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Quantitative evaluation of macroscopic longitudinal dispersivity for one-dimensional flow

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Abstract Macroscopic dispersivity is the most important factor for analysing the convection–dispersion equation (CDE) at the field scale, and it is well known that macroscopic dispersivities vary with the scale of observation. In this study, artificial heterogeneous hydraulic conductivity fields were generated with the stochastic fractal model ($f^{-\zeta}$ model). Macroscopic dispersivities were evaluated for two-dimensional stochastic isotropic and anisotropic fields by performing dimensionless CDE simulations. The results showed that macroscopic dispersivity depends on the length of the contaminant source and the travel distances, as well as on field characteristics such as variability of hydraulic conductivity for one-dimensional flow. We proposed simple models for quantitatively evaluating the average values of macroscopic longitudinal dispersivity by performing two-dimensional numerical experiments. Further, we showed that macroscopic longitudinal dispersivities calculated by these models generally corresponded with that obtained from the field study.

Key words macroscopic longitudinal dispersivity; stochastic fractal model; groundwater

INTRODUCTION

Macroscopic dispersivity is the most important factor for analysing the convection–dispersion equation (CDE) at the field scale, and it is well known that macroscopic dispersivities vary with the scale of observation (Gelhar *et al*., 1992, Dentz *et al*., 2000). In this study, artificial heterogeneous hydraulic conductivity fields were generated with the stochastic fractal model ($f^{-\zeta}$ model) that was proposed by Saito & Kawatani (2000), and macroscopic dispersivities were evaluated for two-dimensional stochastic isotropic and anisotropic fields by performing dimensionless-CDE simulations.

FORMULATION

The governing equation of a two-dimensional (2D) flow field in the dimensionless form may be written as follows:

$$\frac{\partial}{\partial X}\left(K\frac{\partial H}{\partial X}\right)+\frac{\partial}{\partial Y}\left(K\frac{\partial H}{\partial Y}\right)=0 \tag{1}$$

where $X = x/l_0$, $Y = y/l_0$, $H = h/l_0$, $K = k/k_0$, h is the hydraulic head, k is the hydraulic conductivity, l_0 is the characteristic length, and k_0 is mean value of the hydraulic conductivity.

The governing equation of 2D solute transport in the dimensionless form may be written as follows:

$$\frac{\partial C}{\partial T}+U'\frac{\partial C}{\partial X}+V'\frac{\partial C}{\partial Y}=\frac{\partial}{\partial X}\left(D_{XX}\frac{\partial C}{\partial X}+D_{XY}\frac{\partial C}{\partial Y}\right)+\frac{\partial}{\partial Y}\left(D_{YX}\frac{\partial C}{\partial X}+D_{YY}\frac{\partial C}{\partial Y}\right) \tag{2}$$

where $C = c/c_0$, $T = tk_0/l_0$, $D_{XX} = d_{xx}/l_0k_0$, $D_{XY} = d_{xy}/l_0k_0$, $D_{YX} = d_{yx}/l_0k_0$, $D_{YY} = d_{yy}/l_0k_0$, $U' = u'/k_0$, $V' = v'/k_0$, $A_L = \alpha_L/l_0$, $A_T = \alpha_T/l_0$, c is the concentration of the contamination source, t is the time, u' and v' are components of the pore velocity vector, α_L is the longitudinal dispersivity, α_T is the transversal dispersivity. Then, the components of the dispersion coefficient tensor are given as follows:

$$d_{xx} = \frac{\alpha_L u'^2}{\sqrt{u'^2 + v'^2}} + \frac{\alpha_T v'^2}{\sqrt{u'^2 + v'^2}} \;,\; d_{yy} = \frac{\alpha_T v'^2}{\sqrt{u'^2 + v'^2}} + \frac{\alpha_L v'^2}{\sqrt{u'^2 + v'^2}} \;,\; d_{xy} = d_{yx} = \frac{(\alpha_L - \alpha_T) u'v'}{\sqrt{u'^2 + v'^2}} \tag{3}$$

$$D_{xx} = \frac{A_L U'^2}{\sqrt{U'^2 + V'^2}} + \frac{A_T V'^2}{\sqrt{U'^2 + V'^2}} \;,\; D_{yy} = \frac{A_T V'^2}{\sqrt{U'^2 + V'^2}} + \frac{A_L V'^2}{\sqrt{U'^2 + V'^2}} \;,\; D_{xy} = D_{yx} = \frac{(A_L - A_T) U'V'}{\sqrt{U'^2 + V'^2}} \tag{4}$$

SPATIAL DISTRIBUTION MODEL OF HYDRAULIC CONDUCTIVITY

We generated the spatial distribution of hydraulic conductivity using a model based on the stochastic fractal model proposed by Saito & Kawatani (2000). In this model, the equation of the power spectral density function of the logarithmic transformation (κ = log(k)) of hydraulic conductivity takes the following form with $f^{-\zeta}$.

$$S(|\boldsymbol{f}|) \propto |\boldsymbol{f}|^{-\zeta} \tag{5}$$

where $\boldsymbol{f}$ is the wave number vector, $S(|\boldsymbol{f}|)$ is the power spectral density, and ζ is a parameter representing the spatial correlation. When $\zeta = 2$ is used in the 2D field, the distribution of hydraulic conductivity has self-similarity and can be used in the dimensionless form as expressed by equation (1).

We consider the f_x and f_y components of $\boldsymbol{f}$ from equation (5) as follows:

$$|\boldsymbol{f}| = \sqrt{f_x^{\,2} + f_y^{\,2}} \tag{6}$$

Then, to introduce anisotropy between the x- and y-directions, we add the parameter ω ($0 < \omega \leq 1$) and modify equation (6) as follows:

$$|\boldsymbol{f}| = \sqrt{f_x^{\,2} + \left(\omega f_y\right)^2} \tag{7}$$

The variance of κ (variance of $\kappa = \sigma^2$) in this model is in proportion to the resolution (resolution = number of elements, n), and it can be expressed by the following equation using the parameter λ (Saito & Kawatani, 2001):

$$\sigma^2 = \lambda \log_{10} n \tag{8}$$

ANALYTICAL CONDITION

The analysis domain and boundary conditions are shown schematically in Fig. 1.

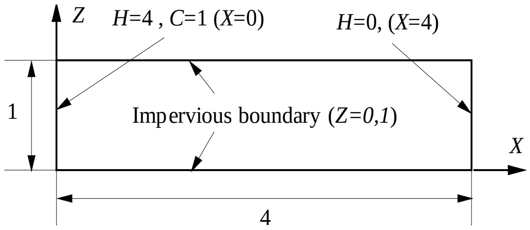

Fig. 1 Analysis domain and boundary conditions.

The characteristic length l_0 was defined as the length of the contamination source. When the domain was divided by a square element that has sides of length L_e equal to $1/2^{N-2}$ ($N > 2$), the resolution n was given as follows:

$$n = 4^{N-1} (N = 3, 4, \ldots) \tag{9}$$

In this study, N, λ, and ω were used as the parameters. In addition, 1000 non-uniform hydraulic conductivity distributions were generated for each combination of the parameters, and the concentration distributions were calculated. Then, the ensemble mean of the change in the contaminant concentration at the several sections were obtained. The dispersivity used in equation (4) was considered to be corresponding to microscopic dispersion, and the following values of A_L and A_T were considered: $A_L = 0.1L_e$, $A_T = 0.1A_L$.

Figure 2 shows the examples of the hydraulic conductivity distribution generated by using equation (5).

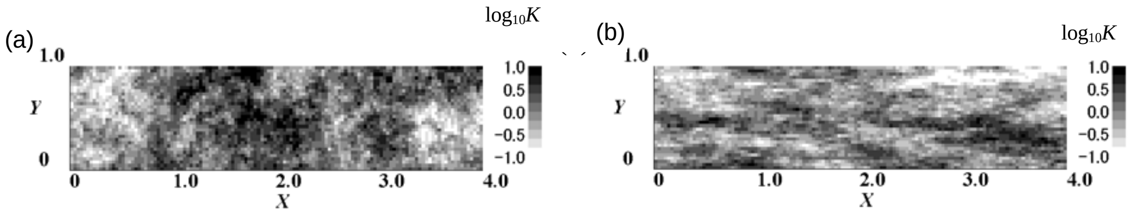

Fig. 2 Distribution of hydraulic conductivity. (a) $\omega = 1.0$, (b) $\omega = 0.2$.

IDENTIFICATION OF MACROSCOPIC DISPERSIVITY

Figure 3 show the examples of the ensemble mean of the change in the cross-sectional average concentration at several cross sections. The dimensionless macroscopic dispersivity A_L' at each section was identified by curve fitting of the theoretical solution that is expressed by equation (10):

$$C = \frac{1}{2}\operatorname{erfc}\left(\frac{X - U_m T}{2\sqrt{DT}}\right) + \frac{1}{2}\exp\left(\frac{U_m X}{D}\right)\operatorname{erfc}\left(\frac{X + U_m T}{2\sqrt{DT}}\right) \tag{10}$$

where D is the dimensionless macroscopic dispersion coefficient ($= A_L'U_m$) and U_m is the dimensionless porous velocity.

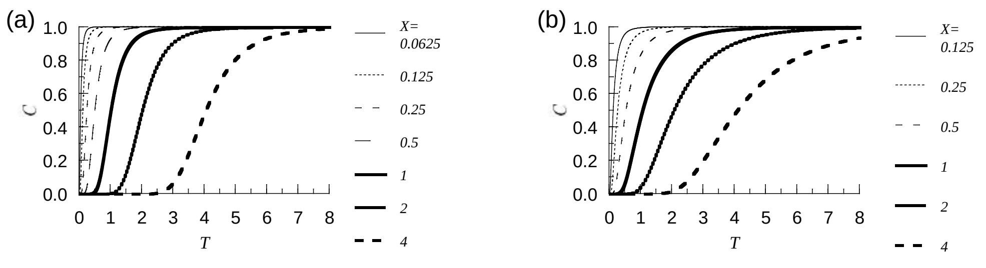

Fig. 3 Temporal changes in cross-sectional averaged concentration. (a) $\lambda = 0.05$, $\omega = 1.0$, (b) $\lambda = 0.04$, $\omega = 0.2$.

RESULTS AND DISCUSSION

The dependence of the macroscopic dispersivity on the distance from the contamination source (in the case of $\omega = 1.0$)

Figure 4 shows the relationship between the distance from the contamination source and the macroscopic dispersivity at each resolution on the semi-log graph. While curves for the different N values are widely separated at short distances from the contamination source, they eventually converge to a straight line. This relationship can be expressed by the following equation using the parameters γ and δ:

$$A_L' = \gamma \log\left(\frac{X}{\delta}\right) \tag{11}$$

This means that the macroscopic dispersivity A_L' is in proportion to the logarithmic value of the distance from the contamination source.

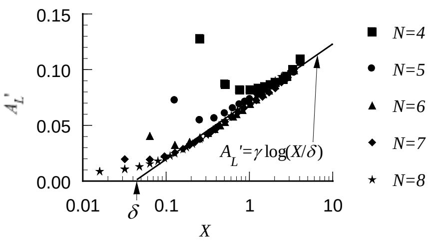

Fig. 4 Relationship between macroscopic dispersivity and travel distance.

The dependence of the macroscopic dispersivity on the parameter λ

Figure 5 shows the relationship between λ in equation (8) and γ in equation (11) on the log–log graph. From this result, the following equation is obtained by means of collinear approximation.

$$\gamma = 1.74 \times \lambda^{1.16} \tag{12}$$

Figure 6 shows the relationship between λ in equation (8) and δ in equation (11). The parameter δ remains almost constant, except when λ is extremely high or low. Thus, it can be estimated that macroscopic dispersion may occur from a distance equal to 0.04–0.05 times the length of the contamination source, l_0.

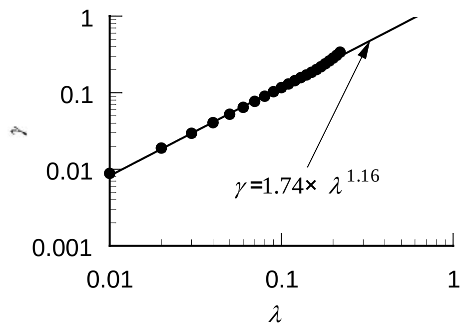

Fig. 5 Relationship between λ and γ_0.

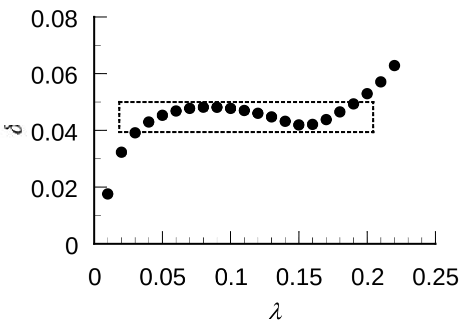

Fig. 6 Relationship between λ and δ.

The relationship between the macroscopic dispersivity and the length of the contamination source

The macroscopic dispersivity considered here has been normalized by the length of the contamination source, l_0. Thus, the macroscopic dispersivity in a real scale, α_L', is given by equation (13):

$$\alpha_L' = l_0 \gamma \log\left(\frac{x}{l_0 \delta}\right) \tag{13}$$

These results indicate that the macroscopic dispersivity is dependent on the length of the contamination source, l_0, distance from the source, x, and the dispersion of saturated hydraulic conductivity, λ.

Figure 7 demonstrates the relationship between x and a_L'. The macroscopic longitudinal dispersivity calculated by this model generally corresponded with that obtained in the field study reported by Gelhar *et al*. (1992).

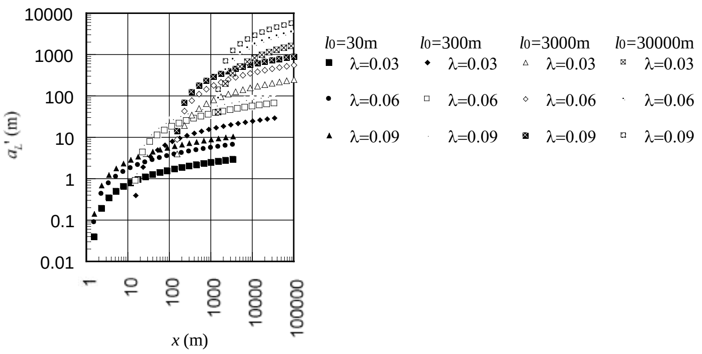

Fig. 7 Relationship between the macroscopic dispersivity and the travel distance in the field scale.

The dependence of the macroscopic dispersivity on the distance from the contamination source (in the case of 0 < ω < 1.0)

Figure 8 shows the relationship between the normalized distance from the contamination source, X, and the square root of the normalized macroscopic dispersivity A_L' in the case of $\omega = 0.2$ and $\omega = 0.8$ on the semi-log graph. It appears that this relationship is linear and can be expressed by the following equation using the parameters γ and δ (similar to equation (11)):

$$\sqrt{A_L'} = \gamma \log_{10}\left(\frac{X}{\delta}\right) \tag{14}$$

Then, the parameter Γ is introduced and defined as $\Gamma = \gamma^2$. By substituting Γ in equation (14), A_L' is expressed as follows:

$$A_L' = \Gamma \left\{\log_{10}\left(\frac{X}{\delta}\right)\right\}^2 \tag{15}$$

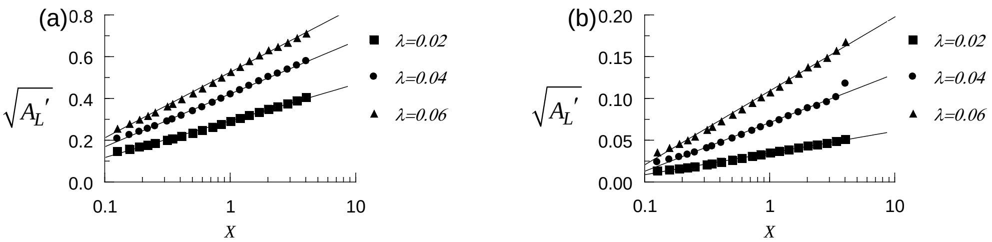

Fig. 8 Relationship between the macroscopic dispersivity and the travel distance. (a) $\omega = 0.2$, (b) $\omega = 0.8$.

The dependence of the macroscopic dispersivity on the parameter λ

Figure 9(a) shows the relationship between λ in equation (8) and Γ in equation (15) for different values of ω. This relationship can be expressed by the following equation obtained by means of collinear approximation on the log–log graph:

$$\Gamma = \varepsilon\lambda^{\theta} \tag{16}$$

where ε and θ are the fitting parameters.

Figures 9(b) and (c) show the relationship between ω and θ or ε. Although the parameter θ is slightly dependent on ω, it could be assumed to be constant. However, the parameter ε is strongly dependent on ω, and it can be assumed to be co-linear on the semi-log graph. Thus, the following are obtained:

$$\theta = 1.08 \tag{17}$$

$$\varepsilon = -1.92\log_{10}\omega + 0.334 \tag{18}$$

The parameter δ is not dependent on λ, similar to the case of $\omega = 1$. However, it could be assumed to be co-linear on the log–log graph, as shown in Fig. 9(d), and the following equation is obtained by means of co-linear approximation:

$$\delta = 4.54\times10^{-3}\omega^{-0.911} \tag{19}$$

Therefore, in the case of anisotropic fields ($0 < \omega < 1$), the macroscopic dispersivity in a real scale, α_L', is given by equation (20):

$$\alpha_L' = l_0\Gamma\left\{\log_{10}\left(\frac{x}{l_0\delta}\right)\right\}^2 \tag{20}$$

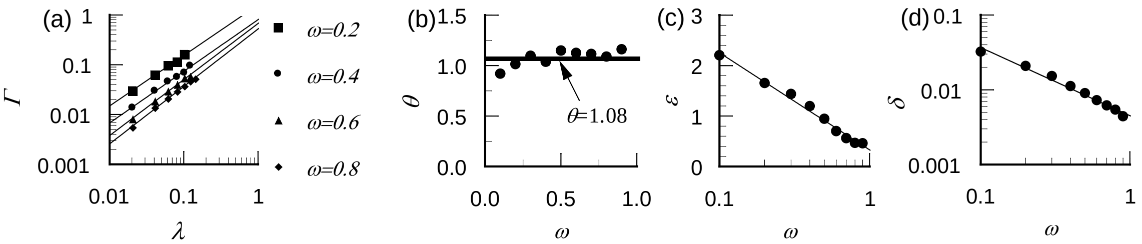

Fig. 9 Relationship between the parameters: plots of (a) λ *versus* Γ, (b) ω *versus* θ, (c) ω *versus* ε, (d) ω *versus* δ.

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