The Simulation of Pore Size Distribution from Unsaturated Hydraulic Conductivity Data Using the Hydraulic Functions

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Until now, the pore size distribution, PSD, of soil profile has been calculated from soil moisture characteristic data by water release method or mercury porosimetry using the capillary rise equation. But the current methods are often difficult to use and time consuming. Thus, in this work, theoretical framework for an easy and fast technique was suggested to estimate the PSD from unsaturated hydraulic conductivity data in an undisturbed field soil profile. In this study, unsaturated hydraulic conductivity data were collected and simulated by the variation of soil parameters in the given boundary conditions (Brooks and Corey soil parameters, α_{BC} = 1 - 5 L^{-1}, b = 1 - 10; van Genuchten soil parameters, α_{VG} = 0.001 - 1.0 L^{-1}, m = 0.1 - 0.9). Then, K_s (1.0 cm h^{-1}) was used as the fixed input parameter for the simulation of each models. The PSDs were estimated from the collected $K(h)$ data by model simulation. In the simulation of Brooks-Corey parameter, the saturated hydraulic conductivity, K_s, played a role of scaling factor for unsaturated hydraulic conductivity, $K(h)$. Changes of parameter b explained the shape of PSD curve of soil intimately, and a α_{BC} affected on the sensitivity of PSD curve. In the case of van Genuchten model, K_s and α_{VG} played the role of scaling factor for a vertical axis and a horizontal axis, respectively. Parameter m described the shape of PSD curve and $K(h)$ systematically. This study suggests that the new theoretical technique can be applied to the *in situ* prediction of PSD in undisturbed field soil.

Key words: *Soil pore size distribution, Hydraulic conductivity, Matric potential, Soil moisture characteristic curve, Simulation*

Introduction

Hydraulic properties such as soil moisture characteristics curve (SMCC) and pore size distribution (PSD) are very important for the interpretation of soil physical characteristics and for the management of agricultural practices. The relationships between soil water content and water tension or infiltration rate are used to describe water flow in soil commonly. The hydraulic conductivity of a soil is affected by soil structure and pore size distribution. In the comprehension of soil hydraulic properties, the relationships of the hydraulic conductivity and water content, $K(\theta)$, and of the matric potential and the water content, $\Psi(\theta)$, are very important. Especially $\Psi(\theta)$ can be used to predict $K(\theta)$ and pore size distribution in soil is characterized from its soil moisture characteristics curve, indirectly (Childs, 1969). The measurement of $K(\theta)$ is very difficult and time consuming. Therefore many researches that utilize physical and empirical relation between hydraulic properties and other soil parameters have been studied. As an alternative to measurements, pedo-transfer functions have predicted water retention characteristics and hydraulic properties from the input variables that could be measured more easily such as soil texture, bulk density, or other soil variables (Rawls and Brakensiek, 1985; Ahuja et al., 1989; Vereecken et al., 1989, Saxton et al., 1986).

Recent development and application of tension disc infiltrometer (Ankeny et al., 1988; Perroux and White, 1988) has provided a simple, fast, and *in situ* method measuring infiltration rate. Tension disc infiltrometer is useful instrument that offer estimating methods of soil hydraulic properties at the soil surface. The most widely used method based on tension disc infiltrometer measurement is the Wooding's (1968) solution of approximate steady-state

water flow from a surface circular source. Other methods include the determination of sorptivity, macroscopic capillary length (White et al., 1992) and the numerical inversion (Vogeler et al., 1996). Reynolds and Elrick (1991) have attempted to assess the accuracy of soil hydraulic parameters estimated with tension infiltrometer using Wooding's approximate solution. They have reported that the estimated values of hydraulic conductivity from saturated soil were found to be 5 to about 300% of comparing to numerical simulation or other laboratory methods. But despite of large variation, it was thought that the measurement of unsaturated hydraulic conductivity by tension infiltrometer was useful since the other methods were not available in direct field measurement or needed to further validate the estimating technique (White and Perroux, 1989; Ankney et al., 1991).

Soil pores are very difficult to observe and characterize, bearing that the pore networks are complex 3-dimensional structure in variety of size, shape, connectivity. Burdine (1953) and Mualem (1976) have reported the pore size distribution models that were inferred from water retention characteristic making assumptions of pore continuity and connectivity. But the advanced analyzing of soil structure are very expensive and time consuming.

A few researchers, such as Everts and Kanwar (1993), Timlin et al. (1994), and Logsdon et al. (1993) have interpreted the relationship of soil pore size distribution and water flow using tension infiltrometer data without any quantification of the soil pore size distribution. Recently, Yoon et al. (2007) have attempted to estimate the characteristics of soil water retention and pore size distribution using tension infiltrometer data.

Goal of this research is to propose a simple theoretical approach to estimate pore size distribution from soil unsaturated hydraulic conductivity data using the tension disc infiltrometer technique that may provide a simple, rapid, and accurate soil hydraulic conductivity measurement. In order to investigate the feasibility of this theoretical approach, two hydraulic conductivity functions of Brooks and Corey (1964) and van Genuchten (1980) were adjusted, through the proposed theoretical approach, pore size distributions were simulated from unsaturated hydraulic conductivity data in each hydraulic function.

Materials and methods

Brooks and Corey model   Using a multiple regression analysis on soil water retention data, Campbell (1974)

developed the equation to describe water retention as follows;

$$h = h_e \left(\frac{\theta(h)}{\theta_s} \right)^{-b} \qquad \text{(Eq. 1)}$$

where, θ is the volume wetness (L^3 L^{-3}), θ_s is the saturated volume wetness (L^3 L^{-3}), h is the matric potential (L), h_e is the air-entry potential (L) of soil, and b is Campbell's water retention parameter. Similar to the prediction of unsaturated soil hydraulic conductivity (K) as proposed by Brooks and Corey (1966), the hydraulic conductivity function was proposed as

$$K = K_s \left(\frac{\theta(h)}{\theta_s} \right)^{2b+3} \qquad \text{(Eq. 2)}$$

where, K_s is the saturated hydraulic conductivity (L T^{-1}). By assuming that the effect of residual volumetric water content is negligible (i. e., $\theta(h) \gg \theta_r$ or $\theta_r \cong 0$), the effective saturation ($S_e(h)$, L^3 L^{-3}) would be equal to $S_e(h)/S_s$ and thus can be expressed in terms of matric potential as follows;

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \cong \frac{\theta(h)}{\theta_s} \qquad \text{(Eq. 3)}$$

By rearranging Eq. 1, the effective saturation will be given as

$$S_e(h) = \frac{\theta(h)}{\theta_s} = |\alpha_{BC} h|^{-1/b} \qquad \text{(Eq. 4)}$$

where, α_{BC} is the reverse of an air entry potential (h_e^{-1}, L^{-1}). Through substitution of Eq. 4 into Eq. 2, the relationship between K and h can be obtained as follows;

$$K(h) = K_s |\alpha_{BC} h|^{-2-3/b} \qquad \text{(Eq. 5)}$$

van Genuchten model   The hydraulic conductivity function of van Genuchten (1980) was known to perform better to predict a soil hydraulic properties. These functions were usually written as

$$K(\theta) = K_s S_e^l \left[1 - (1 - S_e^{1/m})^m \right]^2 \qquad \text{(Eq. 6)}$$

where S_e is the scaled water content (-), K_s is the

saturated hydraulic conductivity (L T^{-1}), θ_r and θ_s indicate the residual and saturated water contents (L^3 L^{-3}), respectively, l is a pore connectivity parameter (-), and n (-) and m ($= 1 - 1/n$) (-) are empirical parameters. The pore connectivity parameter l in the hydraulic conductivity function was estimated by Mualem (1976) to be 0.5 as an average for most soils.

The effective saturation by van Genuchten soil model will be given as

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \cong \frac{\theta(h)}{\theta_s} = \frac{1}{(1 + |\alpha_{VG} h|^n)^m} \quad \text{(Eq. 7)}$$

and van Genuchten soil parameters were confined as follows;

$$n = \frac{1}{1 - m} \qquad 0 < m < 1$$

$$\alpha_{VG} = \frac{1}{h_e}(2^{1/m} - 1)^{1-m}$$

where α_{VG} (L^{-1}) is the empirical parameter and h_e is the air-entry potential (L) of soil. Through substitution of Eq. 7 into Eq. 6, the relationship between K and h can be obtained as follows;

$$K(h) = K_s \left(\frac{1}{(1 + |\alpha_{VG} h|^n)^m} \right)^l \left[1 - \left(1 - \left(\frac{1}{(1 + |\alpha_{VG} h|^n)^m} \right)^{1/m} \right)^m \right]^2$$

(Eq. 8)

Estimation of PSD from unsaturated hydraulic conductivity data The soil moisture characteristic curve is the plot θ versus h. The effective water saturation ($S_e(h)$) is equivalent to the fraction of total pore space filled with water ($\theta(h)/\theta_s$), which can be obtained by inputting the values of α_{BC} and b into Eq. 4 in the case of Brooks and Corey model. Therefore, soil moisture characteristic curve (SMCC, $\theta(h)$) can be obtained by multiplying the effective water saturation by soil porosity (f, which was equal to θ_s);

$$S_e(h) \times f = \theta(h) = \theta_s \times |\alpha_{BC} h|^{-1/b} \quad \text{(Eq. 9)}$$

In the similar manner, soil moisture characteristic curve (SMCC, $\theta(h)$) can be obtained using the van Genuchten soil model as follows;

$$S_e(h) \times f = \theta(h) = \theta_s \times \frac{1}{(1 + |\alpha_{VG} h|^n)^m} \quad \text{(Eq. 10)}$$

In addition, the effective water saturation ($S_e(h)$) is the fraction of accumulative volume of a water filled soil pores as a function of h. Upon assuming that the pores were capillary tube shape and the contact angle of water to pore to be zero, the largest water filled soil pore with a radius (r) at given matric pressure h could be expressed by applying well known capillary equation;

$$r(h) = \frac{2\gamma}{\rho_w g h} \quad \text{(Eq. 11)}$$

where, γ is the surface tension (kg sec^{-2}) of water, ρ_w is the density of water (kg m^{-3}), and g is the gravitational acceleration (9.81 m sec^{-2}). The cumulative fraction of pore space filled with water, therefore, can be plotted with respect to soil pore size by plugging Eq. 11 into Eq. 3 and Eq. 7 for Brooks and Corey model and van Genuchten model, respectively.

Simulation of PSD In each models, unsaturated hydraulic conductivity data were collected and simulated by the variation of soil parameters in the given boundary conditions (Brooks and Corey soil parameters, $\alpha_{BC} = 1 - 5$ L^{-1}, $b = 1 - 10$; van Genuchten soil parameters, $\alpha_{VG} = 0.001 - 1.0$ L^{-1}, $m = 0.1 - 0.9$). Then, K_s (1.0 cm h^{-1}) was used as the fixed input parameter for the simulation of each models. This fixed value of 1.0 cm h^{-1} was within the range of K_s in sandy loam or sandy clay loam soils. The PSDs were estimated from the collected $K(h)$ data by model simulation using the Eq. 10 and Eq 11 for Brooks and Corey model and van Genuchten model, respectively.

Results and Discussion

Simulation of PSD by Brooks-Corey parameters The Eq. 5 ($K(h) = K_s |\alpha_{BC} h|^{-2-3/b}$) was the function that explains the relationship of unsaturated hydraulic conductivity ($K(h)$) and hydraulic pressure head (h). In Eq. 5 the role of K_s has been easily understood as the scaling factor of $K(h)$. The effects of α_{BC} and b on $K(h)$ were more complex.

Figure 1 and 2 showed the effects on PSD and $K(h)$ by the variation of b when α_{BC} was 1.0, and 5.0, respectively. Figure 3 and 4 showed the effects on PSD and $K(h)$ by the variation of α_{BC} when b was 1.0, and 5.0, respectively. In the changes of Brooks-Corey soil parameters, data points were plotted on a log-log scale in relationship between $K(h)$ and pressure head (h) as the declined straight lines in
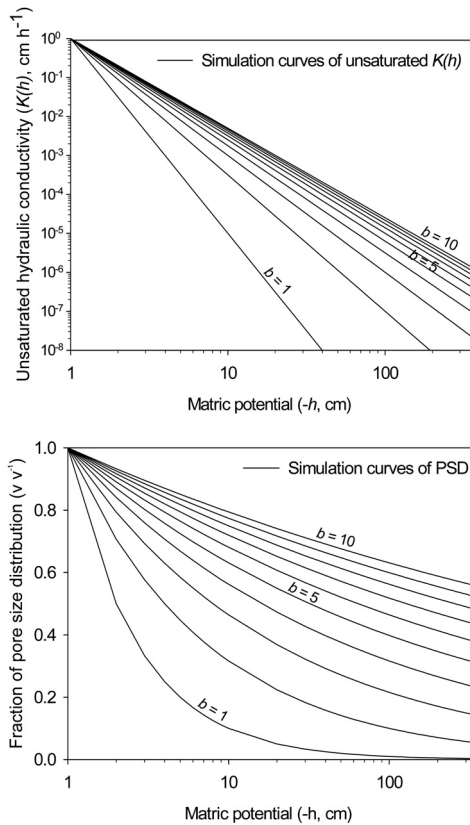
Fig. 1. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in parameter b in Eq. 5. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the α_{BC} is 1.0 cm^{-1}.
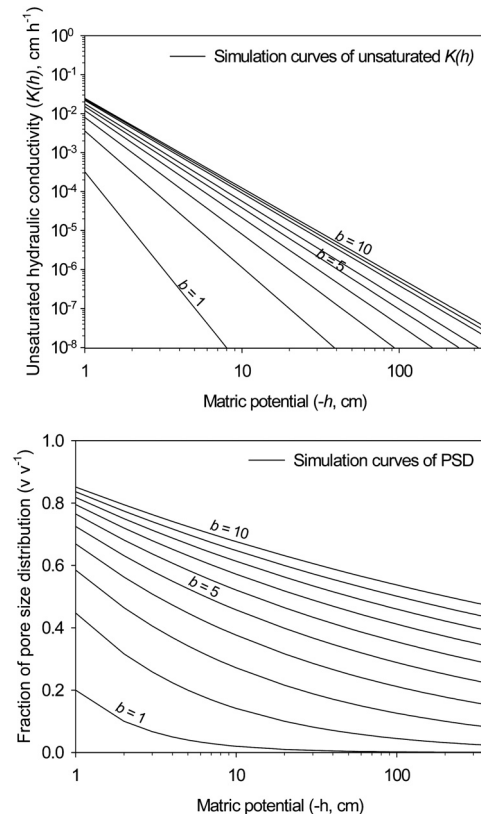

Fig. 2. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in parameter b in Eq. 5. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the α_{BC} is 5.0 cm^{-1}.

decreasing of h. Low b led to a stronger reduction in the simulations of PSD and $K(h)$, but the effect on $K(h)$ of b was more meager than that of α_{BC}. The reduction of PSD and $K(h)$ also showed a same tendency successively in the sequential variation of soil parameter b. Campbell (1974) has defined the soil parameter b as PSD factor in hydraulic function (Eq. 5). In the simulated curves of PSD by h, the variation of parameter b caused the high variations on PSD. Nachabe (1996) has reported that small variation of soil parameter b did not affect the infiltration rate significantly in the research of shape factor modeling the infiltration rate. In this study, The small variation in b gave a small effect for $K(h)$, too.

Low α_{BC} caused a strong reduction in $K(h)$ apparently but gave a little effect for the reduction of PSD. Variation of b was enough to explain the curve shape of PSD in a full range of pore space. Parameter b was closely concerned with PSD and affected on the sensitivity of $K(h)$. The α_{BC} may not express the PSD of variable textured soils directly.

Nachabe (1996) reported that the shape factor, b, could not be measured directly in the field, also, b was difficult

to estimate accurately because it varied within a narrow range, and it involved many other soil parameters. White and Sully (1987) suggested that the using of setting b value ($b = 0.55$) was practical for most field. But the suggestion of White and Sully (1987) was not proper to estimate PSD from measured $K(h)$ data set, because soil parameter b was strongly related with the shape of PSD curve. The opinion that the using $b = 0.55$ was practical for most field was possible when parameterization procedure was simplified in the estimation of $K(h)$ for field soils.

In the adjustment of Brooks and Corey model for the simulation of PSD and unsaturated $K(h)$, pore volume fractions and hydraulic conductivity might be overestimated at high pressure head. It was thought that overestimation was resulted from the nature of Brooks-Corey hydrological model adopting exponential type function, and K_s was seem to be increased exponentially in high water content. It has been reported that developed model to describe hydraulic properties in homogeneous porous media cannot account for significant impact of the structural pores on water retention and hydraulic conductivity close to saturation
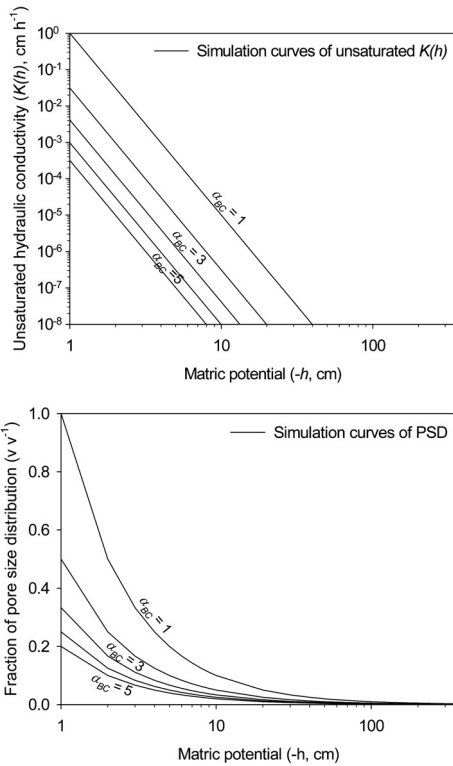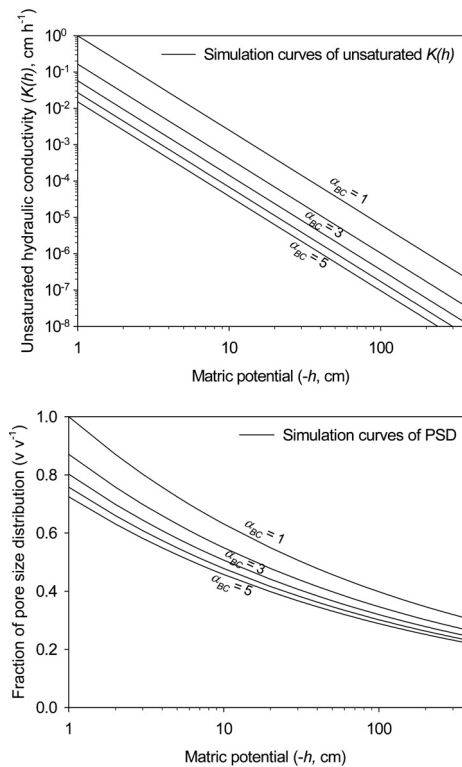
Fig. 3. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in α_{BC} in Eq. 5. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the b is 1.0.
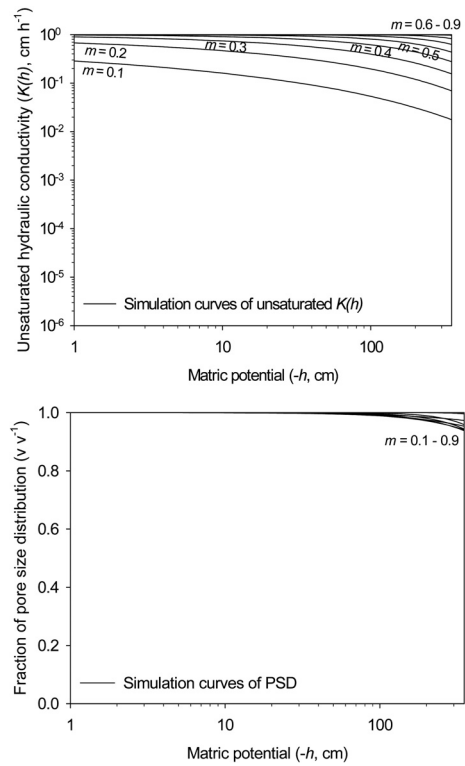

Fig. 5. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in parameter m in Eq. 8. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the α_{VG} is 0.001 cm^{-1}.

(Mualem, 1976; van Genuchten, 1980). Since Brooks-Corey hydrological model is assuming soil matrix as homogeneous media, the prediction of PSD in saturated condition may be difficult. In recently for further improvement of hydraulic conductivity two or multi-domain models have been proposed (Smettem and Kirkby, 1990; Othmer et al., 1991; Durner, 1992; Ross and Smettem, 1993). To characterize PSD in saturated condition more correctly, it is possible to adopt recent works such as multi-domain model in the estimation model of pore size distribution.

Simulation of PSD by van Genuchten soil parameter
The Eq. 8 is the relationship between $K(h)$ and hydraulic pressure head (h) from the van Genuchten model. In order to understand the shape variation of PSD and $K(h)$ according to changes of van Genuchten soil parameters (α_{VG}, m, n), simulation data in variation of α_{VG} and m were plotted in Fig. 5, 6, and 7. In simulation of PSD and $K(h)$, K_s and α_{VG} played the role of scaling factors about a vertical axis and a horizontal axis. The m is a soil parameter which describes systematically the shape sensitivity of PSD curves and $K(h)$. The systematic

Fig. 4. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in α_{BC} in Eq. 5. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the b is 5.0.

scheme of simulation curves may be caused by the closed boundary condition of equation variables. The hydrological model of van Genuchten has included some constraints as closed form equation (van Genuchten, 1980). Schaap and Leij (2000) imposed the following constraints during the optimization to avoid fitted parameters with unreasonable values, $0.0001 < \alpha_{VG} < 1.000$ cm^{-1}, $1.0001 < n < 10$ ($n = 1/(1-m)$).

The van Genuchten hydrological model may explain PSD and $K(h)$ in near saturated condition as shown in simulation results. But Schaap and Leij (2000) reported that prediction of $K(h)$ was physically unrealistic but it occasionally occurred while fitting van Genuchten's hydrological model equation because of random or systematic errors in unsaturated conductivity data.

In this simulation results we can confirm the reversion of $K(h)$ having one breakpoint by variations in m on the $K(h)$ in Eq. 8. And Fig. 6 and 7 showed the reversion range below the breakpoint during the simulation of $K(h)$. In reversion of $K(h)$, reduction of total pore space in

variation of m may lead to more enhanced $K(h)$. This effect may be physically unrealistic but imply theoretical concept.

Also Nachabe (1996) has reported that the α_{BC} and b of Brooks and Corey model and α_{VG} and m of van Genuchten model had physical implications, but that K_s in van Genuchten model had no physical meaning, because estimation of K_s by the van Genuchten model could have several fit. van Genuchten and Nielson (1985) and Luckner et al. (1989) have argued that K_s might not be especially suitable matching point because K_s was sensitive to macropore flow. However, the K_s was used with matching point for the estimation of other parameters since it could be measured in a simple experiment commonly. But the use of measured K_s might be not always correct in parameter estimation procedure, because a measured K_s was determined apart from the determining of $K(h)$ in field. In the procedure of van Genuchten parameter estimation for the estimation of PSD, the using of K_s as matching point may mislead reasonable parameter estimation.
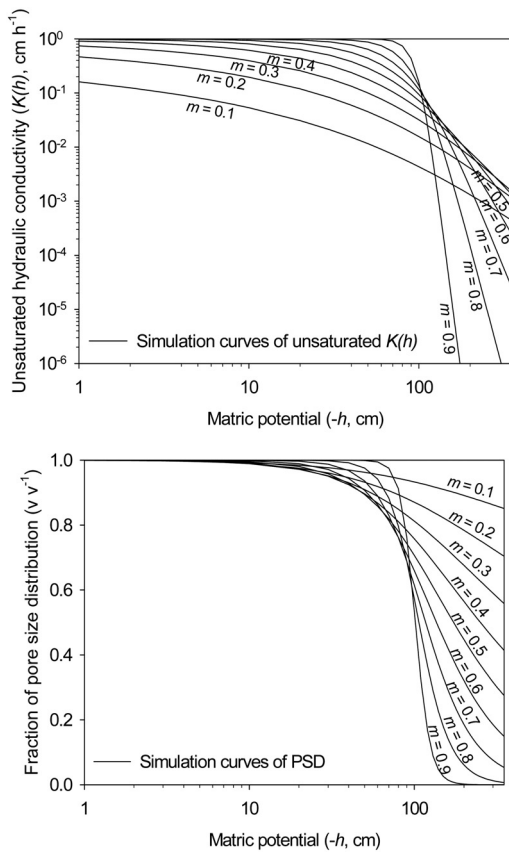

Fig. 6. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in parameter m in Eq. 8. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the α_{VG} is 0.01 cm^{-1}.
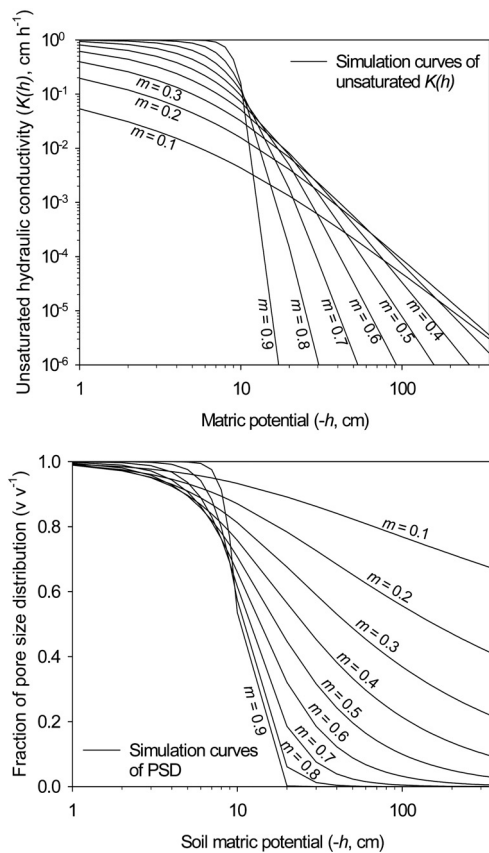
Fig. 7. The effect on PSD and unsaturated hydraulic conductivity, $K(h)$, of the variations in parameter m in Eq. 8. Straight lines indicate the simulation curves of PSD and $K(h)$ when the K_s is 1.0 cm h^{-1}, and the α_{VG} is 0.1 cm^{-1}.

Conclusion

In the simulation of Brooks-Corey parameter, the K_s played a role of scaling factor for $K(h)$. Changes of parameter b explained the shape of PSD curve of soil intimately, and a α_{BC} affected on the sensitivity of PSD curve. In the case of van Genuchten model, K_s and α_{VG} played the role of scaling factor for a vertical axis and a horizontal axis, respectively. Parameter m described the shape of PSD curve and $K(h)$ systematically.

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토양 수리학적 함수를 이용한 불포화 수리전도도로부터
공극크기분포의 모사

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토양의 공극 크기별 분포는 토양중 수분의 함량과 수분퍼텐셜의 관계를 나타내는 토양수분특성 자료로부터 계산된다. 그러나 기존의 토양수분특성 측정방법들은 교란된 토양을 이용하거나 코어시료를 채취한다 하여도 동역학적으로 변화하는 현장 토양 공극분포를 반영하는 데는 많은 어려움이 있었다. 또한 이러한 토양수분특성 자료를 얻기 위해서는 많은 시간과 노력이 요구되어 왔다. 따라서 본 연구에서는 교란되지 않은 현장 토양에서 측정한 불포화 수리전도도 자료로부터 토양의 공극 크기별 분포 곡선을 추정하는 이론적 체계를 제시하고자 하였다. 이를 위해 Brooks-Corey와 van Genuchten의 수리학적 모델을 이용하여 토양의 불포화 수리전도도 자료로부터 공극의 크기별 분포를 추정하는 이론적 모델을 전개하였으며, 이러한 이론적 모델에 근거하여 Brooks-Corey와 van Genuchten의 soil parameter들의 변화에 따른 불포화수리전도도와 공극 크기별 분포곡선의 모사하였다. 공극크기별 분포곡선의 모사는 토성별 불포화수리전도도 곡선의 scaling factor 역할을 하는 K_s를 1.0 cm h^{-1}로 설정하고, 수리학적 모델별로 일정한 경계조건 (Brooks-Corey soil parameters, α_{BC} = 1 − 5 L^{-1}, b = 1 − 10; van Genuchten soil parameters, α_{VG} = 0.001 − 1.0 L^{-1}, m = 0.1 − 0.9)에서 수행하였다. Brooks-Corey 모델을 이용한 공극 크기별 분포곡선의 모사에서는 parameter b가 공극분포곡선의 형태에 영향을 주었으며, α_{BC}는 공극분포곡선의 민감도에 영향을 주었다. 또 van Genuchten 모델을 이용한 공극 크기별 분포곡선의 모사에서는 α_{VG}가 scaling factor의 역할을 하였으며, parameter m은 공극분포곡선의 형태에 영향을 주었다. 따라서 경계조건 안에서 불포화 수리전도도 자료로부터 공극의 크기별 분포 모사가 가능하였으며, 토양 parameter들이 토성, 입자분포 등의 물리적 특성을 잘 반영하는 경우 이론적으로 현장 토양의 공극 크기별 분포의 추정이 가능할 것으로 판단되었다.