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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 behaviour 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.

Key words: Diffusion equation, Fick's law, parabolic equation, infinite speed, integro-differential equation, coupled problem for the concentration and mass flux.
MSC 2000: AMS 65M06, 65M20, 65M15

1 Introduction

The diffusion process is usually simulated using the classical diffusion equation

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

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

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

where the mass flux is split into $J = J_a + J_F$, J_a denotes the advection flux

$$J_a = vc, \tag{3}$$

and J_F is given by Fick's law

$$J_F = -D\nabla c. \tag{4}$$

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

$$D = D_m I + D_d \tag{5}$$

where D_m is associated with molecular diffusion and D_d represents the dispersive tensor that depends on the velocity v. It was observed in this case that (1) gives accurate results in laboratory environment for perfectly homogeneous media and a deviation of Fickian behaviour is presented when nonhomogeneous media are used (see for instance [5], [9], [8]). 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 [9] for some examples. In this paper we consider the use of differential equations for the mass flux J or for J_F that replaces 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 consider that the memory effect is only introduced in time and we present several mathematical models to replace the classical diffusion equation depending on the smoothness of the data. If the memory effect is introduced is space and time then the classical diffusion equation is replaced by a set of models presented in Section 3.

2 Memory in time

A common approach introduced in the literature to avoid the infinite propagation speed observed when the classical diffusion equation is used, is the replacement of Fick's law for J by differential relations.

2.1 Non Fickian contribution

We start by considering the replacement of Fick's law for the flux J by the following differential equation

$$\tau \frac{\partial J}{\partial t} + J = -D\nabla c, \tag{6}$$

where τ is a delay parameter (see [8]). This relation leads to

$$J(t) = -\frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D\nabla c(s)\, ds + J(0)e^{-\frac{t}{\tau}}. \tag{7}$$

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We remark that (6) can be obtained from

$$J(t+\tau) = -D\nabla c, \tag{8}$$

neglecting second order terms in a Taylor's expansion of J in τ. Equation (8) means that the dispersion mass flux is induced by the gradient of the concentration but at a delay time which means that a memory effect in time is introduced following this approach.

Combining (6) with (2) the following integro-differential equation is obtained

$$\frac{\partial c}{\partial t} + v \cdot \nabla c - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} \nabla \cdot (D\nabla c(s))\, ds + \nabla \cdot J(0) e^{-\frac{t}{\tau}} = f \ \text{ in } \Omega \times (0,T]. \tag{9}$$

The case when $J(0) = 0$ in equation (9) was largely studied from a mathematical point of view. Without being exhaustive we mention [1], [2], [3], [6], [7], [10], [11] and [12].

It should be pointed out that this approach requires the smoothness in space of J at $t = 0$. Moreover the integro-differential equation (9) is equivalent to an hyperbolic equation if the initial concentration is smooth enough. In fact, it can be shown that (9) is equivalent to

$$\frac{\partial^2 c}{\partial t^2} + v \cdot \nabla \frac{\partial c}{\partial t} + \frac{1}{\tau}\left(\frac{\partial c}{\partial t} + v \cdot \nabla c\right) = \frac{1}{\tau}\nabla \cdot (D\nabla c) + \frac{\partial f}{\partial t} + \frac{f}{\tau} \text{ in } \Omega \times (0,T], \tag{10}$$

with the initial conditions

$$\begin{cases} c(0) = c_0 \\ \dfrac{\partial c}{\partial t}(0) = -v \cdot \nabla c_0 + f(0) \end{cases} \text{ in } \Omega \tag{11}$$

where c_0 denotes the initial concentration.

In presence of nonsmooth data, the simulation of the concentration is obtained considering the coupled problem

$$\begin{cases} \dfrac{\partial c}{\partial t} + v \cdot \nabla c + \nabla \cdot J = f \\ \tau \dfrac{\partial J}{\partial t} + J = -D\nabla c \end{cases} \text{ in } \Omega \times (0,T], \tag{12}$$

defined in $\Omega \times (0,T]$, with the initial conditions

$$\begin{cases} J(0) = J_0 \\ c(0) = c_0 \end{cases} \text{ in } \Omega, \tag{13}$$

and convenient boundary conditions. Coupled problem (12), (13) can be easily discretized in space and time using an implicit-explicit approach.

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2.2 Fickian and non Fickian contributions

In what follows we assume that the mass flux admits the decomposition $J = J_F + J_{nF}$ where J_F is defined by Fick's law with a diffusion tensor D_F and a non Fickian contribution J_{nF} defined by (6) with a diffusion tensor D_{nF}. In this case J admits the integro-differential representation

$$J(t) = -D_F \nabla c(t) - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D\nabla c(s)\, ds + J_{nF}(0) e^{-\frac{t}{\tau}}. \tag{14}$$

and the integro-differential equation (9) is replaced by

$$\frac{\partial c}{\partial t} + v\cdot\nabla c - \nabla\cdot(D_F\nabla c) - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} \nabla\cdot(D_{nF}\nabla c(s))\, ds + \nabla\cdot J_{nF}(0)e^{-\frac{t}{\tau}} = f \ \text{ in } \Omega\times(0,T]. \tag{15}$$

Moreover (12) is in this case replaced by

$$\begin{cases} \dfrac{\partial c}{\partial t} + v\cdot\nabla c - \nabla\cdot(D_F\nabla c) - \nabla\cdot J_{nF} = f \\ \tau\dfrac{\partial J_{nF}}{\partial t} + J_{nF} = -D_{nF}\nabla c \end{cases} \quad \text{in } \Omega\times(0,T]. \tag{16}$$

3 Memory in time and space

3.1 Non Fickian contribution

To introduce memory in space and time, it is necessary to introduce in equation (6) spatial derivatives. In [5] the following equation for one dimensional domain was considered

$$\tau\frac{\partial J}{\partial t} + \tau(v\cdot\nabla)J + J = -D\nabla c. \tag{17}$$

If we neglect the two first terms of the first member of (17) then we recover the classical Fick's law.

Using the method of characteristics in (17) we obtain for the dispersion mass flux the following expression

$$J(x,t) = e^{-\frac{t}{\tau}} J(0) - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D\nabla c(x + v(s-t), s)\, ds. \tag{18}$$

This equation can be obtained from

$$J(x+\tau v, t+\tau) = -D\nabla c(x,t) \tag{19}$$

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neglecting second order terms in a convenient Taylor's expansion. Equation (19) reflects the memory effect in space and time: the mass flux at $x + \tau v$ at time $t + \tau$ is related with the gradient of the concentration at a delayed position x and at a delayed time t.

From equation (2) and (19) we obtain the following integro-differential equation

$$\frac{\partial c}{\partial t} + v \cdot \nabla c - \frac{1}{\tau} \int_0^t e^{-\frac{t-s}{\tau}} \nabla \cdot (D \nabla c(x + v(s-t), s))\, ds + \nabla \cdot J(0) e^{-\frac{t}{\tau}} = f \text{ in } \Omega \times (0, T], \quad (20)$$

which requires smoothness on J at $t = 0$. The numerical simulation of (20) 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.

We establish in what follows an hyperbolic equation combining (17) with the mass conservation equation (2). From (2) we obtain

$$\nabla \cdot J = -\frac{\partial c}{\partial t} - v \nabla c + f, \quad (21)$$

$$\nabla \cdot ((v \cdot \nabla) J) = -v \cdot \nabla \frac{\partial c}{\partial t} - v \cdot \nabla (v \cdot \nabla c) + v \cdot \nabla f, \quad (22)$$

and

$$\nabla \cdot \frac{\partial J}{\partial t} = -\frac{\partial^2 c}{\partial t^2} - v \cdot \nabla \frac{\partial c}{\partial t} + \frac{\partial f}{\partial t}. \quad (23)$$

Furthermore, from (17) we also have

$$\nabla \cdot J + \tau \nabla \cdot \frac{\partial J}{\partial t} + \tau \nabla \cdot ((v \cdot \nabla) J) = -\nabla \cdot (D \nabla c). \quad (24)$$

Replacing (21)-(23) in (24) we obtain the following third order hyperbolic equation with mixed derivatives

$$\frac{\partial^2 c}{\partial t^2} + 2v \cdot \nabla \frac{\partial c}{\partial t} + \frac{1}{\tau} \Big(\frac{\partial c}{\partial t} + v \cdot \nabla c - \nabla \cdot (D \nabla c) \Big) + v \cdot \nabla (v \cdot \nabla c) = \frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{f}{\tau} \quad (25)$$

in $\Omega \times (0, T]$. We point out that the establishment of (25) requires smooth data and it should be complemented with the initial conditions

$$\begin{cases} \dfrac{\partial c}{\partial t}(0) = v_0 \\ c(0) = c_0 \end{cases} \text{ in } \Omega. \quad (26)$$

In presence of non-smooth data, the simulation of the concentration and mass flux is obtained considering the coupled problem

$$\begin{cases} \dfrac{\partial c}{\partial t} + v \cdot \nabla c + \nabla \cdot J = f \\ J + \tau \dfrac{\partial J}{\partial t} + \tau (v \cdot \nabla) J = -D \nabla c \end{cases} \text{ in } \Omega \times (0, T], \quad (27)$$

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defined in $\Omega \times (0, T]$, with the initial conditions (13) and convenient boundary conditions. Coupled problem (27), (13) can be easily discretized in space and time using an implicit-explicit approach.

3.2 Fickian and non Fickian contributions

In what follows we assume that the mass flux admits the decomposition $J = J_F + J_{nF}$ where J_F is defined by Fick's law with a diffusion tensor D_F and a non Fickian contribution J_{nF} defined by (17) with a diffusion tensor D_{nF}. In this case J admits the integro-differential representation

$$J(x,t) = e^{-\frac{t}{\tau}} J_{nF}(0) - D_F \nabla c(x,t) - \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D_{nF} \nabla c(x + v(s-t), s)\, ds, \qquad (28)$$

and the integro-differential equation (20) is replaced by the following one

$$\begin{aligned} \frac{\partial c}{\partial t} + v \cdot \nabla c - \nabla \cdot (D_F \nabla c) \quad & -\frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} \nabla \cdot (D_{nF} \nabla c(x + v(s-t), s))\, ds \\ & + \nabla \cdot J_{nF}(0) e^{-\frac{t}{\tau}} = f \ \text{ in } \Omega \times (0,T]. \end{aligned} \qquad (29)$$

In this case the hyperbolic equation (25) is replaced by

$$\begin{aligned} \frac{\partial^2 c}{\partial t^2} + 2v \cdot \nabla \frac{\partial c}{\partial t} \quad & -\nabla \cdot \left(D_F \nabla \frac{\partial c}{\partial t} \right) + \frac{1}{\tau}\left(\frac{\partial c}{\partial t} + v \cdot \nabla c - \nabla \cdot (D_F \nabla c) - \nabla \cdot (D_{nF} \nabla c) \right) \\ & + v \cdot \nabla (v \cdot \nabla c) - v \cdot \nabla (\nabla \cdot (D_F \nabla c)) = \frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{f}{\tau} \ \text{ in } \Omega \times (0,T], \end{aligned} \qquad (30)$$

and (27) takes the form

$$\left\{ \begin{array}{l} \dfrac{\partial c}{\partial t} + v \cdot \nabla c - \nabla \cdot (D_F \nabla c) + \nabla \cdot J = f \\ \dfrac{\partial J}{\partial t} + (v \cdot \nabla) J + \dfrac{1}{\tau} J = -\dfrac{D_{nF}}{\tau} \nabla c \end{array} \right. \quad \text{in } \Omega \times (0,T]. \qquad (31)$$

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References

[1] A. Araújo, J.R. Branco and J.A. Ferreira, *On the stability of a class of splitting methods for integro-differential equations*, Appl. Numer. Math. **59** (2009) 436–453.

[2] J.R. Branco, J.A. Ferreira and P. de Oliveira, *Numerical methods for the generalized Fisher-Kolmogorov-Petrovskii-Piskunov equation*, Appl. Numer. Math. **57** (2007) 89– 102.

[3] J.A. Ferreira and P. de Oliveira, *Memory effects and random walks in reaction transport systems*, Appl. Anal., **86** (2007) 99–118.

[4] J.A. Ferreira and P. de Oliveira, *Qualitative analysis of a delayed non Fickian model*, Appl. Anal. **87** (2008) 873–886.

[5] S.M. Hassahizadeh, *On the transient non-Fickian dispersion theory*, Transp. Porous Media **23** (1996) 107–124.

[6] Y. Lin, *Semi-discrete finite element approximations for linear parabolic integrodifferential equations with integrable kernels*, J. Integral Equations Appl. **10** (1998) 51–83.

[7] Y. Lin, V. Thomée and L.B. Wahlbin, *Ritz-Volterra projections to finite-element spaces and applications to integrodifferential and related equations*, SIAM J. Numer. Anal., **28** (1991) 1047–1070.

[8] C. Maas, *A hyperbolic dispersion equation to model the bounds of a contaminated groundwater body*, J. Hydrol. **226** (1999) 234–241

[9] S. P. Neuman and D.M. Tartakowski *Perspective on theories of non-Fickiantransport in heterogeneous media*, Adv. Water. Resour. **32** (2009) 670–680.

[10] A.K. Pani and T.E. Peterson, *Finite element methods with numerical quadrature for parabolic integro-differential equations*, SIAM J. Numer. Anal. **33** (1996) 1084–1105.

[11] R.K. Sinha, R.E. Ewing and R.D. Lazarov, *Some new error estimates of a semidiscrete finite volume method for a parabolic integro-differential equation with non-smooth initial data*, SIAM J. Numer. Anal. **43** (2006) 2320–2344.

[12] V. Thomée and N-Y. Zhang, *Error estimates for semidiscrete finite element methods for parabolic integro-differential equations*, Math. Comp. **53** (1989) 121–139.