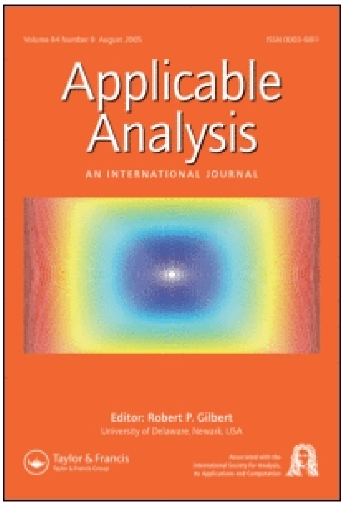

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Qualitative analysis of a delayed non-Fickian model

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Qualitative analysis of a delayed non-Fickian model

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This article focusses on the mathematical analysis of a delayed integro-differential model in which flux does not obey the classical Fick's law. The well-posedness of the integro-differential model in the Hadamard's sense is established. The dependence on the delay parameter of the total amount of desorpted/sorpted mass is studied. Numerical results that show the effectiveness of the model are included.

Keywords: Fick's law; non-Fickian flux; delayed integro-differential equation; well-posedness in Hadamard sense; sorption; desorption

AMS Classifications: 35B35; 35B40; 35C10; 35K65

1. Introduction

Diffusion phenomena are described by

$$\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x} \tag{1}$$

where, u is the concentration of the diffusing substance and J stands for the flux that is the rate of transfer of the diffusing substance through unit area of a section. Equation (1) is a consequence of mass conservation law. Assuming that the flux is proportional to the concentration gradient,

$$J(x,t) = -D\frac{\partial u}{\partial x}(x,t). \tag{2}$$

where, $D > 0$ denotes the diffusion coefficient, the classical diffusion equation is obtained.

However, experimental evidence of diffusing phenomena within different field of applications shows that (1)–(2) does not represent an accurate model. Several results reported in the literature show that numerical simulations of concentration and total amount of released mass, provided by the classical diffusion equation, does not fit with experimental data [1–6] because it can be observed that experimental curves exhibit a delay. In fact in the absorption or desorption in polymers, the polymeric matrix

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reacts to the presence of the penetrant molecules with a certain delay that is the flux at time t is related to the gradient of the concentration at a time $t-\tau$. This delay τ can be explained, in the case of polymers, by the entrapment of the diffusing substance caused by the particular molecular structure of the matrix. The assumption of a Brownian motion underlying Fick's law is not also compatible with biological barriers as in the case of diffusion through the human skin. In fact, the transport of substances across it is a complex phenomenon involving physical, chemical and biological interactions that cause a delay in the diffusion (see [1], [17], [23]).

Precise control over diffusion is paramount in the development of advanced delivery systems. Important tools in this development are mathematical models with good theoretical properties where the role of the delay parameter τ is completely understood and which lead to accurate numerical simulation. This is the problem addressed in this article.

Let us define the flux J such that

$$J(x, t+\tau) = \frac{D}{\tau}\frac{\partial u}{\partial x}(x, t). \tag{3}$$

Assuming that τ is small enough we have from (3)

$$\frac{\partial J}{\partial t} + \frac{1}{\tau}J(x, t) = -\frac{D}{\tau}\frac{\partial u}{\partial x}(x, t)$$

and integrating this first order equation we obtain

$$J(x, t) = -\frac{D}{\tau}\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(x, s)\mathrm{d}s. \tag{4}$$

With this new definition for the flux, mass conservation law leads to an integro-differential equation, which coupled with initial and boundary conditions reads

$$\begin{cases} \dfrac{\partial u}{\partial t}(x, t) = \dfrac{D}{\tau}\displaystyle\int_0^t e^{-(t-s)/\tau}\frac{\partial^2 u}{\partial x^2}(x, s)\mathrm{d}s, \quad x \in (0, L), t \in (0, T], \\ u(0, t) = u_\ell, \quad u(L, t) = u_r, t \in (0, T], \\ u(x, 0) = f(x), \quad x \in (0, L). \end{cases} \tag{5}$$

The initial boundary value problem (IBVP) (5) was introduced first independently in [10] and [11], to model a heat conduction problem. In fact if the classical model (1)–(2) is considered, a sudden change in the temperature made at a point of a bar, will be felt instantly everywhere. To overcome this pathological behaviour Cattaneo replaced the Fourier law for the heat flux by (4). A modified version of (5) was considered in [23]. We point out that for reaction–diffusion systems a delayed integro-differential equation of type (5) was considered for instance in [12–19].

But does (5) lead to an accurate expression of the total amount M of diffusing substance? What is the effect of the delay parameter τ on M? Does it decreas the concentration and the mass of diffusive substance? To answer such questions we organize the article as follows. In Section 2, we establish the existence of a solution of the IBVP (5). The regularity of such solutions is also studied in this section. In Section 3, the uniqueness and the well-posedness of the IBVP (5) is concluded. As (5) depends on the delay parameter τ, the asymptotic behaviour of this model is also studied. In Section 4, we establish that the solution of the delayed model converges to the solution of the classical diffusion model (1)–(2). Section 4 focusses on the behaviour of the total amount of diffusing substance defined by the integro-differential model. Finally, in Section 5 some numerical illustrations are included.

2. Existence of a solution

In this section, we establish the existence of a solution of the IBVP (5). By $L^2[0, L]$, we denote the vector space of all functions defined in $[0, L]$ such that $\int_0^L f^2(x)\mathrm{d}x < \infty$. In $L^2[0, L]$, we consider the usual L^2 inner product $(.,.)$ and by $\|.\|$ we denote the corresponding norm.

Due to its particular structure it is possible to compute the solution of (5) by using Fourier analysis. We remark that the existence of a solution for IBVP (5) was considered in [20]. However, the special expression established in this article is needed to prove the convergence results in Section 4.

THEOREM 1 *If* $f(0) = u_\ell$, $f(L) = u_r$ *and* $f''' \in L^2[0, L]$, *then*

$$u(x,t) = \sum_{n=1}^{[L/2\pi\sqrt{D\tau}]} A_n \left(\frac{1+\delta_n(\tau)}{2\delta_n(\tau)} e^{(t/2\tau)\left(-1+\delta_n(\tau)\right)} + \frac{-1+\delta_n(\tau)}{2\delta_n(\tau)} e^{(t/2\tau)\left(-1-\delta_n(\tau)\right)} \right) \sin\left(\frac{n\pi}{L}x\right)$$
$$+ \sum_{[L/2\pi\sqrt{D\tau})]+1}^{\infty} A_n e^{-(t/2\tau)} \left(\cos\left(\frac{t\delta(n\tau)}{2\tau}\right) + \frac{1}{\delta_n(\tau)} \sin\left(\frac{t\delta(n\tau)}{2\tau}\right) \right) \sin\left(\frac{n\pi}{L}x\right)$$
$$+ \frac{u_r - u_\ell}{L} x + u_\ell \tag{6}$$

for $x \in [0, L]$, $t \in [0, T]$, *where* $[(L/2\pi\sqrt{D\tau})]$ *represents the integer part of* $(L/2\pi\sqrt{D\tau}) \notin \mathbb{N}$ *and*

$$A_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi}{L}x\right)\mathrm{d}x + \frac{2}{n\pi}\left(u_r(-1)^n - u_\ell\right), \quad n \in \mathbb{N}, \tag{7}$$

$$\delta_n(\tau) = \begin{cases} \sqrt{1 - 4D\dfrac{n^2\pi^2}{L^2}\tau}, & n \le \left[\dfrac{L}{2\pi\sqrt{D\tau}}\right] \\ \sqrt{-1 + 4D\dfrac{n^2\pi^2}{L^2}\tau}, & n \ge \left[\dfrac{L}{2\pi\sqrt{D\tau}}\right] + 1. \end{cases} \tag{8}$$

Proof Let us consider the auxiliary function

$$w = u - \left(\frac{u_r - u_\ell}{L}x + u_\ell\right)$$

Solution of the auxiliary homogeneous problem:

$$\begin{cases} \dfrac{\partial w}{\partial t}(x,t) = \dfrac{D}{\tau}\displaystyle\int_0^t e^{-(t-s)/\tau}\dfrac{\partial^2 w}{\partial x^2}(x,s)\mathrm{d}s, & x \in (0,L), t \in (0,T], \\ w(0,t) = w(L,t) = 0, & t \in (0,T], \\ w(x,0) = f(x) - \dfrac{u_r - u_\ell}{L} - u_\ell, & x \in (0,L). \end{cases} \tag{9}$$

After some tedious but straightforward computations we can establish that

$$w(x,t) = \sum_{n=1}^{[L/2\pi\sqrt{D\tau}]} A_n\Big(\frac{1+\delta_n(\tau)}{2\delta_n(\tau)}e^{(t/2\tau)\big(-1+\delta_n(\tau)\big)} + \frac{-1+\delta_n(\tau)}{2\delta_n(\tau)}e^{(t/2\tau)\big(-1-\delta_n(\tau)\big)}\Big)\sin\Big(\frac{n\pi}{L}x\Big)$$
$$+ \sum_{n=[L/2\pi\sqrt{D\tau}]+1}^{\infty} A_n e^{-(t/2\tau)}\left(\cos\Big(\frac{t\delta(n\tau)}{2\tau}\Big) + \frac{1}{\delta_n(\tau)}\sin\Big(\frac{t\delta(n\tau)}{2\tau}\Big)\right)\sin\Big(\frac{n\pi}{L}x\Big), \tag{10}$$

where, A_n and $\delta_n(\tau)$ are defined, respectively, by (7) and (8).

From (10) it is easy to show that (6) is a formal solution of IBVP (5).

In order to conclude that (6) is in fact a solution of IBVP (5) we establish that u has first- and second-order continuous derivatives with respect to time and space variables. The proof is divided into following three steps:

1. We start by proving that (6) defines a continuous function. We note that for n such that $n \geq [(L/2\pi\sqrt{D\tau})] + 1$, we have

$$|u_n(x,t)| \leq |A_n|\Big(1 + \frac{1}{\delta_n(\tau)}\Big), \quad x \in [0,L], t \in [0,T], \tag{11}$$

where,

$$u_n(x,t) = A_n e^{-(t/2\tau)}\Big(\cos\Big(\frac{t\delta(n\tau)}{2\tau}\Big) + \frac{1}{\delta_n(\tau)}\sin\Big(\frac{t\delta(n\tau)}{2\tau}\Big)\Big)\sin\Big(\frac{n\pi}{L}x\Big).$$

For A_n the representation holds

$$A_n = \frac{2}{n\pi}\int_0^L f'(x)\cos\Big(\frac{n\pi}{L}x\Big)\mathrm{d}x,$$

and as

$$S_m = \sum_{n=1}^{m}\frac{1}{n}\Big(1+\frac{1}{\delta_n(\tau)}\Big)\int_0^L f'(x)\cos\Big(\frac{n\pi}{L}x\Big) \leq C\left(\sum_{n=1}^{m}\frac{1}{n^2\big(1+\delta_n(\tau)\big)^2}\right)^{1/2}\|f'\|_{L^2[0,L]}$$

for some positive constant C n-independent, then $\sum_n |A_n|(1+(1/\delta_n(\tau)))$ is convergent. This fact leads to the uniform convergence of the series

$$\sum_{n\geq[L/2\pi\sqrt{D\tau}]+1} u_n(x,t)$$

in $[0,L]\times[0,T]$. Consequently, u is continuous in $[0,L]\times[0,T]$.

2. Let us now show that u is differentiable with respect to t, by proving that

$$\sum_{n\geq[L/2\pi\sqrt{D\tau}]+1} \frac{\partial u_n}{\partial t}(x,t)$$

converges uniformly in $[0,L]\times[0,T]$. As

$$\left|\frac{\partial u_n}{\partial t}(x,t)\right| \leq C|A_n|\Big(1+\frac{1}{\delta_n(\tau)}+\delta_n(\tau)\Big)$$

for some positive constant C n-independent, we prove that

$$\sum_{n \geq [L/2\pi\sqrt{D\tau}]+1} |A_n|\delta_n(\tau) \tag{12}$$

converges.

In fact it can be shown that

$$A_n = \frac{-2L}{n^2\pi^2}\int_0^L f''(x)\sin\left(\frac{n\pi}{L}x\right)\mathrm{d}x$$

which implies that for some positive constant C n-independent

$$S_m = \sum_{n \geq [L/2\pi\sqrt{D\tau}]+1}^{m} |A_n|\delta_n(\tau) \leq C\left(\sum_{n \geq [L/2\pi\sqrt{D\tau}]+1}^{m} \frac{\delta_n(\tau)^2}{n^4}\right)^{1/2} \|f''\|_{L^2[0,L]}$$

is a convergent sequence. Thus, (12) converges.

3. Using the same kind of arguments it can be shown that $(\partial u/\partial x)$ and $(\partial^2 u/\partial x^2)$ exist and are continuous in $[0, L] \times [0, T]$. This concludes the proof. ■

Solution (6) is composed by three terms: a finite sum, a sum with an infinite number of terms and a third term coming from the boundary conditions. We note that the terms in the finite sum recall the terms in the solution of the parabolic diffusion Equations (1) and (2); the terms in the infinite sum recall the solution of a wave type hyperbolic equation. From a formal view point as $\tau \to 0$ we have $(L/2\pi\sqrt{D\tau}) \to \infty$ and consequently the infinite sum disappears. In this case, the solution $u(x, t)$ given by (6) converges formally to the solution of (1)–(2). We postpone to a later section the rigorous proof of this result.

In order to simplify expression (6) it was assumed that $(L/2\pi\sqrt{D\tau}) \notin \mathbb{N}$. If this assumption does not hold then in the expression of $u(x, t)$ we should consider the term $e^{-(t/2\tau)}A_m(1 + (t/2\tau))\sin((m\pi/L)x)$ where, $m = (L/2\pi\sqrt{D\tau})$. Nevertheless this last term does not imply any substantial change in Theorem 1. Attending to this fact we suppose in what follows that $(L/2\pi\sqrt{D\tau}) \notin \mathbb{N}$.

3. Unicity of solution

For the classical diffusion equation the uniqueness of its solution is a consequence of the stability of the IBVP

$$\begin{cases} \dfrac{\partial u}{\partial t}(x, t) = D\dfrac{\partial^2 u}{\partial x^2}(x, t) & x \in (0, L), t \in (0, T], \\ u(0, t) = u_\ell, \quad u(L, t) = u_r, t \in (0, T], \\ u(x, 0) = f(x), \quad x \in (0, L), \end{cases} \tag{13}$$

with respect to perturbations of the initial condition. Such stability is established by using the maximum principle [21].

For the delayed IBVP (5) the proof of stability is based on the following estimate [14] for the energy functional:

$$E(u)(t) = \|u(t)\|^2_{L^2[0,L]} + \frac{D}{\tau}\left\| \int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s \right\|^2_{L^2[0,L]}, \quad t \geq 0. \tag{14}$$

THEOREM 2 *Let u be a solution of the delayed IBVP* (5) *with homogeneous boundary conditions. Then,*

$$E(u)(t) \leq \|f\|^2_{L^2[0,b]}, \quad t \geq 0. \tag{15}$$

Proof Multiplying the delayed integro-differential equation of (5) by u, with respect to the L^2 inner product $(.,.)$, we easily get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{L^2} = -\frac{D}{\tau}\left(\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s, \frac{\partial u}{\partial x}(t)\right). \tag{16}$$

As

$$\left(\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s, \frac{\partial u}{\partial x}(t)\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\|\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s\right\|^2_{L^2} + \frac{1}{\tau}\left\|\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s\right\|^2_{L^2},$$

we deduce from (16) the differential inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u\|^2_{L^2} + \frac{D}{\tau}\left\|\int_0^t e^{-(t-s)/\tau}\frac{\partial u}{\partial x}(s)\mathrm{d}s\right\|^2_{L^2}\right) \leq 0 \tag{17}$$

which lead to (15). ∎

As a corollary of Theorem 2 we conclude the stability of model (5).

COROLLARY 1 *Let u and $\tilde{u}$ be solutions of the delayed IBVP* (5) *with initial conditions f and $\tilde{f}$, respectively. Then,* $w = u - \tilde{u}$ *satisfies*

$$\|w(t)\|^2_{L^2[0,L]} + \frac{D}{\tau}\left\|\int_0^t e^{-(t-s)/\tau}\frac{\partial w}{\partial t}(s)\mathrm{d}s\right\|^2_{L^2[0,L]} \leq \|f - \tilde{f}\|^2_{L^2[0,b]}, \quad t \geq 0. \tag{18}$$

The existence of a solution for (5) was established in Theorem 1 by a constructive approach. The uniqueness of such solution in L^2 is now a consequence of Corollary 1. Moreover, as by Corollary 1, the delayed IBVP (5) is stable with respect to perturbations of the initial condition, we conclude that the integro-differential model (5) is well-posed in Hadamard sense.

4. Asymptotic behaviour of the model

4.1. *Asymptotic behaviour of the solution*

In this section, we study the dependence on the parameter τ of the solution u of (5). We point out that the asymptotic behaviour of the solution of the homogeneous version of IBVP (5) where the integro-differential equation

$$\frac{\partial u}{\partial t}(x,t) = \alpha(\tau)\frac{\partial^2 u}{\partial x^2}(x,t) + \frac{D}{\tau}\int_0^t e^{-(t-s)/\tau}\frac{\partial^2 u}{\partial x^2}(x,s)\mathrm{d}s$$

is considered has been studied in [22]. As it is assumed that $\alpha(\tau) > 0$, the approach used in such a paper cannot be followed here.

In what follows we represent the solution of the IBVP (5) by $u(x, t, \tau)$. This solution can be written in the equivalent form

$$u(x,t,\tau) = \frac{u_r - u_\ell}{L} x + u_\ell + \sum_{n=1}^{\infty} u_n(x,t,\tau) \sin\Big(\frac{n\pi}{L} x\Big)$$

with

$$u_n(x,t,\tau) = \begin{cases} A_n\Big(e^{(t/2\tau)\left(-1+\delta_n(\tau)\right)} \dfrac{1+\delta_n(\tau)}{2\delta_n(\tau)} + e^{(t/2\tau)\left(-1-\delta_n(\tau)\right)} \dfrac{-1+\delta_n(\tau)}{2\delta_n(\tau)}\Big), & n \leq \Big[\dfrac{L}{2\pi\sqrt{D\tau)}}\Big], \\ A_n e^{-(t/2\tau)}\Big(\cos\Big(\dfrac{t\delta_n(\tau)}{2\tau}\Big) + \dfrac{1}{\delta_n(\tau)}\sin\Big(\dfrac{t\delta_n(\tau)}{2\tau}\Big)\Big), & n \geq \Big[\dfrac{L}{2\pi\sqrt{D\tau}}\Big] + 1, \end{cases}$$

where, A_n and $\delta_n(\tau)$ are defined by (7) and (8), respectively.

As

$$\lim_{\tau\to 0} \frac{-1+\delta_n(\tau)}{2\delta_n(\tau)} = 0, \quad \text{for } n \leq \Big[\frac{L}{2\pi\sqrt{D\tau}}\Big],$$

and

$$\lim_{\tau\to 0} \frac{1}{2\tau}\big(-1+\delta_n(\tau)\big) = -D\frac{n^2\pi^2}{L^2}, \quad \text{for } n \leq \Big[\frac{L}{2\pi\sqrt{D\tau}}\Big],$$

we deduce that, for some τ_0 and $\tau \in (0, \tau_0]$, there exists $\varepsilon > 0$ such that

$$|u_n(x,t,\tau)| \leq e^{-\epsilon D(\pi^2/L^2)} |A_n|, \quad \text{for } n \leq \Big[\frac{L}{2\pi\sqrt{D\tau}}\Big],\ x \in [0, L],\ t \in [\epsilon, T]. \tag{19}$$

Let us consider now $n \geq [(L/2\pi\sqrt{D\tau})] + 1$ and $t \in [\epsilon, T]$ with $\epsilon > 0$. We have successively

$$|u_n(x,t,\tau)| \leq |A_n| e^{-(t/2\tau)}\Big(1 + \frac{1}{\delta_n(\tau)}\Big),$$

$$e^{-(t/2\tau)} \frac{1}{\delta_n(\tau)} \leq e^{-(\epsilon/2\tau)} \frac{1}{\sqrt{-1 + \gamma\tau[1/\sqrt{\gamma\tau}]^2 + 2\gamma\tau[1/\sqrt{\gamma\tau}] + \gamma\tau}}$$

with $\gamma = (4D\pi^2/L^2)$.

As $\lim_{\tau\to 0} \gamma\tau[(1/\sqrt{\gamma\tau})]^2 = 1,\ \lim_{\tau\to 0} \gamma\tau[(1/\sqrt{\gamma\tau})] = 0$ we conclude that

$$\lim_{\tau\to 0} e^{-(\epsilon/2\tau)} \frac{1}{\sqrt{-1 + \gamma\tau[1/\sqrt{\gamma\tau}]^2 + 2\gamma\tau[1/\sqrt{\gamma\tau}] + \gamma\tau}} = 0.$$

This last convergence implies that, for some τ_1 and for $\tau \in (0, \tau_1]$,

$$|u_n(x,t,\tau)| \leq C|A_n|, \quad \text{for } n \geq \Big[\frac{L}{2\pi\sqrt{D\tau}}\Big] + 1,\ x \in [0, L], t \in [\epsilon, T], \tag{20}$$

where, C is a positive constant τ-independent and n-independent.

In the proof of Theorem 1 it was shown that if $f(0) = u_\ell$, $f(L) = u_r$ and $f' \in L^2[0, L]$, then $\sum_n |A_n|$ converges. Then from (19) and (20) we conclude that u is τ-continuous for $x \in [0, L]$ and for $t \in (0, T]$. Moreover, as $\sum_{n=1}^{\infty} u_n(x, t, \tau)$ converges uniformly for $\tau \in (0, \tau_0]$, for some positive τ_0, and for $x \in [0, L], t \in [\epsilon, T]$ for every positive $\epsilon < T$, then $u(x, t, \tau) \to u(x, t)$ when $\tau \to 0$, where u and u_F are the solutions of IBVPs (5) and (13), respectively.

As a consequence of the previous arguments we easily establish the next result.

THEOREM 3 *If $f(0) = u_\ell$, $f(L) = u_r$ and $f' \in L^2[0, L]$ then $u(x, t, \tau)$ is τ-continuous and*

$$\lim_{\tau \to 0} u(x, t, \tau) = u_F(x, t) \text{ uniformly for } x \in [0, L], t \in (0, T], \tag{21}$$

where, u and u_F are the solutions of IBVPs (5) *and* (13), *respectively.*

In the previous result and in what follows the uniform convergence on $(0, T]$ means that the convergence is uniform on $[\epsilon, T]$ for every $\epsilon > 0$, $\epsilon < T$.

4.2. *Asymptotic behaviour of the mass*

The delayed IBVP (5) can be used to model sorption or desorption diffusion phenomena depending on the relation between the concentrations at the boundary points and the initial distribution. In this model, a time memory effect was introduced to delay the diffusion phenomenon. Consequently, it should be observed that a delayed effect on the sorpted or desorpted mass is computed by using IBVP (5). We prove this result in what follows.

Let $M(t, \tau)$ be the total amount of diffusing substance at time t defined by

$$M(t, \tau) = \int_0^L u(x, t, \tau) \mathrm{d}x. \tag{22}$$

As u is given by (6) we obtain

$$M(t, \tau) = \frac{u_r + u_\ell}{2} L + \sum_{n=1}^{\infty} M_n(t, \tau)$$

where, $M_n(t, \tau)$ is defined by

$$M_n(t, \tau) = \begin{cases} A_n \dfrac{L((-1)^{n+1} + 1)}{n\pi} \Big(e^{(t/2\tau)\left(-1+\delta_n(\tau)\right)} \dfrac{1 + \delta_n(\tau)}{2\delta_n(\tau)} \\ \quad + e^{(t/2\tau)\left(-1-\delta_n(\tau)\right)} \dfrac{-1 + \delta_n(\tau)}{2\delta_n(\tau)} \Big), \quad n \leq \left[\dfrac{L}{2\pi\sqrt{D\tau})} \right], \\ A_n \dfrac{L((-1)^{n+1} + 1)}{n\pi} e^{-(t/2\tau)} \Big(\cos\Big(\dfrac{t\delta_n(\tau)}{2\tau} \Big) \\ \quad + \dfrac{1}{\delta_n(\tau)} \sin\Big(\dfrac{t\delta_n(\tau)}{2\tau} \Big) \Big), \quad n \geq \left[\dfrac{L}{2\pi\sqrt{D\tau}} \right] + 1, \end{cases}$$

where, A_n and $\delta_n(\tau)$ are defined by (7) and (8), respectively.

Following the proof of Theorem 3, it can be shown that if $f \in L^2[0, L]$, then $\sum_{n=1}^{\infty} M_n(t, \tau)$ converges uniformly for $t \in (0, T]$ and for $\tau \in (0, \tau_0]$, for some positive τ_0. Furthermore,

$$M(t, \tau) \to M_F(t) \quad \text{as}\, \tau \to 0, \quad \text{for}\, t \in (0, T], \tag{23}$$

where, $M_F(t)$ is the total amount of diffusing substance at time t defined by the classical diffusion model (13).

In order to quantify the delayed effect introduced in the IVBP (5), we compute the total amount of diffusing substance entering or emerging at the right boundary point $x = L$

$$M_R(t, \tau) = \int_0^t J(L, s, \tau) \mathrm{d}s, \tag{24}$$

where, $J(L, s, \tau)$ represents the flux defined by (4). It can be shown that $J(L, s, \tau)$ admits the representation

$$J(L, t, \tau) = D\frac{u_\ell - u_r}{L}\left(1 - e^{-(t/\tau)}\right) + \sum_{n=1}^{\infty} J_n(t, \tau), \tag{25}$$

with

$$J_n(t, \tau) = DA_n(-1)^{n+1}\frac{n\pi}{L}\hat{J}_n(t, \tau)$$

where,

$$\hat{J}_n(t, \tau) = \frac{1}{\delta_n(\tau)}\left(e^{(t/2\tau)\left(-1+\delta_n(\tau)\right)} - e^{(t/2\tau)\left(-1-\delta_n(\tau)\right)}\right),$$

for $n \le [(L/2\pi\sqrt{D\tau})]$, and

$$\hat{J}_n(t, \tau) = 2e^{-(t/2\tau)}\frac{1}{\delta_n(\tau)}\sin\left(\frac{t\delta_n(\tau)}{2\tau}\right)$$

for $n \ge [(L/2\pi\sqrt{D\tau})] + 1$.

For $n \le [(L/2\pi\sqrt{D\tau})]$ we have

$$|J_n(t, \tau)| \le C|A_n|n, \quad \text{for } \tau \in (0, \tau_0], \ t \in [0, T], \tag{26}$$

for some positive constant C τ-independent and n-independent.

Let ϵ be a positive constant and let $t \in [\epsilon, T]$. As

$$|e^{-(t/2\tau)}\frac{1}{\delta_n(\tau)}\sin\left(\frac{t\delta_n(\tau)}{2\tau}\right)| \le e^{-(\epsilon/2\tau)}\frac{1}{\delta_n(\tau)} \to 0 \text{ when } \tau \to 0$$

holds we conclude that, for $n \ge [(L/2\pi\sqrt{D\tau})] + 1$,

$$|J_n(t, \tau)| \le C|A_n|n, \quad \text{for } \tau \in (0, \tau_1], \ t \in (0, T], \tag{27}$$

for some positive constant C τ-independent and n-independent and for some τ_1.

If the initial distribution f is such that $f(0) = u_\ell$, $f(L) = u_r$ and $f'' \in L^2[0, L]$, then it can be shown that

$$\sum_{n=1}^{\infty} |A_n|n$$

converges. Consequently,

$$\sum_{n=1}^{\infty} J_n(t, \tau) \tag{28}$$

converges uniformly for $t \in (0, T]$ and for $\tau \in (0, \tau_0]$ for some τ_0. Moreover,

$$J(L, t, \tau) \to J(L, t), \quad \text{when } \tau \to 0, \quad \text{for } t \in (0, T],$$

where, $J(L, t)$ is the Fickian flux at $x = L$ defined by $J(L, t) = -D(\partial u/\partial x)(L, t)$, where, u is the solution of the IBVP (13).

By using (25) we easily obtain

$$M_R(t, \tau) = D\frac{u_\ell - u_r}{L}\left(t - \tau(1 - e^{-(t/\tau)})\right) + \sum_{n=1}^{\infty} M_n(t, \tau),$$

with

$$M_n(t, \tau) = DA_n(-1)^{n+1}\frac{n\pi}{L}\hat{M}_n(t, \tau)$$

where,

$$\hat{M}_n(t, \tau) = \frac{2\tau}{\delta_n(\tau)}\left(\frac{1}{-1 + \delta_n(\tau)}e^{(t/2\tau)\left(-1-\delta_n(\tau)\right)} + \frac{1}{1 + \delta_n(\tau)}e^{(t/2\tau)\left(-1+\delta_n(\tau)\right)}\right) - \frac{4\tau}{\delta_n(\tau)^2 - 1}$$

for $n \le [(L/2\pi\sqrt{D\tau})]$, and

$$\hat{M}_n(t, \tau) = -\frac{4\tau e^{-t/2\tau}}{\delta_n(\tau)\left(1 + \delta_n(\tau)^2\right)}\left(\cos\left(\frac{t\delta_n(\tau)}{2\tau}\right) + \frac{1}{\delta_n(\tau)}\sin\left(\frac{t\delta_n(\tau)}{2\tau}\right)\right) + \frac{4\tau}{1 + \delta_n(\tau)^2}$$

for $n \ge [(L/2\pi\sqrt{D\tau})] + 1$.

As

$$\begin{aligned}&\left|\frac{4\tau e^{-t/2\tau}}{\delta_n(\tau)\left(1 + \delta_n(\tau)^2\right)}\left(\cos\left(\frac{t\delta_n(\tau)}{2\tau}\right) + \frac{1}{\delta_n(\tau)}\sin\left(\frac{t\delta_n(\tau)}{2\tau}\right)\right)\right| \\ &\quad \le \frac{4\tau e^{-(\epsilon/2\tau)}}{1 + \delta_n(\tau)^2}\left(1 + \frac{1}{\delta_n(\tau)}\right) \to 0, \quad \text{when} \quad \tau \to 0, \qquad \text{for} \quad t \in [\epsilon, T],\end{aligned}$$

for $\epsilon > 0$, and

$$\frac{4\tau}{1 + \delta_n(\tau)^2} \to 0 \quad \text{when} \quad \tau \to 0,$$

it can be shown following the convergence analysis of (28) that $\sum_{n=1}^{\infty} M_n(t, \tau)$ converges uniformly in $(0, T] \times (0, \tau_0]$, for some τ_0, and

$$M_R(t, \tau) \to M_{R,F}(t), \quad \text{when } \tau \to 0, \quad \text{for } t \in (0, T], \tag{29}$$

where, $M_{R,F}(t)$ denotes the total amount of substance entering or emerging at the right boundary point $x = L$ defined by the IBVP (13).

5. Numerical simulation

In this section, we present some numerical illustrations of the results obtained in the previous sections, namely the convergences (21), (23) and (29). The numerical approximations for the solution $u(x, t, \tau)$ defined by (6), for the total amount of diffusing

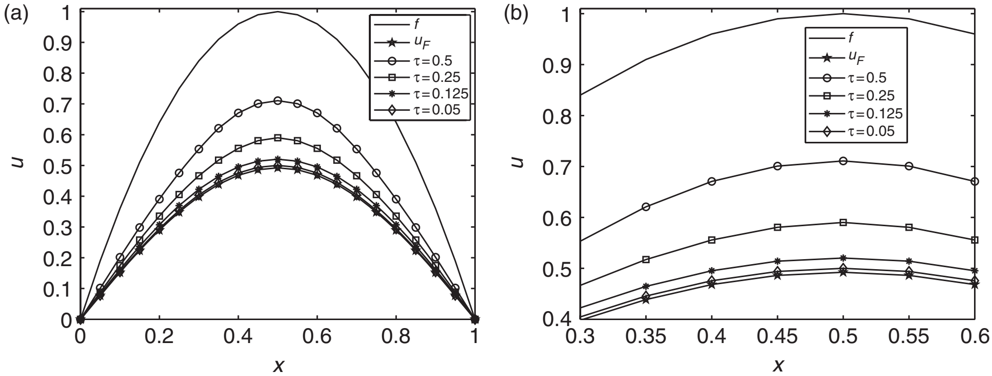

Figure 1. The effect of τ on the solution of (5).

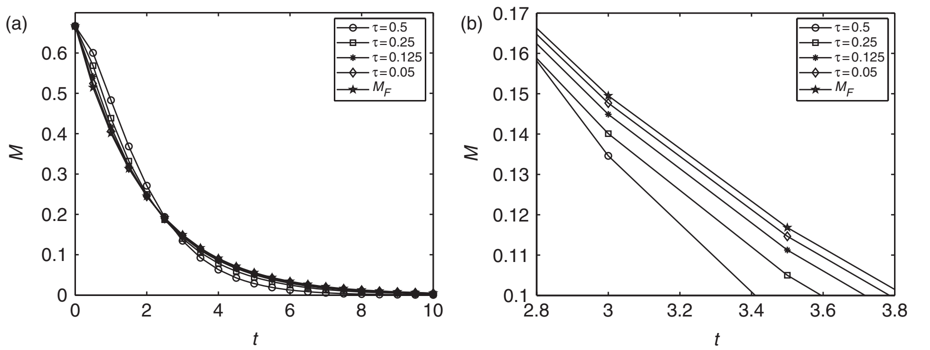

Figure 2. The effect of τ on the total amount of diffusing substance defined by (5).

substance at time t, $M(t, \tau)$, defined by (22), and for the total amount of diffusing substance emerging at the right boundary point $x = L$, $M_R(t, \tau)$, defined by (24), are computed truncating the Fourier series and by considering 1000 terms.

In all experiments, we consider a polymeric matrix containing a diffusing substance whose initial concentration is defined by $f(x) = 4(1 - x)x$ for $x \in [0, 1]$. The substance at the boundaries $x = 0$ and $x = 1$ is immediately removed and consequently boundary conditions $u_\ell = u_r = 0$, are considered.

In Figure 1, the graphs of the solution of (5) are plotted for $D = 0.1$, $t = 1$ and for different values of τ. The convergence (21) is illustrated in this figure and the delay effect of parameter τ can be clearly observed.

The behaviour of $M(t, \tau)$ when $t \in [0, 10]$, is illustrated in Figure 2 for $D = 0.05$. Convergence (23) is also illustrated by Figure 2. In Figure 2(b) the delay effect of parameter τ can be clearly observed.

The delay effect of τ on the total amount of the diffusing substance emerging at $x = 1$ for $t \in [0, 10]$ can be observed in Figure 3. Convergence (29) is clearly depicted.

The effect of the diffusion coefficient on the total amount of diffusing substance $M(t, \tau)$ defined by (22) for $\tau = 0.125$ and in the correspondent Fickian quantity M_F is illustrated in Figure 4(a). The increase of D implies as expected a decrease on $M(t, \tau)$ and on M_F. Consequently such increase implies an increase on the total amount of the diffusing

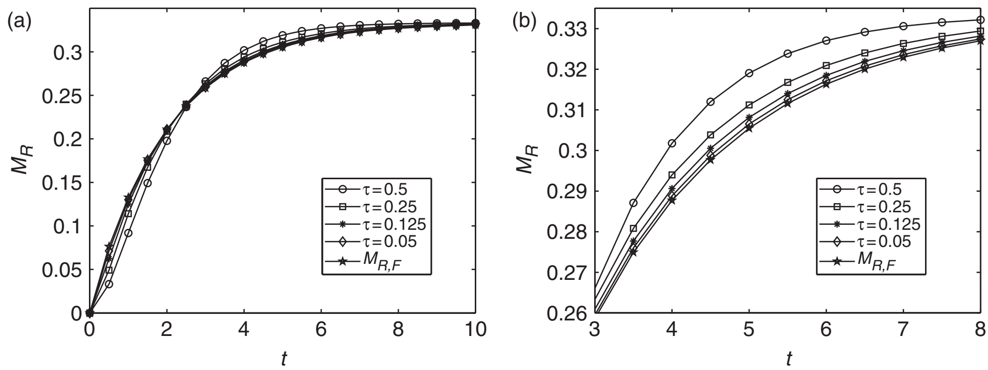

Figure 3. The effect of τ on the total amount of the diffusing substance emerging at $x=1$ defined by (5).

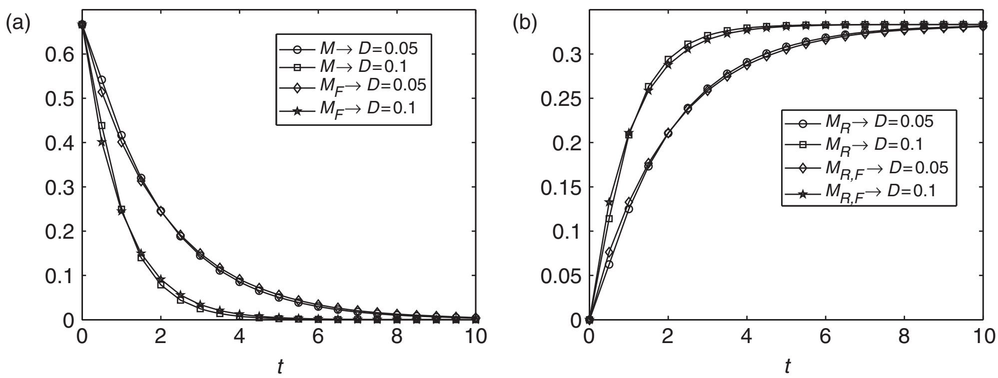

Figure 4. The effect of the diffusion coefficient D on the total amount of the diffusing substance in [0, 1] and on the total amount of the diffusing substance emerging at $x=1$.

substance emerging at $x=1$, $M_R(t,\tau)$, defined by (5) and on the correspondent Fickian quantity $M_{R,F}$. This behaviour is illustrated in Figure 4(b).

6. Conclusions

Diffusion phenomena are traditionally modelled by the diffusion equation. In certain phenomena, the numerical results obtained by simulation exhibit a certain delay effect when compared with experimental data. In order to take into account the delay effect in such phenomena integro-differential models depending on a delay parameter were considered in this article.

The well-posedness of the new diffusion IBVP was established. The existence of a solution was proved by construction.

As we mentioned before, the delay parameter τ was introduced to retard the diffusion phenomenon. Intuitively, when $\tau \to 0$ the solution of the integro-differential model should converge to the solution of the classical diffusion model. This fact was rigorously proved and the delay effect was numerically illustrated.

The total amount of diffusing substance and the total amount of diffusing substance entering or emerging on some boundary of the domain also depend on the delay parameter τ. The behaviour of these quantities when the delay parameter goes to zero has been studied and the convergence to the correspondent quantities obtained with the classical diffusion model was established. The delay effect of τ was numerically illustrated.

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