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Use of water retention curves predicted from particle-size distribution data for simulation of transport of Benzo[a]pyrene in soil

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요 약 문

Water retention curve (WRC), one of soil hydraulic properties, is often approximated by property-transfer models (PTMs). Using the PTMs, we can estimate the WRCs from other physical properties such as particle-size distribution (PSD). The objective of this work was to investigate the performance of two PTMs with different origins for numerical simulations on transport of Benzo[a]pyrene in a soil. To do this, we chose both PTMs with different origins, i.e., (1) the lognormal distribution model (L and NL models), and (2) the modified Kovács model (MK model). The MK model showed the worse performance in estimation of the WRCs. When transport of B[a]P was simulated, the MK model predicted to move farther than the L and NL models did, indicating that transport of B[a]P in a soil can be greatly influenced by the choice of PTMs.

key word : water retention curve, particle-size distribution, property-transfer model. Benzo[a]pyrene, lognormal distribution model, modified Kovács model

1. Introduction

Persistent organic pollutants (POPs) such as Benzo[a]pyrene have been widespread in the environment. Especially, to analyze transport phenomena of POPs in soils, we need to perform numerical simulations using soil hydraulic properties and physico-chemical properties of target POPs. Water retention curve (WRC) which is one of soil hydraulic properties and can be used to estimate unsaturated hydraulic conductivities is often approximated by property-transfer models (PTMs). Using the PTMs, we can estimate the WRCs from other physical properties such as particle-size distribution (PSD) (Dane and Hopmans, 2002).

The objective of this work is to investigate the performance of two PTMs with different origins for numerical simulations on transport of Benzo[a]pyrene in a soil. To do this, we chose both PTMs with different origins, i.e., (1) the lognormal distribution model (Hwang and

Powers, 2003; Hwang and Choi, 2005), and (2) the modified Kovács model (Aubertin et al., 2003).

2. Theory

Lognormal distribution model

Recently, Hwang and Powers (2003) has developed a lognormal distribution model for estimating the WRC directly from the PSD, by applying a lognormal distribution law to the PSD and void-size distribution (VSD) and then combining them with the WRC function developed by Kosugi (1996). Parameters of the WRC have physical significance and are related directly to the statistics of the PSD and VSD. They applied the model to sandy soils and found that it performed reasonably well for estimating the WRC. They also found that the nonlinear model (NL model), which assumes a nonlinear relation between the PSD and VSD, performed better than the linear model (L model). Hwang and Choi (2005) evaluated the predictive potential of the lognormal distribution model for a broader range of soil textures.

Modified Kovács model

Kovács (1981) proposed a model for which the WRC equation is based on physical characteristics of porous media. The Kovács (1981) model assumes that water is held by both capillary and adhesive forces. In the model, both components act simultaneously to induce suction. The equation for capillary component is developed from a cumulative VSD function, while the adhesive component equation is based on an interaction law with van der Waals type attraction between solid surface and water dipoles. The capillary component become dominant at relatively low suction values, while the adhesive component is more important at higher suction when most capillary water has been withdrawn.

The original Kovács model (Kovács, 1981) did not easily lend itself to practical engineering applications because some of the key parameters were not completely defined. Aubertin et al. (1998) modified the original Kovács model and applied the modified model to the WRC of tailings and silts. For general applications from coarse- to fine-textured soils, Aubertin et al. (2003) did further modify the model of Aubertin et al. (1998). The final modified version of the original Kovács model (Aubertin et al., 2003) is named herein as the modified Kovács (MK) model.

3. Simulation scenario

The 113 ‘undisturbed’ sandy soil samples (sand, loamy sand, and sandy loam textures) were chosen from the UNSODA database. These data were used to test which model shows better performance for estimating the WRC.

A scenario was simulated in this study, i.e., downward transport of benzo[a]pyrene (B[a]P) pulse in a homogeneous and isotropic soil (UNSODA No. 1015 soil) with a soil depth of 100 cm. Numerical simulations using HYDRUS-1D were carried out during 3,650 days (10 years) for water and B[a]P movement downward to a water table (h = 0) located at z = 100 cm. The soil surface was held at a low h = 500 cm. A B[a]P pulse was added with its concentration of 5 mmol during $0 < t < 5$ days.

4. Results and discussion

Figure 1 shows comparison of predicted and observed water contents for three models (i.e., L, NL, and MK models). The MK model showed the worst performance among the models. Especially, it over-predicted water contents at the wet range. On the other hand, all three models under-predicted water contents at the dry range.

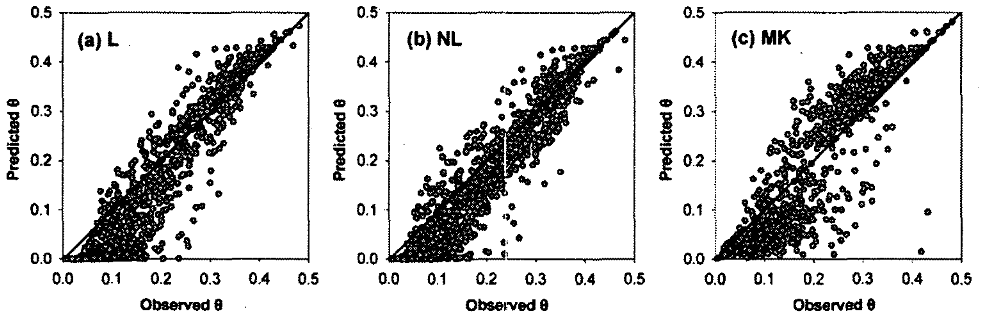

Figure 1. Scatter plot for predicted vs. observed water contents for (a) L, (b) NL, and (c) MK models

Figure 2 shows B[a]P concentration profile along soil depth at 10 years. The MK model predicted that B[a]P moves to z = 30 cm. On the other hand, the L and NL models predicted shorter movement and its concentration was smaller. It indicates that transport of B[a]P in a soil can be greatly influenced by the choice of PTMs.

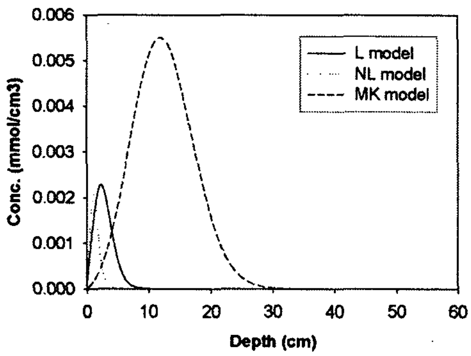

Figure 2. Benzo[a]pyrene concentration profile along soil depth after 10 years.

5. Conclusions

The MK model showed the worse performance in estimation of the WRC. Especially, it over-predicted water contents at the wet range. And the NL model showed slightly better performance than other models. However MK model has better performance compared to L, NL model in adhesion zone.

When transport of B[a]P was simulated for the same scenario, the MK model predicted to move farther than the L and NL models did, indicating that transport of B[a]P in a soil can be greatly influenced by the choice of PTMs.

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