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Probabilistic Characteristics of Effective Diffusion Coefficient in the Porous Media

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ABSTRACT

To check the variability of the effective diffusion coefficient in the unsaturated porous soil media, a Monte Carlo simulation was done for the equation suggested by Millington and Quirk(1961). The results shows that the probability density function of D_e/D_o is positively skewed. It means the chance of having less effective diffusion coefficient values in the soil media than mean value is high. Also, the distribution types of D_e/D_o are about same regardless of assumed distribution types of input parameters.

Introduction

Even though, the transport of gas and vapor in the vadose zone of the soil media can occur by many different mechanisms such as density induced convective flow, thermal gradient, pressure gradient by barometric pumping, diffusion is the most important process in the soil media in description of the gas transport. For the description of the diffusion in the porous media, the effective diffusion coefficient is often used. Understanding the variability of the effective diffusion coefficient is essential in the understanding of the gas behavior in the porous soil media. In this paper, effective diffusion coefficient will be discussed and Monte Carlo simulation will be used to evaluate the variability of the effective diffusion coefficient.

Effective Diffusion Coefficient

In 1855, Adolph Fick introduced a theory, now known as Fick's first law of diffusion, which stated the diffusion of chemicals within various media was analogous to heat and electrical conduction as follows:

$$J = -D\frac{\partial C}{\partial x} \qquad (1)$$

where J = diffusion flux ($M/L^2/T$), D = diffusion coefficient (L^2/T), C = chemical potential or concentration (M/L3), and x = distance (L).

To describe the diffusive transport of gaseous pollutants through soil, Fick's law can be used. However within a soil matrix, not every cross sectional area is available for diffusion process, and diffusion occurs along irregular and tortuous paths and this is presented in the Fig. 1. Fick's First Law, as applied to the tortuous channel of in Fig. 1, and for the block considered as a whole, those can be written as:

$$Q = -D_o\frac{A_e\Delta C}{L_e} \text{ : for the tortuous path} \qquad Q = -D\frac{A\Delta C}{L} \text{ : for the block as a whole} \qquad (2)$$

where Q = diffusive mass flow (M/T), A_e = area perpendicular to the direction of the tortuous path of length L_e , ΔC = concentration difference, and D_o = diffusion coefficient for open gaseous transport.

Solving for D/D_o yields the following:

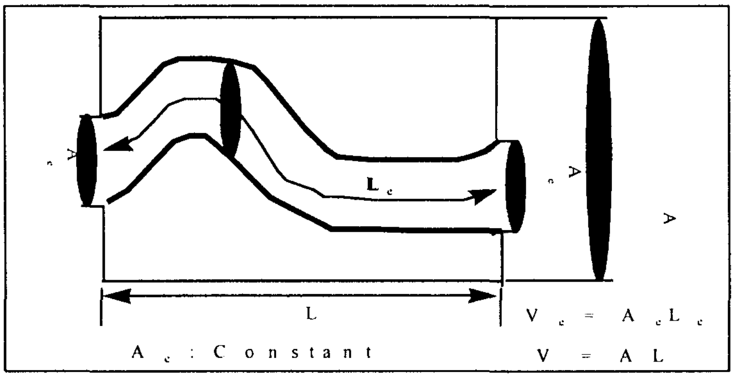

Fig. 1 Tortuosity model; diffusion length (L_e) and area (A_e) as related to the block length and cross section.

$$D = D_o \varepsilon_a \left(\frac{L}{L_e}\right)^2 \quad \text{and} \quad Q = -D_o \varepsilon_a \left(\frac{L}{L_e}\right)^2 A \frac{\Delta C}{L} \qquad (3)$$

where ε_a = air-filled porosity.

If we want to rewrite the equation (1),

$$J = -D_e \frac{\partial C}{\partial x} = -D_e \frac{\Delta C}{L} \qquad (4)$$

where D_e = effective diffusion coefficient and also τ = tortuosity;

then we can get the relationships of $D_e = D_o \varepsilon_a \tau$ and $\tau = \left(L/L_e\right)^2$.

Many investigators(Lai, 1976; Curie, 1970; Grable, 1968) have sought to determine a general relationship between effective diffusion coefficient and the total porosity, air-filled porosity, or both for the diffusion of a gas in a porous medium.

Among these, the expression of Millington and Quirk (1961) is the most frequently, almost exclusively, used equation in VOC emission models in the literature. Based on the Fick's first principles, Millington and Quirk derived the following relationship for the effective vapor diffusion coefficient:

$$\frac{D_e}{D_o} = \frac{\varepsilon_a^{10/3}}{\varepsilon_t^2} \qquad (5)$$

where ε_a = air-filled porosity and ε_t = total porosity.

Monte Carlo Method

A Monte Carlo simulation essentially consists of repetitively performing a set of model calculations with different combinations of input parameters, where each variable has its own characteristic distribution from which random values are generated. This repeated calculation using randomly generated input data generates a distribution of output values, and the statistics of the output parameter characterize the variability or uncertainty associated with the prediction. The general schematic representation of a Monte Carlo simulation is given in the Fig. 2. In the simulation, the random number generation algorithms by Press et al. (1992) and the sampling number of 5000 are used.

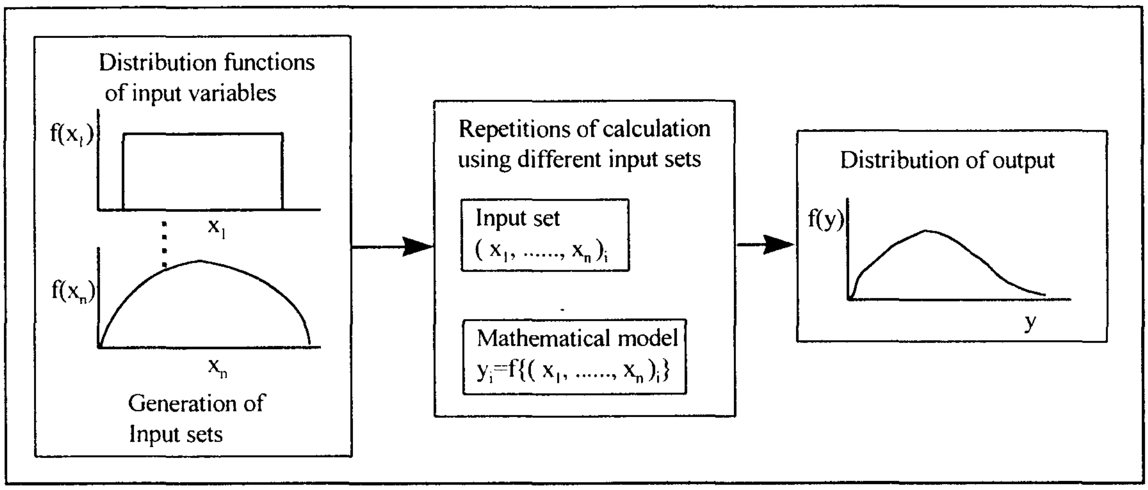

Fig.2 A schematic representation of the Monte Carlo simulation

Input Data

To check the variability of the effective diffusion coefficient with variabilities of air filled porosity and total porosity using Monte Carlo simulation, two variables are assumed to be independent. An assumed mean values are picked up first, and then for the uniform distribution, the upper and lower bounds are assumed. For the normal, the standard deviation of the distribution which gives about the 95% of the values are in the range of upper bound and lower bound of the uniform distribution is assumed. For the lognormal distribution, the mean and standard deviation of the distribution are assumed to be same as those of normal distribution. Under that condition, the variables for the lognormal distribution are calculated. The summary of the input data is given in the Table 1.

Table1 Input Data for the Monte Carlo Simulation

	air filled porosity	total porosity
uniform distribution	upper bound : 0.348 lower bound : 0.152 mean : 0.25	upper bound : 0.548 lower bound : 0.312 mean : 0.43
normal distribution	mean : 0.25 standard deviation : 0.050	mean : 0.43 standard deviation : 0.060
lognormal distribution	mean : 0.25 standard deviation : 0.050	mean : 0.43 standard deviation : 0.060

Results and Discussions

The results from the Monte Carlo simulation are summarized and shown in the Table2 and the probability density functions of the D_e/D_o is given in the Fig. 3.

The first thing we can do is compare these results with the deterministic method. The deterministic calculation gives 0.053 for D_e/D_o with air filled porosity of 0.25 and total porosity of 0.43. The probabilistic methods give slightly higher mean values for D_e/D_o than those of deterministic method.

Table2 Statistics of D_e/D_o from the Monte Carlo simulation

	mean	standard deviation	skewness coefficient
uniform distribution	0.069	0.054	1.258
normal distribution	0.065	0.048	1.916
lognormal distribution	0.066	0.055	3.092

The statistics of the Monte Carlo simulation show that there are not much differences in the mean values and standard deviations from the different distributions of input variables. It means the statistics of D_e/D_o is mainly controlled by the equation itself rather than the assumed distribution types. It also partly comes from the input values which was adjusted to have same mean values and standard deviations for each variable. So, it may be more important for the variability of the effective diffusion coefficient to evaluate the variability of the mean and standard deviations of the porosities than the distribution type of input variables.

Another thing we can recognize from the Table 2 is the high positive skewness coefficient The high positive skewness coefficient represents the situations which the tail of the distribution is on the right. It means the chances of having less effective diffusion coefficient values in the soil media than mean value is relatively high. As the mean value of the distribution is from the product of the variable and its probability terms as follows,

$$\mu = \int_{-\infty}^{\infty} x f(x) dx \quad : \text{continuous function}$$

$$= \sum_i x_i P(x_i) \quad : \text{discrete function}$$

The chances of having low value is high and thus low emission rates possibly, even though the mean value for the effective diffusion coefficient may be same.

The probability density function of the D_e/D_o shows the lognormal distribution type as in the Fig. 3. This results show that the variability or uncertainty analysis of the effective diffusion coefficient should be carefully done considering the final distribution type. Without the information about the distribution type, the normal distribution is usually assumed, but from the Monte Carlo simulation results, that is not the case for the effective diffusion coefficient. Therefore, these kind of probabilistic characteristics of the effective diffusion coefficient should be carefully considered in the understanding of the gas behavior in the porous soil media.

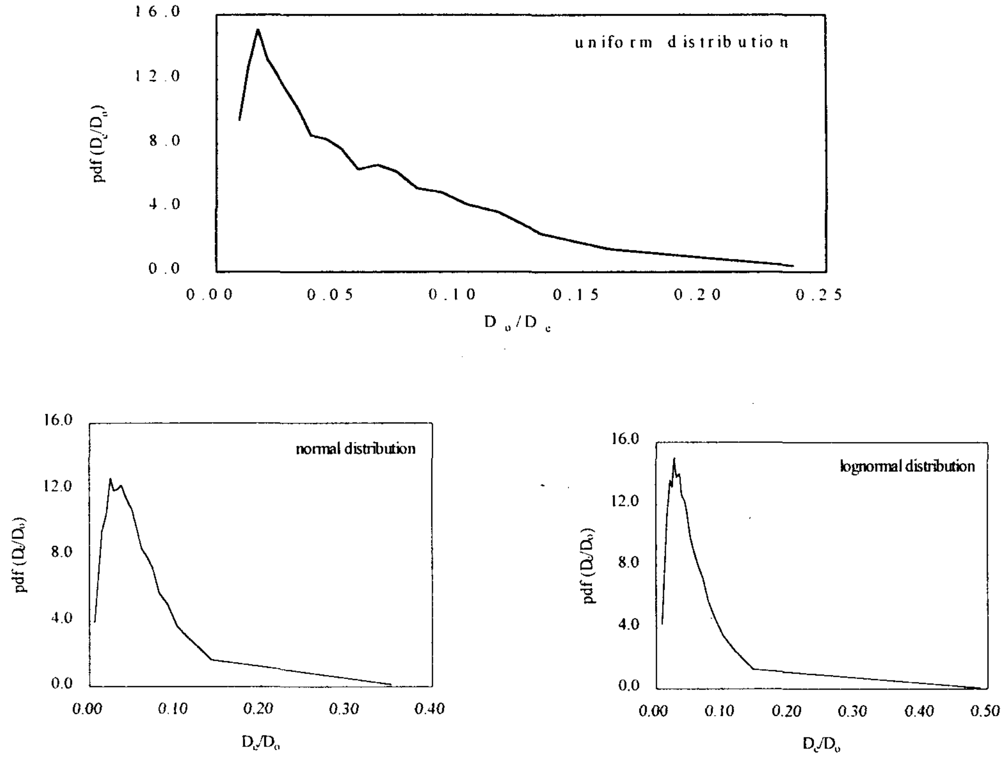

Fig3. Probability density functions(pdf) of D_e/D_o from the Monte Carlo simulation.

References

Currie, J. A. "Movement of soil gases in soil respiration," *Sorption and Transport Processes in Soils,* Soc. Chem. 37, pp152-171 (1970).

Freeze, R. A. and Cherry, J. A. Groundwater, Prentice-Hall, Inc., Englewood Cliffs, NJ, US (1979).

Grable, A. R., and Siemer, E. G. "Effects of bulk density, aggregate size, and soil water suction on oxygen diffusion, redox potentials, and elongation of corn roots," *Soil Sci. Soc. Am. Proc.*, 32:180-186, (1968).

Lai, S. H., Tiedje, J. M., and Erickson, A. E. "In situ measurement of gas diffusion coefficient in soil," *Soil Sci. Soc. Am. Proc.*, 40(1), pp 3-6 (1976).

Marshall, T. J. and Holmes, J. W. Soil Physics, Cambridge University Press, New York, (1979).

Mendoza, C. A. and Frind, E. O. "Advective-dispersive transport of dense ogranic vapors in the unsaturated zone: 1, model development, 2, sensitivity analysis," *Water Resources Res.*, 26(3), pp 379-98 (1990).

Millington, R. J., and Quirk, J. P. "Permeability of porous solids," *Trans. Faraday Soc.*, 57, pp 1200-120, (1961).

Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P. Numerical Recipes in Fortran, Cambridge University Press, NY, (1992).