Temperature dependence of large-scale water-retention curves: a case study

Hui-Hai Liu · G. S. Bodvarsson · J. H. Dane

Abstract A local-scale model for temperature-dependence of water-retention curves may be applicable to large scales. Consideration of this temperature dependence is important for modeling unsaturated flow and transport in the subsurface in numerous cases. Although significant progress has been made in understanding and modeling this temperature effect, almost all the previous studies have been limited to small scales (on the order of several centimeters). Numerical experiments were used to investigate the possibility of extending a local-scale model for the temperature-dependence of water retention curves to large scales (on the order of meters). Temperature effects on large-scale hydraulic properties are of interest in many practical applications. Numerical experiment results indicate that the local-scale model can indeed be applicable to large-scale problems for special porous media with high air entry values. A typical porous medium of this kind is the porous tuff matrix in the unsaturated zone of Yucca Mountain, Nevada, the proposed geologic disposal site for national high-level nuclear wastes. Whether this finding can approximately hold for general cases needs to be investigated in future studies.

Resumé Un modèle à l'échelle locale pour la dépendance à la température des courbes de rétention de l'eau, pourrait être appliqué à de grandes échelles. Dans de nombreux cas cette dépendance est un facteur considérable de la modélisation des écoulements en milieux non–saturés et le transport en sub-surface. Bien que des progrès significatifs ont été réalisés pour comprendre et modéliser l'effet de la température, la plus part des études existantes se sont limitées aux petites échelles (quelques centimètres). L'expérimentation numérique a été utilisée pour étudier la possibilité d'étendre un modèle local à une échelle pluri-métrique. L'effet de la température sur les propriétés hydrauliques est non négligeable dans plusieurs cas. Les résultats des tests numériques indiquent que les modèles sur les petites échelles pourraient être appliqués à des échelles plus grandes, dés lors que le milieu poreux serait caractérisé par une importante pression de l'air à l'entrée. Un milieu poreux typique de cette sorte est le tuf à matrice poreuse de la zone non-saturée dans le Yucca Mountain, Nevada, un site géologique proposé pour le stockage des déchets nucléaires hautement radioactifs. L'application de ces résultats à d'autres cas devrait être étudiée dans de futures études.

Resumen Un modelo en pequeña escala para la dependencia de temperatura que muestran las curvas de retención de agua puede ser aplicable a escalas grandes. La consideración de la dependencia de la temperatura es importante en muchos casos para el modelizado de transporte y flujo no saturado en el subsuelo. Aunque se ha logrado un avance significativo en el entendimiento y modelizado del efecto de la temperatura, casi todos los estudios previos se han limitado a escalas pequeñas (en el orden de varios centímetros). En este estudio se utilizaron experimentos numéricos para investigar la posibilidad de extender un modelo de escala pequeña para la dependencia de temperatura de las curvas de retención de agua a escalas mayores (en el orden de metros). Los efectos de la temperatura en las propiedades hidráulicas a gran escala son de interés en muchas aplicaciones prácticas. Los resultados de los experimentos numéricos indican que los modelos de escala pequeña pueden efectivamente ser aplicables a problemas en gran escala en medios porosos especiales con altos valores de entrada de aire. Un medio poroso típico de esta clase lo constituye la toba porosa intersticial en la zona no saturada de la Montaña Yuca, Nevada, el sitio geológico propuesto para el depósito nacional de residuos nucleares de alto nivel. Es necesario investigar con estudios futuros si los resultados de esta investigación pueden ser válidos para otros casos generales.

Keywords Unsaturated zone · Thermal conditions · Scale effects · General hydrogeology · Yucca Mountain

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Introduction

In many cases, considerable temperature variation occurs during water flow in unsaturated geologic media. One example is the thermo-hydrologic processes expected to occur in the unsaturated zone of Yucca Mountain, Nevada. The US Department of Energy is evaluating the feasibility of using Yucca Mountain as the geologic disposal site for national high-level nuclear wastes. These wastes could emit a significant amount of radioactive decay heat resulting in coupled processes including heat transfer, water flow in the liquid and vapor phases, and solute transport (Bodvarsson and Tsang 1999; Buscheck et al. 2002). During these thermo-hydrologic processes, temperature variation near the potential repository can give rise to both water vaporization in the high temperature zone and condensation in the low temperature zone. To understand and model these processes is critical for assessing the performance of the repository. Other typical examples involving temperature effects on unsaturated flow include steam flushing for removal of non-aqueous phase fluids from the subsurface (e.g., She and Sleep 1998).

It is well known that hydraulic properties of porous media such as hydraulic conductivity and water retention, are temperature-dependent (e.g., Philip and de Vries 1957; Nassar and Horton 1989a,b; Zhang et al. 2003) and that ignoring these effects can result in substantial prediction errors for water movement (e.g., Hopmans and Dane 1985). Considerable experimental and theoretical efforts have been made in understanding and predicting these temperature effects. While the effect of temperature on the hydraulic conductivity function has been well explained by changes in viscosity (Haridasan and Jensen 1972; Hopmans and Dane 1986a,b), the recent focus has been on the temperature dependence of water-retention curves (Liu and Dane 1993; Grant and Salehzadeh 1996; She and Sleep 1998). A more detailed discussion of this temperature dependency and the relevant models is given in the next section of this paper.

All previous experimental and theoretical studies of temperature effects on water-retention curves have been performed at the local (core) scale (on an order of several centimeters). Many field-scale modeling studies have shown more interest in temperature effects on large-scale water-retention curves. For example, the size of a single grid block in the site-scale unsaturated zone model of Yucca Mountain is at least on the order of meters. Because of the subsurface heterogeneity, water-retention curves are scale-dependent (Bodvarsson et al. 1999; Liu and Bodvarsson 2003). An important question for field-scale modeling studies is: Can predictive models of the temperature effects developed at local scales be applicable to large-scale water-retention curves? This important issue has not been addressed in the literature and simply ignored in some field studies. The major objective of this paper is to call attention to this issue by reporting results of recent studies concerning the temperature effects on water-retention curves of the porous tuff matrix in the unsaturated zone of Yucca Mountain.

Models for temperature effects on local water-retention curves

Before discussing temperature dependency of large-scale water-retention curves, models for temperature effects on local water-retention curves are briefly reviewed. Philip and de Vries (1957) proposed the first model for predicting temperature effects on water-retention curves. Their model implies that for a given volumetric water content (θ)—cubic meters of water per cubic meter of porous media ($m^3 m^{-3}$)—soil water geometric configurations (including the contact angle, which is the angle between water–air and solid–air interfaces at their intersection) at the pore scale are identical for different temperatures. In this case, the only factor that alters the corresponding capillary pressure is the air–water surface tension which is a function of temperature. Therefore, their theoretical model can be expressed as (Philip and de Vries 1957):

$$\frac{P_c(\theta,T)}{P_c(\theta,T_r)}=\frac{\sigma(T)}{\sigma(T_r)} \tag{1}$$

where P_c is the capillary pressure (Pa), σ is the surface tension at the air–water interface (N/m), T is the temperature (K), and the subscript r refers to the reference values.

However, the temperature effects predicted with Eq. (1) are consistently smaller than those observed during laboratory experiments. To account for additional potential factors that contribute to the temperature effects, Liu and Dane (1993) hypothesized that for a given water content, pore-scale soil water distributions are not identical, but temperature-dependent. They argued that because of the complicated structure of the porous medium, in combination with the surface tension of water, not all soil water is effectively interconnected and isolated packages may exist either as thin water films on solid surfaces or as entrapped water. Therefore, the total water content (θ) can be expressed as a combination of an isolated water content (θ_i) and a continuous water content (θ_c) as

$$\theta=\theta_i(T)+\theta_c(T) \tag{2}$$

For a given total water content, the soil hydraulic properties are determined only by the continuous water content which, however, is temperature dependent. As demonstrated in Liu and Dane (1993), the new model gives better prediction as supported by the experimental data of Hopmans and Dane (1986a) and is also consistent with other experimental observations (Liu and Dane 1993).

Liu and Dane's (1993) concept regarding the isolated water phase is supported by some experimental studies (Harris and Morrow 1964; Wildenschild et al. 2001). Harris and Morrow (1964) studied pendular rings in packs

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of relatively large uniform spheres, and found that some of the pores in the sphere pack remained full and became isolated from the bulk liquid during the drainage process. Wildenschild et al. (2001) also used the concept of entrapment of water as one plausible mechanism for the flow rate dependence of soil hydraulic characteristics.

Based on an in-depth discussion within the context of thermodynamics, Grant and Salehzadeh (1996) developed a model to consider the additional effects resulting from temperature dependence of the contact angle. They were able to relate the temperature dependence of the contact angle to the enthalpy of immersion. Their model can be expressed as

$$\frac{P_c(\theta, T)}{P_c(\theta, T_r)} = \frac{\beta + T}{\beta + T_r} \tag{3}$$

where β (K) is a parameter related to temperature dependence of surface tension and contact angle. A detailed discussion of the parameter β (K) can be found in Grant and Salehzadeh (1996).

She and Sleep (1998) considered all the three mechanisms mentioned above (temperature dependence of surface tension, water distribution and contact angle) and developed a generalized model given by

$$\frac{P_c(S_e, T)}{P_c(S_e, T_r)} = \frac{\beta + T}{\beta + T_r} \tag{4}$$

where S_e is the effective saturation defined by

$$S_e = \frac{S - S_r}{1 - S_r} \tag{5}$$

In Eq. (5), S is water saturation, and S_r is the residual water saturation and is here considered to be a function of temperature.

She and Sleep (1998) provided a critical examination of the relevant mechanisms governing the temperature-dependence of water-retention curves. They also conducted experiments on silica sand, and found, for temperature less than 60°C, that the residual water content decreases with increasing temperature, which is consistent with Liu and Dane (1993). However, they noticed that the residual water content actually increases with temperature at relatively high temperatures, viz., between 60 and 80°C, a range not covered in previous investigations. In addition to some practical issues (such as measurement errors in the data and fitting errors in calculating residual water content θ_r, or S_r), this may result from that fact that Liu and Dane (1993) did not consider the effects of contact angle change on θ_r . Other factors that may need further investigation are the effects of vaporization-condensation processes at the pore-scale on the isolated liquid water phase, especially at high temperatures where these processes should become more significant. On the other hand, Liu and Dane (1993) simply assumed that the isolated water content is a linear function of total water content, which may not be the case in reality. She and Sleep (1998) also calculated the contact angle as a function of temperature based on the model of Grant and Salehzadeh (1996). They found that the calculated contact angle increases with increasing temperature while literature studies suggest that contact angles should decrease with increasing temperature. Therefore, they concluded that other effects, in addition to those mentioned above, play a role in the temperature dependence of water-retention curves. Nevertheless, they could use Eq. (4) to represent their observations very well when the parameter values were determined (or fitted) using some of measured values. In practical applications, it seems to be adequate to use Eq. (4) for describing the temperature effects on local water-retention curves.

Large-scale water-retention curves for a special porous medium

Almost all experimental and modeling studies on the temperature dependence of water-retention curves have been limited to local (or core) scales. In field-scale modeling studies, information is needed regarding temperature effects on large-scale water-retention curves.

For porous media with large air-entry pressure values, capillary forces are generally strong (Liu and Bodvarsson 2003). The tuff matrix in the unsaturated zone of Yucca Mountain is a porous medium of this kind and has air-entry pressure values that are about two to three orders of magnitude higher than for most common soils (Liu and Bodvarsson 2003). The water distribution at a core scale is conventionally determined by a capillary-equilibrium model, assuming that capillary pressure is uniform for liquid water in different pores for a given core sample (e.g., Mualem 1976). When the capillary force is very strong, this capillary-equilibrium model can be approximately extended to large scales under steady-state flow conditions. Giving this assumption, Liu and Bodvarsson (2003) proposed the following formulation to determine large-scale water-retention curves, $S_{\mathrm{lg}}(P_{\mathrm{c}})$, using small-scale ones, $S_{\mathrm{lc}}(P_{\mathrm{c}})$,

$$S_{\mathrm{lg}}(P_c) = \frac{\int S_{lc}(P_c)\phi dV}{\int \phi dV} \tag{6}$$

where S_{lg} and S_{lc} are the water saturation at the large and the local (core) scales, respectively, V is the porous-medium volume under consideration, and ϕ is the porosity. Note that Eq. (6) is valid for a general porosity distribution (Liu and Bodvarsson 2003) and, for simplicity, a uniform distribution of porosity is used in this study. A comprehensive evaluation of Eq. (6) was presented by Liu and Bodvarsson (2003). They compared the water-retention curves simulated for two-dimensional porous media, characterized by very different heterogeneous structures, with the results directly calculated from Eq. (6) and found excellent agreements between them.

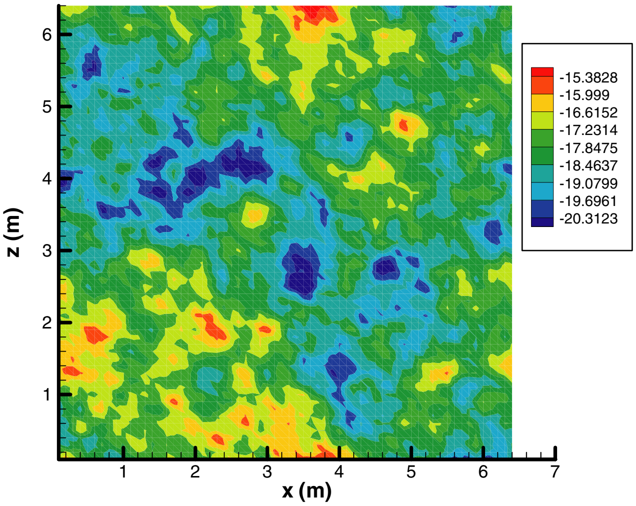

Fig. 1 Numerically generated distributions for log permeability (m^2). The *x* and *z* refer to the horizontal and vertical distances, respectively

It should be emphasized that Eq. (6) is only valid for porous media with large air entry values. For most other porous media, a closed-form relation for upscaling water-retention curves has not yet been established. Previous studies on the temperature effects are limited to $S_{lc}(P_c)$ (local water-retention curves). The focus of this study is on the temperature effects on $S_{lg}(P_c)$ (upscaled water-retention curves in Eq. (6)).

Calculation of temperature effects on large-scale water-retention curves

In this study, whether Eq. (4), which is known to be valid for the local retention curve–$S_{lc}(P_c)$ in Eq. (6)—is applicable to the large-scale (upscaled) water-retention curve—$S_{lg}(P_c)$ in Eq. (6)—for predicting the temperature dependence will be evaluated. Numerical experiments were performed for this evaluation purpose.

Numerical experiments were performed for a two-dimensional vertical heterogeneous porous medium. The heterogeneous distribution for log(permeability) was generated as a stochastic fractal with a 64×64 small grid (Fig. 1), the total size of which roughly corresponds to that for a grid block near the repository in the corresponding field-scale modeling studies for the unsaturated zone of Yucca Mountain. Fractional Brownian motion (fBm) was used to generate permeability fields with a Hurst coefficient value of 0.7. Detailed discussions on the fundamental properties of the stochastic fractal and procedures to generate the fractal distribution with the spectral method can be found in Molz et al. (1997) and Liu and Molz (1996). The mean value for log(permeability) is consistent with the mean value of core measurement for the middle non-lithophysal unit of the unsaturated zone of Yucca Mountain (Table 1) (CRWMS 2000). The variance of log(permeability) is 1.0 for the porous medium domain. The repository for geological disposal of high-level nuclear wastes is partially located in this unit. The effective water-retention curve is determined from Eq. (6).

Table 1 Representative tuff matrix property values for the middle non-lithophysal unit of the unsaturated zone of Yucca Mountain (CRWMS 2000)

Log of permeability (m^2)	−18.12
Porosity (−)	0.11
α (Pa^{-1})	3.69×10^{-6}
m (−)	0.325
S_r (−)	0.19

A number of empirical relations are available for local (core) scale constitutive relations (e.g., Brooks and Corey 1964; van Genuchten 1980). Flint et al. (1999) demonstrated that core-scale constitutive relations for tuff matrix at Yucca Mountain could be represented by van Genuchten (1980) relations:

$$S_e = \left[1 + |\alpha P_c|^n\right]^{-m} \tag{7}$$

where α (Pa^{-1}), n (−), and m (−) are empirical fitting parameters with $m = 1 - 1/n$. Based on Eqs. (4) and (7), parameter α may be treated as a function of temperature such that the form of Eq. (7) can be applied for different temperatures:

$$\alpha(T) = \alpha(T_r)\frac{\beta + T_r}{\beta + T} \tag{8}$$

Based on the β values reported in Grant and Salehzadeh (1996) and She and Sleep (1998), it is assumed that the β value ranges from −400 K to −500 K for the tuff matrix at Yucca Mountain. It is unknown how the β factor is correlated with the hydraulic properties (such as permeability) in natural porous media. Therefore, different degrees of correlation of β with hydraulic properties were assumed in this study. To calculate the saturation S from effective saturation S_e, one needs to define the relationship between temperature and the residual saturation S_r. Based on the study of Liu and Dane (1993), it was assumed that

$$S_r(T) = S_r(T_r) + 0.001(T_r - T) \tag{9}$$

For simplicity, the above equation was also assumed to be applicable through the whole porous medium domain in Fig. 1, and S_r is uniformly distributed in the domain. Note that other distributions of local S_r are not expected to alter the conclusions of this study. Because of the linearity of Eq. (6), these assumptions allow Eq. (9) to hold also for the large-scale water-retention curve defined in Eq. (6). Note that the assumed relation (Eq. 9) and the β values were needed for this study because the relevant measured data are not available for the tuff matrix in the unsaturated zone of Yucca Mountain.

Once a heterogeneous permeability field was generated, local-scale capillary pressure-saturation curves were assigned to each small grid block (0.1×0.1 m) based on Miller–Miller similarity (Miller and Miller 1956). Therefore, the van Genuchten parameter m is the same for all small grid blocks as given in Table 1. The van Genuchten

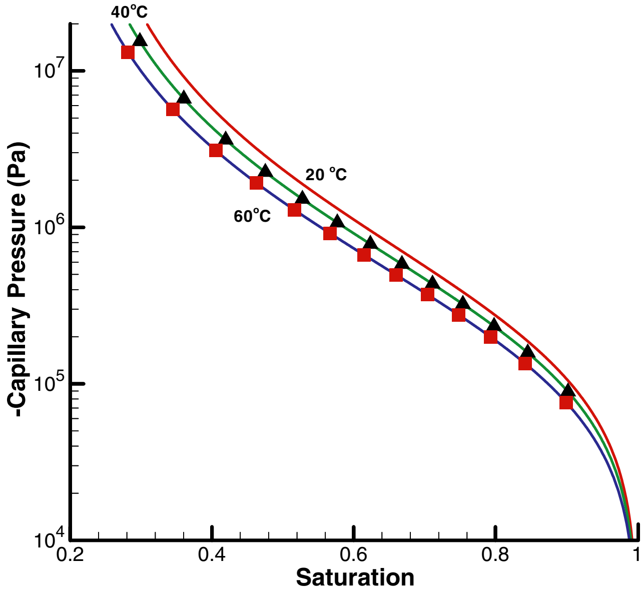

Fig. 2 Comparisons between calculated large-scale water-retention curves (Eq. 6) and the predicted ones (Eq. 4) for different temperatures. The reference temperature is 20°C and the factor β is a constant (-450 K) for the porous medium domain shown in Fig. 1

parameter α at a small grid block is related to the permeability (for the reference temperature) by

$$\alpha = \alpha_{ref}\sqrt{\frac{k_{p,ref}}{k_p}} \tag{10}$$

where k_p is the permeability of the small grid block in Fig. 1 and subscript 'ref' refers to reference values given in Table 1. The porosity and residual saturation values (for reference temperature T_r) were assumed to be the same for all grid blocks in a two-dimensional porous medium block shown in Fig. 1. Their values are also given in Table 1.

Based on Eqs. (7, 8, 9, 10), local water-retention curves (for each small grid block) can be generated for different temperatures. If it is further assumed that the temperature is uniformly distributed within the porous medium domain (Fig. 1), for a given temperature, the large-scale water-retention curve for the porous medium can be determined, based on Eq. (6), from these local curves. Note that the uniform temperature distribution at a scale on the order of several meters is a reasonable approximation for the unsaturated zone of Yucca Mountain because liquid water flow in the tuff matrix is very slow (as a result of small permeability) and heat conduction is the major mechanism for the heat transfer process. However, in cases where heat advection is the major heat transfer mechanism, this may be a poor assumption because of physical non-equilibrium occurring within the porous medium.

Results and discussion

Figure 2 shows upscaled (large-scale) water-retention curves (solid lines) calculated using Eq. (6) for the vertical heterogeneous porous medium domain (Fig. 1). As previously discussed, this porous medium domain may be considered as a single numerical grid block for large-scale modeling studies for the unsaturated zone of Yucca Mountain. A constant β value of −450 K was used in determining temperature dependence of local water-retention curves (Eqs. 7 and 8). To evaluate whether Eq. (4), originally developed for small-scales (e.g., core-scale), can be used for the large-scale curves, Fig. 2 also shows predicted large-scale water-retention curves for temperatures of 40 and 60°C. The prediction uses Eq. (4) and the same constant β value (−450 K) as used at the local scale, and treats the water-retention curve with a temperature of 20°C as the reference curve (the reference temperature is 20°C). Specifically, for a given point at the reference water-retention curve, the effective saturation $S_\mathrm{e}(T_\mathrm{r})$ could be calculated based on Eq. (5) and the value for $S_\mathrm{r}(T_\mathrm{r})$. Because Eq. (4) is applied for the same S_e value corresponding to different temperatures, $S_\mathrm{e}(T)$ was assigned to be $S_\mathrm{e}(T_\mathrm{r})$ and the saturation $S_\mathrm{lg}(T)$ was calculated based on $S_\mathrm{e}(T)$ and $S_\mathrm{r}(T)$ (Eq. 9). The corresponding capillary pressure at temperature T was then calculated using Eq. (4). In this way, a point in Fig. 2 for a temperature T is predicted from the corresponding point at temperature T_r. The comparison between predicted data points and the calculated water-retention curves is in a very good agreement.

In Fig. 2, a constant β value was used. To examine the effects of a heterogeneous distribution of β on the temperature dependence of large-scale water-retention curves, a case in which β was randomly distributed in the porous medium domain (Fig. 1) was considered. The random distribution was generated with a uniform distribution between −400 to −500 K. The simulated water-retention curves are almost identical to those shown in Fig. 2 for a given temperature. Again, an excellent agreement was obtained between the simulated curves and those predicted using the average β value (−450 K). Two extreme cases in which β is a linear function of log (permeability), and either increases or decreases with log (permeability), were also considered. The linear functions were determined in such a way that β ranged from −400 to −500 K in the simulation domain. Excellent agreements (cf. Fig. 2) were obtained when the predictions were made using the averaged β values for the two cases.

One important implication from the above comparisons is that both the parameter β and the relationship given in Eq. (4) may not be scale-dependent (or weakly scale-dependent). In other words, the β values determined at the small scale and the corresponding relation for the temperature dependence of local water-retention curves can be directly used for large-scale modeling studies (if there is a spatial variation of β, the average value should be used for the large-scale modeling).

The above conclusion was obtained for a special porous medium that has a large air entry value and is characterized by capillary equilibrium under steady-state flow conditions. For a heterogeneous porous medium, strong physical non-equilibrium may exist during unsaturated flow processes. In these cases, interplay between subsurface heterogeneity and coupled water flow and heat transfer may make the situation more complicated. On the other hand, one may argue that subsurface heterogeneity is generally the largest uncertainty for most field-scale studies. Compared with the effects of subsurface heterogeneity on subsurface flow and transport, the temperature effects resulting from the temperature dependence of water-retention curves may be secondary. In the other words, the effects of temperature on water-retention curves are expected to be much less significant that those of the subsurface heterogeneity. Therefore, based on the current study results and practical considerations, it seems to be reasonable to consider that the models developed for temperature dependence of local water-retention curves may be practically applied to the large-scale modeling studies. However, the validity of this hypothesis needs to be investigated in future studies.

Summary and conclusions

Consideration of the temperature-dependence of water-retention curves is important for modeling unsaturated flow in the subsurface. Although significant progress has been made in understanding and modeling this temperature effect, almost all previous studies have been limited to small scales. In this study, numerical experiments were used to investigate the possibility of extending local-scale models for temperature effects to large scales. Temperature effects on large-scale hydraulic properties are of interest for many practical applications.

This study indicates that local-scale models for temperature-dependence of water-retention curves can indeed be used for large-scale modeling studies for special porous media with high air entry values. A typical porous medium of this kind is the tuff matrix in the unsaturated zone of Yucca Mountain. Whether this finding can approximately hold in general cases needs to be investigated in future studies.

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