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ANOMALOUS DIFFUSION IN POROUS MEDIA

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Abstract: In this paper, an incompressible single phase and single component flow in a porous media presenting a nonfickian behaviour is studied. The model is composed by a parabolic equation for the pressure, with homogeneous Dirichlet or Neumann boundary conditions, coupled with a mass conservation equation for the concentration, a transport equation for the mass flux and by a Darcy's law for the velocity. The transport equation for the mass flux takes into account a nonfickian behaviour both in space and time. An IMEX finite element method is proposed to solve numerically the coupled system of equations and the behaviour of the physical unknowns is illustrated.

Keywords: porous media, nonfickian diffusion, darcy law, imex method, numerical simulation.

1. Introduction

Traditionally, the behaviour of a miscible displacement of one fluid by another in a porous medium $\Omega \subset \mathbb{R}^2$ is described by the following set of equations: a parabolic pressure equation

$$\frac{\partial}{\partial t}(\phi\rho) + \nabla \cdot (\rho \mathbf{v}) = q \text{ in } \Omega \times (0, T], \tag{1}$$

where ρ, ϕ, q and $\mathbf{v}$ represent the density of the mixture, the porosity of the medium, the source or sink term and the flow velocity given by Darcy's law

$$\mathbf{v} = -\frac{1}{\mu}\mathbf{K}\nabla p \text{ in } \Omega \times (0, T], \tag{2}$$

where $\mathbf{K}$ and μ represent the permeability tensor and the viscosity of the mixture; and by a mass conservation equation

$$\frac{\partial}{\partial t}(\phi\rho c) + \nabla \cdot (\rho c \mathbf{v}) + \nabla \cdot \mathbf{J} = qc^* \text{ in } \Omega \times (0, T], \tag{3}$$

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where c and $\mathbf{J}$ represent the concentration of the injected fluid and the mass flux. In (3) c^* denotes the prescribed concentration at sources or $c^* = c$ at sinks.

For incompressible fluids, under the assumption that the mass flux $\mathbf{J}$ is described by Fick's law

$$\mathbf{J} = -\mathbf{D}(\mathbf{v})\nabla c, \tag{4}$$

and by using a constant density ρ, equation (3) is replaced by the advection-diffusion equation

$$\rho\frac{\partial}{\partial t}(\phi c) + \rho\nabla\cdot(c\mathbf{v}) - \nabla\cdot(\mathbf{D}(\mathbf{v})\nabla c) = qc^* \text{ in } \Omega\times(0,T], \tag{5}$$

with the diffusion-dispersion tensor $\mathbf{D}(\mathbf{v})$ that is defined by

$$\mathbf{D}(\mathbf{v}) = D_m\phi\mathbf{I} + d_t\|\mathbf{v}\|\mathbf{I} + \frac{d_\ell - d_t}{\|\mathbf{v}\|}\mathbf{v}\mathbf{v}^t, \tag{6}$$

where $\|\mathbf{v}\|$ is the magnitude of the velocity, D_m is the molecular diffusion coefficient, and d_t, d_ℓ are the transverse and longitudinal dispersivities, respectively.

In order to compute the unknowns $\rho, p, \mathbf{v}, \phi$ and c, equations (1), (2), (3) are complemented by some state equations or constitutive relations. For instance in [1], different state equations are summarized for the following scenarios: the density is constant and the fluid is incompressible, the fluid is compressible with constant compressibility, or the porous media is deformable with a high gradient of pressure.

The parabolic equation (5) has been largely considered in the numerical simulation of fluid flows in several contexts as can be seen for instance in [1–6] and in the references therein. The main theoretical objection to use equation (5) is its parabolic character which induces an infinite speed of propagation for the concentration, that is phisically unacceptable [7]. Another objection to (5), observed in [7], is related with definition (6) of the diffusion-dispersion tensor $\mathbf{D}(\mathbf{v})$ where the transversal and longitudinal dispersions are assumed to be constant. In fact it is often observed in applications that they increase with the distance and/or with time. A third objection is the linear dependence of the mass flux $\mathbf{J}$ on the gradient of the concentration given by (4). This is because, when a large concentration gradient exists, nonlinear effects become important and (4) should then be replaced by a nonlinear relation between $\mathbf{J}$ and ∇c that includes additional terms. This problem was also observed when high pressure gradients are present [8–10]. Several approaches

have been considered in the literature to overcome these objections to use (5). We mention, without being exhaustive, the papers [7, 8, 10–22].

In this paper we start in Section 2 by presenting some mathematical models that were introduced in the literature to avoid some of the limitations of the classical diffusion equation mentioned above. Between these models, a coupled model for the evolution of a mixture in a porous medium is described at the end of this section and it will be used in the rest of this work. In Section 3 we propose an implicit-explicit method, based on finite element methods, to discretize this coupled model. Section 4 is devoted to the numerical simulation, we start by presenting some numerical experiments showing the accuracy of the proposed method. The qualitative behaviours of the relevant quantities for a diffusion process in a porous medium are compared in fickian and nonfickian contexts. It should be stressed that, to the best of our knowledge, such comparison has not yet been illustrated. Finally, in Section 5 we summarize the main conclusions.

2. Modelling memory in diffusion on porous media

2.1. Memory in time on dispersive mass flux. A common approach to overcome the infinite propagation speed for the concentration in the advection-diffusion equation (5) is its replacement by the following nonlocal time integro-differential equation

$$\frac{\partial c}{\partial t}(t) + \mathcal{A}c(t) + \int_0^t K_{er}(t-s)\mathcal{B}(s,t)c(s)ds = f \text{ in } \Omega \times (0,T] \tag{7}$$

where $\mathcal{A}$ and $\mathcal{B}$ are second order differential operators with respect to the spatial variables, K_{er} represents a time convolution kernel and f is a reaction term [11–16, 18]. Numerical methods for initial values problems defined by (7) were largely studied and a huge collection of methods is now available, see for example [23–36].

This type of integro-differential equation with memory in time can be obtained by assuming that the mass flux admits the decomposition

$$\mathbf{J} = \mathbf{J}_m + \mathbf{J}_d \tag{8}$$

where $\mathbf{J}_m = -\phi D_m \nabla c$ is the molecular diffusion and $\mathbf{J}_d$ is the dispersive mass flux that satisfies the following differential equation

$$\mathbf{A}\frac{\partial \mathbf{J}_d}{\partial t} + \mathbf{J}_d = -\mathbf{D}_{dis}(\mathbf{v})\nabla c, \tag{9}$$

where $\mathbf{A}$ is a tensor and $\mathbf{D}_{dis}(\mathbf{v})$ is the dispersive tensor

$$\mathbf{D}_{dis}(\mathbf{v}) = d_t\|\mathbf{v}\|\mathbf{I} + \frac{d_t - d_\ell}{\|\mathbf{v}\|}\mathbf{v}\mathbf{v}^t.$$

Equation (9) was proposed in [18] in the case that the porous medium presents small-scale heterogeneities. In particular, when $\mathbf{A}$ is an invertible matrix, the dispersive mass flux $\mathbf{J}_d$ solution of (9) admits the representation

$$\mathbf{J}_d(t) = e^{-\mathbf{A}^{-1}t}\mathbf{J}_d(0) - \int_0^t e^{-\mathbf{A}^{-1}(t-s)}\mathbf{A}^{-1}\mathbf{D}_{dis}(\mathbf{v})\nabla c(s)ds. \tag{10}$$

If the molecular mass flux $\mathbf{J}_m$ is given by Fick's law (4) with $\mathbf{D}(\mathbf{v})$ replaced by $\phi D_m\mathbf{I}$, that is

$$\mathbf{J}_m(t) = -\phi D_m\nabla c(t),$$

from (3), (8) and (10) we obtain

$$\begin{aligned}\frac{\partial}{\partial t}(\phi\rho c) + \nabla\cdot(\rho c\mathbf{v}) &= \nabla\cdot(\phi D_m\nabla c)\\ &\quad + \int_0^t e^{-\mathbf{A}^{-1}(t-s)}\nabla\cdot\left(\mathbf{A}^{-1}\mathbf{D}_{dis}(\mathbf{v})\nabla c(s)\right)ds + qc^*\end{aligned}$$

in $\Omega\times(0,T]$, when $\mathbf{J}_d(0)$ is constant. We observe that using a one dimensional domain Ω, equation (9) is a first order approximation of $\mathbf{J}_d(t+\mathbf{A})$, when

$$\mathbf{J}_d(t+\mathbf{A}) = -\mathbf{D}_{dis}(\mathbf{v})\nabla c(t),$$

that describes then the memory effect in time of a nonlocal approach, see [18]. A second order differential equation in time and space was also obtained in [18], that has finite velocity of propagation under convenient assumptions on the model parameters used.

2.2. Memory in time and space on dispersive mass flux. In what follows we take into account the memory effect both in time and space of the dispersive mass flux $\mathbf{J}_d(\mathbf{x},t)$. The resulting total mass flux $\mathbf{J}$ will be then replaced accordingly in the advection-diffusion mass conservation equation (5) that will be added to a system of differential equations describing the flux $\mathbf{J}$ itself.

For incompressible flows, [7] introduced the following equation for the mass flux

$$\mathbf{A}\frac{\partial\mathbf{J}}{\partial t} + \mathbf{A}(\mathbf{J}\cdot\nabla)\mathbf{v} + \mathbf{A}(\mathbf{v}\cdot\nabla)\mathbf{J} + \mathbf{J} = -\mathbf{D}(\mathbf{v})\nabla c \text{ in } \Omega\times(0,T], \tag{11}$$

where $\mathbf{A}$ is a dispersion tensor and $\mathbf{D}(\mathbf{v})$ is the diffusion-dispersion tensor given by (6).

We highlight in what follows the meaning of equation (11). When velocity $\mathbf{v}$ is constant and $\mathbf{A} = \tau\mathbf{I}$, equation (11) has the form

$$\tau\frac{\partial \mathbf{J}}{\partial t} + \tau(\mathbf{v}\cdot\nabla)\mathbf{J} + \mathbf{J} = -\mathbf{D}(\mathbf{v})\nabla c \tag{12}$$

that is similar to (9), where only the dispersive flux was considered. Assuming that $\mathbf{J}$ is zero at $t = 0$, the solution of (12) is

$$\mathbf{J}(\mathbf{x}, t) = -\int_0^t e^{-\tau(t-s)}\mathbf{D}(\mathbf{v})\nabla c(\mathbf{x} - \mathbf{v}(t-s), s)\, ds.$$

This last expression means that the mass flux $\mathbf{J}(\mathbf{x}, t)$ at point $\mathbf{x}$ and at time t depends on the behaviour of the concentration gradient at previous times and previous positions, that is, it accounts for a memory effect in time and space. In fact, (12) can also be obtained by the linear expansion of

$$\mathbf{J}(\mathbf{x} + \tau\mathbf{v}, t + \tau) = -\mathbf{D}(\mathbf{v})\nabla c,$$

which further shows the existence of memory in time and space for the mass flux. Energy estimates for the coupled model (3), (12) have been obtained in [37], for the case of constant porosity, velocity and density and an extra term of fickian diffusion in equation (3).

An equivalent form for equation (11) appears also in [19, 20] where slow moving incompressible fluids are considered. In these works, it is assumed that the mass flux is decomposed as in (8) with $\mathbf{J}_d$ that satisfies

$$\frac{\partial \mathbf{J}_d}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{J}_d + (\mathbf{J}_d\cdot\nabla)\mathbf{v} = -\mathbf{D}_0(\mathbf{v})\nabla c + D_m\mathbf{s}, \tag{13}$$

where

$$\mathbf{s} = -\boldsymbol{\eta}\mathbf{J}_d, \tag{14}$$

D_m is the usual molecular diffusion coefficient, and

$$\mathbf{D}_0(\mathbf{v}) = \beta_1\|\mathbf{v}\|^2\mathbf{I} + \beta_2\mathbf{v}\mathbf{v}^T$$

with $\beta_i,\ i = 1, 2$, that are medium constants and $\boldsymbol{\eta}$ that is a positive definite tensor that depends on the velocity. Combining (13) with (14) we obtain

$$\frac{\partial \mathbf{J}_d}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{J}_d + \big(\nabla\mathbf{v} + D_m\boldsymbol{\eta}\big)\mathbf{J}_d = -\mathbf{D}_0(\mathbf{v})\nabla c.$$

As pointed out in [7], the proposed models avoid some of the limitations of the classical diffusion model, namely the dispersive mass flux is influenced by the weighted contribution from all previous values of the gradient of the concentration. This fact implies that the dispersive mass flux is scale-dependent and the longitudinal-transversal dispersivities are time dependent.

2.3. Differential model. In this paper, the model used is described by a constant density $\rho = 1$, the parabolic pressure equation (1), the Darcy's law (2), the mass conservation equation (3) in nonconservative form and by equation (11) provided with $\mathbf{A} = \tau\mathbf{I}$. This leads to the following model

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{v} = q & \text{in } \Omega \times (0,T], \\ \mathbf{v} = -\dfrac{1}{\mu}\mathbf{K}\nabla p & \text{in } \Omega \times (0,T], \\ \dfrac{\partial}{\partial t}(\phi c) + \mathbf{v}\cdot\nabla c + \nabla \cdot \mathbf{J} = f(c) & \text{in } \Omega \times (0,T], \\ \tau\dfrac{\partial \mathbf{J}}{\partial t} + \tau(\mathbf{J}\cdot\nabla)\mathbf{v} + \tau(\mathbf{v}\cdot\nabla)\mathbf{J} + \mathbf{J} = -\mathbf{D}(\mathbf{v})\nabla c & \text{in } \Omega \times (0,T], \end{cases} \tag{15}$$

where $\mathbf{D}(\mathbf{v})$ is given by (6), τ is a parameter controlling the memory effect of the mass flux (see the discussion done in the previous section) and $f(c) = qc^*$.

In this scenario, the porosity ϕ can be either known or calculated by using a constitutive law, as done in [6]. Indeed, when the porosity is not known for a certain media, it can be assumed a relationship between the porosity and the pressure. For instance if the media is slightly compressible, then it can be assumed that

$$\phi(p) = \phi^o e^{c_R(p-p^o)} \tag{16}$$

where c_R denotes the rock compressibility constant of the medium, p^o is a reference pressure and ϕ^o is the reference porosity (see [38]).

In the context of porous media, it is common, see [1], to consider a viscosity μ dependent on the concentration through the standard quarter power law

$$\mu(c) = (\mu_s^{-0.25}c + (1-c)\mu_0^{-0.25})^{-4}. \tag{17}$$

The system of equation (15) is complemented with boundary conditions for pressure, concentration and flux. We consider Dirichlet and Neumann boundary conditions for the pressure, concentration and flux. To formalize our setting, we first introduce two, possibly different, nonempty disjoint

partitions of the boundary

$$\partial\Omega = \Gamma_{D,p} \cup \Gamma_{N,p} \quad \text{and} \quad \partial\Omega = \Gamma_{D,c} \cup \Gamma_{N,c}.$$

We assume that the pressure profile is known on $\Gamma_{D,p}$

$$p = p_D \text{ on } \Gamma_{D,p}, \tag{18}$$

and that satisfies a Neumann boundary condition on $\Gamma_{N,p}$

$$-\frac{1}{\mu(c)}\mathbf{K}\nabla p \cdot \mathbf{n} = 0 \text{ on } \Gamma_{N,p},$$

where $\mathbf{n}$ denotes the outer unit normal. For the Darcy's law (2), we have that this last boundary condition can be recast as

$$\mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \Gamma_{N,p}. \tag{19}$$

The concentration and mass flux's boundary conditions are then imposed as follows

$$c(\mathbf{x}, t) = g(\mathbf{x}, t),\ \forall \mathbf{x} \in \Gamma_{D,c} \quad \text{and} \quad \mathbf{J}(\mathbf{x}, t) \cdot \mathbf{n} = 0,\ \forall \mathbf{x} \in \Gamma_{N,c}, \tag{20}$$

where $g(\mathbf{x}, t)$ is a known function defined in $\Gamma_{D,c}$. System (15) is also complemented with initial data for the pressure, concentration and flux

$$c(0) = c_0, \quad p(0) = p_0, \quad \mathbf{J}(0) = \mathbf{J}_0. \tag{21}$$

3. An IMEX finite element method

In this section, we present a continuous Galerkin finite element method to solve the system (15). Let us first introduce some notations used in this and in the next section. We denote by $L^2(\Omega)$ and $H^1(\Omega)$ the standard L^2 and H^1 Sobolev spaces of scalar functions. Given a nonzero measure portion Γ of $\partial\Omega$, $H^1_\Gamma(\Omega)$ denotes the space of $H^1(\Omega)$ of functions that have zero trace on Γ. Also, the equivalent spaces for vectorial functions are represented using the same notation, but with bold letters. With an abuse of notation, we shall denote by the same notation, $(\cdot, \cdot)$, the inner product of L^2 and $\mathbf{L}^2$.

The weak formulation of the differential problem (15), (18), (19), (20) and (21) reads as follows: find

$$p(t) \in H^1(\Omega),\ p(t) = p_D \text{ on } \Gamma_{D,p},$$

$$c(t) \in H^1(\Omega),\ c(t) = g(t) \text{ on } \Gamma_{D,c}$$

and

$$\mathbf{J}(t) \in \mathbf{H}^1(\Omega)$$

such that $\forall w_1 \in H^1_{\Gamma_{D,p}}(\Omega)$, $\forall w_1 \in H^1_{\Gamma_{D,c}}(\Omega)$ and $\forall \mathbf{w}_3 \in H^1(\Omega) \times H^1(\Omega)$

$$\left(\frac{\partial}{\partial t}\phi(p(t)), w_1\right) + \left(\frac{1}{\mu(c(t))}\mathbf{K}\nabla p(t), \nabla w_1\right) = (q, w_1), \tag{22}$$

$$\left(\frac{\partial}{\partial t}(\phi(t)c(t)), w_2\right) + (\mathbf{v}(t)\cdot\nabla c(t), w_2) - (\mathbf{J}(t), \nabla w_2) = (f(c(t)), w_2), \tag{23}$$

$$\begin{aligned}\left(\tau\frac{\partial \mathbf{J}}{\partial t}(t) + \mathbf{D}(\mathbf{v}(t))\nabla c(t) + \tau(\mathbf{J}(t)\cdot\nabla)\mathbf{v}(t), \mathbf{w}_3\right) + \\ + (\tau(\mathbf{v}(t)\cdot\nabla)\mathbf{J}(t) + \mathbf{J}(t), \mathbf{w}_3) \;=\; 0.\end{aligned} \tag{24}$$

We introduce now a finite element discretization of the previous variational problem. Let k denote a positive integer and h a positive real number. We denote by $\mathbb{P}_k$ the space of polynomials of degree less than or equal to k, and by $\mathcal{T}_h$ an admissible triangulation of Ω. We introduce the finite-elements space

$$V_h^k = \{v_h \in C^0(\bar{\Omega}) |\ v_{h|_K} \in \mathbb{P}_k,\ \forall K \in \mathcal{T}_h\}$$

with $k = 1, 2$. The other spaces used in the following are

$$V_h^{k,0} = \{v_h \in V_h^k |\ v_{h|_{\partial\Omega}} = 0\},$$

$$V_h^{k,0,D,p} = \{v_h \in V_h^k |\ v_{h|_{\Gamma_{D,p}}} = 0\}$$

and

$$V_h^{k,0,D,c} = \{v_h \in V_h^k |\ v_{h|_{\Gamma_{D,c}}} = 0\}.$$

A fully discrete Galerkin approximation of the system (15) is now presented. The time discretization divides the time-interval $[0, T]$ in N subintervals with a fixed time step $\Delta t = T/N$. This approximation computes the pressure, concentration and flux following this order at each time t_n with $t_n = t_{n-1} + \Delta t$ starting with $t_0 = 0$.

The fully discrete Galerkin approximation used for the pressure equation (22) at time t_{n+1} is presented below. The variational formulation for the pressure problem reads as: find $p_{n+1} \in V_h^k$ such that $p_{n+1} = p_{D,h}(t_{n+1})$ on $\Gamma_{D,p}$, where $p_{D,h}(t_{n+1})$ is the projection of $p_D(t_{n+1})$ into V_h^k, and for all $v_h \in V_h^{k,0,D,p}$

$$\begin{aligned}&\left(\frac{d\phi}{dp}(p_n)p_{n+1}, v_h\right) + \\ &+\Delta t\left(\frac{\mathbf{K}}{\mu(c_n)}\nabla p_{n+1}, \nabla v_h\right) \;=\; \Delta t(q_{n+1}, v_h) + \left(\frac{d\phi}{dp}(p_n)p_n, v_h\right).\end{aligned} \tag{25}$$

After calculating p_{n+1} we reconstruct the velocity as

$$\mathbf{v}_n = -\frac{\mathbf{K}}{\mu(c_n)}\nabla p_{n+1}. \tag{26}$$

In order to solve the concentration and flux equations, we use the weak formulations (23) and (24), that is, we solve the following problem: find $c_{n+1} \in V_h^k$ such that $c_{n+1} = g_h(t_{n+1})$ on $\Gamma_{D,c}$ (where $g_h(t_{n+1})$ is the projection of $g(t_{n+1})$ into V_h^k) and $\mathbf{J}_{n+1} \in V_h^k \times V_h^k$ such that

$$\begin{aligned} &(\phi(p_{n+1})c_{n+1}, v_h)+ \\ &+\Delta t(\mathbf{v}_n \cdot \nabla c_{n+1}, v_h) \\ &\quad -\Delta t(\mathbf{J}_{n+1}, \nabla v_h) \;&=\; &(\phi(p_n)c_n, v_h) + \Delta t(f_{n+1}, v_h) \end{aligned} \tag{27}$$

and

$$\begin{aligned} &(\tau + \Delta t)(\mathbf{J}_{n+1}, \mathbf{w}_h)+ \\ &\tau\Delta_t((\mathbf{v}_n \cdot \boldsymbol{\nabla})\mathbf{J}_{n+1} + (\mathbf{J}_{n+1} \cdot \boldsymbol{\nabla})\mathbf{v}_n, \mathbf{w}_h) \\ &\quad +\Delta t(\mathbf{D}(\mathbf{v}_n)\nabla c_{n+1}, \mathbf{w}_h) \;&=\; &\tau(\mathbf{J}_n, \mathbf{w}_h) \end{aligned} \tag{28}$$

for all $v_h \in V_h^{k,0,D,c}$ and $\mathbf{w}_h = (w_{1,h}, w_{2,h})^T$ with $w_{1,h}, w_{2,h} \in V_h^k$.

Let $\{\varphi_i^p\}_{i=1,\dots,N_p}$, $\{\varphi_j^c\}_{j=1,\dots,N_c}$ and $\{\boldsymbol{\varphi}_l^{\mathbf{J}}\}_{l=1,\dots,N_{\mathbf{J}}}$ denote the basis functions of the spaces $V_h^{k,0,D,p}$, $V_h^{k,0,D}$ and $V_h^k \times V_h^k$ respectively, the solution of the problem (25)-(28) can be expressed as a linear combinations of the respective basis functions

$$p_{n+1} = \sum_{i=1,\dots,N_p} \alpha_i^p \varphi_i^p, \qquad c_{n+1} = \sum_{j=1,\dots,N_c} \beta_j^c \varphi_j^c, \qquad \mathbf{J}_{n+1} = \sum_{l=1,\dots,N_{\mathbf{J}}} \gamma_l^{\mathbf{J}} \boldsymbol{\varphi}_l^{\mathbf{J}}.$$

Gathering the degrees of freedom for the pressure, concentration and flux in the vectors P_{n+1}, W_{n+1} and $\mathbf{U}_{n+1}$, respectively, these can be calculated by solving the following linear systems

$$M_{n+1}P_{n+1} = F_{p,n+1} \tag{29}$$

and

$$\begin{bmatrix} A_{n+1} & B \\ C_n & D_{n+1} \end{bmatrix} \begin{bmatrix} W_{n+1} \\ \mathbf{U}_{n+1} \end{bmatrix} = \begin{bmatrix} F_{c,n+1} \\ F_{\mathbf{J},n+1} \end{bmatrix} \tag{30}$$

where

$$
\begin{aligned}
M_{n+1}(i,j) &= \left(\tfrac{d\phi}{dp}(p_n)\varphi_j^p, \varphi_i^p\right) + \Delta t \left(\tfrac{\mathbf{K}}{\mu(c_n)}\nabla\varphi_j^p, \nabla\varphi_i^p\right), && \forall i,j = 1,\dots,N_p,\\
A_{n+1}(i,j) &= \left(\phi(p_{n+1})\varphi_j^c, \varphi_i^c\right) + \Delta t \left((\mathbf{v}_n\cdot\nabla\varphi_j^c), \varphi_i^c\right), && \forall i,j = 1,\dots,N_c,\\
B(i,l) &= -\Delta t \left(\boldsymbol{\varphi}_l^{\mathbf{J}}, \nabla\varphi_i^c\right), && \forall i = 1,\dots,N_c,\\
& && \forall l = 1,\dots,N_{\mathbf{J}},\\
C_n(l,i) &= \Delta t \left(\mathbf{D}(\mathbf{v}_n)\nabla\varphi_i^c, \boldsymbol{\varphi}_l^{\mathbf{J}}\right), && \forall l = 1,\dots,N_{\mathbf{J}},\\
& && \forall i = 1,\dots,N_c,\\
D_{n+1}(l,m) &= (\tau+\Delta t)\left(\boldsymbol{\varphi}_m^{\mathbf{J}}, \boldsymbol{\varphi}_l^{\mathbf{J}}\right)\\
&\quad +\tau\Delta t \left((\mathbf{v}_n\cdot\boldsymbol{\nabla})\boldsymbol{\varphi}_m^{\mathbf{J}}, \boldsymbol{\varphi}_l^{\mathbf{J}}\right)\\
&\quad +\tau\Delta t \left((\boldsymbol{\varphi}_m^{\mathbf{J}}\cdot\boldsymbol{\nabla})\mathbf{v}_n, \boldsymbol{\varphi}_l^{\mathbf{J}}\right), && \forall l,m = 1,\dots,N_{\mathbf{J}},\\
F_{p,n+1}(i) &= \left(\tfrac{d\phi}{dp}(p_n)p_n, \varphi_i^p\right) + \Delta t \left(q_{n+1}, \varphi_i^p\right), && \forall i = 1,\dots,N_p,\\
F_{c,n+1}(i) &= \left(\phi(p_n)c_n, \varphi_i^c\right) + \Delta t \left(f_{n+1}, \varphi_i^c\right), && \forall i = 1,\dots,N_c,\\
F_{\mathbf{J},n+1}(l) &= \tau \left(\mathbf{J}_n, \boldsymbol{\varphi}_l^{\mathbf{J}}\right), && \forall l = 1\dots,N_{\mathbf{J}}.
\end{aligned}
$$

We remark that matrix B does not depend on time and can be assembled only once. There are several ways to optimize the assembly of the linear systems (29)-(30). A first possibility lies in the mass counterpart of the pressure associated matrix M_{n+1} and A_{n+1}. These matrices can be assembled using the finite element space corresponding to all the degrees of freedom that steam from the triangulation (boundary conditions are implemented by a simple row elimination procedure) and stored. The mass counterpart of M_{n+1} is nothing more than, up to a constant, the mass counterpart of A_{n+1}.

Notice that the concentration and flux problems are implicitly coupled for stability reasons. Indeed, on the simpler fickian case ($\tau = 0$), an explicit treatment of the flux, either in the concentration equation, or in the flux equation, would lead to a time discretization with an undesirable stability restriction in the time step.

4. Numerical experiments

This section aims to study numerically the accuracy of the IMEX finite element method described by equations (25), (26), (27) and (28), and to illustrate the nonfickian behaviour of the solution of the initial boundary value problem (15), (18), (19), (20) and (21).

In order to proceed with the description of the numerical experiments we make the following assumption on the domain, parameters and functions

used in (15): $\Omega = [0,1]^2$, $f = q = 0$, $\phi(\mathbf{x},t) = e^{p(\mathbf{x},t)}$, $\mu(c) = \frac{1}{((1-M)c+M)^4}$ (where $M = 0.5^{-0.25}$, using $\mu_S = 1$ and $\mu_0 = 0.5$ in (17)).

4.1. Convergence behaviour. We start by studying numerically the convergence properties of the IMEX method introduced before. We take $\mathbf{K} = \mathbf{I}$ (where $\mathbf{I}$ is the two-dimensional identity matrix) and $D_m = d_t = d_l = 0.1$. We use as initial conditions (at time $t = 0$): the pressure $p(\mathbf{x},0) = x_1x_2(x_1-1)(x_2-1)$, the concentration $c(\mathbf{x},0) = e^{((x_1-0.5)^2+(x_2-0.5)^2)/0.05}$ where $\mathbf{x} = (x_1,x_2)$, and the mass flux $\mathbf{J}(\mathbf{x},0) = \mathbf{0}$. As boundary conditions (see (20)) we use

$$p(\mathbf{x},t) = 0, \forall \mathbf{x} \in \partial\Omega, \quad c(\mathbf{x},t) = 0, \forall \mathbf{x} \in \Gamma_{D,c} \quad \text{and} \quad \mathbf{J}(\mathbf{x},t)\cdot\mathbf{n} = 0, \forall \mathbf{x} \in \Gamma_{N,c},$$

where $\Gamma_{N,c} = \{0\} \times [0,1]$ and $\Gamma_{D,c} = \partial\Omega \backslash \Gamma_{N,c}$.

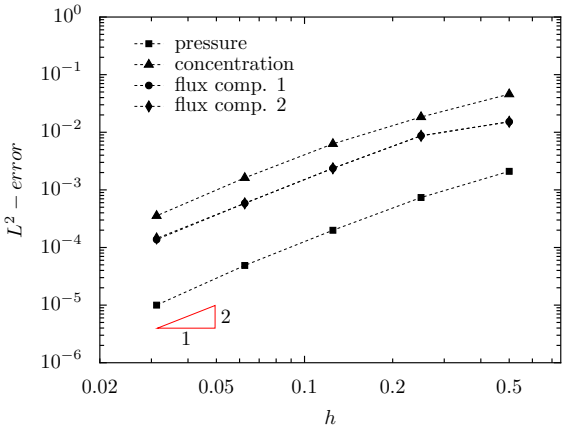
The errors of the numerical pressure, concentration and flux components are measured by using the following time discrete norm

$$||u||_{\Delta t} = \left(\Delta t \sum_{i=0}^{N-1} ||u(t_n)||^2_{L^2(\Omega)} \right)^{\frac{1}{2}}$$

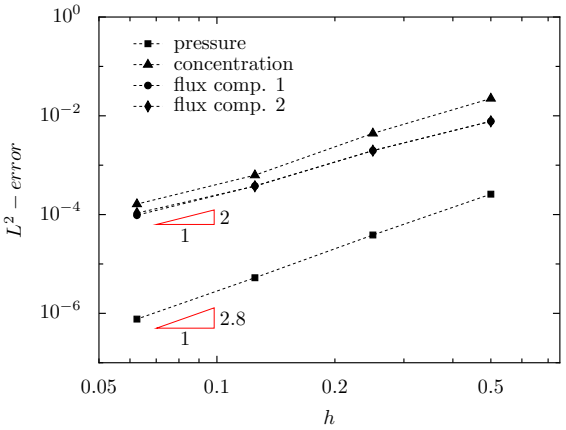
that us just the discrete analogue (by application of the rectangle quadrature rule in time) of the standard norm in $L^2([0,T], L^2(\Omega))$. The errors are defined using reference solutions obtained with $\Delta t = 10^{-5}$ and $h = 0.03125$.

In Figure 1 we plot the error measure in the $\|\cdot\|_{\Delta t}$ norm associated with several simulations. All of the numerical results are computed with piecewise linear, quadratic finite elements or with a mix of both types of elements. The results show that the numerical error decays with unexpected convergence orders. Indeed, it does not seem clear what is the dependence of the numerical convergence orders with respect to the degree of the polynomial approximation spaces used.

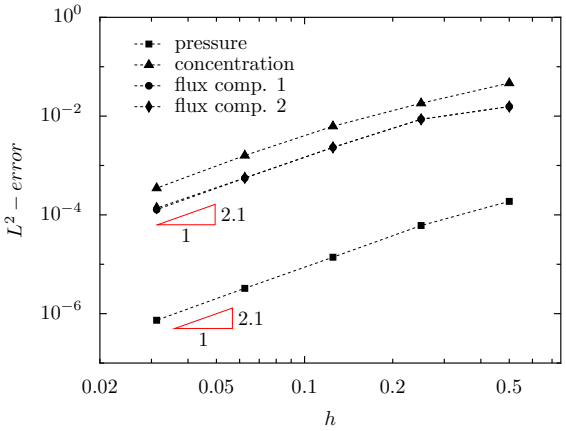
4.2. Qualitative behaviour. Let us consider a numerical example to illustrate the difference in behaviour between the fickian and nonfickian regimes. We assume the following parameters: Ω and $\mu(c)$ are the same as in the previous example, $p^o = 0$, $\phi^o = 0.3$, $c_R = 10^{-7}$, $D_m = 10^{-6}$, $d_l = 4 \cdot 10^{-3}$ and $d_t = 2 \cdot 10^{-3}$. We consider that the medium is isotropic and take the diagonal



(A) Piecewise linear elements



(B) Piecewise quadratic elements



(C) Piecewise linear elements for concentration and flux and piecewise quadratic elements for the pressure

FIGURE 1. L^2-norm error results for $T = 0.1$, time step $\Delta t = 10^{-5}$.

components of the permeability tensor $\mathbf{K} = (k_{ij})_{i,j=1,2}$ as

$$k_{11} = k_{22} = \frac{1}{2}\left(\left(\frac{1-10^{-7}}{2}\right)(\sin(6\cos(x_1)\pi)\cos(4\pi\sin(3x_2)) - 1) + 1\right).$$

The permeability behaviour is illustrated in Figure 2.

As boundary conditions, we use for the concentration $c(\mathbf{x}, t) = 4(1-x_2)x_2$, $\forall \mathbf{x} \in \Gamma_{D,c}$, where $\Gamma_{D,c}$ denotes the left side of the square, and $\mathbf{J} \cdot \mathbf{n} = 0$ on $\partial\Omega \backslash \Gamma_{D,c}$. Defined by $\Gamma_{D,p}$ the union of the left and right sides of the square Ω, we use $p(\mathbf{x}, t) = 1$ on the left side of the square and $p(\mathbf{x}, t) = 0$ on the right side of the square and homogeneous Neumann boundary conditions for the

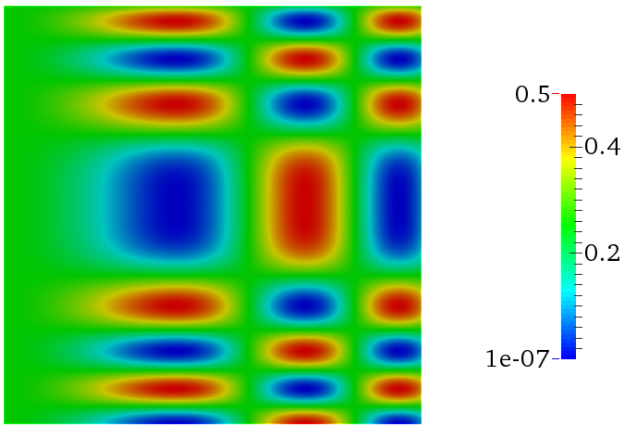


FIGURE 2. The $\|\cdot\|_\infty$ norm of the permeability tensor.

pressure on $\Gamma_{N,p} = \partial\Omega \backslash \Gamma_{D,p}$. The initial profile for the flux and concentration is zero while the initial pressure field is given by

$$p(\mathbf{x}, 0) = 1 - x_1, \ \forall \mathbf{x} \in \Omega.$$

Integrating over $[0, 0.5]$ with $\Delta t = 10^{-3}$ and $h = 0.01$, the pressure (and velocity) remains essentially the same throughout the process. The concentration and the flux, however, exhibit changes, due to convection and diffusion phenomena.

Since the system of equations to solve has with these parameters two equations dominated by convection phenomena, it is necessary to use stabilisation techniques. To accomplish this, the interior penalty method is used for the concentration and mass flux equations. This means that the terms

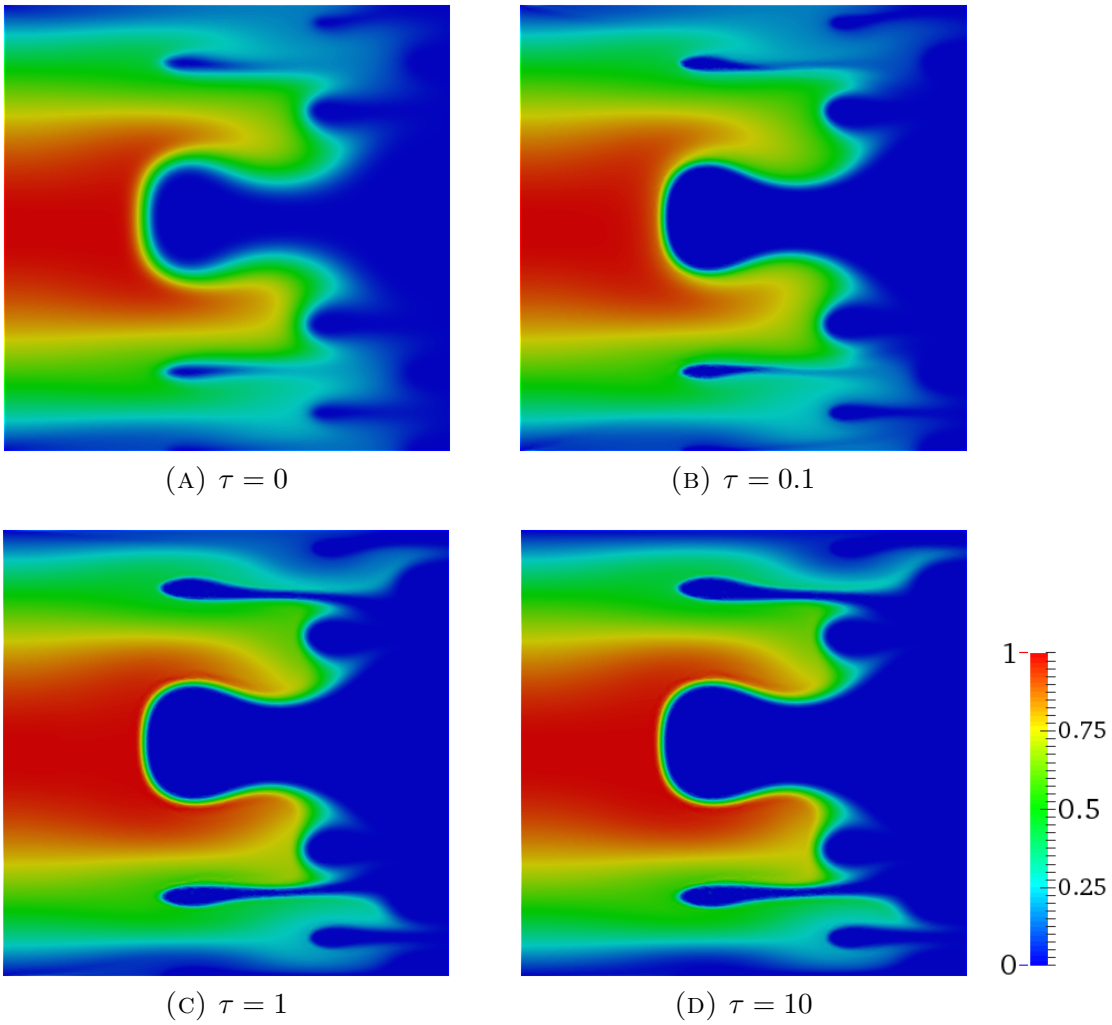
$$j_1(c_{n+1}, v_h; \mathbf{v}_n) := \gamma \sum_{F \in \mathcal{F}_I} \int_F h_F^2 |\mathbf{v}_n \cdot \mathbf{n}| [\![\boldsymbol{\nabla} c_{n+1}]\!]_F \cdot [\![\boldsymbol{\nabla} v_h]\!]_F \, ds, \ \forall v_h \in \mathbf{V}_h^{k,0,D,c}, \tag{31}$$

and

$$j_2(\mathbf{J}_{n+1}, \mathbf{w}_h; \mathbf{v}_n) := \gamma \sum_{F \in \mathcal{F}_I} \int_F h_F^2 |\mathbf{v}_n \cdot \mathbf{n}| [\![\boldsymbol{\nabla} \mathbf{J}_{n+1}]\!]_F \cdot [\![\boldsymbol{\nabla} \mathbf{w}_h]\!]_F \, ds, \ \forall \mathbf{w}_h \in V_h^k \times V_h^k, \tag{32}$$

are added to (27) and (28) and properly discretised. In (31),(32), $\mathcal{F}_I$ denotes the set of interior edges of the triangulation $\mathcal{T}_h$, $[\![\cdot]\!]_F$ denotes the usual jump function across the edge F, h_F is the length of edge F and $\gamma > 0$ is a stabilisation parameter. In all the following simulations, the stabilisation parameter used is $\gamma = 0.01$.

We plot in Figure 3 the concentration profiles at time $t = 0.5$. It is observed that the main difference (with increasing τ) is the increase of the steepness of the concentration front. This indicates that, for nonzero τ, the concentration front advancing on the domain, diffuses less than in the fickian case (Figure 3a). This behaviour is in agreement with the expected finite propagation



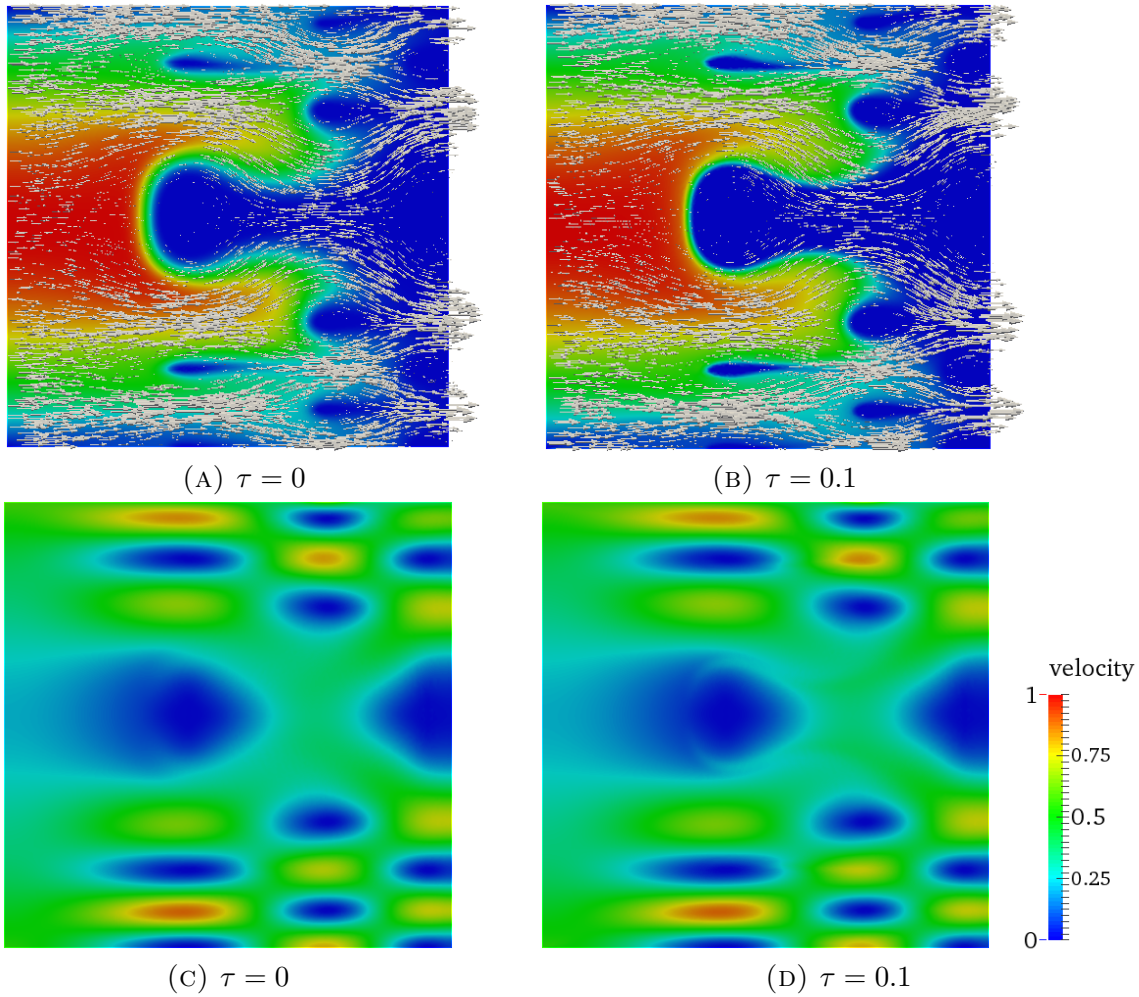
(A) $\tau = 0$ (B) $\tau = 0.1$

(C) $\tau = 1$ (D) $\tau = 10$

FIGURE 3. Concentration profiles for $t = 0.5$ using a time step $\Delta t = 10^{-3}$ and space step $h = 0.01$.

speed for the concentration.

In Figure 4 we plot the fickian and the nonfickian velocity fields at time $t = 0.5$ for $\tau = 0$ and $\tau = 0.1$ respectively. In the nonfickian case, the velocity field presents a steep variation in the front while a smoother behaviour is observed in the fickian case. This fact is consequence of the high variation of the concentration in the front that happens in the nonfickian case.



(A) $\tau = 0$ (B) $\tau = 0.1$

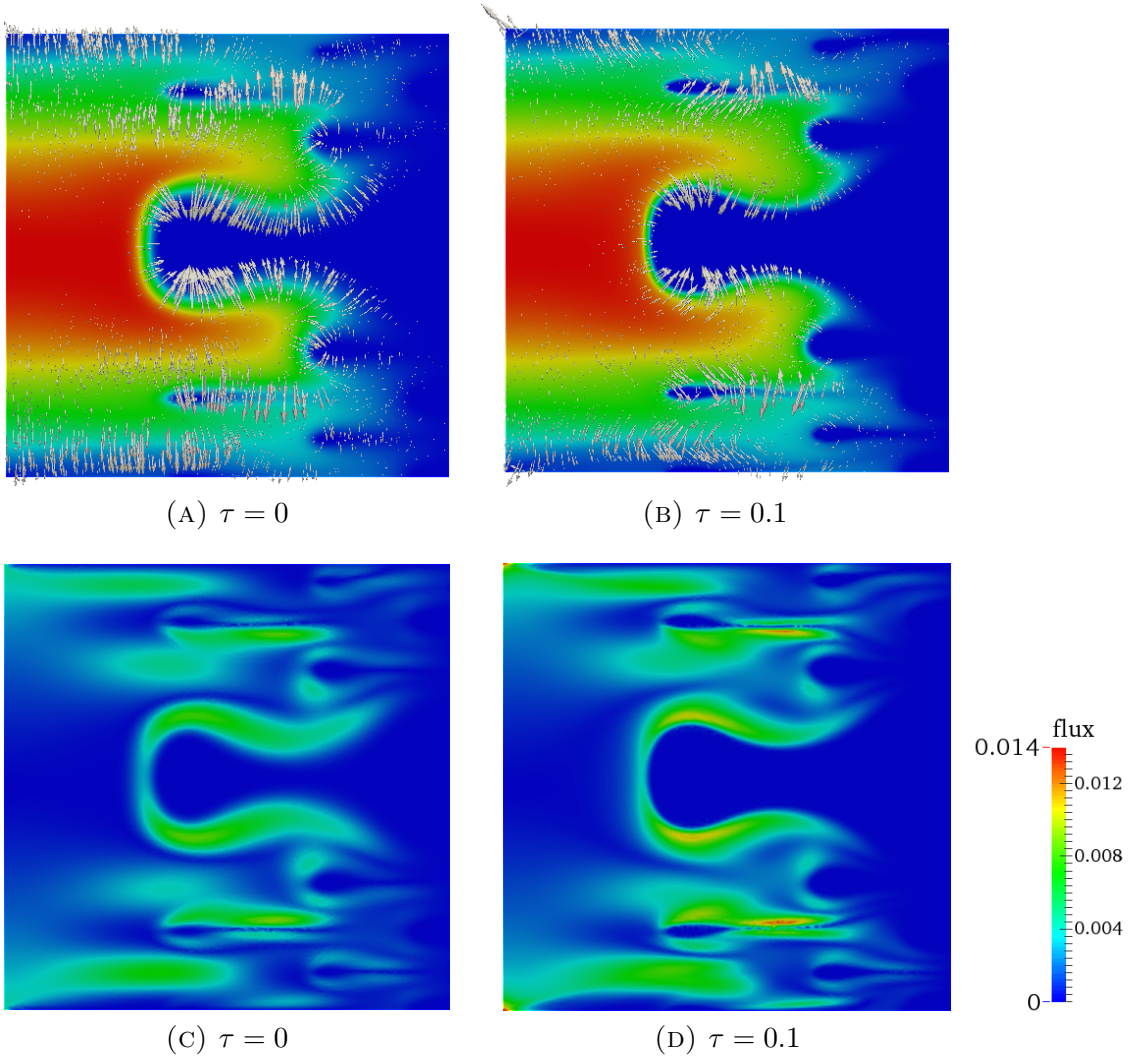
(C) $\tau = 0$ (D) $\tau = 0.1$

FIGURE 4. Concentration profiles and velocity fields ((a),(b)), magnitude of the velocity field ((c),(d)) for $t = 0.5$ using a time step $\Delta t = 10^{-3}$ and space step $h = 0.01$.

In Figure 5 the fickian and nonfickian mass flux fields at time $t = 0.5$ are plotted. In presence of memory in time and space effects, a delayed distribution of the mass fluxes is observed. Also, their magnitude is higher in the regions where the concentration presents steep gradients.

5. Conclusions

In this paper we presented a mathematical model to describe a diffusion process in porous media when the mass flux of the fluid at a specified point depends on the concentration behaviour in a spatial neighborhood and at past times. The model is presented highlighting the main differences with



(A) $\tau = 0$ (B) $\tau = 0.1$

(C) $\tau = 0$ (D) $\tau = 0.1$

FIGURE 5. Concentration profiles and mass flux fields ((a), (b)), magnitude of flux field ((c),(d)) for $t = 0.5$ using a time step $\Delta t = 10^{-3}$ and space step $h = 0.01$.

several models described in the literature. The model can be used to study the evolution of the concentration of an injected fluid in a resident fluid in a porous medium when they are completely mixed and they flow together as one fluid. Traditionally the mass flux of the injected fluid is described by Fick's law. However, to take into account its evolution when a space and time memory effects are presented, Fick's law is replaced by a partial differential equation for the mass flux that is coupled with a mass conservation law and with Darcy's law for the velocity. To simulate the behaviour of this system a IMEX finite element method is proposed which is coupled with a stabilisation

techniques when the problem is dominated by convection. The convergence properties of the method are numerically studied and the behaviour of the concentration, mass flux and velocity are illustrated and compared with the fickian one.

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