

# 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 is established assuming that this quantity at a certain point and at a certain time, depend on the concentration gradient in neighbour points (both in time and space). In order to numerical validate this approach, an IMEX finite element method is proposed to solve the coupled system of equations. The qualitative behaviour of the physical unknowns is illustrated and its dependence on the memory effect is discussed.

## 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

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

where  $\rho, \phi, q$  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

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

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

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

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. In this paper, we represent vectorial and tensorial variables in bold and adopt the notation  $\operatorname{div}(\mathbf{v})$  to represent the divergence operator of the vector variable  $\mathbf{v}$ .

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

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

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

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

with the diffusion-dispersion tensor  $\mathbf{D}(\mathbf{v})$ , see [1], that is defined by

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

where  $\|\mathbf{v}\|$  is the magnitude of the velocity,  $D_m$  is the molecular diffusion coefficient, and  $d_t$ ,  $d_\ell$  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 [2], 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 [3, 4, 5, 6, 7, 2] 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 physically unacceptable [8]. Another objection to (5), observed in [8], 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  $\nabla c$  that includes additional terms. This problem was also observed when high pressure gradients are present [9, 10, 11]. Several approaches have been considered in the literature to overcome these objections to use (5). We mention, without being exhaustive, the papers [12, 13, 14, 9, 15, 16, 8, 17, 11, 18, 19, 20, 21, 22, 23].

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, both for one and two dimensional problems. 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

The model for diffusion in porous media proposed in this paper sits upon two fundamental principles: the first, to use Darcy's law and the fluid's mass conservation to describe the velocity of the fluid; the second, to couple this equation with another for the evolution of the concentration

that can accommodate the nonfickian behaviour of the solute's mass flux. The main reason behind such choice is that there is experimental evidence that Fick's law no longer applies in this context (a particular case where this happens, which is documented in the literature, is tracer transport in porous media), see [24, 25, 26], and alternative models, such as the one derived in [8] from basic principles, seem better suited for this description. It was also shown that simpler models for the evolution of the concentration, as we shall describe in section 2.1, provide more promising results, as it is shown in the work [27].

## 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

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

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 [12, 13, 14, 15, 16, 17, 19]. Numerical methods for initial values problems defined by (7) were largely studied and a huge collection of methods is now available, see for example [28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41].

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

$$\mathbf{J} = \mathbf{J}_m + \mathbf{J}_d \quad (8)$$

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

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

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

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

Equation (9) was proposed in [19] 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

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

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

$$\frac{\partial}{\partial t}(\phi \rho c) + \text{div}(\rho c \mathbf{v}) = \text{div}(\phi D_m \nabla c) + \int_0^t e^{-\mathbf{A}^{-1}(t-s)} \cdot \text{div}(\mathbf{A}^{-1} \cdot \mathbf{D}_{dis}(\mathbf{v}) \cdot \nabla c(s)) ds + qc^* \text{ in } \Omega \times (0, T]$$

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

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

that describes then the memory effect in time of a nonlocal approach, see [19]. A second order differential equation in time and space was also obtained in [19], 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, [8] introduced the following equation for the mass flux

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

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

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

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

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

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 [42], 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 [21, 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

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

where

$$\mathbf{s} = -\boldsymbol{\eta} \cdot \mathbf{J}_d, \quad (14)$$

$D_m$  is the usual molecular diffusion coefficient, and

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

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

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

As pointed out in [8], 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

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

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

In real world applications, the parameter  $\tau$  can assume a wide range of values. For instance, in [27], the values of  $\tau$  range from 67 to 383 in the context of tracer transport in porous media. In other examples, the authors consider  $\tau$  much smaller, in the context of diffusion in polymers, for example. Since the parameter  $\tau$  can assume such a wide range of values, to illustrate numerically the behaviour of the concentration profile for increasing values of  $\tau$ , we shall consider set of representatives with different orders of magnitude, see section 4.1.2.

In this scenario, the porosity  $\phi$  can be either known or calculated by using a constitutive law, as done in [7]. 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

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

where  $c_R$  denotes the rock compressibility constant of the medium,  $p^o$  is a reference pressure and  $\phi^o$  is the reference porosity (see [43]).

In the context of porous media, it is common, see [2], to consider a viscosity  $\mu$  dependent on the concentration through the standard quarter power law

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

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  $\Gamma_{D,p}$

$$p = p_D \quad \text{on} \quad \Gamma_{D,p}, \quad (18)$$

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

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

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

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

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

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

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

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

### 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  $\Gamma$  of  $\partial\Omega$ ,  $H^1_\Gamma(\Omega)$  denotes the space of  $H^1(\Omega)$  of functions that have zero trace on  $\Gamma$ . 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

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

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

and

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

such that

$$\left( \frac{\partial}{\partial t} \phi(p(t)), w_1 \right) + \left( \frac{1}{\mu(c(t))} \mathbf{K} \cdot \nabla p(t), \nabla w_1 \right) = (q, w_1), \quad \forall w_1 \in H^1_{\Gamma_{D,p}}(\Omega), \quad (22)$$

$$\left( \frac{\partial}{\partial t} (\phi(t)c(t)), w_2 \right) + (\mathbf{v}(t) \cdot \nabla c(t), w_2) - (\mathbf{J}(t), \nabla w_2) = (f(c(t)), w_2), \quad \forall w_2 \in H^1_{\Gamma_{D,c}}(\Omega), \quad (23)$$

$$\left( \tau \frac{\partial \mathbf{J}}{\partial t}(t) + \mathbf{D}(\mathbf{v}(t)) \cdot \nabla c(t) + \tau \nabla \mathbf{v}(t) \cdot \mathbf{J}(t) + \tau \nabla \mathbf{J}(t) \cdot \mathbf{v}(t) + \mathbf{J}(t), \mathbf{w}_3 \right) = 0, \forall \mathbf{w}_3 \in H^1(\Omega) \times H^1(\Omega). \quad (24)$$

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  $\Omega$ . We introduce the finite-elements space

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

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

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

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

and

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

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  $v_h \in V_h^{k,0,D,p}$

$$\left( \frac{d\phi}{dp}(p_n) p_{n+1}, v_h \right) + \Delta t \left( \frac{\mathbf{K}}{\mu(c_n)} \cdot \nabla p_{n+1}, \nabla v_h \right) = \Delta t (q_{n+1}, v_h) + \left( \frac{d\phi}{dp}(p_n) p_n, v_h \right). \quad (25)$$

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

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

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

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

and

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

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  $\{\varphi_l^J\}_{l=1,\dots,N_J}$  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

$$p_{n+1} = \sum_{i=1,\dots,N_p} \alpha_i^p \varphi_i^p, \quad c_{n+1} = \sum_{j=1,\dots,N_c} \beta_j^c \varphi_j^c, \quad \mathbf{J}_{n+1} = \sum_{l=1,\dots,N_J} \gamma_l^J \varphi_l^J.$$

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

$$M_{n+1}P_{n+1} = F_{p,n+1} \quad (29)$$

and

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

where

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

We remark the 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 stem 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), both in a one and two-dimensional framework.

### 4.1 Two-dimensional case

The numerical results obtained in this section are obtained make the following assumptions (unless stated otherwise):  $\Omega = [0, 1]^2$ ,  $f = q = 0$ ,  $\phi(\mathbf{x}, t) = e^{p(\mathbf{x}, t)}$ ,  $\mu(c) = \frac{1}{((1-M)c+M)^4}$  (where  $M = 0.5^{-0.25}$ , using  $\mu_S = 1$  and  $\mu_0 = 0.5$  in (17)).



### 4.1.1 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  $p(\mathbf{x}, 0) = x_1 x_2 (x_1 - 1)(x_2 - 1)$ , 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  $\Gamma_{D,c} = \partial\Omega \setminus \Gamma_{N,c}$ .

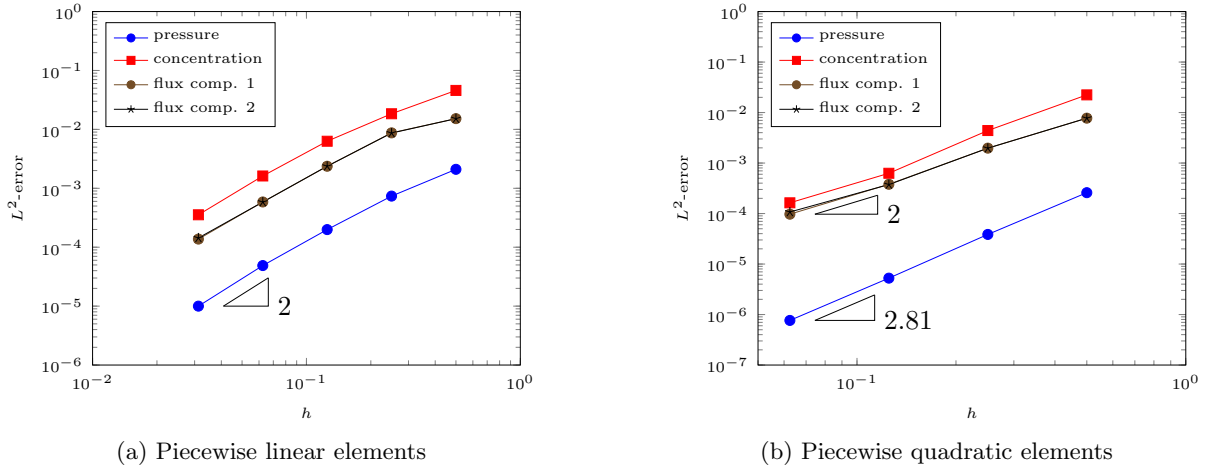


Figure 1:  $L^2$ -norm error results for  $T = 0.1$ , time step  $\Delta t = 10^{-5}$ .

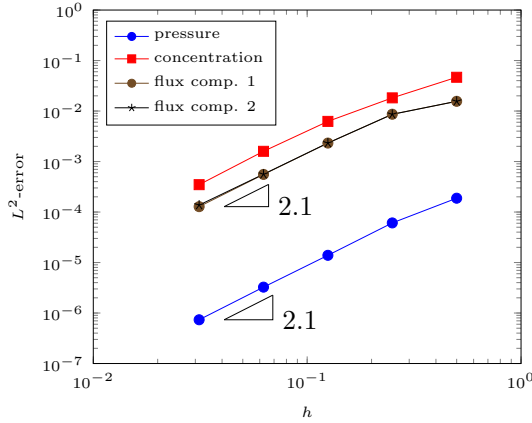


Figure 2:  $L^2$ -norm error results for  $T = 0.1$ , time step  $\Delta t = 10^{-5}$  (piecewise linear elements for concentration and flux and piecewise quadratic elements for the pressure).

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

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

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 Figures 1-2 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.

#### 4.1.2 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:  $\Omega$  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 components of the permeability

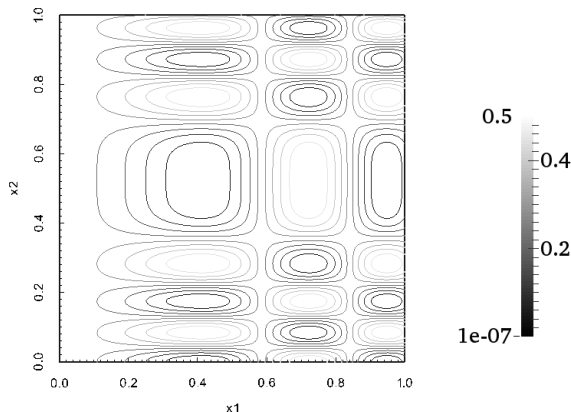


Figure 3: The  $\|\cdot\|_{\infty}$  norm of the permeability tensor.

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 3.

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  $\partial\Omega \setminus \Gamma_{D,c}$ . Defined by  $\Gamma_{D,p}$  the union of the left and right sides of the square  $\Omega$ , 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 pressure on  $\Gamma_{N,p} = \partial\Omega \setminus \Gamma_{D,p}$ . 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.

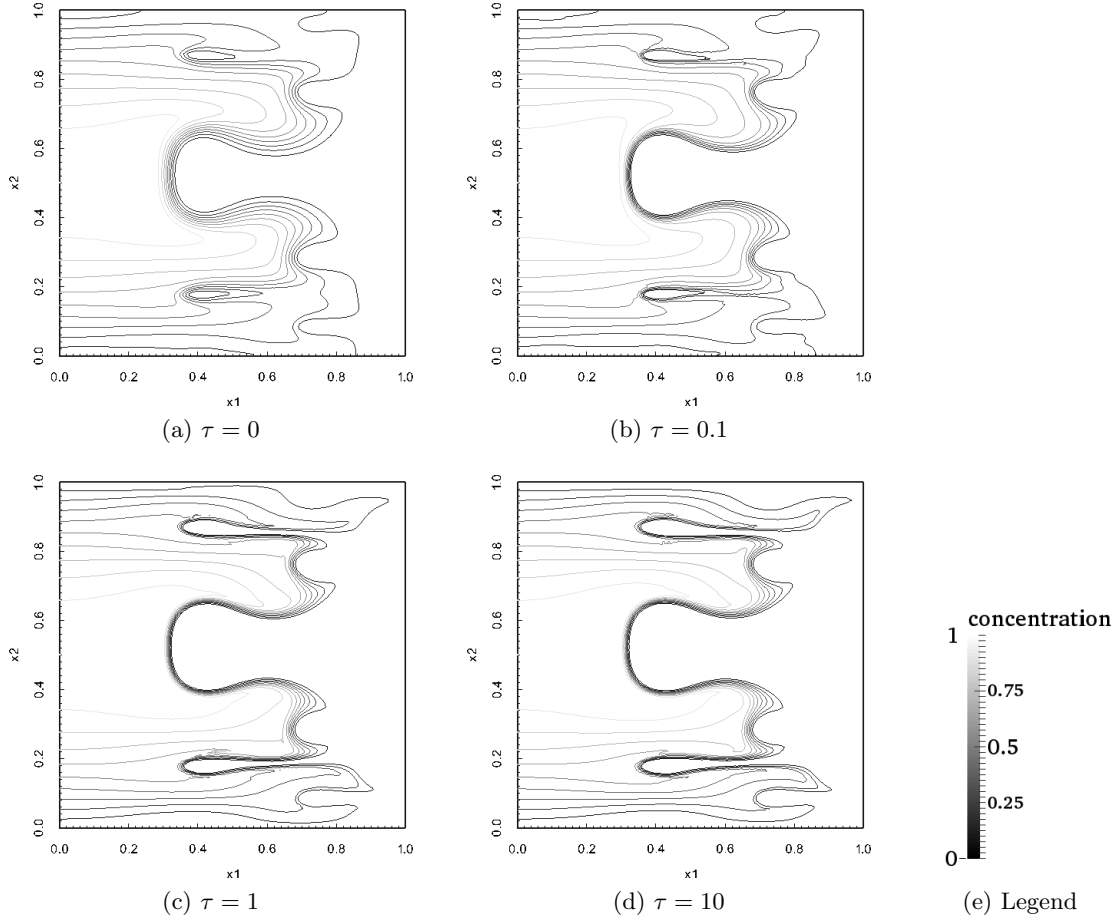


Figure 4: Concentration profiles for  $t = 0.5$  using a time step  $\Delta t = 10^{-3}$  and space step  $h = 0.01$ .

Since the system of equations to solve has 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

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

and

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

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 4 the concentration profiles at time  $t = 0.5$ . It is observed that the main difference (with increasing  $\tau$ ) is the increase of the steepness of the concentration front. This indicates that, for nonzero  $\tau$ , the concentration front advancing on the domain, diffuses less than in the fickian case (Figure 4a). This behaviour is in agreement with the expected finite propagation speed for the concentration.

In Figure 5 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.

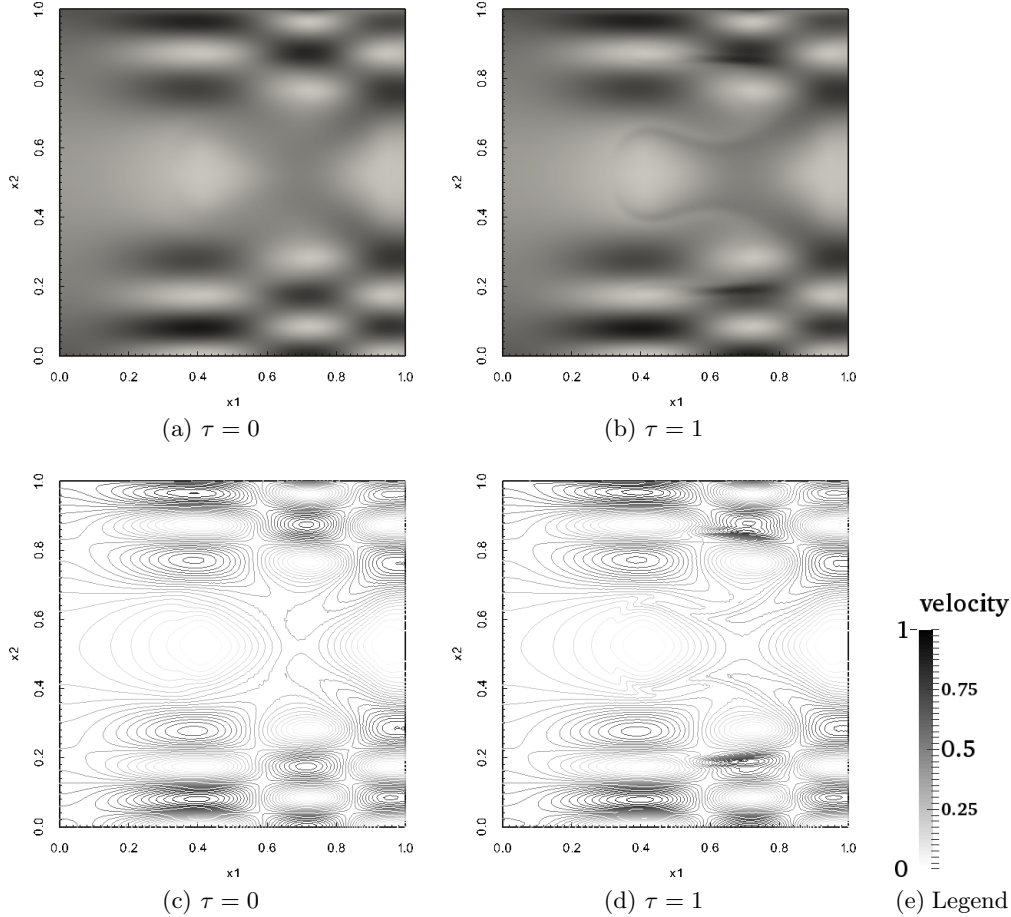


Figure 5: Magnitude of the velocity field profiles ((a),(b)) and contour plots ((c),(d)) for  $t = 0.5$  using a time step  $\Delta t = 10^{-3}$  and space step  $h = 0.01$ .

In Figure 6 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.

## 4.2 One-dimensional (simpler) case: qualitative behaviour

The conclusions drawn from the previous example regarding the qualitative behaviour of the numerical solution, in respect to the increase of the  $\tau$  parameter, can be further illustrated with a simpler one dimensional problem. We rewriting the previous numerical method in a one dimensional simpler setting and perform similar numerical experiments as in section 4.1.2. We consider now the following parameters (we drop the bold notation, since all quantities are scalar):  $\Omega = (0, 1)$ ,  $T = 0.2$ ,  $\mu = 1$ ,  $K = 10^{-3}$ ,  $D = 1$ ,  $p^o = 0$ ,  $\phi^o = 0.3$ ,  $c_R = 10^{-7}$ . The system of equations has initial conditions  $c(x, t) = 0$ ,  $p(x, t) = 1 - x$ ,  $J(x, t) = 0$ , and boundary

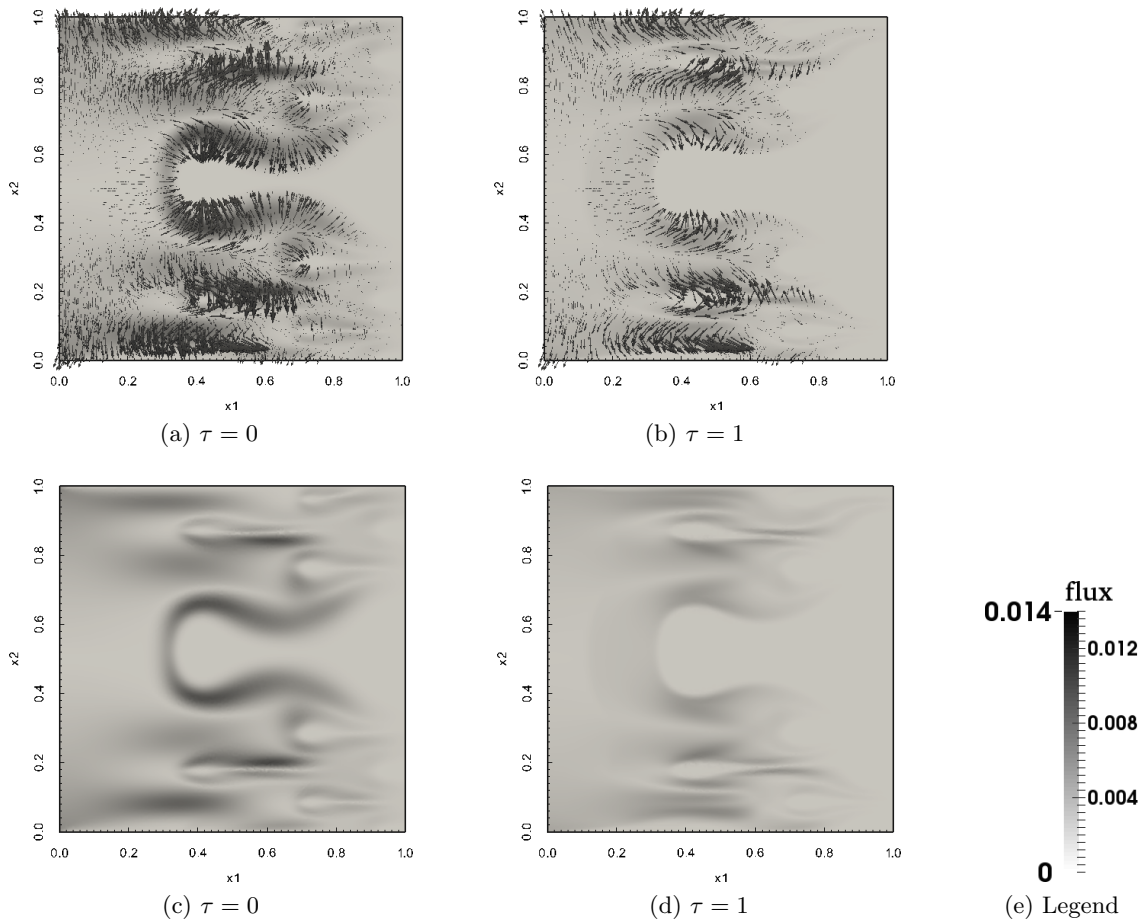


Figure 6: Plots of mass flux field ((a),(b)) and magnitude of the mass flux field ((c),(d)) for  $t = 0.5$  using a time step  $\Delta t = 10^{-3}$  and space step  $h = 0.01$ .

conditions  $p(0, t) = 1$ ,  $p(1, t) = 0$ ,

$$c(0, t) = \frac{4t}{T} H\left(\frac{T}{4} - t\right) + H\left(t - \frac{T}{4}\right)$$

and  $J(1, t) = 0$ ,  $t \in [0, 0.2]$ . The function  $H$  denotes the Heaviside function.

The numerical solution of the previous problem has a constant velocity field. This choice is made with the purpose of decreasing the complexity involved in the simulation, thus allowing to grasp the dependence of the concentration on  $\tau$ .

We plot in Figure 7 the concentration profile, for several values of  $t$  and different values of  $\tau$ . As in the two dimensional case, increasing  $\tau$  delays the evolution of the concentration front entering the domain, especially when comparing with the pure fickian regime. It is also visible that the front is sharper for increasing values of  $\tau$ , which is a standard behaviour with nonfickian diffusion. These results are in agreement with the discussion in [44].

## 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 neighbourhood and at past times. The model is presented highlighting the main differences with 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. This approach for the mass flux is motivated by experimental results that show that Fick's law no longer holds for certain contexts. 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 show that this tool can be used to accurately simulate the system's dynamics. From the numerical simulation, as expected, we observe that diffusion processes in media with strong memory properties (both in time and space) lead to concentration's moving fronts presenting steep gradients. This is observed both in the (simple) one-dimensional case study, as well as in the two-dimensional one.

## 6 Acknowledgements

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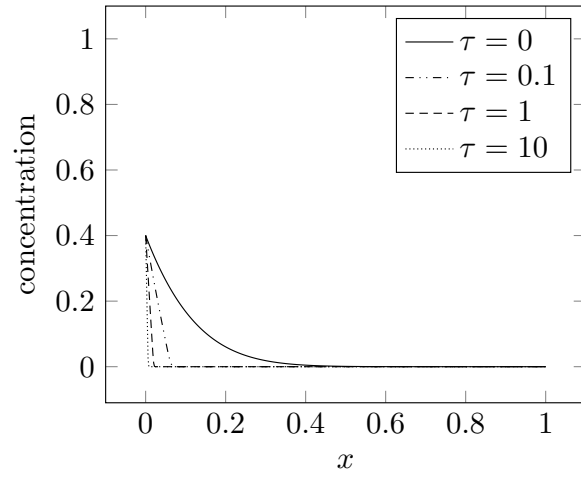
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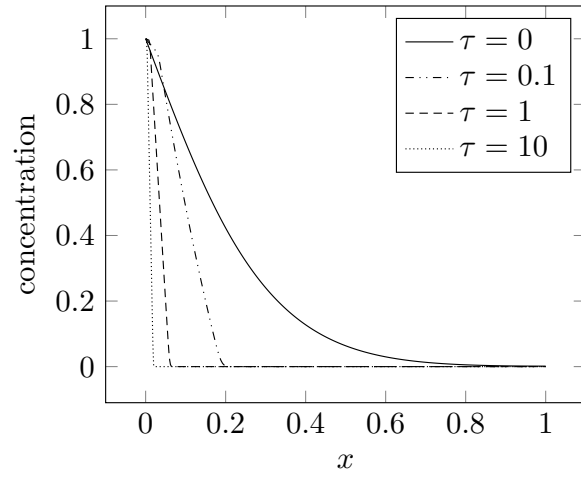
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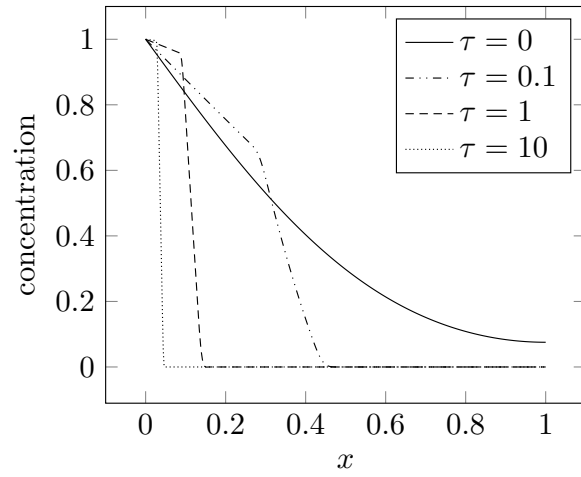
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(a)  $t = 0.02$



(b)  $t = 0.06$



(c)  $t = 0.14$

