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Anomalous diffusion in porous media

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ABSTRACT

In this paper, an incompressible single phase and single component flow in a porous media presenting a non-Fickian 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 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:

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

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

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

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

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

where c and $\mathbf{J}$ represent the concentration of the injected fluid and the mass flux, respectively. 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,

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

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

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

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

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

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

In order to compute the unknowns ρ, p, $\mathbf{v}$, ϕ and c, Eqs. (1)–(3) are complemented by some state equations or constitutive relations. For instance in [2], different state equations are summarised 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 Eq. (5) has been largely considered in the numerical simulation of fluid flows in several contexts as can be seen for instance in [2–7] and in the references therein.

The main theoretical objection to use Eq. (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 ∇c that includes additional terms. This problem was also observed when high pressure gradients are present [9–11]. Several approaches have been considered in the literature to overcome these objections to use (5). We mention, without being exhaustive, the papers [8,9,11–23].

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 discretise 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 non-Fickian 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 summarise 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 non-Fickian 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 [24–26], 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 Eq. (5) is its replacement by the following nonlocal time integro-differential equation:

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

where $\mathcal{A}$ and $\mathcal{B}$ are second order differential operators with respect to the spatial variables, K_{er} represents a time convolution kernel and f is a reaction term [12–17,19]. Numerical methods for initial values problems defined by (7) were largely studied and a huge collection of methods is now available, see for example [28–41].

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

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

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

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