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MEMORY EFFECT IN TIME AND SPACE IN NON FICKIAN DIFFUSION PHENOMENA

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ABSTRACT: Usually diffusion processes are simulated using the classical diffusion equation. In certain scenarios such equation induces anomalous behavior and consequently several improvements were introduced in the literature to overcome them. One of the most popular was the replacement of the diffusion equation by an integro-differential equation. Such equation can be established considering a modification of Fick's mass flux where a delay in time is introduced. In this paper we consider mathematical models for diffusion processes that take into account a memory effect in time and space.

KEYWORDS: Diffusion equation, Fick's law, parabolic equation, infinite speed, integro-differential equation, coupled problem, concentration, mass flux.

1. Introduction

The diffusion process is usually simulated using the classical diffusion equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \nabla \cdot (\mathbf{D}_F \nabla c) = f \text{ in } \Omega \times (0, T], \tag{1}$$

where c denotes the concentration of a solute, $\mathbf{v}$ and $\mathbf{D}_F$ represent, respectively, the velocity field and the diffusion tensor, $\Omega \subset \mathbb{R}^n$, and f denotes a source term. Throughout the paper, the velocity $\mathbf{v}$ is assumed constant in space and time. Equation (1) is established using the mass conservation law

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J}_{total} = f, \tag{2}$$

where the total mass flux $\mathbf{J}_{total}$ is split into $\mathbf{J}_{total} = \mathbf{J}_a + \mathbf{J}_F$, with $\mathbf{J}_a$ being the advection flux

$$\mathbf{J}_a = \mathbf{v}c, \tag{3}$$

and $\mathbf{J}_F$ is given by Fick's law

$$\mathbf{J}_F = -\mathbf{D}_F \nabla c. \tag{4}$$

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For instance, when diffusion processes occur in porous media, the diffusion tensor is replaced by

$$\mathbf{D}_F = \mathbf{D}_m\mathbf{I} + \mathbf{D}_d \tag{5}$$

where $\mathbf{D}_m$ is associated with molecular diffusion and $\mathbf{D}_d$ represents the dispersive tensor that depends on the velocity $\mathbf{v}$. It was observed in this case that (1) gives accurate results in laboratory environments for perfectly homogeneous media and a deviation of Fickian behaviour is presented when nonhomogeneous media are used (see for instance [6], [10], [9]). Fick's law also does not reproduce flux behavior in diffusion in biological tissues or polymeric materials. Indeed, it has been observed in this case that the flux at a certain time t depends on the gradient of the concentration at a previous instant $t-\tau$ (see [3]).

However, the main limitation induced by (1) is the infinite propagation speed which is associated with its parabolic character.

To overcome the deviations observed when (1) is used, several approaches have been introduced in the literature (see [10] for some examples). In this paper we consider the use of differential equations for the mass flux $\mathbf{J}_{total}$ or for $\mathbf{J}_F$ that replace Fick's law (4). We shall see that this induces a memory effect in time or in time and space.

The paper is organized as follows. In Section 2 we introduce the differential model that we intent to study in this paper and derive, under suitable regularity conditions, equivalent formulations. In Section 3, we obtain energy estimates for the formulations introduced in Section 2. Finally, in Section 4, we simulate the evolution of the coupled model and illustrate the different behavior of the variables.

2. Memory in time and space

In this paper we study the following model

$$\frac{\partial c}{\partial t} + \nabla\cdot(\mathbf{v}c) - \nabla\cdot(\mathbf{D}_F\nabla c) + \nabla\cdot\mathbf{J} = f, \text{ in } \Omega\times(0,T] \tag{6}$$

$$\tau\frac{\partial \mathbf{J}}{\partial t} + \tau(\mathbf{v}_\mathbf{J}\cdot\nabla)\mathbf{J} + \mathbf{J} = -\mathbf{D}_{nF}\nabla c, \text{ in } \Omega\times(0,T] \tag{7}$$

to govern the evolution of c on a domain Ω over time. In (6)-(7), $\mathbf{v}_\mathbf{J}$ is the *non Fickian flux velocity* and is assumed constant in time and space, $\mathbf{D}_F$ and $\mathbf{D}_{nF}$ are assumed real symmetric positive definite matrices with a lower positive bound α_F and α_{nF}, respectively. Furthermore, we assume that all entries of these tensors are $L^\infty(\Omega)$ functions.

This system is complemented with initial data

$$c(\mathbf{x},0)=c_0(\mathbf{x}) \text{ and } \mathbf{J}(\mathbf{x},0)=\mathbf{J}_0(\mathbf{x}), \mathbf{x}\in\Omega.$$

Regarding boundary conditions, let us first introduce a disjoint decomposition of the boundary: $\partial\Omega=\partial\Omega^+\cup\partial\Omega^-$, where

$$\partial\Omega^-=\{\mathbf{x}\in\partial\Omega:\ \mathbf{v_J}\cdot\mathbf{n}(\mathbf{x})<0\}$$

and $\mathbf{n}(\mathbf{x})$ represents the unit outer normal vector at $\mathbf{x}\in\partial\Omega$.

We complement (6)-(7) with the following boundary conditions:

$$\frac{\partial c}{\partial \mathbf{n}}=0 \text{ on } \partial\Omega^-, \quad c=0 \text{ on } \partial\Omega^+$$

and

$$\mathbf{J}=\mathbf{0} \text{ on } \partial\Omega^-.$$

Remark 1. *The coupled system* (6)-(7) *comprises three components for the mass flux: the advective mass flux, the Fickian mass flux (modeling, for instance, the molecular mass flux) and a non Fickian component (through* (7)*). The* total mass flux *admits the representation*

$$\mathbf{J}_{total}=\mathbf{v}c-\mathbf{D}_F\nabla c+\mathbf{J}.$$

It is clear that if $\tau=0$, (6)-(7) *is equivalent to* (1)*. However, when $\tau>0$, the term $\nabla\cdot\mathbf{J}$ in* (6)*, induces a different flux for this variable.*

Equation (7) has already been proposed in the literature in the context of porous media. In fact, Strack [15] and Tompson [17] proposed a similar equation to model the dispersive mass flux in a porous media. These contributions did not include the convective term $\tau(\mathbf{v_J}\cdot\nabla)\mathbf{J}$ although such a model had already been proposed by Scheidegger [13]. We point the reader to Hassanizadeh [6] for an overview on these models.

In order to understand and study the diffusion process in a system like (6)-(7), we will now limit our analysis to the case $\mathbf{v}=\mathbf{0}$.

We can follow two approaches to derive, under certain regularity conditions, equivalent formulations of (6)-(7) that will be detailed in the next sections.

2.1. Integro-differential formulation. Using the method of characteristics in (7) we obtain for the dispersion mass flux the following expression

$$\mathbf{J}(\mathbf{x},t) = e^{-\frac{t}{\tau}}\mathbf{J}(\mathbf{x},0) - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}}\mathbf{D}_{nF}\nabla c(\mathbf{x}+\mathbf{v_J}(s-t),s)\,ds \tag{8}$$

valid for $(\mathbf{x},t)\in\Omega^*$ where

$$\Omega^* = \{x\in\Omega:\ \mathbf{x}-t\mathbf{v_J}\in\Omega\}\,.$$

A similar expression can be deduced in the case $\mathbf{x}-t\mathbf{v_J}\in\partial\Omega$.

Equation (7) can be obtained also from

$$\mathbf{J}(\mathbf{x}+\tau\mathbf{v_J},t+\tau) = -\mathbf{D}_{nF}\nabla c(\mathbf{x},t) \tag{9}$$

neglecting second order terms in a convenient Taylor's expansion. Equation (9) reflects the memory effect in space and time: the mass flux at $\mathbf{x}+\tau\mathbf{v_J}$ at time $t+\tau$ is related with the gradient of the concentration at a delayed position $\mathbf{x}$ and at a delayed time t.

From equation (6) and (8) we obtain the following integro-differential equation,

$$\begin{aligned}\frac{\partial c}{\partial t} - \nabla\cdot(\mathbf{D}_F\nabla c) + \nabla\cdot\mathbf{J}(0)e^{-\frac{t}{\tau}}&\\ -\frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}}\nabla\cdot(\mathbf{D}_{nF}\nabla c(\mathbf{x}+\mathbf{v_J}(s-t),s))\,ds &= f \ \text{ in } \Omega^*\times(0,T],\end{aligned} \tag{10}$$

which requires smoothness on $\mathbf{J}$ at $t=0$.

Remark 2. *We can observe from the presence of the integral in* (10) *the dependence of the total flux with respect to time and space. Indeed, if* $\mathbf{v_J}=\mathbf{0}$*, the total flux has a term involving the gradient of the concentration at all instants in* $(0,t)$*. In this case we say there is an effect of* memory in time *for the flux. However, if* $\mathbf{v_J}\neq\mathbf{0}$*, then the total flux will depend on the history of the gradient along a characteristic of the flux equation. In this case, we say the flux has* memory in time and space*.*

Remark 3. *While representation* (8) *is valid only on* Ω^* *if* $\mathbf{v_J}\neq\mathbf{0}$*, in the case* $\mathbf{v_J}=\mathbf{0}$ *and* $\tau>0$*, the characteristics cover the whole domain* $\Omega\times(0,T)$ *and* (10) *is valid over* $\Omega\times(0,T)$*.*

Remark 4. *The numerical simulation of (10) with a nonzero velocity* $\mathbf{v_J}$ *imposes several difficulties, namely, the requirement that all data from previous* *time levels be stored to approximate properly the integral, as well as the shift in the space variable in* ∇c.

The simpler case in which $\mathbf{v_J} = \mathbf{J}(0) = \mathbf{0}$ in equation (10) was largely studied from a mathematical point of view. Without being exhaustive, we mention [1], [4], [5], [7], [8], [11], [14] and [16].

2.2. Hyperbolic formulation. We establish in what follows an hyperbolic equation combining (6) with (7). From (7) we obtain

$$\nabla \cdot \mathbf{J} = -\frac{\partial c}{\partial t} + \nabla \cdot (D_F \nabla c) + f, \tag{11}$$

$$\nabla \cdot ((\mathbf{v_J} \cdot \nabla)\mathbf{J}) = -\mathbf{v_J} \cdot \nabla \frac{\partial c}{\partial t} + \mathbf{v_J} \cdot \nabla(\nabla \cdot (\mathbf{D}_F \nabla c)) + \mathbf{v_J} \cdot \nabla f, \tag{12}$$

and

$$\nabla \cdot \frac{\partial \mathbf{J}}{\partial t} = -\frac{\partial^2 c}{\partial t^2} + \nabla \cdot (\mathbf{D}_F \nabla \frac{\partial c}{\partial t}) + \frac{\partial f}{\partial t}. \tag{13}$$

Furthermore, from (7) we also have

$$\nabla \cdot \mathbf{J} + \tau \nabla \cdot \frac{\partial \mathbf{J}}{\partial t} + \tau \nabla \cdot ((\mathbf{v_J} \cdot \nabla)\mathbf{J}) = -\nabla \cdot (\mathbf{D}_{nF} \nabla c). \tag{14}$$

Replacing (11)-(13) in (14) we obtain the following third order hyperbolic equation with mixed derivatives

$$\begin{aligned} \frac{\partial^2 c}{\partial t^2} + \mathbf{v_J} \cdot \nabla \frac{\partial c}{\partial t} - \mathbf{v_J} \cdot \nabla(\nabla \cdot (\mathbf{D}_F \nabla c)) & \\ \frac{1}{\tau}\Big(\frac{\partial c}{\partial t} - \nabla \cdot ((\mathbf{D}_F + \tau \mathbf{D}_{nF})\nabla c)\Big) &= \frac{\partial f}{\partial t} + \mathbf{v_J} \cdot \nabla f + \frac{f}{\tau} \end{aligned} \tag{15}$$

in $\Omega \times (0, T]$. We point out that the establishment of (15) requires smooth data and it should be complemented with the initial conditions

$$\begin{cases} \dfrac{\partial c}{\partial t}(0) = -\nabla \cdot \mathbf{J}_0 + f(0) + \nabla \cdot (\mathbf{D}_F \nabla c_0) \\ c(0) = c_0 \end{cases} \quad \text{in } \Omega. \tag{16}$$

3. Energy estimates

In this section we focus on deducing energy estimates for the different equations introduced in the previous section.

Let us first introduce some notations, necessary for the following sections. 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 $H^1(\Omega)$ 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 $\mathbf{L}^2$.

Finally, given a space V as any of the ones introduces before, we define

$$L^2(0,T;V) = \left\{ u : (0,T) \longrightarrow L^2(\Omega) : \int_0^T \|u(s)\|_0^2 \, ds < \infty \right\}$$

and

$$H^1(0,T;V) = \left\{ u \in L^2(0,T;V) : \frac{\partial u}{\partial t} \in L^2(0,T;V) \right\}.$$

For vectorial functions, the definitions follow the same notation as for the scalar counterparts.

3.1. Fickian diffusion. For the case in which no memory in time and space is present in the model and $\mathbf{v} = 0$, we consider the following weak formulation: given $f \in L^2(0,T;L^2(\Omega))$ and $c_0 \in L^2(\Omega)$, find $c \in L^2\left(0,T;H^1_{\partial\Omega^+}(\Omega)\right)$ such that $\dfrac{\partial c}{\partial t} \in L^2(0,T;L^2(\Omega))$ such that

$$\left(\frac{\partial c}{\partial t}, v\right) + (\mathbf{D}_F \nabla c, \nabla v) = (f, v) \ \text{ a.e. in } (0,T), \quad \forall v \in H^1_{\partial\Omega^+}(\Omega). \tag{17}$$

For a concentration c satisfying (17), it is known that (see, for instance, [12])

Proposition 1. *If $c \in C(0,T;L^2(\Omega))$ then there exists $\varepsilon > 0$ such that*

$$\|c(t)\|_0^2 + \alpha_F \int_0^t \|\nabla c(s)\|_0^2 \, ds \leqslant \exp^{\epsilon t} \left(\|c(0)\|_0^2 + \frac{1}{\epsilon} \int_0^t \|f(s)\|_0^2 \exp^{-\epsilon s} \, ds \right).$$

3.2. Non-Fickian diffusion. In the case of the presence of non Fickian type diffusion, we analyze the two different models deduced in section 2: the integro-differential model (10) and the hyperbolic model (15).

3.2.1. *Integro-differential model.* For the integer-differential model, we consider the weak formulation: given $f \in L^2(0,T;L^2(\Omega))$ and $c_0 \in L^2(\Omega)$, find $c \in L^2\left(0,T;H^1_{\partial\Omega^+}(\Omega)\right)$ such that $\frac{\partial c}{\partial t} \in L^2(0,T;L^2(\Omega))$ and

$$\begin{aligned}&\left(\frac{\partial c}{\partial t}, v\right) + (\mathbf{D}_F \nabla c, \nabla v)\\ &+\frac{1}{\tau}\int_0^t \exp^{-\frac{t-s}{\tau}} (\mathbf{D}_{nF}\nabla c(s), \nabla v)\, ds = (f,v) \text{ a.e. in } (0,T), \quad \forall v \in H^1_{\partial\Omega^+}(\Omega)\end{aligned} \tag{18}$$

for which the following energy estimate holds (see [2]).

Proposition 2. *If $c \in C\left(0,T;L^2(\Omega)\right)$, then for $\epsilon > \tau$,*

$$\begin{aligned}\|c(t)\|_0^2 + \alpha_F \int_0^t \|\nabla c(s)\|_0^2\ ds + \frac{\alpha_{nF}}{\tau}\left\|\int_0^t \exp^{-\frac{t-s}{\tau}}\nabla c(s)\ ds\right\|_0^2 \\ \leqslant \exp^{\epsilon t}\|c(0)\|_0^2 + \frac{1}{\epsilon}\int_0^t \|f\|_0^2 \exp^{\epsilon(t-s)}\ ds\end{aligned} \tag{19}$$

Remark 5. *We highlight that if $\frac{\partial c}{\partial t} \in C^0(0,T;H^1_{\partial\Omega^+}(\Omega))$ then*

$$\frac{\alpha_{nF}}{\tau}\left\|\int_0^t \exp^{-\frac{t-s}{\tau}}\nabla c(s)\ ds\right\|_0^2 \longrightarrow \alpha_{nF}\|\nabla c(t)\|_0^2$$

showing that the term $\tau^{-1}\left\|\int_0^t \exp^{-\frac{t-s}{\tau}}\nabla c(s)\ ds\right\|_0^2$ can be seen a relaxation of $\|\nabla c(t)\|_0^2$. The proof of this result follows from the following equality and then taking the limit on both sides as τ tends to zero:

$$\begin{aligned}\frac{1}{\tau}\int_0^t \exp^{-\frac{t-s}{\tau}}\nabla c(s)\ ds &= \frac{1}{\tau}\left[\frac{\exp^{-\frac{t-s}{\tau}}}{\frac{1}{\tau}}\nabla c(s)\right]_0^t - \frac{1}{\tau}\int_0^t \frac{\exp^{-\frac{t-s}{\tau}}}{\frac{1}{\tau}}\nabla\frac{\partial c}{\partial t}(s)\ ds\\ &= \nabla c(t) - \exp^{-\frac{t}{\tau}}\nabla c(0) - \int_0^t \exp^{-\frac{t-s}{\tau}}\nabla\frac{\partial c}{\partial t}(s)\ ds.\end{aligned}$$

3.2.2. *Hyperbolic model.* We now turn to analyze an energy estimate for equation (15). In order to simplify the derivation of such estimate, we consider the simpler case in which no Fickian component is present, i.e., $\mathbf{D}_F \equiv \mathbf{0}$. The reason for this simplification is related with the term $\mathbf{v_J}\cdot\nabla(\nabla\cdot(\mathbf{D}_F\nabla c))$ which does not seem easily treatable in the context of weak solutions.

The weak formulation for the simplified hyperbolic problem reads as: given $f \in L^2(0,T;H^1(\Omega))$, $\frac{\partial f}{\partial t} \in L^2(0,T;L^2(\Omega))$, $c_0 \in H^2_{\partial\Omega^+}(\Omega)$ and $\nabla \cdot \mathbf{J}_0 \in L^2(\Omega)$, find $c \in H^1\left(0,T;H^1_{\partial\Omega^+}(\Omega)\right)$ and $\frac{\partial^2 c}{\partial t^2} \in L^2(0,T;L^2(\Omega))$ such that

$$\begin{aligned}\left(\frac{\partial^2 c}{\partial t^2}, v\right) + \left(\frac{1}{\tau}\frac{\partial c}{\partial t} + \mathbf{v_J}\cdot\nabla\frac{\partial c}{\partial t}, v\right) & \\ + (\mathbf{D}_{nF}\nabla c, \nabla v) &= (\tilde{f}, v) \text{ a.e. in } (0,T), \quad \forall v \in H^1_{\partial\Omega^+}(\Omega)\end{aligned} \tag{20}$$

where $\tilde{f} = \frac{\partial f}{\partial t} + \mathbf{v_J}\cdot\nabla f + \frac{f}{\tau}$.

To establish an energy estimate for the weak form (20), we need first to introduce some notation: for $u \in H^1(\Omega)$, we define the seminorm

$$|u|_{\mathbf{v_J},\partial\Omega^-} = \int_{\partial\Omega^-} u^2|\mathbf{v_J}\cdot\mathbf{n}|.$$

We can show that c verifies the following estimate:

Proposition 3. *If* $c \in C(0,T;H^1_{\partial\Omega^+}(\Omega))$ *then there exists* $C>0$ *such that*

$$\begin{aligned}&\left\|\frac{\partial c}{\partial t}(t)\right\|_0^2 + \alpha_{nF}\|\nabla c(t)\|_0^2 + \int_0^t \left|\frac{\partial c}{\partial t}(s)\right|^2_{\mathbf{v_J},\partial\Omega^-} ds \\ &\leqslant C\left(\|\nabla\cdot\mathbf{J}_0\|_0^2 + \|f(0)\|_0^2 + \|c_0\|_2^2 + \int_0^t ||\tilde{f}(s)||_0^2\, ds\right).\end{aligned} \tag{21}$$

Proof: Taking $v = \frac{\partial c}{\partial t}$ in (20), it can be shown

$$\frac{1}{2}\frac{d}{dt}\left(\left\|\frac{\partial c}{\partial t}\right\|_0^2 + (\mathbf{D}_{nF}\nabla c, \nabla c)\right) + \frac{1}{\tau}\left\|\frac{\partial c}{\partial t}\right\|_0^2 + \left(\mathbf{v_J}\cdot\nabla\frac{\partial c}{\partial t}, \frac{\partial c}{\partial t}\right) = \left(\tilde{f}, \frac{\partial c}{\partial t}\right). \tag{22}$$

Attending to the boundary conditions, using integration by parts and recalling that $\mathbf{v_J}$ is constant, we can conclude that

$$\begin{aligned}\left(\mathbf{v_J}\cdot\nabla\frac{\partial c}{\partial t}, \frac{\partial c}{\partial t}\right) &= \frac{1}{2}\sum_{j=1}^d \int_{\partial\Omega}\frac{\partial c}{\partial t}\mathbf{v}_{\mathbf{J},j}\mathbf{n}_j\, ds \\ &= \frac{1}{2}\int_{\partial\Omega}\frac{\partial c}{\partial t}(\mathbf{v_J}\cdot\mathbf{n})\, ds\end{aligned}$$

where $\mathbf{n}_j$ denotes the j-th component of $\mathbf{n}$.

From the definition of $\partial\Omega^-$, it follows that

$$\left(\mathbf{v_J}\cdot\nabla\frac{\partial c}{\partial t},\frac{\partial c}{\partial t}\right)\leqslant\frac{1}{2}\left|\frac{\partial c}{\partial t}\right|^2_{\mathbf{v_J},\partial\Omega^-}. \tag{23}$$

Combining (22) with (23) and using Cauchy-Schwarz and Young's inequality, there exists $\epsilon>0$ such that

$$\frac{1}{2}\frac{d}{dt}\left(\left\|\frac{\partial c}{\partial t}\right\|_0^2+(\mathbf{D}_{nF}\nabla c,\nabla c)\right)+\left(\frac{1}{\tau}-\frac{1}{2\epsilon}\right)\left\|\frac{\partial c}{\partial t}\right\|_0^2+\frac{1}{2}\left|\frac{\partial c}{\partial t}\right|^2_{\mathbf{v_J},\partial\Omega^-}\leqslant\frac{1}{\epsilon}||\tilde{f}||_0^2. \tag{24}$$

Choosing $\epsilon>\frac{\tau}{2}$, we obtain (21). ■

Remark 6. *Estimate* (21)*, obtained from our model, considering only non-Fickian diffusion with memory in time and space, is a typical estimate for wave-type equations and not similar to the estimates obtained for the standard Fickian diffusion equation or the integro-differential approach. It is nonetheless interesting to notice that the presence of Neumann boundary conditions for c induces an extra term in the left hand side,*

$$\int_0^t\left|\frac{\partial c}{\partial t}\right|^2_{\mathbf{v_J},\partial\Omega^-}.$$

3.3. Coupled model. The mixed weak formulation for the coupled model reads as: $f\in L^2(0,T;L^2(\Omega))$, $c_0\in L^2(\Omega)$, $\mathbf{J}_0\in\mathbf{L}^2(\Omega)$ find $c\in L^2\left(0,T;H^1_{\partial\Omega^+}(\Omega)\right)$, $\mathbf{J}\in L^2\left(0,T;\mathbf{H}^1_{\partial\Omega^-}(\Omega)\right)$ such that $\frac{\partial c}{\partial t}\in L^2(0,T;L^2(\Omega))$, $\frac{\partial \mathbf{J}}{\partial t}\in L^2(0,T;\mathbf{L}^2(\Omega))$ and

$$\begin{aligned}\left(\frac{\partial c}{\partial t},v\right)&+(\mathbf{D}_F\nabla c,\nabla v)\\ -(\mathbf{J},\nabla v)&=(f,v)\ \text{a.e. in }(0,T),\quad\forall v\in H^1_{\partial\Omega^+}(\Omega)\\ \tau\left(\frac{\partial\mathbf{J}}{\partial t},\mathbf{w}\right)&+(\mathbf{J},\mathbf{w})\\ +\tau\left((\mathbf{v_J}\cdot\nabla)\mathbf{J},\mathbf{w}\right)&=-(\mathbf{D}_{nF}\nabla c,\mathbf{w})\ \text{a.e. in }(0,T),\quad\forall\mathbf{w}\in\mathbf{H}^1_{\partial\Omega^-}(\Omega).\end{aligned} \tag{25}$$

For system (25), the following estimate holds:

Proposition 4.

$$
\begin{aligned}
&\|c(t)\|_0^2 + \tau \|\mathbf{J}(t)\|_0^2 + \alpha_F \int_0^t \|\nabla c(s)\|_0^2 \ ds \\
&\leqslant \exp^{\epsilon t}\left(\|c(0)\|_0^2 + \tau \|\mathbf{J}(0)\|_0^2 + \frac{1}{\epsilon}\int_0^t \|f(s)\|_0^2 \exp^{-\epsilon s} \ ds \right).
\end{aligned} \tag{26}
$$

where $\epsilon = \dfrac{1}{\tau}\left(\dfrac{C}{\min\left(\frac{C}{2}, \frac{\alpha_F}{C}\right)} - 2 \right)$ *and* $C = 1 + \max\limits_{i,j=1,\cdots,d} \|(\mathbf{D}_{nF})_{ij}\|_\infty$.

Proof: We start by taking $v = c$ in the first equation of (25). As the entries of $\mathbf{D}_f$ has a positive lower bound α_F, it follows that

$$\frac{1}{2}\frac{d}{dt}\|c(t)\|_0^2 + \alpha_F \|\nabla c\|_0^2 \leqslant (\mathbf{J}, \nabla c) + (f, c).$$

Applying Cauchy-Schwarz's and Young's inequality, there exists $\epsilon > 0$ such that

$$\frac{1}{2}\frac{d}{dt}\|c(t)\|_0^2 + \alpha_F \|\nabla c\|_0^2 \leqslant \frac{1}{2\epsilon}\|f\|_0^2 + \frac{\epsilon}{2}\|c\|_0^2 + (\nabla c, \mathbf{J}). \tag{27}$$

On the other hand, taking $\mathbf{w} = \mathbf{J}$ in the second equation of (25), we immediately conclude that

$$\frac{\tau}{2}\frac{d}{dt}\|\mathbf{J}(t)\|_0^2 + \|\mathbf{J}\|_0^2 = -\left(\mathbf{D}_{nF}\nabla c, \mathbf{J}\right) - \tau\left((\mathbf{v}_\mathbf{J}\cdot\nabla)\mathbf{J}, \mathbf{J}\right). \tag{28}$$

Denoting $\mathbf{J}_i$ and $\mathbf{v}_{\mathbf{J},i}$ as the i-th component of $\mathbf{J}$ and $\mathbf{v}_\mathbf{J}$, respectively, we notice that the term $((\mathbf{v}_\mathbf{J}\cdot\nabla)\mathbf{J}, \mathbf{J})$ can be written as

$$((\mathbf{v}_\mathbf{J}\cdot\nabla)\mathbf{J}, \mathbf{J}) \ = \ \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\mathbf{J}_i, \frac{\partial \mathbf{J}_i}{\partial x_j}\mathbf{v}_{\mathbf{J},i}\right).$$

Following the same reasoning as to obtain (23), we conclude that

$$-\left((\mathbf{v}_\mathbf{J}\cdot\nabla)\mathbf{J}, \mathbf{J}\right) \leqslant 0. \tag{29}$$

Therefore, combining (29) and (28) we get

$$\frac{\tau}{2}\frac{d}{dt}\|\mathbf{J}(t)\|_0^2 + \|\mathbf{J}\|_0^2. \leqslant -\left(\mathbf{D}_{nF}\nabla c, \mathbf{J}\right). \tag{30}$$

Summing (27) with (30) and attending to the regularity of the entries of $\mathbf{D}_{nF}$, Cauchy-Schwarz and Young's inequalities, there exist constants

$C, \eta > 0$ such that

$$\begin{array}{c} \frac{1}{2}\frac{d}{dt}\left(\|c(t)\|_0^2 + \tau\,\|\mathbf{J}\|_0^2\right) \\ +\left(\alpha_F - \frac{C\eta}{2}\right)\|\nabla c\|_0^2 + \left(1-\frac{C}{2\eta}\right)\|\mathbf{J}\|_0^2 \;\leqslant\; \frac{1}{2\epsilon}\|f\|_0^2 + \frac{\epsilon}{2}\|c\|_0^2 \end{array} \tag{31}$$

Choosing $\eta = \min\left(\frac{C}{2}, \frac{\alpha_F}{C}\right)$ and defining $\gamma = \frac{C}{\eta} - 2 \geqslant 0$, we arrive at

$$\frac{d}{dt}\left[\|c(t)\|_0^2 + \tau\,\|\mathbf{J}\|_0^2\right]\alpha_F\,\|\nabla c\|_0^2 + \leqslant \frac{1}{\epsilon}\|f\|_0^2 + \epsilon\,\|c\|_0^2 + \gamma\,\|\mathbf{J}\|_0^2 .$$

Assuming $\epsilon = \frac{\gamma}{\tau}$, integrating over $(0,t)$ and applying Gronwall's lemma, we finally conclude (26). ■

Remark 7. *Estimate* (26) *is similar to the estimates obtained for Fickian diffusion process and the integro-differential formulation. In fact, in both cases when we consider only Fickian flux or we consider memory in time for the flux, the estimates are of the same type.*

4. Numerical simulation

In this section we apply a finite element method to approximate the solution of (25) in a one dimensional setting. This will serve to illustrate the behavior of the solution of the coupled model, under different choices of parameters.

We start by introducing the numerical method. Let $\Delta t, h > 0$. We denote by $\mathcal{T}_h$ a uniform grid on $\Omega = (0,1)$ with mesh size h and V_h the space of piecewise linear polynomials built on $\mathcal{T}_h$. Let $x \in \{0,1\}$ and

$$V_h^x = \{v_h \in V_h :\; v_h(x) = 0\}.$$

Let $P_h : L^2(\Omega) \longrightarrow V_h$ denote the L^2 projection operator onto V_h.

4.1. Numerical method. The finite element approximation of (25) reads as: given $J_h^0 = P_h J_0$ and $c_h^0 = P_h c_0$, find $c_h^{n+1} \in V_h^1$ and $J_h^{n+1} \in V_h^0$ such that

$$\begin{aligned} \left(c_h^{n+1}, v_h\right) + \left(D_F\frac{\partial c_h^{n+1}}{\partial x} - J_h^{n+1}, \frac{\partial v_h}{\partial x}\right) &= (P_h f(t_{n+1}), v_h) \\ &\quad + (c_h^n, v_h), \qquad \forall v_h \in V_h^1 \\ \left(\frac{\tau}{\Delta t}+1\right)\left(J_h^{n+1}, w_h\right) & \\ + \left(D_{nF}\frac{\partial c_h^{n+1}}{\partial x} + \tau v_J \frac{\partial J_h^{n+1}}{\partial x}, w_h\right) &= \frac{\tau}{\Delta t}(J_h^n, w_h), \qquad \forall w_h \in V_h^0 \end{aligned} \tag{32}$$

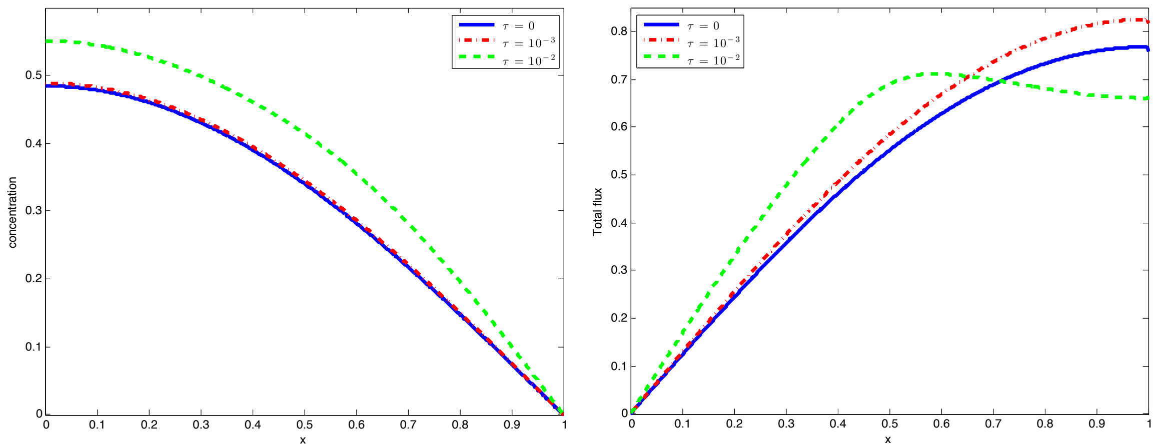
Remark 8. *Method* (32) *treats coupled problem* (25) *fully implicitly and we expect that this scheme benefits from reasonable stability properties. It can be shown that* (32) *satisfies a discrete version of* (26).

4.2. Comparison of different flux behaviors. In order to illustrate the effect of non Fickian flux in the evolution of c, we shall conduct a few numerical simulations.

Let us consider an initial condition

$$c_0(x) = \begin{cases} 1, & x \in [0, 0.4] \\ 1 - 5(x - 0.4), & x \in (0.4, 0.6) \\ 0, & x \in [0.6, 1] \end{cases}$$

and $D_F = D_{nF} = 1$. We start by performing two simulations: the first, considering $\tau = 0$; in the second, we take two nonzero values for τ. We plot the corresponding approximate concentration profiles at time $t = 0.125$ on Figure 1(a). It seems that varying the parameter τ induces a delayed effect

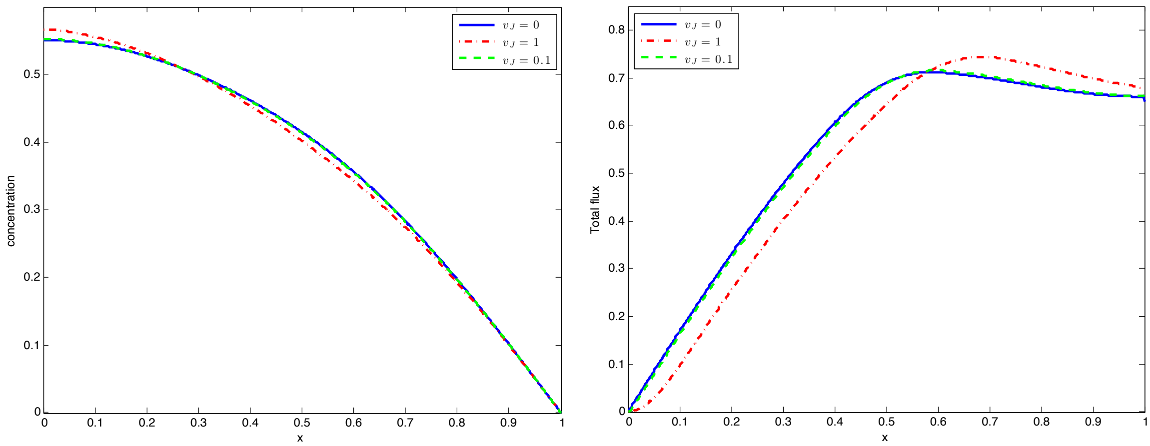


(a) Concentration plot (b) Total flux plot

FIGURE 1. Plots of concentration and flux profile at $t = 0.125$ for different values of τ and $v_J = 0$.

in the diffusion process (as compared with Fickian diffusion only). We report also as different total flux profiles.

In Figure 2 we plot the same variables, but now fixing τ and varying the flux velocity v_J, i.e., considering a model where only memory in time is present, and another with memory in time and space. As in the previous simulation, the choice of the parameter v_J has an impact on the profile of the concentration c.



(a) Concentration plot (b) Total flux plot

FIGURE 2. Plots of concentration and total flux profile at $t = 0.125$ for different values of v_J and $\tau = 0.1$.

5. Conclusions

We have considered a coupled system of equations to model a diffusion process presenting a Fickian and non Fickian mass flux contributions. This model introduces a memory effect in time and space for the flux.

In some special cases, we showed that the coupled problem is the same as others already proposed in the literature. Also, the energy estimate obtained for the coupled problem are consistent with the ones found for those other equivalent formulations. A finite element method was implemented to illustrate the different behavior of the various effects of memory in time and space.

It is our goal to apply the model studied in this paper to model diffusion (and advection) in porous media. In this case, this system should be coupled with Darcy's law for the velocity and an elliptic equation for the pressure (for incompressible flows).

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