A Travelling Wave Solution for Nonlinear Colloid Facilitated Mass Transport in Porous Media

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Abstract. Colloid facilitated solute transport through porous media is investigated. Sorption on the matrix is modelled by the linear equilibrium isotherm whereas sorption on colloidal sites is regulated by nonlinearly equilibrium *vs* nonequilibrium. A travelling wave-type solution is obtained to describe the evolution in both the liquid and colloidal concentration.

Keywords: Nonlinear transport · Colloids · Travelling wave

1 Introduction

Aquifers' contamination and adverse effects on the environment have become a matter of considerable concern. Hence, it would be desirable having a predicting model to asses the effects of such a contamination risk [13]. A large number of mathematical models have been developed in the past [11,12,15]. Current models often emphasize either physical or chemical aspects of transport [2,8]. However, a general approach relies upon multicomponent transport modelling, and it has been only recently formulated in [6]. In this case, both adsorption and complexation in solution were taken into account along with precipitation/dissolution phenomena. In particular, being concerned with complex chemistry, such a model comes with non linear transport equations. The main interest related to the solution for such a system of `PDE`s is that it allows one to analyze the sensitivity of mass transport to the variation of different parameters. Unfortunately, generally analytical (closed form) solutions are not achievable, and concurrently one has to resort with numerical approximation. However, such a stand point may arise two serious issues. One is about the discretization in order to suppress instability and numerical dispersion [9]. The other is that in some situations (typically at the very beginning of the transport process) very steep concentration(s) gradients may develop. To accurately monitor these gradients, very fine discretizations may be necessary: an undesirable

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situation in view of computational times [4]. Alternatively, one can introduce a few approximations which enable one to gain analytical solution. In particular, in the present paper a travelling wave solution is derived for the case of colloid facilitaed mass transport with nonlinear sorption/desorption.

2 The Transport Model

We consider steady flow with constant velocity U in a one dimensional porous medium that carries simultaneously solute and colloidal particles. In such a system the mass flux vectors for the colloids and solute are

$$J_c\left(z,t\right)=nC_c\left(z,t\right)U_c\left(z,t\right), \quad J\left(z,t\right)=nC\left(z,t\right)U\left(z,t\right)-\overline{D}\,\frac{\partial C\left(z,t\right)}{\partial z} \tag{1}$$

respectively, where C_c and C are the concentrations (per unit volume of fluid) of colloidal and solute particles, $\overline{D}$ is the pore scale dispersion and n the porosity. Generally, advection colloidal velocity U_c is larger than U, due to “exclusion phenomena”. We model this ‘exclusion’ process by assuming that U_c depends linearly upon U through a constant coefficient $R_e \geq 1$, i.e. $U_c = R_e U$. Colloidal generation/removal is quantified by the mass balance equation for colloidal particles. However, in the context of the present paper we neglect both generation and removal, such that one can assume that the concentration C_c of colloidal particles is uniform. The applicability of such an assumption is throughly discussed in [5].

Let S denote the solute concentration on colloids, defined per unit colloidal concentration; the actual solute concentration C_c^s on colloidal particles is SC_c. Furthermore, we denote with N the solute concentration (mass of sorbed solute per unit bulk volume) sorbed on the porous matrix. Thus, the total solute concentration writes as $C_t = n\left(C + C_c^s\right) + N$, and concurrently the (solute) mass balance equation is

$$\frac{\partial}{\partial t}\left[n\left(C+C_c^s\right)+N\right]+\frac{\partial}{\partial z}\left(J_c+J\right)=0. \tag{2}$$

Substitution of (1) into (2) leads to the reaction diffusion equation

$$\frac{\partial C}{\partial t}+\frac{\partial C_c^s}{\partial t}+U\frac{\partial}{\partial z}\left(R_e C_c^s+C\right)=-\frac{1}{n}\frac{\partial N}{\partial t}+D\frac{\partial^2 C}{\partial z^2} \qquad \left(D=\frac{\overline{D}}{n}\right) \tag{3}$$

where, for simplicity, we have regarded n and $\overline{D}$ as constant. Generally, both C_c^s and N depend upon C in a very complex fashion, however we shall assume that sorption on the porous medium is governed only by the linear equilibrium model, i.e. $N = nK_d\,C$ (K_d is the linear partitioning coefficient between the fluid and sorbed phase), and we mainly focus on the effect of mass exchange between the fluid and colloidal solute concentration. For this reason, we consider a quite general dependence of C_c^s upon C accounting for a nonlinear mass exchange, i.e.

$$\frac{\partial}{\partial t} C_c^s = L\left[\varphi\left(C\right) - C_c^s\right], \tag{4}$$

being L a given rate transfer coefficient. We assume that solute is continuously injected at $z = 0$:

$$C\left(0, t\right) = C_0, \tag{5}$$

whit zero initial C-concentration. The nonlinear reaction function φ describes the equilibrium between the two phases, and its most used expressions are those of Langmuir and Freudlich [8]. When kinetics is fast enough, i.e. $L \gg 1$, the left hand side of (4) may be neglected, up to a transitional boundary layer [10], therefore leading to a non linear equilibrium sorption process.

3 Travelling Wave Solution

Overall, the system of Eqs. (3)–(4) can not be solved analytically. To obtain a simple solution (which nevertheless keeps the main physical insights), we consider a travelling wave type solution. Specifically, we assume that a travelling wave solution, that generally occurs after a large time. This allows one to assume that C at the inlet boundary is approximately equal to the feed concentration C_0, so that the initial/boundary conditions may be approximate as follows

$$C(z,t) \simeq \begin{cases} C_0 & \text{for } z = -\infty \\ 0 & \text{for } z = +\infty, \end{cases} \tag{6}$$

for any $t \geq 0$. We introduce the moving coordinate system $\eta = z - \alpha t$, where α represents the constant speed of the travelling wave (that will be determined later on). We assume that each concentration, both in the liquid and in the colloidal phase, moves with the same velocity α, which authorizes to write $C\left(z,t\right) = C\left(\eta\right)$ and $C_c^s\left(z,t\right) = C_c^s\left(\eta\right)$. Of course this approximation works better and better as the time increases. With these assumptions, the system (3)–(4) is reduced to an `ODE`-problem

$$\begin{cases} -\alpha \dfrac{\mathrm{d}}{\mathrm{d}\eta}\left(RC + C_c^s\right) + U\dfrac{\mathrm{d}}{\mathrm{d}\eta}\left(C + C_c^s\right) = 0 \\[2ex] -\alpha \dfrac{\mathrm{d}}{\mathrm{d}\eta} C_c^s = L\left[\varphi\left(C\right) - C_c^s\right] \end{cases} \tag{7}$$

with boundary conditions given by

$$C\left(-\infty\right) = C_0, \qquad C\left(+\infty\right) = 0 \tag{8}$$

$$C_c^s\left(-\infty\right) = \varphi_0, \qquad C_c^s\left(+\infty\right) = \varphi\left(0\right) = 0, \tag{9}$$

where $\varphi_0 \equiv \varphi\left(C_0\right)$. We now identify the wave velocity α by integrating the first of (7) over η

$$-\alpha\left(RC+C_c^s\right)+U\left(C+C_c^s\right)=A=\text{const.} \tag{10}$$

From boundary conditions (8)–(9), one has

$$A=0 \quad \Rightarrow \quad \alpha=U\left(\frac{C_0+\varphi_0}{RC_0+\varphi_0}\right). \tag{11}$$

that inserted in (7) yields, after some algebra, the following boundary value problem for C:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}\eta}C=\tau_0\left[\dfrac{\varphi_0}{C_0}C-\varphi\left(C\right)\right] \\ C\left(-\infty\right)=C_0, \quad C\left(+\infty\right)=0, \end{cases} \tag{12}$$

with the constant τ_0 defined as:

$$\tau_0=\frac{L}{\alpha}=\frac{L}{U}\left(\frac{\varphi_0+RC_0}{\varphi_0+C_0}\right). \tag{13}$$

Solution of (12) is possible if $\varphi\equiv\varphi\left(x\right)$ is a "convex" isotherm (i.e. $\mathrm{d}^2\varphi/\mathrm{d}x^2<0$). This is always the case for Freundlich/Langmuir type φ-function. Moreover, the presence of the reaction rate L gives smooth concentration profiles that become steeper and steeper as L increases, in particular for $L\to\infty$ solution of (12) asymptotically behaves as the one pertaining to the (nonlinear) equilibrium [8]. For the application to the quantification of the pollution risk, it is important to quantify the extent of the concentration front S_f. This latter exists if and only if

$$\int_0^{\varepsilon}\frac{\mathrm{d}x}{\varphi\left(x\right)}<\infty \qquad \text{for any} \quad \varepsilon>0. \tag{14}$$

The differential equation in (12) is expressed in integral form upon integration with respect to an arbitrary reference $C\left(\eta_r\right)=C_r$. The final result is

$$\tau_0\left(\eta_r-\eta\right)=\int_C^{C_r}\frac{\mathrm{d}x}{\dfrac{\varphi_0}{C_0}x-\varphi\left(x\right)}=G\left(C,C_r\right), \tag{15}$$

being the shape of the G-function depending upon the structure of the reaction function φ. Since the solution (15) is given as function of an arbitrary reference value $C_r\equiv C\left(\eta_r\right)$, it is important to identify the position η_r pertaining to such a concentration value. The adopted approach relies on the method of moments [1, 3,7]. In particular, we focus on the zero-order moments [L], i.e.

$$\eta_X=\frac{1}{C_0}\int_{-\infty}^{+\infty}\mathrm{d}\eta\, C\left(\eta\right), \qquad \eta_Y=\frac{1}{\varphi_0}\int_{-\infty}^{+\infty}\mathrm{d}\eta\,\varphi\left(\eta\right). \tag{16}$$

Before proceeding further, we wish noting here that when the number (say n) of unknown parameters is greater than 1, one has to sort with moments of order $0, 1, \ldots, n-1$. The moment η_X can be regarded as the distance along which C has increased from 0 to C_0 (at a fixed time t). A similar physical insight can be attached to the moment η_Y pertaining to the sorbed concentration on colloidal sites. While integrals (16) are not bounded, their difference it is. Indeed, integration from $\eta = -\infty$ to $\eta = +\infty$ of the `ODE` in (12) by virtue of (16) leads to $\eta_Y - \eta_X = \frac{C_0}{\tau_0\,\varphi_0}$. We can now focus on how to use moments (16) to identify the reference point η_r. Thus, we integrate (15) from 0 to C_0, and division by C_0 results in $\eta_r - \eta_X = \frac{\widetilde{G}}{\tau_0\,C_0}$, with $\widetilde{G} = \int_0^{C_0} \mathrm{d}x\, G\,(x, C_r)$. Once $\widetilde{G}$ has been computed, the reference position is uniquely fixed.

4 Concluding Remarks

A travelling wave solution for colloid facilitated mass transport through porous media has been obtained. A linear, reversible kinetic relation has been assumed to account for mass transfer from/toward colloidal particles. This leads to a simple `BV`-problem, that can be solved by means of a standard finite difference numerical method. The present study is also the fundamental prerequisite to investigate the dispersion mechanisms of pullatants under under (more complex) flow configurations along the lines of [14]. Some of them are already part of ongoing research projects.

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