m_{H,c}\|^2_H + \Delta t \sum_{\ell=1}^{m} \|\nabla_H e^{\ell}_{H,c}\|^2_{H,+}\Big)^{1/2},$$

where p and c are solutions of the coupled problem (4), (6) with boundary and initial conditions (7), (8), respectively, and where p^m_H and c^m_H are numerical solutions obtained with the IMEX method (31)-(34). To evaluate the convergence rate we use the formula

$$\text{Rate}_g = \frac{\log\left(\dfrac{\text{Error}_{g,1}}{\text{Error}_{g,2}}\right)}{\log\left(\dfrac{H_{1,max}}{H_{2,max}}\right)},$$

for $g = p$, c, and where H_1 and H_2 are two grid vectors with $\text{Error}_{g,1}$ and $\text{Error}_{g,2}$ the corresponding errors. The initial grid Ω_H is randomly generated. The new grids are defined considering the midpoints of the intervals $[x_{i-1}, x_i]$ and $[y_{j-1}, y_j]$. Moreover, we fix $T = 0.01$ and $\Delta t = 10^{-7}$.

Example 1. *In this example, we consider the system (4), (6) with the following coefficients*

$$A(c) = \begin{bmatrix} 1+c & 0 \\ 0 & 2+c \end{bmatrix}, \quad D(c,\nabla p) = \begin{bmatrix} 1+2c+\dfrac{\partial p}{\partial x} & 0 \\ 0 & 1+c+2\dfrac{\partial p}{\partial y} \end{bmatrix},$$

$$B(c,\nabla p) = \begin{bmatrix} c\dfrac{\partial p}{\partial x} \\ \\ 3c\dfrac{\partial p}{\partial y} \end{bmatrix}, \quad E(c,\nabla p) = \begin{bmatrix} -\dfrac{\partial p}{\partial x} & 0 \\ 0 & -\dfrac{\partial p}{\partial y} \end{bmatrix}, \quad \text{and} \quad K_{er}(s) = e^{-s}.$$

We choose q_1, q_2, and the initial conditions (8) so that the exact solution is

$$p(x,y,t) = e^t xy(x-1)(y-1)\sin(xy) \quad \text{and} \quad c(x,y,t) = e^t xy(x-1)(y-1).$$

In Table 1 we present the results of our simulation. We observe that the solutions p and c belong to $H_0^3(\Omega)$ and the numerical results illustrate the convergence estimates (70) and (71).

H_{max}	$Error_p$	$Rate_p$	$Error_c$	$Rate_c$	N_x	N_y
1.316e-01	2.615e-04	1.981	2.841e-05	1.975	9	8
6.579e-02	6.625e-05	1.995	7.227e-06	1.993	18	16
3.290e-02	1.662e-05	1.999	1.815e-06	2.000	36	32
1.645e-02	4.158e-06	2.000	4.538e-07	2.009	72	64
8.224e-03	1.040e-06	2.000	1.127e-07	2.018	144	128
4.112e-03	2.600e-07	-	2.783e-08	-	288	256

Table 1. Numerical errors and convergence rates for Example 1.

For further illustration, we solve Example 1 using a considerable number of randomly generated spatial grids. In Figure 2 we plot the logarithmic norm of all errors $Error_g$, $g = p, c$, versus the logarithmic norm of all H_{max}. The slop of the least-square straight line (shown in green) is an approximation of the convergence order, and the values obtained, which are also displayed in Figure 2, again confirm the convergence estimates (70) and (71).

■

In the next example we consider that $p(t) \in H_0^2(\Omega)$ but it doesn't belong to $H_0^3(\Omega)$. Following the lines of Theorem 1 and using the results of [16], we

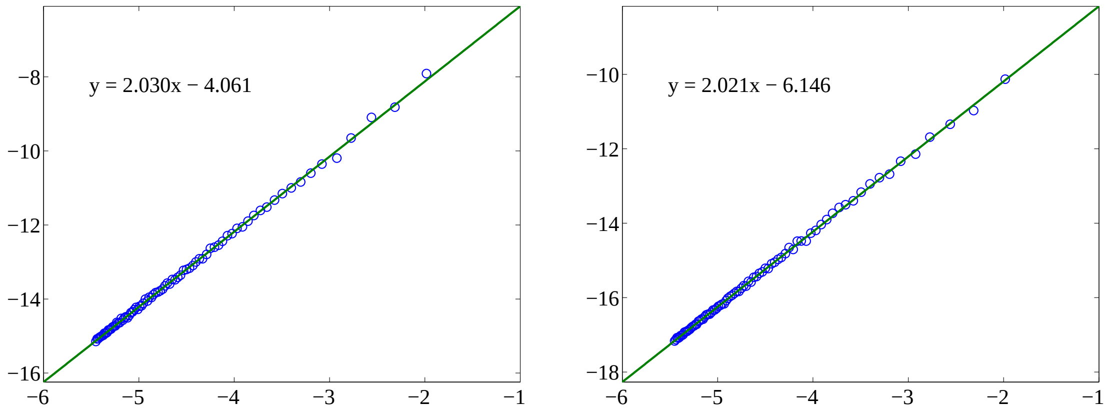

FIGURE 2. From left to right: Plot of $\log(\mathrm{Error}_p)$ and $\log(\mathrm{Error}_c)$ versus $\log(H_{max})$.

anticipate that the second order convergence rate will be lost for both $p(t)$ and $c(t)$

Example 2. *We now consider system (4), (6) with the coefficient functions used in Example 1 but we choose q_1, q_2, and the initial conditions (8) so that the exact solution is*

$$p(x, y, t) = e^t 2xy(x^2-1)(y^2-1)|x-0.5|^{2.1} \quad \textit{and} \quad c(x, y, t) = e^t xy(x-1)(y-1).$$

The numerical results presented in Table 2 agree with expectations, since the convergence rate for both p and c is of order $O(H_{max})$.

H_{max}	$Error_p$	$Rate_p$	$Error_c$	$Rate_c$	N_x	N_y
1.381e-01	9.708e-03	1.050	7.783e-05	1.293	8	10
6.906e-02	4.688e-03	1.051	3.177e-05	1.121	16	20
3.453e-02	2.263e-03	1.079	1.461e-05	1.084	32	40
1.726e-02	1.071e-03	1.093	6.888e-06	1.086	64	80
8.632e-03	5.024e-04	1.009	3.246e-06	1.001	128	160
4.316e-03	2.497e-04	-	1.622e-06	-	256	320

TABLE 2. Numerical errors and convergence rates for Example 2.

In Figure 3, we repeat the same type of experiments plotted on Figure 2. The slop of the least-square straight line, close to one, again confirms the first order convergence rate for Example 2.

■

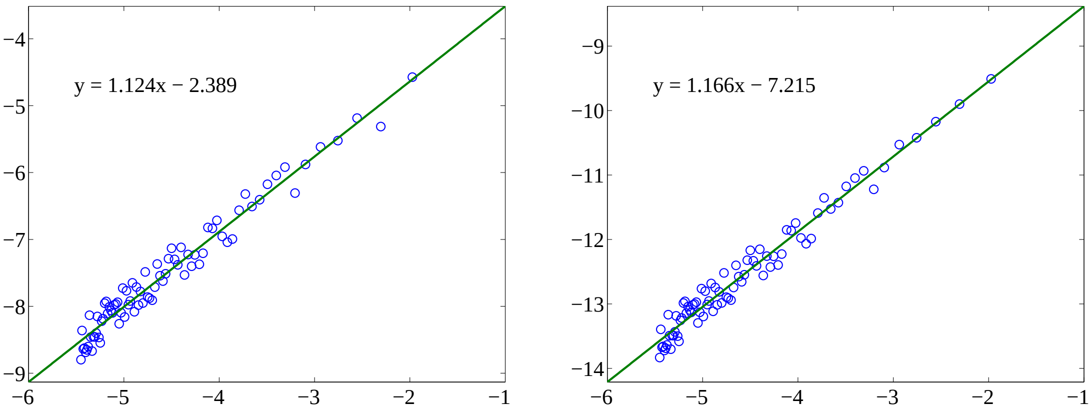

FIGURE 3. From left to right: Plot of $\log(\text{Error}_p)$ and $\log(\text{Error}_c)$ versus $\log(H_{max})$.

In what follows we present one example that intent to illustrate not only the differences between Fickian and non-Fickian models, in the case of miscible displacement in porous media, but also the fact the non-Fickian model can replicate key properties observed in real world experiments.

Example 3. *Let us consider the miscible displacement problem in porous media. We suppose that the resident fluid and the injected fluid are fully miscible and flow together as a unique fluid. We assume that there are no source or sink terms, i.e.,* $q_1 = q_2 = 0$, *and that the initial distribution of the injected fluid is as given in Figure 4 (on the right). In the pressure equation (3) we take* $K = I$, $\mu = 1$, *and the Dirichlet boundary conditions:* 0.4 *(bottom boundary),* 0.2 *(left and right boundaries) and* 0 *(top boundary). The obtained pressure field is shown in Figure 4 (on the left). Let* c *represent the concentration of the injected fluid. For both Fickian and non-Fickian model we define the diffusion tensor* $D = d_m \phi I$ *with* $d_m = 5 \times 10^{-3}$ *and* $\phi = 1$, *meaning that the longitudinal* (α_ℓ) *and transversal* (α_t) *dispersivity coefficients are zero. For the non-Fickian model we also take* $\tau = 10^{-1}$ *and* $E = d_{m,nF} I$ *with* $d_{m,nF} = 10^{-2}$. *The coupled problem is complemented with Dirichlet homogeneous boundary conditions for the concentration. This is equivalent to assume that the fluid is removed when it reaches the boundary.*

In Figure 5 we show the evolution of the concentration in the Fickian and non-Fickian case. As can be seen from the figures, the non-Fickian model is able to reproduce key features reported in experimental studies, such as

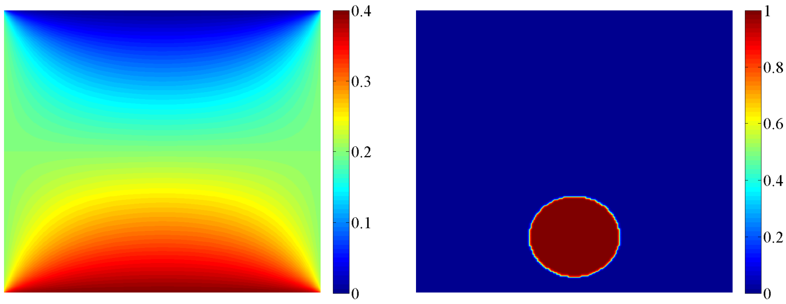

FIGURE 4. From left to right: Pressure and initial concentration.

highly asymmetric plumes with steep fronts and long and low concentration tails. Note that, for simplicity, in this example we omit physical units.

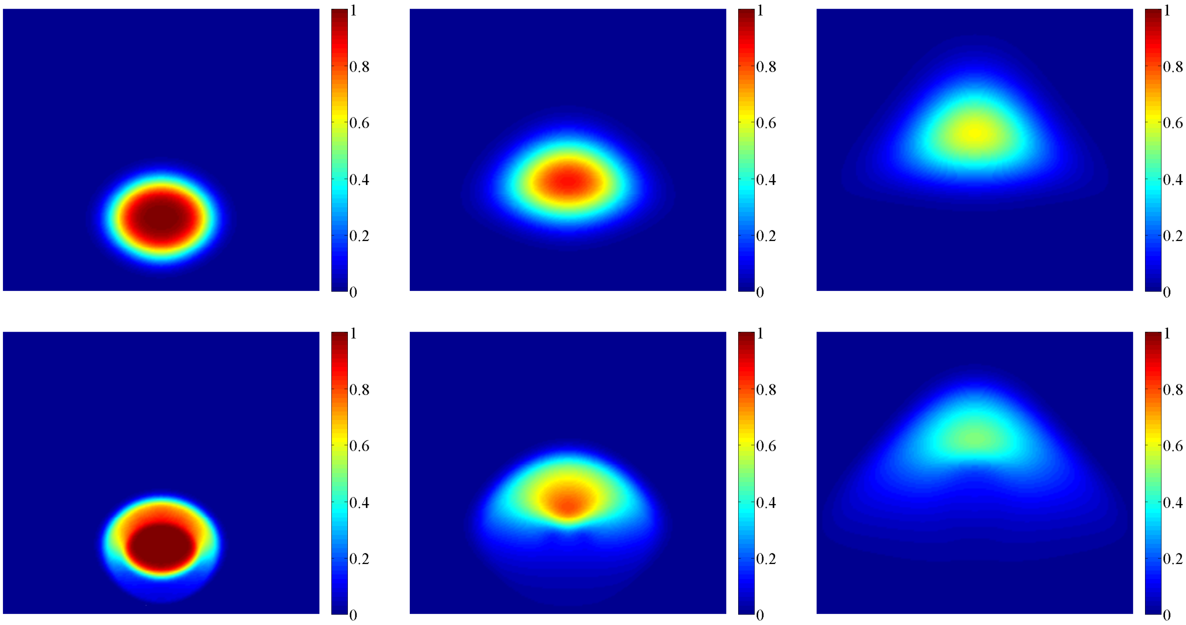

FIGURE 5. From left to right: Fickian concentration (first row) and non-Fickian concentration (second row) at time 0.15, 0.5, and 1.

6. Conclusion

This paper deals with the numerical approximation of a coupled initial boundary value problem formed by the elliptic equation (6) and the integro-differential equation of Volterra type (4). This system can be used to describe diffusion in porous media where a memory effect in time is present.

To solve the coupled system (6), (4) we proposed the IMEX method (31), (32) which can be seen as a fully discrete in time and space piecewise linear finite element method (35), (36). The convergence properties of the method were studied. We proved in particular that the numerical pressure and concentration are second order convergent in space with respect to a discrete H^1-norm and L^2-norm, respectively. The convergence estimates (70) and (71) are somehow unexpected because (31), (32) is a finite difference method with first order truncation error with respect to the L^∞-norm. Moreover, we also proved that the IMEX method (31), (32) is first order accurate in time.

We point out that the convergence analysis was made avoiding the usual approach, introduced by Wheeler in [34], and where the error is split into two terms with the aid of an auxiliary stationary problem. This alternate technique relies on the analysis of a convenient error equation and allows to relax the smoothness assumptions required by the technique in [34].

Numerical experiments were also performed. The results of Example 1 illustrate the error estimates (70) and (71), while Example 2 shows the sharpness of these estimates, since the reduction of the smoothness of the solutions p, c imply losing the second order convergence rate. At last, in Example 3, we used the problem of miscible displacement in porous media to highlight the differences between Fickian and non-Fickian model.

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