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Letter to the Editor

Dispersion of components in transport processes: Velocity dispersion model

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Abstract

This paper presents a new model of dispersion of components in transport processes. It is suggested that the flow velocity may be specified by a Gauss function with relative dispersion of flow velocity $\beta = \sigma_v/v$; the overall dispersion of inert component (in porous as well as in homogeneous medium) may be calculated from the equation $\sigma = (2Dt/\tau^2 + (\beta vt)^2)^{0.5}$, where D is the diffusion coefficient, t is time, τ is tortuosity, and v is flow velocity. The most common range of variability of relative dispersion of flow velocity in natural soils is 8–32%. The model is well applicable to column and field experiments.

Keywords: Transport phenomena; Porous media; Diffusion; Dispersion; Dispersivity; Porosity; Tortuosity; Gauss function

1. Introduction

It is known that diffusion, as affected by movement of a solution, may be characterized by a "conditional" or "effective" diffusion coefficient (more commonly "coefficient of hydrodynamic dispersion" or simply "dispersion coefficient"). The effective diffusion coefficient increases linearly with flow velocity:

$$D_{\text{eff}} = D + \alpha v. \tag{1}$$

Here D is the diffusion coefficient, v is flow velocity, and α is an empirical parameter known as dispersivity. There are some ideas that dispersivity is related in some manner to the heterogeneity of the medium (e.g., grain or pore size, size of the flow cells), but a quantitative theory of dispersivity is absent. This is a basis of the model of hydrodynamic dispersion. The numerical values of dispersivity correlate with the scale of an experiment. They range from 0.1–10 mm for column experiments up to 1–100 m for field experiments. This fact lies at the basis of the so-called scale-dependent dispersion model [1–4]:

$$D_{\text{eff}} = D + \varepsilon x v. \tag{2}$$

Here x is distance, and ε is an empirical parameter known as "dispersivity-to-distance ratio." The physical sense of this parameter is more enigmatic than that of "dispersivity." So, let us try to construct a more clear theory.

2. Model description

The classic theory of diffusion is based on statistical laws. If we have numerous results of measurements of some constant X, the density of probability of some result of measurement x is defined by a Gauss function (Fig. 1),

$$P(x) = \left[(1/2\pi)^{0.5}/\sigma_x\right] \exp\left(-0.5\left((x - X)/\sigma_x\right)^2\right). \tag{3}$$

Here σ is the parameter known as standard deviation or dispersion. The integral of the Gauss function from minus infinity to plus infinity is the unit. The integral from $X - x$ to $X + x$ is 0.683; i.e., the value x is located in the range $X \pm \sigma_x$ with probability 68.3%.

If we try to estimate the sum or difference of two constants $X \pm \sigma_x$ and $Y \pm \sigma_y$, the overall standard deviation

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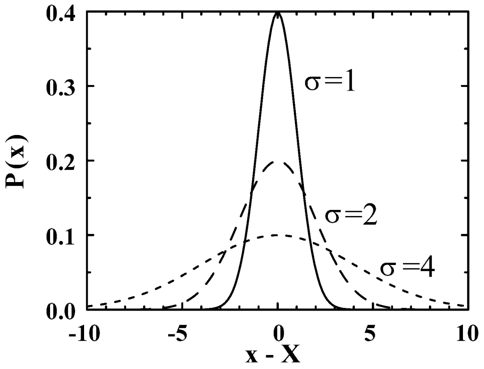

Fig. 1. The Gauss function.

(dispersion) for $Z = X \pm Y$ is

$$\sigma_z = \left(\sigma_x^2 + \sigma_y^2\right)^{0.5}. \quad (4)$$

This is a common law of addition for standard deviations (dispersions).

The location of molecules changes accidentally due to heat fluctuation. Because of this, the laws of diffusion and statistics coincide. The mobility of a molecule in a medium is characterized by the diffusion coefficient D, which is defined by Fick's law:

$$J = D \operatorname{grad} C. \quad (5)$$

Here J is the flux of a component through the elementary surface, and $\operatorname{grad} C$ is the gradient of concentration of the component. The diffusion coefficients of ions and molecules in water are on the order of 10^{-5} cm^2/s. Knowing the diffusion coefficient D, the dispersion may be calculated from Einstein's law:

$$\sigma_x = (2Dt)^{0.5}. \quad (6)$$

The molecule, located at point $x = 0$ at time $t = 0$, should be observed within the range of $0 \pm \sigma_x$ with probability 68.3% at time $t > 0$.

If we consider some unit quantity of molecules (e.g., 1 mol), the concentration of these molecules as a function of x and t coincides with the Gauss function. For the one-dimensional case, the diffusion from some layer should be considered (axis x is perpendicular to the plane of the layer). Using the value of dispersion σ_x from Eq. (6), the concentration profile may be calculated from the equation

$$\begin{aligned} C(x,t)/(C_0\Delta x) &= C(x,t)S/M_0 \\ &= \left[(1/2\pi)^{0.5}/\sigma_x\right]\exp\left(-0.5(x/\sigma_x)^2\right). \quad (7) \end{aligned}$$

Here C_0 is the initial concentration, Δx is the thickness of the layer, S is surface area of the layer (e.g., πr^2 for a tube of radius r), and M_0 is the total amount of the component.

Equations (6) and (7) describe the diffusion of a component from an infinitely thin layer (with infinitely high initial concentration). In reality, at time $t = 0$ the component is distributed in space in some manner; e.g., $C = C_0$ at $x = 0 \pm 0.5\Delta x$, and $C = 0$ at $|x| > 0.5\Delta x$, where Δx is the width of the layer. This initial distribution of the component may be approximated by a Gaussian distribution with $\sigma_x^0 = (1/2\pi)^{0.5}\Delta x$. Thus, the overall dispersion should be calculated from the equation

$$\sigma_x = (\Delta x^2/2\pi + 2Dt)^{0.5}. \quad (8)$$

Equation (8) is more convenient than Eq. (6), since Eq. (6) gives $C(x = 0) > C_0$ at $\sigma_x < \Delta x$. Both Eqs. (6) and (8) are erroneous within some range of time, since the initial conditions are approximated. In Eq. (6), the layer Δx with initial concentration C_0 is approximated by an infinitely thin layer with infinite concentration, whereas in Eq. (8), this layer is approximated by a Gaussian function with maximum $C = C_0$. However, the approximation of initial conditions given by Eq. (8) is closer, and if at some time t dispersion σ_x becomes larger than the initial thickness of the layer Δx, the error becomes negligible.

Staying at the bridge, one may see that the water flow is not uniform, but is disturbed by numerous eddies. So the velocity of any water molecule may be characterized by $v \pm \sigma_v$, where σ_v is velocity dispersion. One may assume that the velocity dispersion is proportional to velocity, and the velocity of a molecule may be defined as $v \pm \beta v$, where β is the relative velocity dispersion. If the medium moves with a velocity v, the middle of the layer Δx passes a distance vt during time t, and the most probable position of any molecule of this layer is vt, but the initial uncertainty of molecule location is $\pm(1/2\pi)^{0.5}\Delta x$, the displacement due to diffusion is $\pm(2Dt)^{0.5}$, the displacement due to velocity fluctuation is $\pm\beta vt$, and the overall dispersion is

$$\sigma_x = \left(\Delta x^2/2\pi + 2Dt + (\beta vt)^2\right)^{0.5}. \quad (9)$$

Applying $\Delta x = 0$, one may calculate the "effective diffusion coefficient" (dispersion coefficient):

$$D_{\text{eff}} = D + (\beta v)^2 t/2. \quad (10)$$

At $x = vt$, "dispersivity" α is $\beta^2 x/2$, whereas "dispersivity-to-distance ratio" ε is $\beta^2/2$ (see Eqs. (1), (2)).

All the above considerations are valid for a homogeneous medium. In a porous medium, some part of space is filled by solid, and this should be taken into account. The fraction of space which may be filled by solution (or gas) is called the porosity, θ. For instance, the porosity of sand is close to 40%. It should be noted that if a solution moves in a tube with velocity 1 m/h, it moves through the part of this tube filled by sand with a velocity $1/\theta = 2.5$ m/h. Similarly, 1 m^3 of porous solution occupies 2.5 m^3 of aquifer. And if a solution moves through a sandwich of layers of different porosity, the velocity of the porous solution is different in each layer (as in a tube constructed from parts of different diameter).

Another important parameter of a porous medium is tortuosity, τ. The porous solution passes through the column by a tortuous way, and covers a distance larger than the column length, and their ratio is the tortuosity. Within the range of