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GROWTH OF THE DISPERSION COEFFICIENT WITH THE MEAN TRAVELLED DISTANCE IN POROUS MEDIA

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ABSTRACT

A general formulation of the transport equation of solutes in porous media is developed theoretically for a slug injection, with the assumption that the distribution of the velocities in the medium is gaussian, and that molecular diffusion is negligible.

The equivalent of the dispersion coefficient in the equation is then shown to be a function of time. Tracer experiments performed both in situ and in the lab seem to be in accordance with this hypothesis; as an example, this model is shown to give an excellent fit for the data published by Coats & al. in 1964, and for which these authors had developed the "dead end pore" model.

INTRODUCTION

The transport of solute in non-uniform porous media is currently described by the dispersion equation, which writes:

$$\operatorname{div}\,(\overline{\overline{D}}\ \operatorname{grad} C - UC) = \frac{\partial C}{\partial t} \qquad (1)$$

$\overline{\overline{D}}$: dispersion tensor, with principal directions parallel and orthogonal to the velocity,
C: concentration,
U: microscopic velocity.

The dispersion coefficients of the tensor $\overline{\overline{D}}$ are assumed to be functions of the velocity U only. However, a large number of authors (e.g. ref. 1,2,3) have recently questioned the validity of this model, both on the basis of theoretical developments and experimental data. It is well known, for instance, that the interpretation of a tracer test gives dispersion coefficients which increase as the distance between the input well and the observation well is increased: such a deviation from the classical model is refered to as the "scale effect".

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In this paper, we will first develop a different equation to represent the transport of solute in porous media, under certain simplifying assumptions, using a stochastic approach. We will then try to support this different formulation by interpreting tracer tests performed in the laboratory or in situ.

A SIMPLIFIED TRANSPORT EQUATION IN A STOCHASTIC FRAMEWORK

We will develop our equation in the ordinary space $\mathbb{R}^n$ (n = 1,2 or 3) with the *three following assumptions:*

a) the transport is governed by the velocity variations of the fluid in the porous medium, molecular diffusion is negligible;

b) the microscopic velocity field, U, which is unknown, can be regarded as a stationary random process, i.e. U is a vectorial stationary random function (SRF). We will further assume that the probability distribution function (PDF) of U is gaussian with n variables, and that U is conservative (div U = 0). This means that the flow is in steady state, with a constant porosity;

c) a slug of tracer is injected at time t = 0 at the origin $X_o = 0$ of the system.

In our notations, U and X are vectors, and U^i or X^i represent one of their components:

$$X = \begin{pmatrix} X^i \\ \vdots \\ X^n \end{pmatrix}$$

The lower index of a vector will denote the time: X_t.

The transport can be described by giving, as a function of time, the position X_t of a particle injected at t = 0 at the origin. As discussed in ref.3, this method of representing transport is equivalent to the determination, in the case of a slug injection, of the concentration C as a function of time and space, as in (1): C(X,t) is equal to the probability density of the particle at location X and time t.

With our assumption (a), the transport equation writes:

$$\frac{dX_t}{dt} = U(X_t) \tag{2}$$

Using the assumptions (b) for the velocity U, we will develop the differential equation which is verified by the probability density $\rho(X,t)$ of the particle (or by the concentration C in the case of a slug injection).

Let: $$V(t) = U(X_t)$$

Matheron (ref.4) has shown that if U is a SRF with a given PDF, then the condition div U = 0 is sufficient to insure that V is also a SRF with the same PDF as U in the time domain.

We can write (2) as:

$$X_t = \int_0^t V(\tau)\,d\tau \tag{3}$$

We then have:

$$E(X_t) = E\left[\int_0^t V(\tau)\,d\tau\right] = \int_0^t E[V(\tau)]\,d\tau = t\,E[V] = t\,E[U] = t\,\bar{U} \tag{4}$$

where $\bar{U} = E[U]$

$$K_t = \mathrm{var}\,[X_t] = E\,[(X_t - E(X_t))^T (X_t - E(X_t))]$$

$$= E\,(X_t^T X_t) - E\,(X_t)\,E\,({}^T X_t)$$

where ${}^T X = (X^1, \dots, X^n)$ is the transpose of X. Note that this variance is a n×n matrix.

$$K_t = E\left[\int_0^t V(\tau)\,d\tau \int_0^t {}^T V(\tau)\,d\tau\right] - t^2 \bar{U}^T \bar{U}$$

$$= \iint_0^t \{E[V(\tau)^T V(\tau')] - \bar{U}^T \bar{U}\}\,d\tau\,d\tau'$$

$$= \iint_0^t E\{[V(\tau) - \bar{U}]^T [V(\tau') - \bar{U}]\}\,d\tau\,d\tau'$$

$$K_t = \iint_0^t C(\tau - \tau')\,d\tau\,d\tau' = 2\int_0^t (t-\tau)\,C(\tau)\,d\tau \tag{5}$$

where C(t) is the n×n covariance matrix of the components of the velocity V, taken with a time lag t.

As we assume the SRF, U, to be a gaussian function with n variables, V is also gaussian and the integral X_t of V in (3) is also gaussian. Then, the PDF of the particle at location X and time t is given by:

$$\rho(X,t) = \frac{1}{(2\Pi)^{n/2}\sqrt{d}}\, e^{-P/2} \tag{6}$$

where d is the determinant of the variance matrix K_t given in (5),

$P = {}^T(X - t\bar{U})\, K_t^{-1} (X - t\bar{U})$

P is a positive quadratic form, the matrix of which is the inverse of the variance matrix K_t.

We will establish the partial differential equation which $\rho(X,t)$ verifies using the Fourier analysis of (6).

The Fourier transform over space of the PDF $\rho(X,t)$ is given by:

$$\mathcal{F}_S[\rho(X,t)] = \int_{\mathbb{R}^n} \rho(X,t)\, e^{iSX} dX = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \rho(X^1, \dots, X^n, t)\, e^{i(S_1 X^1 + \dots + S_n X^n)}\, dX^1 \dots dX^n$$

where $S = (S_1, \dots, S_n)$ is the Fourier variable vector.

One can show that:

$$\mathcal{F}_S[\rho(X,t)] = e^{itS\bar{U} - 1/2\, S K_t {}^T S} \tag{7}$$

The expected value of X_t has been taken here as in (4), and its variance matrix K_t is given in (5).

We can use the following properties of the Fourier transform. In the case of a regular function $f(X,t)$, we have:

$$\frac{\partial}{\partial t} \mathcal{F}_S[f(X,t)] = \mathcal{F}_S\left[\frac{\partial}{\partial t} f(X,t)\right] \tag{8}$$

$$\mathcal{F}_S\left(\frac{\partial f}{\partial X^j}\right) = -iS_j \mathcal{F}_S(f) \tag{9}$$

Here, we can write, according to (7) and (8):

$$\mathcal{F}_S\left(\frac{\partial \rho}{\partial t}\right) = \left(iS\bar{U} - \frac{1}{2} S \frac{\partial K_t}{\partial t} {}^T S\right) \mathcal{F}_S(\rho) \tag{10}$$

Applying (9) twice to (7):

$$\mathcal{F}_S\left(\frac{\partial \rho}{\partial X^j}\right) = -iS_j \mathcal{F}(\rho) \tag{11}$$

$$\mathcal{F}_S\left(\frac{\partial^2 \rho}{\partial X^j \partial X^k}\right) = -S_j S_k \mathcal{F}(\rho) \tag{12}$$

Combining equations (10) to (12), we obtain:

$$\mathcal{F}_S\left(\frac{\partial \rho}{\partial t}\right) = -\mathcal{F}_S\,(\text{grad}\,\rho\,\bar{U}) + \frac{1}{2}\mathcal{F}_S\left[\text{div}\left(\text{grad}\,\rho\,\frac{\partial K_t}{\partial t}\right)\right]$$

where grad ρ is the vector $\left(\frac{\partial \rho}{\partial X^1} \dots \frac{\partial \rho}{\partial X^n}\right)$ and div is the operator $\sum_j \frac{\partial}{\partial X^j}$

By applying $\mathcal{F}_S^{-1}$, we obtain:

$$\boxed{\frac{\partial \rho}{\partial t} = -\,\text{grad}\,\rho\bar{U} + \frac{1}{2}\,\text{div}\left(\text{grad}\,\rho\,\frac{\partial K_t}{\partial t}\right)} \tag{13}$$

which can also be written as:

$$\boxed{\frac{\partial \rho}{\partial t} = -\sum \bar{U}^j \frac{\partial \rho}{\partial X^j} + \frac{1}{2}\sum_j \sum_k \frac{\partial K^{jk}}{\partial t} \frac{\partial^2 \rho}{\partial X^j \partial X^k}} \tag{14}$$

where K^{jk} are the coefficients of the covariance matrix given in (5)

$$K^{jk} = \int_0^t\!\!\int_0^t E\{[V^j(\tau) - \bar{U}^j][V^k(\tau') - \bar{U}^k]\}\,d\tau\,d\tau' = 2\int_0^t (t-\tau)\,C^{jk}(\tau)\,d\tau$$

C^{jk} is a function of time, not of space, and:

$$\frac{1}{2}\frac{\partial K^{jk}}{\partial t} = \int_0^t C^{jk}(\tau)\,d\tau \tag{15}$$

$C^{jk}(\tau)$ is the covariance function of the components j and k of the velocity V, with a time lag τ.

This equation is only valid for a slug injection at t = 0 and X = 0, and not for any other initial conditions.

It is reasonable to assume that, in general:

$$\int_0^t C^{jk}(\tau)\,d\tau \rightarrow A^{jk} \quad \text{as} \quad t\rightarrow\infty$$

Transport will therefore be, in general, asymptotically diffusive, with a constant dispersion tensor, but only for a transient time sufficient for this integral to converge. This will normally be a function of the "correlation length" of the medium, i.e. the distance over which the velocities are correlated.

For early times, equations (13), (14) and (15) show that the "dispersion tensor" $\frac{\partial K_t}{\partial t}$ will vary with time, both in magnitude and in principal directions, as there is a priori no reason why these directions should remain constant when the coefficients vary.

A constant dispersion tensor could only occur if the covariance functions $C^{jk}(\tau)$ of the velocity components were Dirac functions, i.e. a medium displaying no correlations of the velocity components even for small time lags.

Can the theoretical tool developed here for the description of tracer movements be used in practice ? We will examine tracer tests in the field or in the lab which have been interpreted using this approach. For a slug injection, it has been found that equivalent dispersion coefficients seemed to be indeed a function of time, and not of space.

TIME DEPENDENCE OF DISPERSION COEFFICIENTS DURING TRACER TESTS

In situ

In 1978, A. Dieulin conducted a tracer test in the alluvial aquifer of the river Marne, at Torcy. After a slug injection of an electrolytic solution, observations were made at 5, 10 and 15 m from the injection point in the direction of the velocity, under natural flow conditions. Measurements were made by sampling and by in situ resistivity logging. These results have been interpreted, and presented in ref. 5, 6, 7. It was shown that the permeable base of each sedimentary sequence forms a "guide" in which the tracer plume moves forward. Each "guide" (height ∿ 0,30 m) can be regarded as an independent isotropic 2D medium, where an average spatial velocity $\bar{U}$ can be defined.

As a first hypothesis, it was assumed that the direction x of the velocity in each guide was the first principal direction of the dispersion tensor for all time, and that the distribution of the tracer in the medium X_t was gaussian with two variables, as in the above theory. Type curves were computed to determine the variance as a function of time of this distribution at each observation point. As observations were only available in the longitudinal direction, it was further assumed that:

$\bar{x} = t\,\bar{U}$ (movement of the centroïd of the plume)

$K_{xx} = 2t\,D_L(t)$ ($D_L(t)$ "temporal function" of longitudinal dispersion)

$K_{yy} = 2t\,D_T$ (D_T transverse dispersion coefficient, assumed constant)

It was found that $D_L(t)$ was unique for all observation points whereas the usual interpretation would give a different dispersion coefficient for each observation distance (Fig.1). Instead of a "scale effect", the present theory provides a more coherent "time effect" for the variation of the dispersion coefficients.

Other in situ tests performed earlier at Bonnaud (ref.8) were also interpreted with the same hypothesis, providing a more coherent explanation of the data with one unique "temporal function of longitudinal dispersion", instead of a scale effect (ref.5).

Laboratory tests on sediments columns

By integration of the distribution in y and z, the concentration is assumed to follow a 1D gaussian distribution, along the x longitudinal axis of the column for a slug injection. However, tests are usually done with a continuous injection of tracer. As our theory was established for the slug injection only, we assumed, with Gelhar and al. (ref.2), that a continuous injection can approximately be considered as a space convolution, from x = 0 to x = -∞, of slug injections in the medium. Assuming the existence of a longitudinal "temporal function" of dispersion, we then have:

$$C(X,t) = \frac{C_o}{2}\,\mathrm{erfc}\left[\frac{X-\bar{U}t}{2\sqrt{D_L(t)\cdot t}}\right] \qquad (16)$$

Data from Martin (ref.9) have shown that $D_L(t)$ can be decomposed as (ref.5):

$$D_L(t) = f(\bar{U})\,g(\bar{X})$$

f being only a function of $\bar{U}$, with $\bar{X} = \bar{U}t$ (mean travel distance) and g being only a function of $\bar{X}$, which we have defined as the "intrinsic function of dispersion".

This formulation has been applied to experimental data obtained by Coats et al. (ref.10) on a core made of consolidated sediments. They interpreted these data with the "dead end pore" model, but could not fit the experiments with the same model parameters at different velocities.

We chose the Coats et al. data as their "dead end pore" model can be regarded as a special case of our theory, the velocity distribution which they assumed in the medium being very simple: (i) zone with uniform velocity (mobile water); (ii) zone with zero velocity (dead end pores).

In our approach, the average velocity is L/t_o (core length divided by the time when $C/C_o = 0.5$). One can then determine the "temporal function of dispersion" as:

$$D(t) = \frac{(L-\bar{U}t)^2}{4t}\left[\mathrm{erfc}^{-1}\left(\frac{2C}{C_o}\right)\right]^{-2} \qquad (17)$$

Results are given Fig.2 for three different velocities ($\bar{U}_1 = .009$ cm/s, $\bar{U}_2 = .0525$ cm/s and $\bar{U}_3 = .202$ cm/s).

Assuming again that $D(t) = f(\bar{U})g(\bar{X})$, and taking $f(\bar{U}_2)/f(\bar{U}_1) = 4.1$ and $f(\bar{U}_3)/f(\bar{U}_1) = 20.66$, the three functions $g(\bar{X})$ can be shown to be almost identical (Fig.3). It should be noted that $f(\bar{U}_2)/f(\bar{U}_1) = (\bar{U}_2/\bar{U}_1)^{0.8}$ and $f(\bar{U}_3)/f(\bar{U}_1) = (\bar{U}_3/\bar{U}_1)^{0.97}$. The dependence of D(t) on velocity is almost linear, as it is for the usual dispersion coefficient. We will therefore take $f(\bar{U}_1) = \bar{U}_1$.

A unique intrinsic function of dispersion $g(\bar{x})$ has been selected in Fig.3 (solid line). Assuming the exact dependence on velocity, we compute the "temporal dispersion function" as:

$$D_i(t) = f(\bar{U}_i)\ g(\bar{X}) \qquad i = 1,2,3 \qquad \text{(3 runs)}$$

We were able to compute the theoretical responses for the three runs, using equation (16) in Fig. 4,5,6. We have also shown in these figures the best fit for the classical dispersion model, and for Coat's dead end pore model. Whereas our results almost identically follow the observations, the classical model gives very poor results, and Coat's model is also less good, especially for runs 2 and 3, even when using different parameters for each run, which our model does not need to do.

CONCLUSION

A number of limiting assumptions have been necessary to develop the theory (e.g. gaussian distribution of velocity, no molecular diffusion, etc...). However, a few experimental results seem to support our conclusions, namely that for a slug injection of tracer, the equivalent of the dispersion coefficient, what we called the "temporal function of dispersion", is indeed a function of time, or of the mean travelled distance of the tracer.

We intend to continue the research along this line by achieving the following questions:
- validity of time convolution,
- introduction of molecular diffusion,

- determination of the covariance functions of each component of the velocity, and of the principal directions of the covariance matrix.

Work should progress both theoretically and experimentally.

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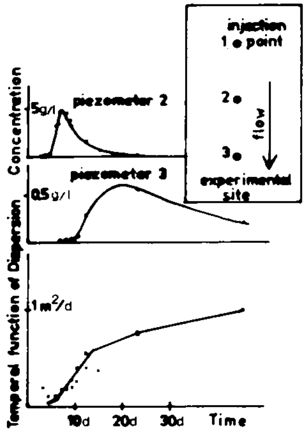

Fig.1. Field experiment: temporal function of dispersion for one of the guides. Calculated curves and experimental data.

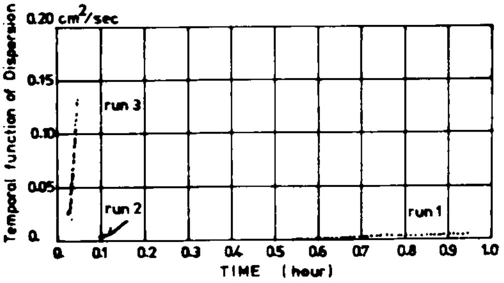

Fig.2. Laboratory experiment (Coats & al., 1964): temporal functions of dispersion (three runs).

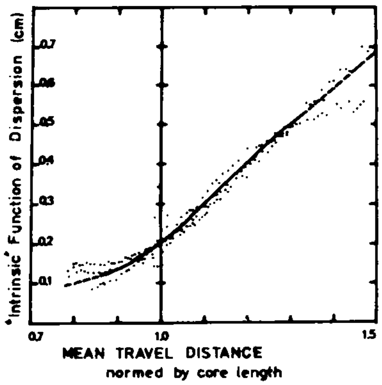

Fig.3. Laboratory experiment (Coats & al., 1964): "intrinsic" function of dispersion (three runs).

Fig. 4

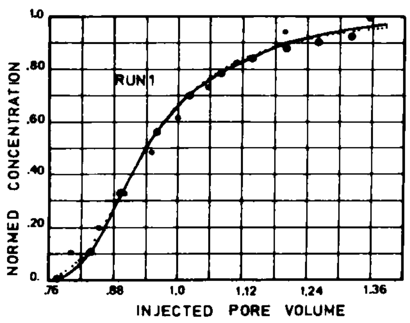

Fig. 5

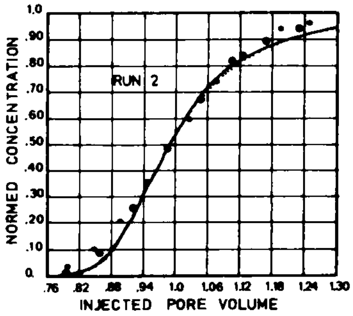

Fig. 6

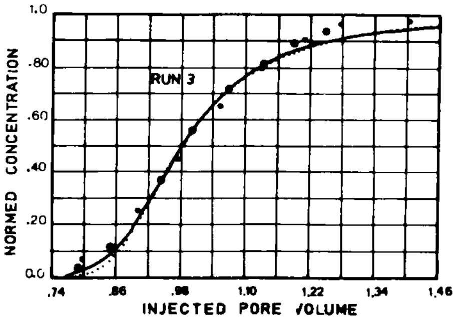

FIG. 4,5 and 6. Laboratory experiment (Coats & al., 1964).
Experimental curve: ——
"Classical" solution: •
Coats' solution: ●
Solution with a temporal
function of Dispersion: ·