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ESTIMATING UNSATURATED HYDRAULIC PROPERTIES OF SOFT ROCK BY THREE DIFFERENT FLOW MODELS

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Several countries utilize the sedimentary soft rock for nuclear waste disposal because it has a potential to use as a host rock. Therefore, the analytical researches on the unsaturated flow of this type of rocks have been increased to assure the safety of the disposal. In this study, the applicability of three models; Brooks-Corey/Burdine (BC), Campbell (CB) and van Genuchten (VG) that have been used commonly for soil was studied, by applying these to one dimensional flow induced by evaporation in six disk shaped soft rock samples. The best parameters in each model were inversely estimated by adopting genetic algorithm (GA). It was clearly found that the best parameters in BC and CB models can be easily estimated and the measured evaporation change could be well analyzed. However, the parameters in VG model could not be estimated easily. It was found that BC and CB models are more robust than the VG model for the analysis of unsaturated flow in soft rock.

Key Words : *sedimentary soft rock, unsaturated flow, inverse estimation, genetic algorithm*

1. INTRODUCTION

As a possible and safe way of hazardous waste disposal, it is isolated in tunnels excavated in deep underground of sedimentary soft rock (mudstone, sandstone, tuff, etc.) which is considered as one of the preferable types of host rock. The reason is that the hydraulic conductivity of soft rock is generally low and it contains clay minerals which have high ability to absorb the radionuclide. However, many reasons such as the unsaturated zone which was created during the excavation, the stress condition change of the tunnel wall and the settlement of waste under the ventilation conditions may cause the generation of many fractures that can form a ‘damaged zone’. This ‘damaged zone’ thus formed around the tunnel becomes high permeable because of many fractures created in it. As a result, the groundwater and hazardous waste flow easily through this high permeable zone. It is crucial to estimate the unsaturated hydraulic properties and the thickness of this zone precisely because the drying mechanism of rock is one of the essential mechanisms to create fractures. For the estimation, the relationship among the relative hydraulic conductivity, saturation and suction pressure of the soft rock should be well evaluated. Although many theoretical/empirical models have been used for the approximation of unsaturated properties of soil, the suitable model for soft rock has not been clarified yet. Therefore, it is essential to study more in detail on a proper model fitting for soft rock. In this study, three different models; Brooks-Corey/Burdine (BC) model1), Campbell (CB) model2) and van Genuchten (VG) model3) which were originally proposed for soils, were utilized to investigate the applicability to the soft rock.

2. THREE MODELS ADOPTED

Three models which are adopted to estimate unsaturated hydraulic properties in this study are summarized as follows.

(1) Brooks-Corey/Burdine (BC) Model

$$\theta(\varphi) = \theta_r + (\theta_{sat} - \theta_r)\left(\frac{\varphi}{\varphi_b}\right)^{-\lambda} \quad \text{if } \varphi < \varphi_b \quad (1)$$

$$k = k_{sat}\left(\frac{\varphi}{\varphi_b}\right)^{-2-3\lambda} \quad \text{if } \varphi < \varphi_b \quad (2)$$

where θ (m^3m^{-3}) is the volumetric water content, θ_{sat} and θ_r are the saturated and residual water content respectively (m^3m^{-3}). φ (Jkg^{-1}) is the matric potential, φ_b (Jkg^{-1}) is the bubbling pressure and λ is the Brooks-Corey's pore size distribution index. k (ms^{-1}) is the unsaturated hydraulic conductivity and k_{sat} (ms^{-1}) is the saturated hydraulic conductivity.

(2) Campbell (CB) Model

$$\theta(\varphi) = \theta_{sat}\left(\frac{\varphi_e}{\varphi}\right)^{1/b} \quad \text{if } \varphi < \varphi_e \quad (3)$$

$$k(\theta) = k_{sat}\left(\frac{\theta}{\theta_{sat}}\right)^{m} \quad \text{if } \varphi < \varphi_e \quad (4)$$

where, φ_e (Jkg^{-1}) is the air entry potential. b and m are shape parameters related to the pore size distribution of the porous media and $m=2b+3$.

(3) van Genuchten (VG) Model

$$S_e = \frac{(\theta - \theta_r)}{(\theta_{sat} - \theta_r)} = \left(1 + \left|\alpha\varphi\right|^n\right)^{-l} \quad \text{if } (0 \le S_e \le 1) \quad (5)$$

$$k(\theta) = k_{sat} S_e^{1/2}\left[1 - (1 - S_e^{1/l})^l\right]^2 \quad (6)$$

where S_e (m^3m^{-3}) is the effective water content, α (m^{-1}), l and n are curve shape factors and $n=1/(1-l)$.

In BC model and VG model, θ_r is approximated as 0.01[4] from the drying test in the laboratory.

The BC and CB models have similar form and the hydraulic property relations are presented in exponential type equations. Both these models have threshold values φ_b and φ_e which indicate the pressure for entering air into the soft rock. On the other hand, VG model has no such value. The major objectives of this research were mainly focused to clarify the effect of the air entry value on the basis of unsaturated flow in soft rock and to investigate the differences among the three utilized models.

3. THE BASIC CONCEPT

The previous authors[4] have studied the inverse estimation technique to estimate the parameters of VG model by analyzing the transient evaporation from a standard soil and a soft rock sample. In this study, the evaporation change from several soft rock samples were analyzed by using above mentioned models and the best parameter combinations in each model were estimated.

(1) Samples used and the evaporation experiment

The rock specimens were sampled from Rokkasho Low-Level Radio-active Waste disposal site in Aomori prefecture of Japan[5]. The Takahoko formation which distributed over this area is mainly consists of sandstone and pumice tuff. In this study, three sandstone specimens and three pumice tuff specimens were used for the unsaturated hydraulic property estimation. The sandstone specimens were homogenous in texture whereas the pumice tuff specimens were consisted with pumice particles (**Fig. 1**). The physical properties and the saturated hydraulic conductivity of these specimens are shown in **Table 1**[5]. The saturated hydraulic conductivity was measured by the falling head test. According to the **Table 1**, the saturated hydraulic conductivities (k_s) of sandstone specimens are almost one order smaller than the pumice tuff specimens.

One dimensional unsaturated flow was generated in the disk shaped specimens by giving

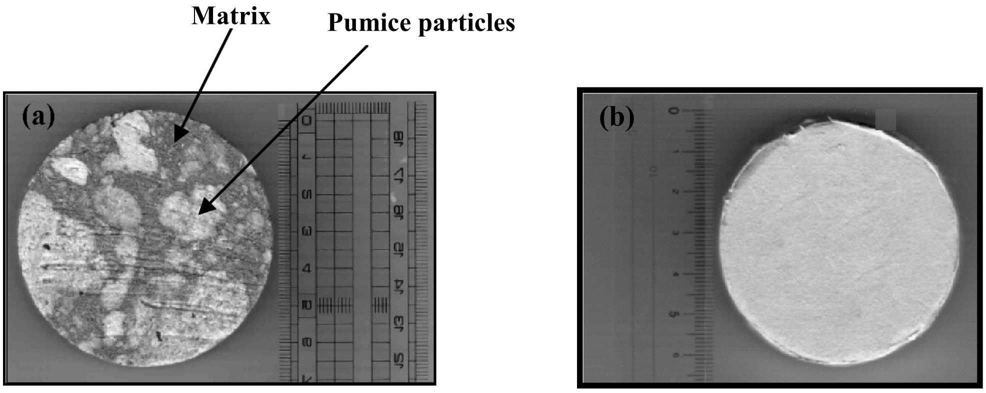

Fig. 1 (a) Appearance of a pumice tuff specimen **(b)** Texturally homogenous sandstone specimen (Maung et al. 2008)

Table 1 Physical property of soft rock specimens
L= Length,D= Diameter,ρ_b=Bulk density,ϕ= Porosity
k_s= Saturated hydraulic conductivity

Sample Name	L (cm)	D (cm)	ρ_b (gcm^{-3})	ϕ (%)	k_s (cm/sec)
Sandstone-1	3	9	1.81	0.42	4.0E-7
Sandstone-2	2	6	1.61	0.46	6.5E-7
Sandstone-3	2	6	1.56	0.46	7.5E-7
Pumice Tuff-1	3	9	1.70	0.52	4.2E-6
Pumice Tuff-2	2	7	1.46	0.58	4.8E-6
Pumice Tuff-3	2	7	1.53	0.52	3.6E-6

the transient evaporation from the upper surface. Initially, the specimens were fully saturated by submerging in a distilled water container and sucking air by a vacuum pump. Then the samples were completely sealed with Silicon sealant except for the upper surface. Evaporation was allowed only from the upper surface. The experiment was conducted in a constant humidity (40%) and air temperature (25^0C) chamber. The evaporation rate was determined by the weight change of the specimen. When it is less than 0.01 g/hour, the experiment was terminated.

(2) Analysis of transient evaporation rate

The transient evaporation rate of soil/rock has been used to inversely estimate hydraulic properties by previous researchers using water and vapor fluxes[4),5),6)].

a) One dimensional upward flow induced by evaporation

Campbell[6)] proposed that the actual evaporation (E_v) in mm/day can be obtained at the soil/rock surface, when the potential evaporation (E_p) rate is known.

$$E_v = E_p \frac{(h_s - h_a)}{(1 - h_a)} \tag{7}$$

where h_s is the soil/rock surface humidity and h_a is the atmospheric humidity. According to this equation, evaporation is a function of h_s under constant h_a. Moreover, h_s indicates only the saturation at the top surface.

$$h_s = \exp\left(\frac{M_w \varphi}{RT}\right) \tag{8}$$

where M_w is the molar mass of water (0.018 Kgmol^{-1}), R is the universal gas constant (8.3143 Jmol^{-1}K^{-1}) and T is the rock surface temperature (K).

b) Two phase transport in rock

The vertical liquid flow through the unsaturated porous media is described by Darcy's law[7)]. According to this, the unsaturated water flux q_l can be written as Eq. (9).

$$q_l = -k(\theta)\left[\left(\frac{\partial \varphi}{\partial z}\right) + 1\right] \tag{9}$$

where q_l is water flux (ms^{-1}), k is soil hydraulic conductivity (ms^{-1}), φ is soil/rock matric head and z is the vertical co-ordinate (m, positive upward).

According to Fick's law[6)], the vapor flow in isothermal porous media can be written with some rearrangements[6)] as Eq. (10)

$$q_v = -k_v \frac{d\varphi}{dz} \tag{10}$$

where q_v is vapor flux (ms^{-1}) and k_v is vapor conductivity (ms^{-1}).

(3) Inverse estimation technique

The inverse technique was applied for the estimation of model parameters[8)]. Further, the genetic algorithm (GA) was adopted as an optimization tool. GA was used by many previous researchers in the parameter estimation by evaporation method[4),5), 9)]. It is a promising solution for the problems occurred in inverse estimation technique such as non-uniqueness and local minima problem. It is well known that the inclusion of many parameters in inverse estimation tends to result non-uniqueness[9)]. Therefore, only two parameters of each model were focused in this study.

The basic theory of GA has been explained by many previous researchers[4),5),9),10)]. Therefore, only the application procedure of GA in this study is summarized as follows.

a) The unknown parameter gene combination was assumed as a chromosome (i.e. BC model φ_b and λ; CB model φ_e and b; VG model l and α)
b) These chromosomes consist of genes which were encoded as binary digits (0 and 1) according to random numbers and they have 22 length binary digits.
c) The population size was fixed as 50 and initially the fitness value (F) was calculated according to the Eq. (11) for every chromosome in this population. E_m and E_c are measured and calculated evaporation respectively.

$$F = \sum_{t=1}^{n} \left[E_m(t) - E_c(t)\right]^2 \tag{11}$$

d) The roulette wheel selection method was carried to select the best chromosomes which had the largest F value (i.e. parents).
e) The crossover and mutation operations in the GA process were done to select the new

chromosomes which are called children. In this study we used 0.6 as crossover rate and 0.005 as mutation probability.

f) The parent combinations and children combinations were compared according to the *F* values and the combinations having the maximum value was selected. This criterion was repeated until the population size reaches to 50 in new generation.

g) The total procedure was repeated until the *SSD* value (Eq. (12a)) becomes lower than a critical value of *SSD* given (i.e. this value is not change with iteration and it is specimen specific) and the difference (D_{SSD}) between the maximum *SSD* (SSD_{max}) and minimum *SSD* (SSD_{min}) becomes constant (see Eq. (12b)).

$$SSD = \frac{1}{F} \tag{12a}$$

$$D_{SSD} = SSD_{\max} - SSD_{\min} \tag{12b}$$

4. ANALYTICAL RESULTS

(1) Performance of Genetic Algorithm

In this study, GA was used to minimize the *SSD* value during the simulation. The three basic operations; the selection, crossover and mutation were repeated for 100 generations to produce the best fit parameters. According to previous studies[4),5)], it has shown that the GA technique is a promising optimization method for the parameter estimation.

(2) Simulation of Evaporation Change

To measure the moisture content in rock specimens is one way to estimate the flux in the specimens. However, the rock specimens were thin to measure the moisture content. Therefore, the transient evaporation method was used in this study.

The three models were used to fit the measured evaporation change. **Fig. 2** shows the measured and calculated evaporation for the sandstone specimens with the selected best combinations of model parameters. According to this figure, it can be seen that the measured evaporation rates for sandstone specimens are nearly constant (~ 12 mm/day) in the initial evaporation conditions. According to the fitted curves, the CB and BC models gave good accordance. The evaporation rate of pumice tuff samples is shown in **Fig. 3**. This figure shows that the initial evaporation rate varies with the samples (~ 12-18 mm/day). This may be due to the variation of pumice distribution in those samples. Similarly, the CB and BC models fitted well with the measured evaporation data of pumice tuff specimens. The obtained model parameters were shown in **Table 2**.

The relationship between the relative hydraulic

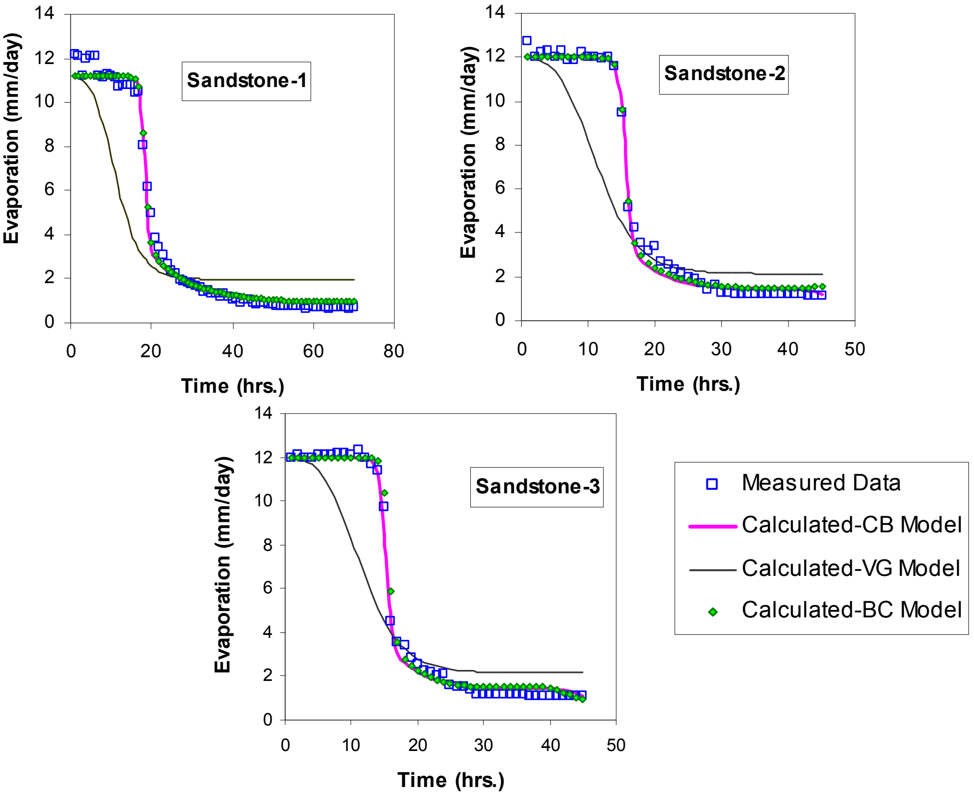

Fig. 2 Measured and calculated evaporation rates for the sandstone specimens

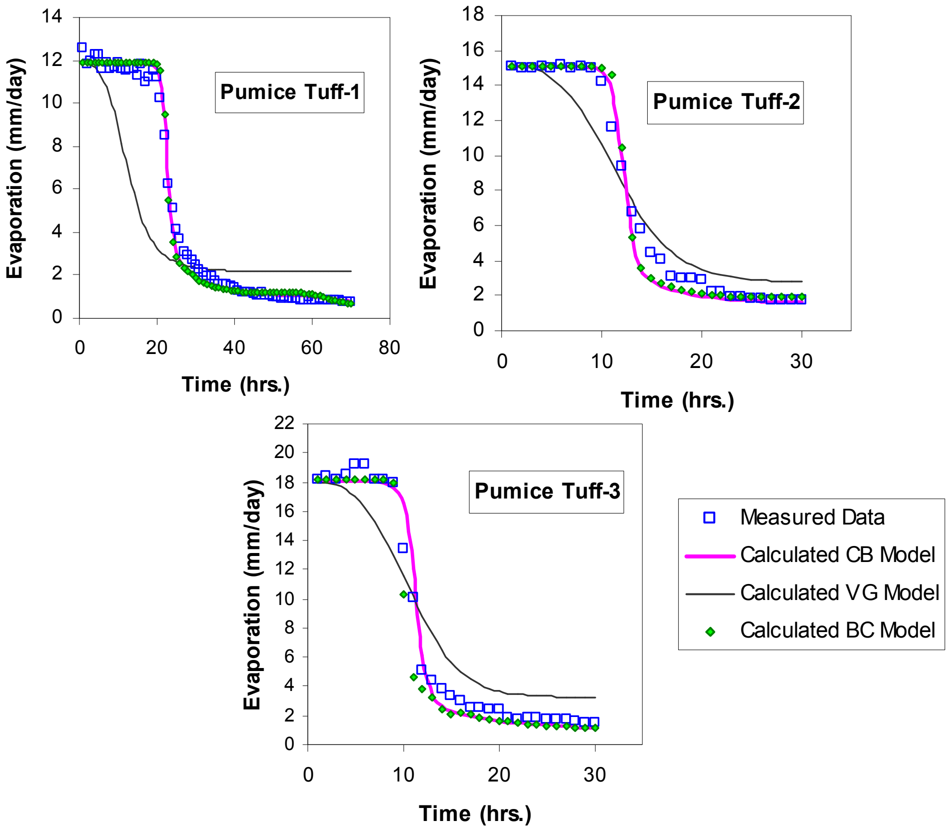

Fig. 3 Measured and calculated evaporation rates for the pumice tuff specimens

Table 2 Optimized model parameters for soft rock specimens

Sample Name	BC Model		CB Model		VG Model	
	φ_b (m)	λ -	b -	φ_e (m)	α (m^{-1})	l -
Sandstone-1	-3.69	1.60	1.63	-4.00	0.01	0.40
Sandstone-2	-2.80	1.90	1.94	-3.90	0.01	0.30
Sandstone-3	-3.80	1.90	2.10	-3.90	0.01	0.40
Pumice Tuff-1	-2.40	2.86	2.90	-3.99	0.01	0.30
Pumice Tuff-2	-1.50	3.59	3.87	-1.71	0.06	0.20
Pumice Tuff-3	-2.50	4.00	3.88	-1.78	0.06	0.21

conductivity, saturation, and suction pressure can be obtained by applying the optimized parameters of the three models (see **Table 2**) to these model equations. These relationships obtained by three models for a sandstone specimen and a pumice tuff specimen are shown in **Fig. 4**. According to this figure, the trends of the unsaturated hydraulic property curves of the soft rock specimens are not so different. Nevertheless, in the 100% saturation condition near the bubbling/air entry pressure, the largest difference in VG model can be observed. Therefore, the relationships can be estimated precisely using CB and BC models as these two models have a threshold value which shows the entering air into the rock sample. Further, in **Fig. 2** and **3** it is clearly seen the fitting of the measured evaporation by VG model is difficult and the reason for this should be considered.

(3) Simulation of parameters in VG model

In the case of VG model, the fitting of evaporation curve is much difficult than the CB and BC models. In such a case, the VG parameter ranges were changed and tried to fit the curves with minimum error. **Fig. 5** shows the difference when the *l* value has changed from 0.2 to 0.9 and the *α* value changed from 0.06 (simulation-1), 0.05 (simulation-2) and to 0.02 (simulation-3) for pumice tuff 2. From this, it is clear that the fitting of VG model is difficult and this model is not robust for soft rock. Therefore, the air entry/bubbling value should be considered as the threshold pressure for soft rock.

5. CONCLUSIONS

The selection of a proper model to estimate unsaturated hydraulic properties for soft rock is very important. In this study, the performance of Brooks-Corey/Burdine, Campbell and van Genuchten models were compared with each other by estimating the best parameters in each model. The obtained results can be summarized as follows.

1. The transient evaporation change can be estimated and the model parameters can be

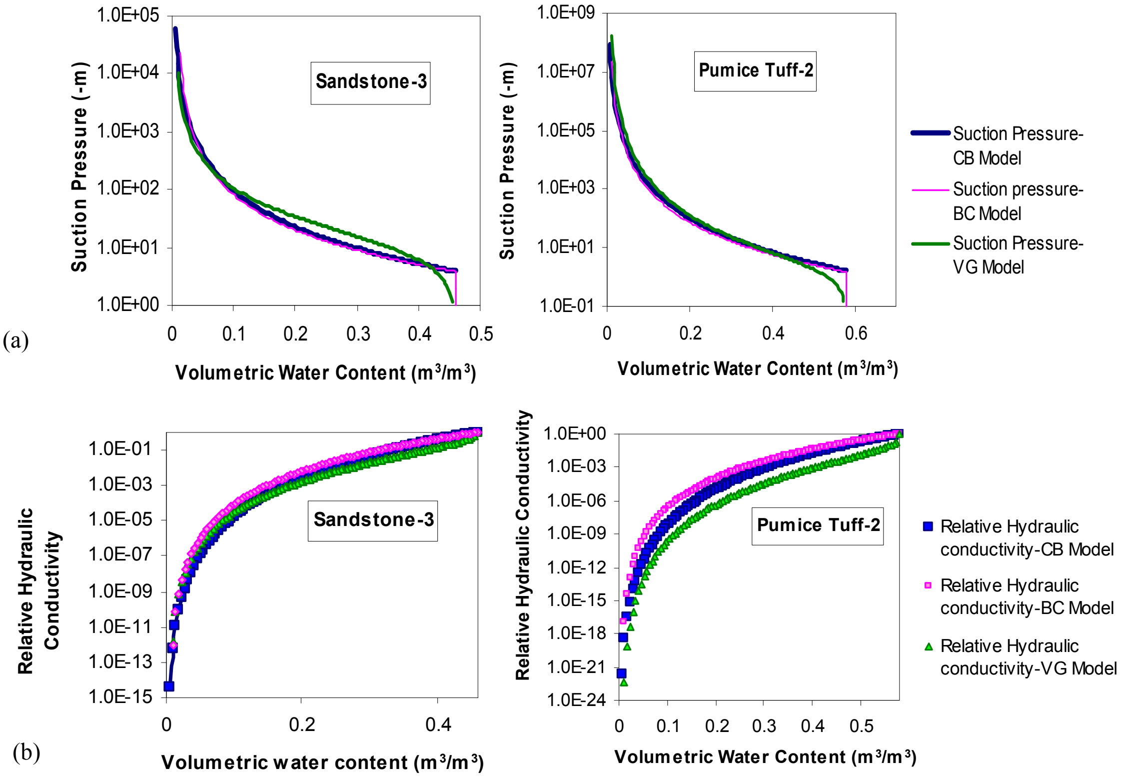

Fig. 4 (a) Relative hydraulic conductivity curves for sandstone-3 and pumice tuff-2 specimens (b) Retention curves for sandstone-3 and pumice tuff-2 specimens

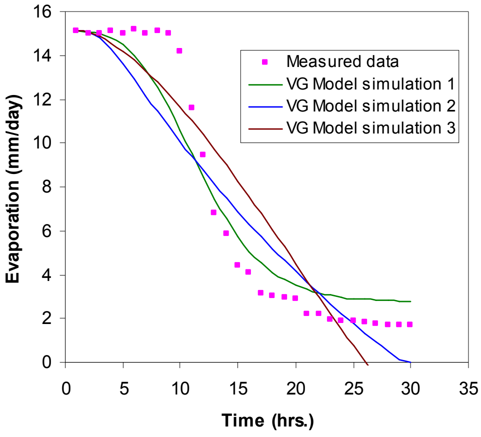

Fig.5 van Genuchten fitting curves for pumice tuff-2 using different parameter ranges

obtained precisely by Brooks-Corey/Burdine and Campbell models.

2. It is difficult to estimate hydraulic parameters by simulating the measured evaporation by van Genuchten model.
3. The Brooks-Corey/Burdine and Campbell models are more robust than the van Genuchten model to analyze the unsaturated flow in soft rock.

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