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Evaluation of the transition characteristics of macroscopic dispersion and estimation of the non-uniform hydrogeological structure

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Abstract In general, a natural aquifer has a hydrogeologically non-uniform structure. The movement of pollutants in groundwater is affected by such structural properties during transport by local advection and microscopic dispersion. The macroscopic dispersion coefficient increases linearly with travel distance or travel time at the initial stage after the pollutant is released, and then converges asymptotically to a constant value after a sufficient travel distance, longer than the integral scale of heterogeneity. For practical applications it is important to know how such macroscopic dispersion increases, when the prediction of pollutant spread is required in the transient stage. In the present study, a method for judging the convergence of macroscopic dispersion is discussed for the analytical and observed average concentration, by numerical simulations. The chi-square test for convergence of the macroscopic dispersivity is applied. Also, an evaluation procedure for the auto-regressive parameters in the model generating the random hydraulic conductivity field is proposed. This evaluation is applied for the case in which the macroscopic dispersion is estimated to be still in the growing stage. The characteristics of the proposed method are examined through application to synthetically generated random fields of hydraulic conductivity.

INTRODUCTION

In numerical simulations of mass transport, the dispersion coefficient plays an important role. Natural aquifers have a hydrogeologically non-uniform structure. A tracer is affected by such non-uniformity and consequently macroscopic dispersion will occur. In general, the macroscopic dispersion coefficient increases linearly with travel distance in the initial stage. After the transition period, the coefficient tends to converge to a constant value, when the longitudinal velocity is constant (Fig. 1; Gelhar, 1993; Dagan, 1984).

However, in practice it is more important to check whether or not we can assume a constant macroscopic dispersion coefficient for the analytical solution of pollutant spread, if the monitoring wells are located close to the source of pollution, within a travel distance of less than the integral scale.

This paper introduces a method for judging the convergence of the macroscopic dispersion coefficient, using the measured concentration of pollutant in a borehole. An evaluation procedure for the auto-regressive parameters used in the random field model of hydraulic conductivity, is also presented.

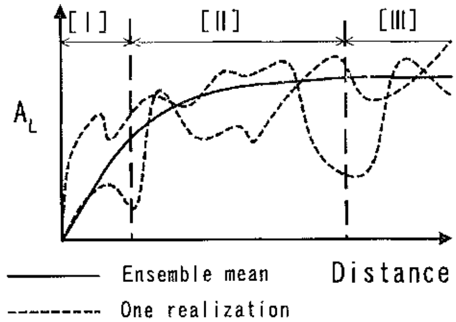

Fig. 1 Schematic diagram of longitudinal dispersivity A_L *vs* travel distance.

JUDGEMENT OF THE TRANSIENT CHARACTERISTICS OF THE MACROSCOPIC DISPERSION COEFFICIENT

Method of judgement

Figure 2 shows the flow chart for judging the transient characteristics of the macroscopic dispersion coefficient. In this study, one injection well and two downstream observation wells are considered in the two-dimensional flow field. The non-reactive tracer is injected instantaneously along the upstream injection well. The analytical solution given by equation (1) (Kinzelbach, 1986) is compared with the averaged concentration at observation well no. 1:

$$C(x,t) = \frac{C_0}{2\sqrt{\pi A_L U t}} \exp\left(-\frac{(x-Ut)^2}{4A_L U t} \right) \tag{1}$$

where x is the distance from the injection well, t is the time, C_0 is the initial concentration at the injection well, U is the average pore velocity, and A_L is the dispersivity.

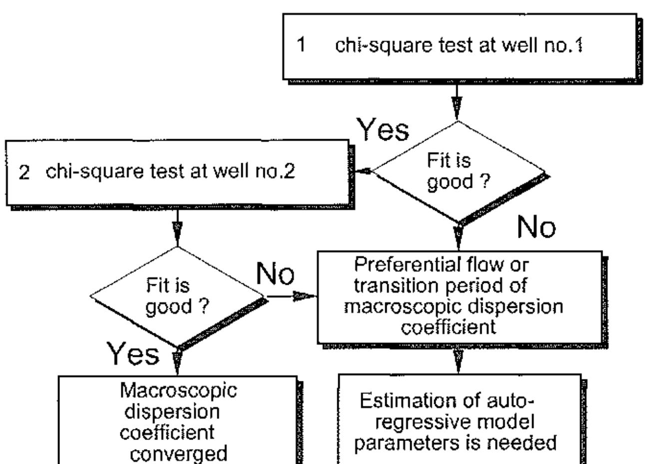

Fig. 2 Method for evaluating macroscopic dispersion using two observation wells.

Before the chi-square test is adapted, U and A_L are evaluated by minimizing H as shown in equation (2):

$$H = \sqrt{\frac{1}{N}\sum_{k=1t}^{N}[C_{obs}(t_k) - C_{cal}(t_k)]^2} \quad (2)$$

where $C_{cal}(t_k)$ and $C_{obs}(t_k)$ is the calculated concentration (equation (1)) and the observed value at time t_k, respectively, k is the observation step number, and N is the total number of observations.

After comparing the fit of the analytical solution breakthrough curve and the observed curve at observation well no. 1, the fit of the breakthrough curves at well no. 2 is also checked. At both wells, when the degree of fit is considered satisfactory, the macroscopic dispersion coefficient is assumed to have converged, i.e. the macroscopic dispersion coefficient is in stage III of Fig. 1 and the field can be considered uniform. Otherwise, the dispersion coefficient is still changing, i.e. in stage I or II of Fig. 1.

To check the goodness of fit of the analytical solution and the observed breakthrough curves, the concentration time series is converted into the histograms (C_i', E_i') as shown in Fig. 3. The time axis is divided into I segments and the concentration axis is divided into J segments. In this study, I and J are chosen equal to 50. Then, the chi-square test is adapted. The sample statistic is:

$$z = \sum_{i=1}^{I}\frac{(C'_i - E'_i)^2}{E'_i} \quad (3)$$

where i is the time segment number, E_i is the maximum expected concentration in segment i, E_{max} is the maximum value of E_i, and C_i is the maximum observed concentration in segment i. In Fig. 3, E_i' and C_i' are defined as $E_i' = J\,E_i/E_{max}$, and $C_i' = J\,C_i/C_{max}$.

Example of the method

At first, a test field is synthetically generated. For the generation of heterogeneous fields of log-transformed hydraulic conductivity, the following auto-regressive model (equation (4)) is sometimes employed (e.g. Smith & Freeze, 1979). The auto-

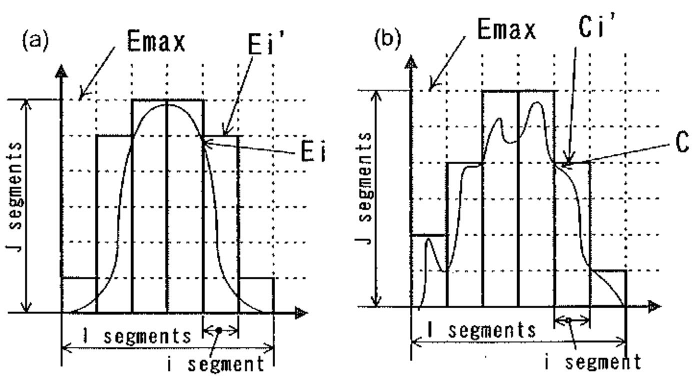

Fig. 3 Schematic illustration of converting the concentrations distribution to histograms: (a) analytical solution, (b) observed value.

regressive parameters a_{xx}, a_{yy}, a_0 and the variance of the Gaussian white noise need to be assigned:

$$a_{xx}\frac{\partial^2 Y}{\partial x^2}+a_{yy}\frac{\partial^2 Y}{\partial y^2}-a_0 Y+\varepsilon(x,y)=0 \tag{4}$$

where Y is the log-transformed hydraulic conductivity K, and $\varepsilon(x,y)$ is the Gaussian white noise. After solving equation (4) by the finite difference method under the appropriate boundary conditions, Y values were assigned to the six different classes of glass bead diameters used in a previous paper by Nakagawa *et al.* (1998). In this model field, the injection well and observation wells are set as shown in Fig. 4.

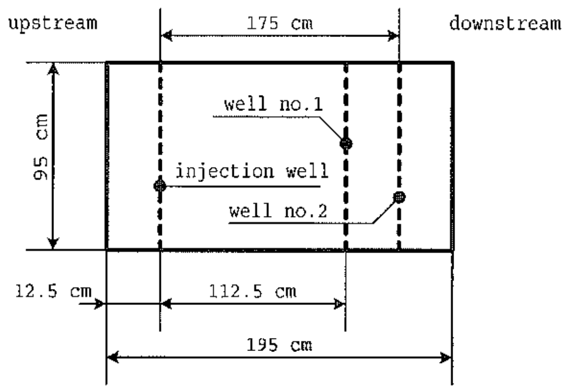

Fig. 4 Model area and the locations of the injection and observation wells.

A numerical simulation of the tracer transport was made. The breakthrough curve of well no. 2 was used as the observed values in the later judgement. In the numerical tracer test, the equations of groundwater flow and non-reactive tracer transport are applied:

$$S_s\frac{\partial h}{\partial t}=\frac{\partial}{\partial x}\left[K\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[K\left(\frac{\partial h}{\partial y}+1\right)\right] \tag{5}$$

$$\frac{\partial C}{\partial t}+\frac{\partial(u'C)}{\partial x}+\frac{\partial(v'C)}{\partial y}=\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}+D_{xy}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y}+D_{yx}\frac{\partial C}{\partial x}\right) \tag{6}$$

where S_s is the specific storage coefficient [L^{-1}], K is the hydraulic conductivity [$L\,T^{-1}$], h is the pressure head [L], u' and v' are the pore velocities [$L\,T^{-1}$], C is the tracer concentration (%), and D is the microscopic dispersion coefficient tensor [$L^2\,T^{-1}$]. As the boundary conditions for equation (5), constant heads were given at the upper and downstream boundaries, and no flux condition was given at the top and bottom of the model area. For equation (6), an instantaneous pulse at the upstream injection well was given and no flux conditions were given for all model area boundaries. The method details and the validity of the numerical model are presented in Nakagawa *et al.* (1998). The parameters of the model field are set to a_{xx} = 10 cm^2, a_{yy} = 10 cm^2, and a_0 = 1, and the generated field of K is shown in Fig. 5(a). The best-fit values of U and A_L for well no. 1 are 0.04 cm s^{-1} and 2.74 cm, respectively. Figure 5(b) shows the histograms converted from the observed concentration and analytical solution in well no. 1. The result of the chi-square test shows that the degree of fit is accepted at a 5% level of significance. Figure 5(c) shows the histograms in well no. 2. When the validity of equation (1) with the parameters of well no. 1 is evaluated at well no. 2, the null hypothesis was not accepted, even at the 1% level of significance. Thus, the parameter values obtained from well no. 1 can not be used as parameter values for well no. 2. Therefore, it can be concluded, the macroscopic dispersion coefficient has not converged.

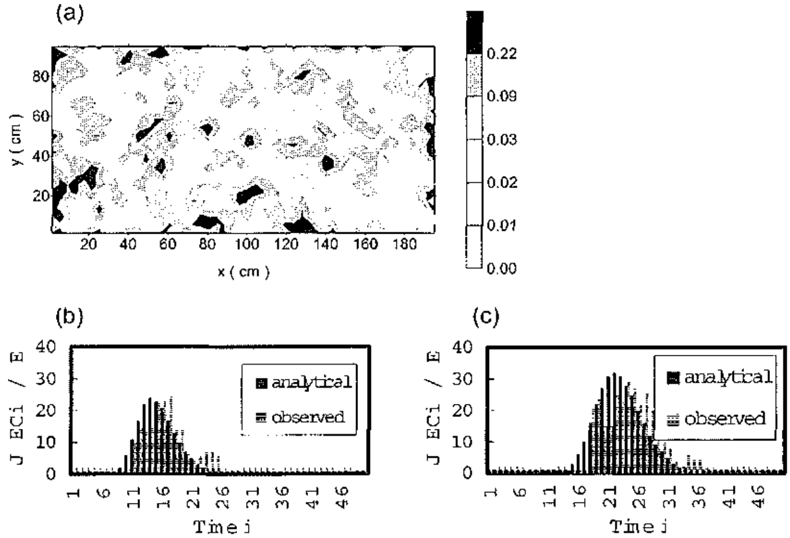

Fig. 5 The characteristics of model field (a_{xx} = 10 cm^2, a_{yy} = 10 cm^2, a_0 = 1, σ_ε^2 = 1.0). (a) generated K-field for the model, (b) observed values and analytical solution after conversion at well no. 1, (c) observed values and analytical solution after conversion at well no. 2.

ESTIMATION OF NON-UNIFORM FIELD CHARACTERISTICS

Figure 6 shows the flow chart of the proposed procedure to estimate the non-uniform field. Information on the vertical distribution of the hydraulic conductivity in both the injection and observation wells are used as boundary conditions in the numerical analysis of equation (4). At first, values of the auto-regressive parameters a_{xx}, a_{yy} and a_0 are assumed. Using the assumed parameters, the non-uniform field is generated and the numerical tracer test is done. This procedure is iterated ten times, and the ensemble average of the breakthrough curves and the observed break-through curve are compared by the chi-square test (in this case, $I = J = 30$). When the agreement is unsatisfactory, the auto-regressive parameters should be re-estimated. Consider the case of Fig. 5(a). In this example, the known data are the vertical distribution of the hydraulic conductivities at the injection well and observation well no. 2. Moreover, the breakthrough curve at well no. 2 is also known. The auto-regressive parameters a_{xx} and a_{yy} are taken to be 0, 5, or 10 cm^2, and a_0 varies between 0 and 1. Therefore, the total parameter combinations are 18 cases.

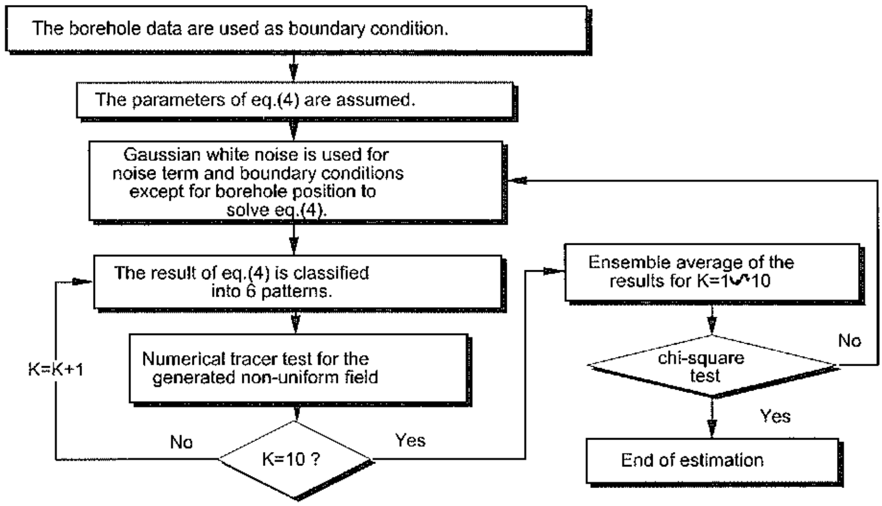

Fig. 6 Estimation procedure for the non-uniform field.

When the level of significance is 5%, the selected combinations were $a_{xx} = 5$ cm^2, $a_{yy} = 10$ cm^2, $a_0 = 1$ and $a_{xx} = 0$ cm^2, $a_{yy} = 10$ cm^2, $a_0 = 1$. That is to say, these combinations represent fields which have a short integral scale in the x direction. One of the fields, for which $a_{xx} = 5$ cm^2, $a_{yy} = 10$ cm^2, and $a_0 = 1$ is shown in Fig. 7(a). This figure is visually very similar to Fig. 5(a). Figure 7(b) compares observed concentrations with the ensemble average concentration from ten calculations using the same parameter values in observation well no. 2. This figure shows good agreement, and thus the presented method is useful for the estimation of the unknown hydrogeological structure of an aquifer.

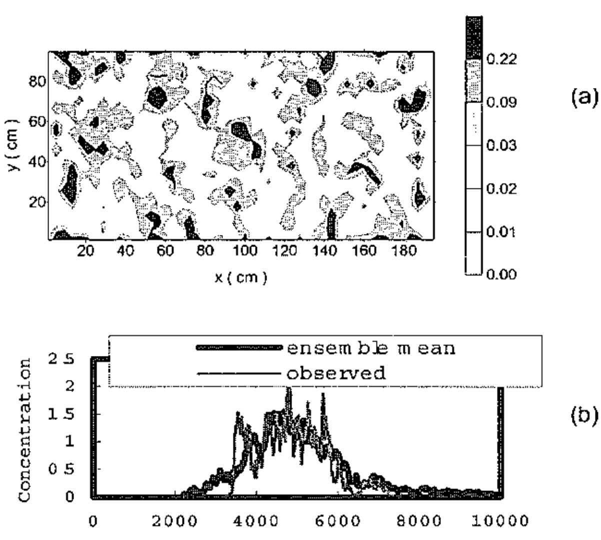

Fig. 7 (a) Example of the estimated field for Fig. 5(a). (b) The concentration distribution at well no. 2 and the ensemble mean.

CONCLUSIONS

The following conclusions can be deduced from the present study.

(a) The first method has proven to be useful for judging the transient stage of the macroscopic dispersion coefficient.

(b) The second method is also useful for evaluating the characteristics of a non-uniform hydraulic conductivity field. The numerical simulation of tracer transport in the evaluated field can reproduce the observed breakthrough curve.

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