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SOLUTE TRANSPORT IN A DUAL POROSITY MEDIUM AND SCALE EFFECT OF DISPERSIVITY: PROPOSAL FOR A PROBABILISTIC EQUATION

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The probabilistic approach is used to simulate particle tracking in a dual porosity medium made of chalk granules with both intergranular and intragranular porosities. Dissolved solutes move by advection-dispersion in the intergranular pore space and may diffuse into intergranular pore space where the advective flux is negligible. It is shown that the particle tracking in the chalky medium is a nonmarkovian process, i.e. that the future position of a particle depends on its former positions. The probability density function of the position of the particle depends on a power of the distance. Using Einstein's rule for the dispersion coefficient, it is shown that the dispersivity exhibits a scale effect according to Mercado's result, i.e. a ballistic dispersion. Experiments by dye tracer tests on a column have been performed for different distances and discharges. The computed results are in good agreement with the experimental data.

INTRODUCTION

The probabilistic approach of particle tracking in the natural environment is not new. It was used successfully in sedimentary transport (Yang and Sayre, 1971), in solute transfer in porous medium without sorption phenomena (Todorovic, 1970) and in solutes transfer in fissured medium (Neretnieks, 2002). The modeling of particle tracking in a porous or fissured medium with mobile/immobile exchanges is very difficult when the partition coefficients are difficult to estimate. The modeling of such a process is carried out by the resolution of the dispersion equation which has to take into account the exchange phenomena between mobile and immobile water (Sudicky and Frind, 1982), (Maloszewski and Zuber ,1991), (Pang et al., 2003). According to these authors, the models are very sensitive to the partition coefficient values. The error on these coefficients must be very weak in order to keep the model reliable. Furthermore, particle tracking modeling using the classical solution of the dispersion equation leads to an increase in apparent dispersivity with the distance if exchange phenomena occur but are not taken into account. The aim of this paper is to derive dispersion equations from a Bayesian point of view which could be an alternative to the traditional numerical models of particle tracking simulation in media with dual porosity.

THEORETICAL ASPECT

According to the definition of conditional probability, the probability of a particle to be in the interval $\{x, x+\Delta x\}$ is:

$$P(x < X \le x + \Delta x) = P\left(X \le x + \Delta x \middle/ X > x\right).P(X > x) \tag{1}$$

If f is the probability density function (PDF) of the random variable x and F the corresponding cumulative distribution function (CDF), (1) can be expressed by :

$$\int_{x}^{x+\Delta x} f(\alpha)\,d\alpha = F(x+\Delta x) - F(x) \tag{2}$$

and

$$P(X > x) = \int_{x}^{+\infty} f(\alpha)\,d\alpha = 1 - \int_{0}^{x} f(\alpha)\,d\alpha = 1 - F(x) \tag{3}$$

The properties of the saturated medium and particularly its exchange capacity must be known to estimate $P\left(X \le x + \Delta x \middle/ X > x\right)$.

If mobile/immobile exchanges occur in a medium with a random distribution of immobile water sites, we consider that the probability $P\left(X \le x + \Delta x \middle/ X > x\right)$, for a particle to meet a site of immobile water when it has covered a distance x, increases when Δx increases and when the distance covered by the particle is longer. That can be expressed by a general probabilistic equation: $P\left(X \le x + \Delta x \middle/ X > x\right) = b.\Delta x.x^{a}$ (4)

By combining (1), (2),(3) and (4), the functions f and F are (Appendix 1) :

$$\begin{cases} F(x) = 1 - e^{-b.\frac{x^{1+a}}{1+a}} \\ f(x) = b.x^{a}.e^{-b.\frac{x^{1+a}}{1+a}} \end{cases} \tag{5}$$

The random variable x does not present a Markovian character (Appendix 2). The future state of the particle depends on the former state and the random variables x_i are dependent. The function f checks:

$$\int_0^{+\infty} f(x)\,dx = 1 \qquad \forall a \tag{6}$$

If one assumes the instantaneous injection of a mass M of particles, the mass conservation equation gives :

$$\int_0^{+\infty} C_R(x,t).S.\omega.dx = M \tag{7}$$

where S (L^2) is the cross section area of the medium and ω the kinematic porosity. $C_R(x,t)$ ($M.L^{-3}$) is the resident concentration at distance x and time t. The flow Q ($L^3.T^{-1}$) is the product of the average velocity U ($L.T^{-1}$), the cross section area and the kinematic porosity.

The following equation checks (7) :

$$C_R(x,t) = \frac{M}{S.\omega}..b..x^{a}.e^{-b.\frac{x^{1+a}}{1+a}} \tag{8}$$

The mass flux $J(t)$ ($M.T^{-1}$) at a time t and a distance x can be expressed by:

$$J(t) = C_R(x,t).\frac{x}{t}.S.\omega \tag{9}$$

x/t is the mean velocity of the particles which reach the distance x at time t.

The flux concentration can be expressed by:

$$C_F = \frac{J(t)}{Q} \tag{10}$$

Combining (8), (9) and (10), the equation of the flux concentration is:

$$C_F(x,t) = \frac{M}{Q.t}..b..x^{a+1}.e^{-b.\frac{x^{1+a}}{1+a}} \tag{11}$$

Equation (8) has to be used to compute the mean and modal distance and the space variance.

By solving $\frac{\partial C}{\partial x} = 0$

for (8), the modal distance, for which the concentration is the strongest, is:

$$x_{\text{mod}} = \left(\frac{a}{b}\right)^{\frac{1}{1+a}} \tag{12}$$

The mean distance, i.e. the centroid of the cloud of particles, is expressed by:

$$\bar{x} = U.t = \int_0^\infty x.f(x).dx = \frac{\Gamma\left(\frac{1}{1+a}\right).b^{-\frac{1}{1+a}}}{(1+a)^{\frac{a}{1+a}}} \tag{13}$$

Γ is the Gamma function. (13) makes it possible to express the coefficient *b*:

$$b = \left(\frac{k}{U.t}\right)^{1+a} \quad with \quad k = \frac{\Gamma\left(\frac{1}{1+a}\right)}{(1+a)^{\frac{a}{1+a}}} \tag{14}$$

Combining (11) and (14), Equation (11) can be rewritten:

$$C_F(x,t) = \frac{M}{Q.t}.\left(\frac{k.x}{U.t}\right)^{a+1}.\ e^{-\frac{\left(\frac{k.x}{U.t}\right)^{1+a}}{1+a}} \tag{15}$$

Equation (15) checks:

$$\int_0^{+\infty} C_F(x,t).Q.dt = M \tag{16}$$

While solving $\frac{\partial C}{\partial t} = 0$ in (15), the average velocity *U* and the maximum concentration can be determined according to *k*, the modal time t_m, the distance *x* and the power number *a*:

$$U = \frac{k.x}{t_m.(2+a)^{\frac{1}{1+a}}} \tag{17}$$

$$C_{\max} = .\frac{M}{Q..tm}.(2+a).e^{-\frac{2+a}{1+a}} \tag{18}$$

EXPERIMENTAL METHOD

We used tracer flow column experiments to test our probabilistic approach. The column length is 1934 mm and its diameter 90 mm. Two piezometers are located in the column; the first one is at 143 mm from the inlet, the second one at 825 mm from the first one. The tracer is injected with a syringe in the first piezometer. The injection is followed by a water flush to approximate a delta function input.

The tracer tests were carried out using a Senonian Chalk. The grain size range between 2 and 3.15 mm. 10.7 kg of chalk were used to fill the 12.2 liters of the column. Using a density value of 1590 kg/m^3 for chalk, the inferred total porosity is 45%.

The tracer tests were carried out for different discharges and masses of fluorescein (Tables 1 and 2). The power number a is computed by Equation (18) and k is computed by Equation (14). An example of comparison between computed concentrations (Equation (15)) and experimental concentrations is given in Figure 1 and shows a good fit between experimental and theoretical values. The k values range between 1.23204 and 1.24000 The a values range between 0.83117 and 0.94628. (Tables 1 and 2)

SCALE EFFECT OF THE DISPERSIVITY

The longitudinal variance of the cloud makes it possible to classify the dispersion:

$$\sigma_x^2 \propto t^{\alpha} \tag{19}$$

If α =1, the dispersion is fickian; if α <1, the dispersion is subdiffusive and if α>1, the dispersion is superdiffusive. In the particular case α = 2, the dispersion is ballistic.

Einstein's equation (Einstein, 1905) makes it possible to express the space variance and the dispersion coefficient:

$$D = \frac{1}{2}.\frac{d\sigma_x^2}{dt} \tag{20}$$

D is the longitudinal dispersion coefficient. Using Equation (5), the variance is:

$$\sigma_x^2 = \int_0^{\infty} \left(x - \bar{x}\right)^2 .f(x).dx = \left(U.t\right)^2.\left(\frac{\Gamma\left(\frac{3+a}{1+a}\right)}{\Gamma\left(\frac{1}{1+a}\right)^2}.\left(1+a\right)^2 - 1\right) \tag{21}$$

Equation (21) shows that the dispersion is ballistic.

According to (20), the longitudinal dispersion coefficient is:

$$D = U^2.t.\left(\frac{\Gamma\left(\frac{3+a}{1+a}\right)}{\Gamma\left(\frac{1}{1+a}\right)^2}.\left(1+a\right)^2 - 1\right) \tag{22}$$

The longitudinal dispersivity is:

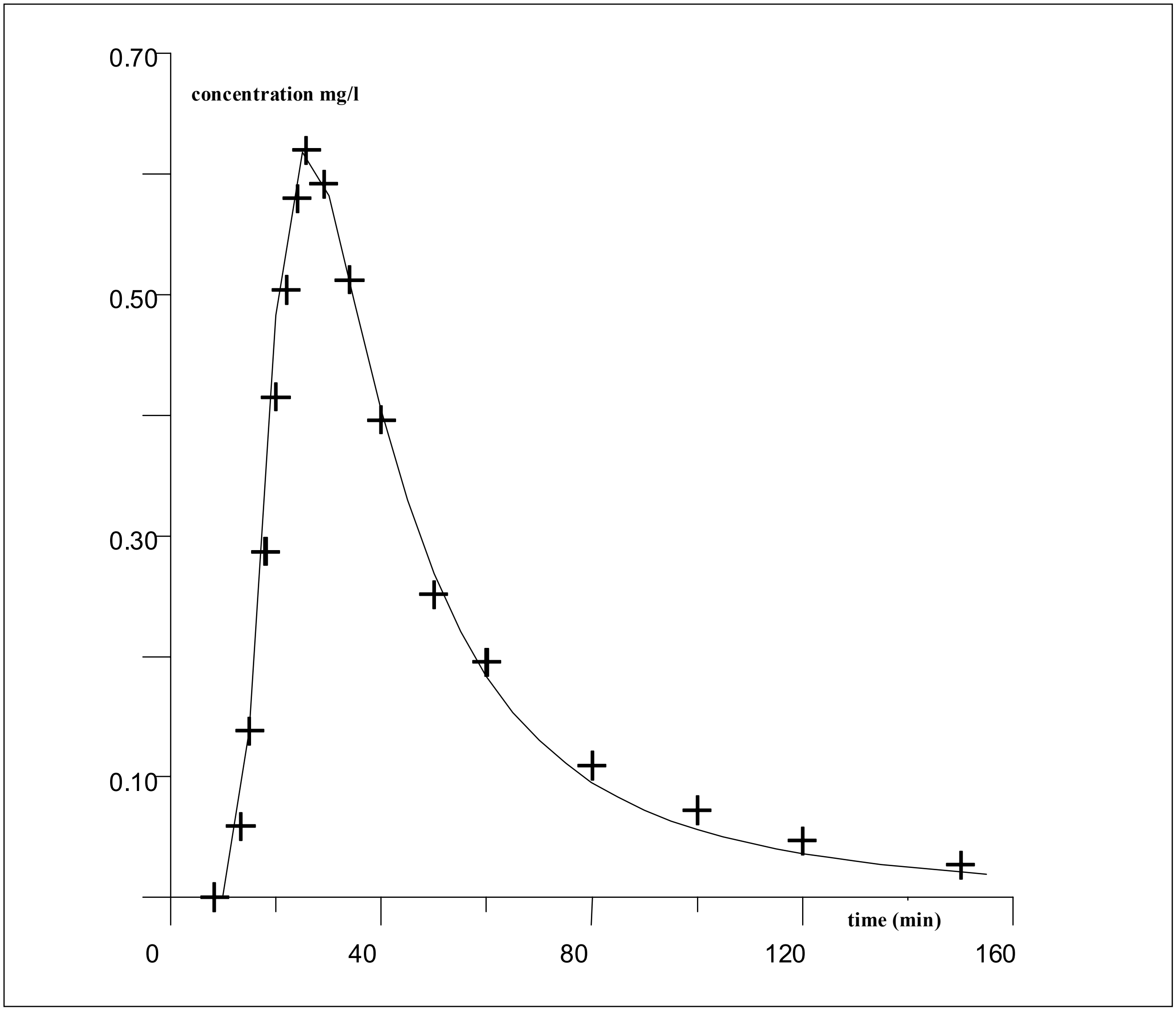

Figure 1. Experimental and computed concentrations versus time for tracer test in chalk. Q=148800 mm^3/min; X=1791 mm.

Table 1. Experimental and computed data for 1791 mm.

Q (mm^3 /min)	M (mg)	t_m (min)	Concentration max (mg/l)	a	k
6310	3.434	67	0.526	0.94628	1.23204
148800	3.892	25.8	0.62	0.85231	1.23890

Table 2. Experimental and computed data for 825mm.

Q (mm^3 /min)	M (mg)	t_m (min)	Concentration max (mg/l)	a	k
63160	3.434	27.6	1.18	0.86293	1.2400
148800	3.892	11.2	1.438	0.83117	1.23645

$$\alpha = \frac{D}{U} = U.t.\left(\frac{\Gamma\left(\frac{3+a}{1+a}\right)}{\Gamma\left(\frac{1}{1+a}\right)^2}.(1+a)^2 - 1 \right) \tag{23}$$

Equation (23) shows that the longitudinal dispersivity increases linearly with the mean travel distance *U.t* which is consistent with Mercado's result (Mercado, 1967) obtained for a stratified aquifer.

CONCLUSION

The probabilistic model presented in this paper reproduces laboratory tracer column experiments for granular materials with a dual porosity. Unlike complex numerical models, the probabilistic model seems not to be very sensitive to the partition coefficients used to calibrate the dispersion and sorption phenomena. However our results do not prejudge of the validity of the model on the field scale. Nevertheless, our experiments suggest that this model could be an alternative to the traditional numerical models. Using the Einstein's equation, the dispersivity has been derived and exhibits a scale effect. It increases linearly with the mean travel distance, that is consistent with Mercado's result (Mercado, 1967) obtained for a stratified aquifer. Work is in progress to test our model on more complex heterogeneous media.

REFERENCES

Einstein, A. 1905. Über die von der Molekularkinetischen Theorie der Wärme gefordete Bewegung von in ruhenden Flüssigkeiten suspendierten Teinchen. Ann. Phys.17: 539-560.

Maloszewski, P. And A. Zuber. 1991. Influence of matrix diffusion and exchange reactions on radiocarbon ages in fissured carbonate aquifers. Water Res. Res., Vol 27(8): 1937-1945.

Mercado, A. 1967. The spreading pattern of injected water in a permeability-stratified aquifer. In Proceedings of the International Association of Science Hydrology, Symposium of Haïfa, Publ. 72, 23-26, GentBrugge, Belgium.

Neretnieks, I. 2002. A stochastic multi-channel model for solute transport-analysis of tracer tests in fractured rock. J. Contam. Hydrol. Vol 55: 175-211

Pang, L., Goltz, M. and M. Close. 2003. Application of the method of temporal moments to interpret solute transport with sorption and degradation. J. Contam. Hydrol. Vol 60: 123-134

Sudicky, E.M and E.O Frind. 1982. Contaminant transport in fractured porous media : analytical solutions for a system of parallel fractures. Water Res. Res., Vol 18(6): 1634-1642.

Todorovic, P. 1970. On some problems involving a random number of random variables. Ann. Math. Statis., Vol 41(3): 1059-1063

Yang, C.T and W.W Sayre. 1971. Stochastic model of sediments dispersion. J. Hydraul, Div. Amer. Soc. Civil. Eng., Vol 97 (HYZ): 265-288

Appendix 1 :

$$P(x < X \le x + \Delta x) = P\left({X \le x + \Delta x} \middle/ {X > x} \right).P(X > x) = \int_x^{x+\Delta x} f(\alpha)\, d\alpha = F(x + \Delta x) - F(x)$$

$$P(X > x) = \int_x^{+\infty} f(\alpha)\, d\alpha = 1 - \int_0^x f(\alpha)\, d\alpha = 1 - F(x)$$

$$P\left({X \le x + \Delta x} \middle/ {X > x} \right) = b.\Delta x.x^a$$

$$F(x + \Delta x) - F(x) = b.\Delta x.x^a \left(1 - F(x)\right)$$

Let $G(x)$ = 1-$F(x)$ and Δx -> 0 :

$$-G'(x) = b.x^a.G(x) \Rightarrow G(x) = A.e^{-b.\frac{x^{1+a}}{1+a}}$$

If $F(0) = P(X \le 0) = 0$ then $F(x) = 1 - e^{-b.\frac{x^{1+a}}{1+a}}$ and $f(x) = b.x^a\, e^{-b.\frac{x^{1+a}}{1+a}}$

Appendix 2 :

$$P(X > x \cap X > x + \Delta x) = P\left({X > x + \Delta x} \middle/ {X > x} \right).P(X > x) = P(X > x + \Delta x)$$

If the cumulative distribution function is $F(x) = 1 - e^{-b.\frac{x^{1+a}}{1+a}}$, then :

$$P\left({X > x + \Delta x} \middle/ {X > x} \right) = \frac{P(X > x + \Delta x)}{P(X > x)} = e^{-\frac{b}{1+a}.\left((x+\Delta x)^{1+a} - x^{1+a}\right)}$$

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