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Influence of pore structure on dispersion coefficient: simulations by equivalent pore-network model

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ABSTRACT

Dispersion is an important phenomenon in solute migration in porous media, which is closely affected by pore structure. Traditional advection-dispersion equation based on continuous porous media assumption ignores the complex pore structure of porous media and is hard to reflect the microscale mechanism of solute migration. Previous studies have reported the observation of the scale effect in dispersion between laboratory experiments and field monitoring. However, the mechanism of the dispersion scale effect has not been fully understood yet. The equivalent pore network model (EPNM) describes the complex pore structure of porous media by statistic parameters, which can be an effective method to study the microscopic mechanism of solute transport. In this study, simulations based on EPNMs are carried out to study the influence of pore structure on dispersion. Influences of pore structure parameters including standard deviation of pore radius, curvature number, and coordination number on dispersion are systematically investigated and discussed. Results show that the increase in the standard deviation of pore body radius, and the decrease in curvature number and coordination number leads to the increase in dispersion coefficient, which can be explained by the distribution of pore throat velocity. The scale effect of dispersion persists even in statistically homogeneous porous media. The change of dispersion coefficient with distance can be fitted by a power function. The results imply that the inhomogeneity of microscopic velocity distribution influences dispersion and its scale effect, which can help to understand the microscopic mechanism of solute transport and determine the parameters used in macroscale simulations.

Keywords: Dispersion, Scale effect, Pore structure, Equivalent pore network model (EPNM)

1 INTRODUCTION

With the development of the economy and industry, the pollution caused by human production activities has been paid more and more attention. The infiltration of polluted surface water into underground aquifers will cause groundwater pollution and eventually produce large-scale pollution. Efficient remediation of polluted groundwater is an important subject in the field of environmental geotechnical engineering. It is of great significance to study solute migration in porous media for groundwater pollution remediation and control (Gong and Piri, 2020).

The pollutant usually exists in the form of solute in groundwater, and its movement process involves convection, mechanical dispersion, and molecular diffusion, which is usually described by the advection-dispersion equation (ADE):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \quad (1)$$

where C is the concentration of the solute in the groundwater, t is time, x is the migration distance, v is the pore velocity of the groundwater, and D is the dispersion coefficient. The ADE is based on the assumption that the porous media is a homogeneous continuous media and has been widely applied in the large-scale simulation of solute transport (Bear, 1972). The transport parameter including D is usually determined by fitting laboratory or field-scale experimental data. Previous studies have reported that the solute transport is closely related to the pore structure of porous media, which has been ignored in this equation, therefore it is hard to use ADE to reflect the mechanism of solute transport in the pore scale. With the development of computing technology, pore-network models (PNMs) have been used to describe the pore structure and to simulate the seepage and solute transport in porous media at the pore scale (Raoof et al., 2010). Based on the PNM, it is possible to study the micromechanics of solute transport in complex pore structures and determine the transport parameter directly from the pore structure parameters (Qin and Hassanizadeh, 2015; Vries, 2021). The statistical parameters used in the PNM can be obtained by pore structure extraction from real porous media samples, including coarse sand and shales (Gao et al., 2012b; Zhang et al., 2021a).

According to previous laboratory and field scale observations, the dispersion of a solute in porous media usually exhibits the scale effect, which refers to the phenomenon that dispersion increases with the increase of solute migration distance (Younes et al., 2020; Zhang et al., 2021b). Due to the scale effect, the dispersion coefficient determined by field tests is generally 2 to 4 orders of magnitude larger than that determined by laboratory tests (Sudicky and Frind, 1982). Previous studies have focused on verifying the existence of scale effects. Although many researchers have reported the observation of the scale effect, the mechanism of this phenomenon is still not fully revealed. One of the accepted explanations of the scale effect of dispersion is that the local inhomogeneity of the aqueous medium (Gao et al., 2012a; Sharma et al., 2015). However, some other researchers have also reported that the scale effect of dispersion also happens in homogenous porous media (Zhang et al., 1994; Pang and Hunt, 2001).

In this study, equivalent pore-network models (EPNMs) are built to simulate the solute transport in the pore structure of porous media. The pore size distribution, the relative size of the pore body and pore throat, and the connectivity are changed in the model to reflect the variation in the pore structure. The influence of the pore structure parameter of the EPNM on the dispersion and its scale effect is discussed.

2 METHOD

In this study, the solute transport process is simulated by EPNM. The geometry of the porous media is described by the statistical parameter of the EPNM. The concentration distribution in the model is then used to calculate the dispersion coefficient.

2.1 The geometry of the EPNM

An EPNM with a maximum coordination number of 26 is adopted to simulate the solute transport in the porous media in this study (Raoof and Hassanizadeh, 2012). An example of the EPNM is shown in Figure 1.

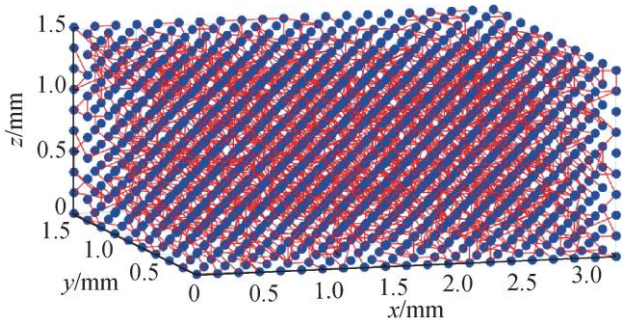


Figure 1. *An example of the EPNM*

In this model, large cavities in porous media are simplified into spherical pore bodies with a variable radius. The positions of the pore bodies are arranged regularly on the grid points. The pore body radius obeys normal distribution (Zhang et al., 2017), which can be described by the mean pore body radius,

μ_{pore}, and the standard deviation of the pore radius, σ_{pore}. The narrow channels in porous media are simplified into cylindrical pore throats. The radius of the pore throat is determined by the size of the pore bodies connected on both sides of it, which follows the BACON bond rules (Acharya et al., 2004). In the BACON rules, the radius of the pore throat is a function of the pore body radius, the length between the centre of the pore bodies and the curvature number, *n*. When the sizes of the pore bodies are constant, a larger *n* leads to a smaller pore throat radius. Detailed functions used in BACON can be found in previous papers (Acharya et al., 2004; Zhang et al., 2017). Therefore the parameter *n* reflects the relative size of the pore body and pore throat. Each pore body is connected to a maximum of 26 adjacent pore bodies (Raoof and Hassanizadeh, 2009), and the number of pore throats connected to each pore body is called the coordination number, ζ. A higher ζ means better connectivity of the model. The parameter ζ reflects the pore connectivity of the model. The length of the grid l_{ele} is determined by iteration calculation to make sure the porosity of the model equals the target value (Hu et al., 2018).

2.2 Solute transport in the EPNM

Based on the uncompressible liquid assumption, the total flux in the pore body *i* should equals the sum of the flux of the upstream pore throats connected to it, which can be written as:

$$Q_i = \sum_{j}^{N_{up}} Q_{ij} \tag{2}$$

where Q_{ij} is the pore throat flux, N_{up} is the number of upstream pore throats connected to this pore body. The flux in pore throat ij, Q_{ij} can be determined by the Hagen-Poiseuille equation:

$$Q_{ij} = \frac{\pi r_{ij}^4}{8\mu l_{ij}}(p_i - p_j) \tag{3}$$

where r_{ij} is the radius of the pore throat, l_{ij} is the length of the pore throat p_i and p_j are the pressure of the pore body connected to this pore throat, and μ is the viscosity of the liquid. By setting a constant pressure boundary to the left and right boundary of the model, the flux of the pore bodies and pore throats can be obtained by solving equation 2 and equation 3.

In this study, the solute is assumed to be conservative and the molecular diffusion is ignored. The mass balance of the solute in the pore body can be written as:

$$V_i \frac{dC_i}{dt} = \sum_{j}^{N_{up}} Q_{ij} C_{ij} - Q_i C_i \tag{4}$$

where V_i is the volume of the pore body, C_i is the liquid concentration in the pore body, C_{ij} is the liquid concentration in the input pore throat, and *t* is time. The mass balance of the conservative solute in the pore throat can be expressed as:

$$V_{ij} \frac{dC_{ij}}{dt} = Q_{ij} C_j - Q_{ij} C_{ij} \tag{5}$$

where V_{ij} is the volume of the pore throat, C_j is the liquid concentration of the input pore body. By solving equations 4 and 5, the concentration of solute in all the pore bodies and pore throats in the EPNM can be obtained.

2.3 Simulation scenarios

EPNMs with a model size of 1000×10×10 are built to simulate the transport of solute in porous media. The porosity of the model is 0.3 and the mean pore body radius is 60 μm, which are used to represent the typical parameters of sand (Horoshenkov and Mohamed, 2006; Lv et al., 2022). To reflect the variation of pore structure, parameters including the standard deviation of pore body radius, curvature number, and coordination number are changed in different models. The simulation scenarios are shown in Table 1. The calculated mean pore throat radius μ_{throat} and element length l_{ele} are also shown in Table

1. It is worth noticing that the value of the parameters here are set to show then influence of pore structure on dispersion. To simulate the solute transport in real porous media samples, pore structure extraction and analysis are needed based on reconstruction process from x-ray computer tomography images (Hu et al., 2018).

The simulation is under a constant flux condition and the Darcy flow velocity of the model is 10^{-5} m/s. A continuous injection boundary with the injection concentration C_0=1000 kg/m³ is set at the left boundary and an outflow boundary is set at the right boundary. For continuous injection conditions, the analytical solution of the solute concentration can be expressed as:

$$\frac{C(x,t)}{C_0} = \frac{1}{2}\mathrm{erfc}\left(\frac{x-ut}{x\sqrt{Dt}}\right) + \frac{1}{2}e^{\frac{ux}{D}}\mathrm{erfc}\left(\frac{x+ut}{x\sqrt{Dt}}\right) \quad (6)$$

where u is the pore velocity. Based on equation 6, an approximate solution for dispersion coefficient D at distance x can be written as:

$$D = \frac{1}{8}\left(\frac{x-ut_{0.1587}}{\sqrt{t_{0.1587}}} - \frac{x-ut_{0.8413}}{\sqrt{t_{0.8413}}}\right)^2 \quad (7)$$

where $t_{0.1587}$ and $t_{0.8413}$ is the time when the concentration at distance x equals $0.1587C_0$ and $0.8413C_0$.

Table 1. *Simulation scenarios*

NO.	σ_{pore} (μm)	n	ζ	μ_{throat} (μm)	l_{ele} (μm)
1	0	0.5	8	17.08	176.25
2	5	0.5	8	17.08	177.50
3	10	0.5	8	17.08	178.91
4	15	0.5	8	17.08	181.88
5	0	0.005	8	22.89	202.50
6	0	1	8	12.84	162.19
7	0	0.5	6	17.08	168.75
8	0	0.5	10	17.08	184.69

3 RESULTS AND DISCUSSIONS

The change of concentration with time at a different distance can be obtained by the EPNM. One example is shown in Figure 2 for scenario NO.1. It can be seen that the EPNM can reflect the transport process solute and its dispersion in porous media effectively.

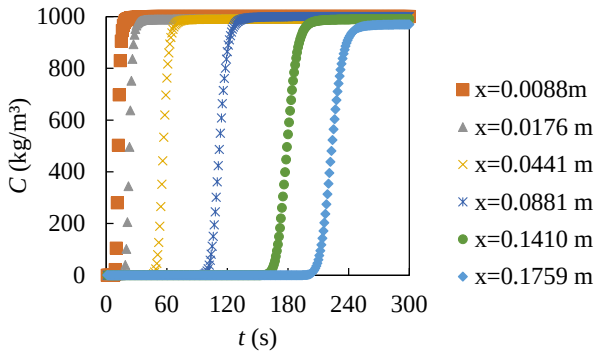
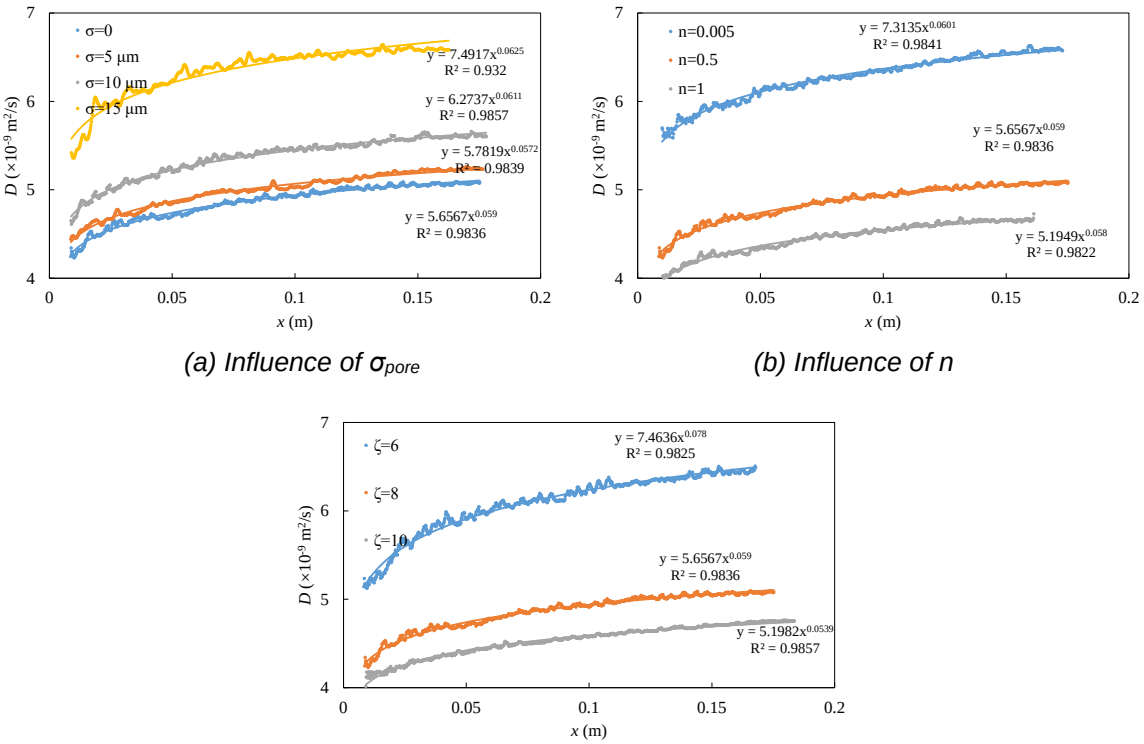


Figure 2. *Change of solute concentration with time at a different distance (scenario NO.1)*

The influence of the pore structure parameters including the standard deviation of pore body radius σ_{pore}, the curvature number n, and the coordination number ζ on the variation of dispersion coefficient D with distance x is exhibited in Figure 3. Results show that D increase with distance in all these simulation

scenarios. It is worth noticing that in the EPNM used in this study, the statistical parameters of the model do not change with distance. This implies that the scale effect of dispersion will also happen in homogeneous porous media, which is also reported in previous experimental observations (Zhang et al., 1994; Pang and Hunt, 2001).



(a) Influence of σ_{pore}

(b) Influence of n

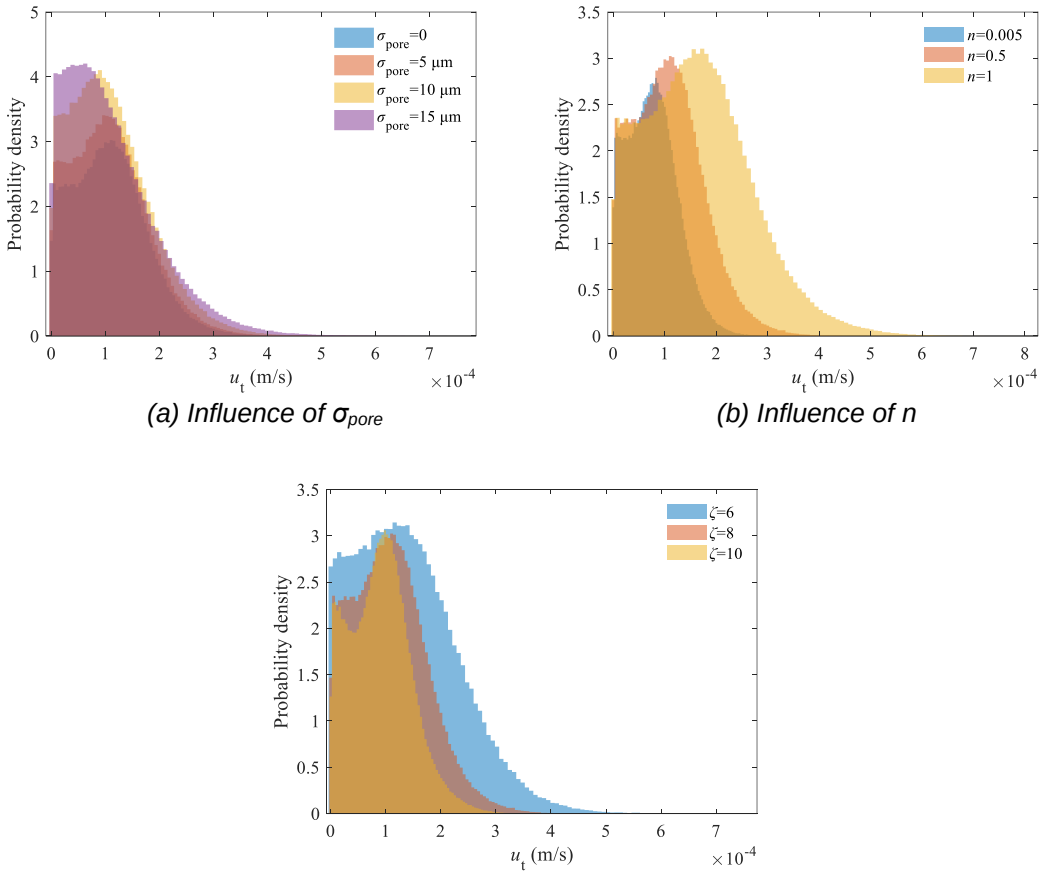
(c) Influence of ζ

Figure 3. *Influence of pore structure parameters on the variation of dispersion coefficient with distance*

Results in Figure 3 can indicate the influence of pore structure parameters on the value of *D* at the same distance. Figure 3a shows that a larger σ_{pore} leads to a larger *D* and this means that the distribution of pore radius can influence the dispersion. The pore radii are more widely distributed with a larger σ_{pore}, and this leads to a more complicated pore velocity distribution, and therefore a higher dispersion. Results in Figure 3b imply that larger *n* results in smaller *D*. The parameter *n* reflects the relative size of the pore body and pore throat, and a larger *n* means that the pore throat is thinner when the pore body radii are constant. Figure 3c shows that an increase in *ζ* leads to a decrease in *D*, and this means models that have better connectivity have lower *D*.

Figure 3 also reflects that the change of *D* with *x* can be fitted by a power function (R^2>0.9), which can be written as $D=Ax^B$. The fitted parameter *A* reflects the relative magnitude of D and *B* reflects the tendency of *D* increases with *x*. The results of Figure 3 imply that the value of *A* and *B* mainly increases with σ_{pore}, and decreases with *n* and *ζ*. However, compared to the change of *A*, the variation of *B* with the pore structure parameter is relatively not significant, which ranges from 0.059 to 0.0625 in this study.

The change of *D* with the pore structure parameters can be explained by the distribution of pore throat velocity in the EPNMs, which is shown in Figure 4. It is worth noticing that although the statistical parameters of the model are the same along distance, the pore throat velocity still has a distribution due to the complex connections between pore bodies. Results in Figure 3 and Figure 4 show that the pore structure parameters can influence the dispersion and its scale effect by influencing the pore throat distribution. A wider pore throat distribution results in higher dispersion and a more significant scale effect.



(a) Influence of σ_{pore}

(b) Influence of n

(c) Influence of ζ

Figure 4. *Influence of pore structure parameters on the distribution of pore throat velocity*

4 CONCLUSIONS

This study aims to investigate the influence of pore structure on dispersion and its scale effect. The equivalent pore network models (EPNMs) with different geometry parameters are built to simulate the solute transport and calculate the change of dispersion coefficient with distance. The main findings of this study include:

(1) The EPNMs can describe the complex pore structure by using statistical parameters and reflect the transport process of solute and its dispersion in porous media effectively, which can be a useful method to study the solute transport mechanism in porous media.

(2) Increase in the standard deviation of pore body radius, decreases in curvature number and coordination number leads to an increase in dispersion coefficient. The change of dispersion coefficient with the pore structure parameters can be explained by the distribution of pore throat velocity in the EPNMs.

(3) The dispersion coefficient shows a scale effect even in statistically homogeneous porous media. The change of dispersion coefficient with distance can be fitted by a power function $D=Ax^B$. The value of A and B mainly increases with the standard deviation of the pore body radius, and decreases with the curvature number and coordination number.

5 ACKNOWLEDGEMENTS

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