

Study of the transport modeling by diffusion of pollutants through porous materials

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ABSTRACT

This paper presents how distance function dispersal produces diffusion range expansion of the contamination. We construct a stratified diffusion model, which describes the dynamics of the size distribution of colonies created by distance migrants of metal ions. The model consists of a Fick's equation combined with a Navier-stokes. The model provides an estimate of range expansion in terms of the rate adsorption due to neighborhood diffusion, the leap time and the geometric form. The results explain various types of nonlinear range expansion observed in materials or biomaterials.

Keywords: Diffusion; Fick's; Navier-Stokes.

1. INTRODUCTION

Mathematical modeling for contamination diffusion constitutes an influential predictive tool to have a basic understanding of bio-transport processes. Although mathematical modeling is theoretical in nature. However, the results established to lead realistic outcomes once compared and verified empirically. In the absence of our experiments, a good number of mathematical models and numerical simulations were carried out with an efficiency up to a large extent.

The theoretical thrust of this paper is within the genre of diffusion model research which presents an efficient methodology for analyzing and predicting diffusion patterns. Our objective is to improve upon standard forecasting methods for pore diffusion, which tend to rely on the premise of analogous diffusion-like effects and patterns across materials or biomaterials [1]. The diffusion model has been applied to different domains from physics, chemicals and biologics essentially including the study of metal ions transport through the pores diffusion is complementary to adsorption [2-5].

2. MATERIALS AND METHODS

2.1. Transport equations.

The governed partial differential equation of pollutant's transport was developed on the basis of the processes for diffusion, and sorption without degradation of pollutants [8]. The equation can be written as follows:

$$\frac{dC_t}{dt} = D_{int} \cdot \frac{d^2C}{dx^2} - v \frac{dC}{dx} - \frac{\rho_p}{\eta} k_p \frac{dC_t}{dt} \quad (1)$$

where C denotes the aqueous phase concentration of the pollutant (mM), t is the operating time (min), x is the vertical distance from the top of column (cm), D_h is the longitudinal or axial hydrodynamic dispersion coefficient (cm²/min), v_{pw} is the pore water velocity or interstitial velocity (cm/min).

The equation can be rearranged to become:

$$\left(1 + \frac{\rho_p}{\eta} k_p\right) \frac{dC_t}{dt} = D_{int} \cdot \frac{d^2C}{dx^2} - v \frac{dC}{dx} \quad (2)$$

Competitive adsorption occurs when some species adsorb to the same adsorption sites on a surface [20-21]. This often happens in infiltration systems where different contaminants can compete for sites on the biomaterial or material [5-6]. Mathematical modeling can be used to resolve these problems and can aid in the design and in predicting future conditions such as distributions of species within a porous.

The diffusion model of metal transport in porous media is computationally more efficient [7]. But, it relies heavily on phenomenological descriptions of transport and adsorption processes and requires knowledge of the effective properties of the medium (geometric form, porosity, effective diffusion coefficient, effective surface area, etc.).

In this paper, we present a [17-18]. particle theoretical model of transport and adsorption. Diffusion is a mesh-free modeling technique that uses a law Fick's to the model fluid dynamics systems as a discrete system of particles.

The expression $\left(1 + \frac{\rho_p}{\eta} k_p\right)$ can be defined as \hbar_f or retardation factor which can be given as:

$$\hbar_f = \left(1 + \frac{\rho_p}{\eta} k_p\right) \quad (3)$$

D_{ef} Is the Effective longitudinal dispersion coefficient which can be expressed as follows:

$$D_{ef} = \frac{D_{int}}{\hbar} \quad (4)$$

v_{ef} Is the Effective pollutant velocity which can be written as follows:

$$v_{ef} = \frac{v}{\hbar} \quad (5)$$

The substitution of Eq. (3), Eq (4), and Eq. (5) into Eq. (2) gives Eq. (6):

$$\frac{dC_t}{dt} = D_{ef} \cdot \frac{d^2C}{dx^2} - v_{ef} \cdot \frac{dC}{dx} \quad (6)$$

By applying an initial condition of $C(x,0) = 0$ for $x > 0$ and boundary conditions of $C(0,t) = C_0$ for $t \geq 0$ and $C(\infty,t) = 0$ for $t \geq 0$ where C_0 is the initial aqueous phase concentration of the pollutant. The analytical solution of eq (7) can then be expressed as

$$\frac{C}{C_0} = \frac{1}{2} \cdot [\operatorname{erfc}\left(\frac{x - v_{ef}t}{2\sqrt{D_{ef}t}}\right) + \exp\left(\frac{v_{ef}x}{D_{ef}}\right) \operatorname{erfc}\left(\frac{x + v_{ef}t}{2\sqrt{D_{ef}t}}\right)] \quad (7)$$

Where

$$\operatorname{erfc}(z) = 1 - \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\mu^2) d\mu$$

At successive times, the concentration distribution is shown in Fig. 1. It is clear that the system cures can be cutted in half by a plane at $x = 0$.

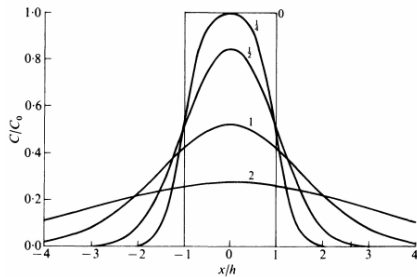


Figure 1. Concentration-distance curves for an extended source of limited extent. Numbers on curves are values of $(Dt/h^2)^{1/2}$.

The distribution is symmetrical about $x = 0$. Therefore eq. 5 also gives the distribution in a semi-infinite system. Such a system is realized in practice in the classical experiment in which a cylinder contains a layer of solution according to [15]. In practice,

3. RESULTS

3.1. Results interpretation.

Fig. 1. Shows the distribution which is symmetrical about $x = 0$. Therefore, eq. 5 also gives the distribution in a semi-infinite system. Such a system is realized in practice in the classical experiment in which a cylinder contains a layer of solution according to ref. [15]. In practice, this means that the concentration changes do not reach the top of the cylinder during the time of the experiment.

The solution of eq. 12 can be extended by superposition to cover a modified surface conditions such as $(j>(t) = C_0 + kt)$ and a non-zero initial concentration. Similar results have been found according to Crank. Fig. 2 is presented as follow:

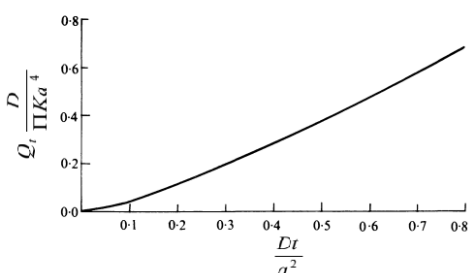


Figure 2. Sorption curve for cylinder with surface concentration kt .

this means that the concentration changes do not reach the top of the cylinder during the time of the experiment.

2.2. Surface concentration constant: initial distribution $f(r)$.

If the cylinder has a radius a the conditions are :

$$C = C_0, \quad r = a, \quad t \geq 0,$$

$$C = f(r) \quad 0 < r < a, \quad t = 0,$$

The solution is :

$$C = C_0 \left(1 - \frac{2}{a} \sum_{n=1}^{\infty} \frac{1}{\alpha_n} \frac{j_0(r\alpha_n)}{j_1(a\alpha_n)} \exp(-D\alpha_n^2 t) \right) + \frac{2}{a^2} \sum_{n=1}^{\infty} \exp(-D\alpha_n^2 t) \frac{j_0(r\alpha_n)}{j_1^2(a\alpha_n)} \int r f(r) j_0(r\alpha_n) dr \quad (8)$$

Where α_n are the positive roots. If the concentration is initially uniform throughout the cylinder $(r)=Ct$ eq. 9 reduces to:

$$\frac{C - C_i}{C_0 - C_i} = \left(1 - \frac{2}{a} \sum_{n=1}^{\infty} \exp(-D\alpha_n^2 t) \frac{j_0(r\alpha_n)}{\alpha_n j_1(a\alpha_n)} \right) \quad (10)$$

Numerical values are given by Williamson and Adams [12-14].

The corresponding expression for Q_t is:

$$Q_t = \left(\Pi K a^2 t - \frac{\Pi K a^4}{8D} + \frac{4\Pi K}{D} \sum_{n=1}^{\infty} \frac{\exp(-D\alpha_n^2 t)}{\alpha_n^4} \right) \quad (11)$$

After the simplification of Eq. (11) gives Eq. (12):

$$\frac{Q_t D}{\Pi K a^2} = \left(\frac{Dt}{a^2} - \frac{1}{8} + \frac{4}{a^4} \sum_{n=1}^{\infty} \frac{\exp(-D\alpha_n^2 t)}{\alpha_n^4} \right) \quad (12)$$

Generally, two major mechanisms, i.e. adsorption and diffusion, govern the transport of pollutants through the porous [19-22]. The Péclet number (R_{ef}), which is a dimensionless parameter, is applied to classify the dominant process of mechanisms between adsorption and diffusion. Where the parameter is defined in this case as:

$$R_{ef} = \frac{v_{ef} x}{D_{ef}} \quad (12)$$

In refs. [8-11] the authors have studied the relationship between R_{ef} and the effects of adsorption and diffusion mechanisms. Their study show that the adsorption process can be neglected when R_{ef} is much smaller than the unity. For R_{ef} , as defined by eq. 12, the computational error between eqs. 7 and 8 is less than 5% for $R_{ef} < 0.3$ and the error is lower than 2% for $R_{ef} < 0.1$. However, there is a wide range of computational errors up to the value 47 % for $R_{ef} > 1$. This means that the adsorption

process cannot be neglected when R_{ef} is equal or greater than the unity.

3.2. Interparticle diffusion.

The relation between the concentration and the adsorbed quantity is given by the eqs. 10 and 11, are shown in Fig.3. If the adsorption process is controlled by the interparticle diffusion, the interparticle diffusion model can be used to predict the diffusion behavior with the approximation that most adsorbent shapes are cylinders Fig.3.

This model assumes constant diffusivity in cylindrical coordinates and can be integrated with appropriate initial and boundary conditions.

The objective of this chapter is to develop a mathematical and an empirical model to study the transfer mechanism of pollutants containing in water through materials or biomaterials like sediments, plants and generally aquatic organisms.

4. CONCLUSIONS

The analytical model is equipped with the law Fick's and Navier-stokes variable diffusivity correlation, which can deal with both increasing and decreasing surface diffusion coefficients with increasing solid loading.

Due to the non-linearity of the boundary condition at the surface of the solid phase, analytical solutions are possible only for constant intraparticle diffusion coefficient. The weaknesses of the analytical diffusion-based models include the assumption of intern and externe surface diffusion coefficient. The application of

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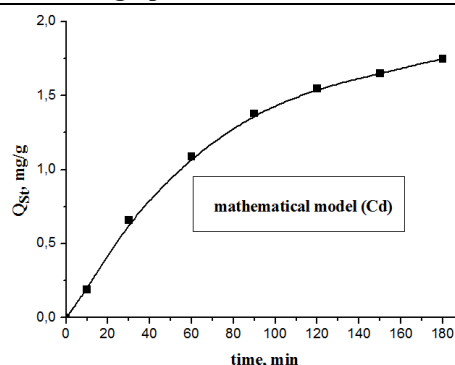


Figure 3. The amount of adsorption of Cadmium (Cd) obtained by mathematical model.

a simplified model, which is not in accordance with the system's physical reality, i.e. the constant diffusion coefficient is justified only when the objective is the estimation of the solid phase diffusion coefficient and conclusions should not be extended to the mechanism of the process.

Despite, reaction kinetics-based of adsorption models are easy to use and can provide some insights into the adsorption mechanism if applied carefully in well-designed experiments.

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