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A constitutive model for water flow in unsaturated fractured rocks

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Abstract:

A conceptual model for describing effective saturation in fractured hard rock is presented. The fracture network and the rock matrix are considered as an equivalent continuum medium where each fracture is conceptualized as a porous medium of granular structure and the rock matrix is assumed to be impermeable. The proposed model is based on the representation of a rough-walled fracture by an equivalent porous medium, which is described using classical constitutive models. A simple closed-form equation for the effective saturation is obtained when the van Genuchten model is used to describe saturation inside fractures and fractal laws are assumed for both aperture and number of fractures. The relative hydraulic conductivity for the fractured rock is predicted from a simple relation derived by Liu and Bodvarsson. The proposed constitutive model contains three independent parameters, which may be obtained by fitting the proposed effective saturation curve to experimental data. Two of the model parameters have physical meaning and can be identified with the reciprocal of the air entry pressure values in the fractures of minimum and maximum apertures. Effective saturation and relative hydraulic conductivity curves match fairly well the simulated constitutive relations obtained by Liu and Bodvarsson. Copyright © 2008 John Wiley & Sons, Ltd.

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INTRODUCTION

Numerical simulation of water flow in fractured hard rocks finds application in many research areas of engineering, geology and geophysics sciences. A typical example is the study of water flow in the vicinity of a geological disposal of high-level nuclear waste in crystalline rock (Flint *et al.*, 2001).

Commonly, numerical simulation of unsaturated flow through a fractured porous medium relies on the continuum approach (Finsterle, 2000; Guarracino and Quintana, 2002). This approach considers mean values of both variables and physical properties defined in a representative elementary volume (REV). In general a REV approach can be justified if a formation contains a dense network of highly interconnected fractures. If a REV can be defined only at a scale similar to the problem of interest, as is the case for poorly connected networks, then this approach is inappropriate (Dagan and Neuman, 1997; Berkowitz, 2002; Liu and Bodvarsson 2003).

Continuum models can consist of single continuum (Liu and Bodvarsson, 2001), double continuum (Bandurraga and Bodvarsson, 1999), or multiple interacting continua (Wu *et al.*, 2004). Single continuum models (or equivalent porous media) are applicable when the fracture network is dense and highly interconnected or when the interaction between fractures and the rock matrix allows sufficient interaction to establish a local equilibrium. In double and multiple overlapping continua models fractures and rock matrix are represented as overlapping, different, but interconnected continua, described by parallel sets of conservation equations. Such models can be considered when the fracture network consists of embedded fracture networks with different properties or scales. An extensive review on conceptual and mathematical models of water flow in fractured rocks can be found in Berkowitz (2002).

In this study, the fracture network and the rock matrix are treated as an equivalent continuum medium while water flow is assumed to obey Richards equation (Richards, 1931). This equivalent medium is characterized by a constitutive model, i.e. relations between capillary pressure, saturation and relative hydraulic conductivity. Accuracy of modelling results is largely determined by the accuracy of these constitutive relations that characterize flow processes at subgrid scale (Liu and Bodvarsson, 2001; Berkowitz, 2002).

Unfortunately, constitutive models for unsaturated fractured rocks are hard to find in the hydrological literature. On the basis of numerical simulation of constitutive relations for fractured rocks, Liu and Bodvarsson (2001) found that the van Genuchten effective saturation curve can match the simulated values and they proposed a relation to estimate the relative hydraulic conductivity from effective saturation. More recently, Guarracino (2006) derived an effective saturation equation based on a fractal

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description of the fracture network and predicted the relative hydraulic conductivity using the classical Burdine model.

The pattern of water flow in unsaturated fractured rocks is highly complex, due to the non-linearity of the processes involved and fracture heterogeneities at different scales. The simplest model for a single fracture is a pair of parallel planes separated by a distance b, called aperture (Berkowitz, 2002). However, when the fractured limiting surfaces are rough and have several contact points this model is rather questionable. Furthermore, the gap between rough walls usually contains fragments of rocks or sediments. In these cases an alternative approach is to model the fracture as a two-dimensional porous medium with hydraulic properties described by classical models as van Genutchen (1980) or Brooks-Corey (1964). This conceptualization of a rough walled fracture has been used in numerical simulation of unsaturated flow by Pruess (1999) and Liu and Bodvarsson (2001).

In this study the theoretical bases of a conceptual model for the calculation of effective saturation curves for fractured hard rocks are presented. The fracture network and the rock matrix are considered as an equivalent continuum medium where each fracture is conceptualized as a porous medium of granular structure and the rock matrix is assumed to be impermeable. The conceptual model is used to obtain a closed-form effective saturation curve for the particular case in which the hydraulic properties of fractures are described with the van Genuchten model and fractal laws are assumed to describe the fracture network. The proposed constitutive model for unsaturated fractured rocks is a combination of the derived effective saturation curve and the hydraulic conductivity relation proposed by Liu and Bodvarsson (2001).

EFFECTIVE SATURATION MODEL

To derive an effective saturation equation for a fractured medium a REV in the form of a cube of volume a^3 is considered. The REV size must be both larger than the scale of microscopic heterogeneities and smaller than the scale of the domain being studied. Fractures of aperture b are represented by vertical two-dimensional porous media of thickness b (Figure 1). Also, it is assumed that fractures are vertical and apertures range from a minimum value b_1 to a maximum value b_2.

At REV scale the pressure head is assumed to be constant. Therefore, all the individual fractures have the same capillary pressure, and water content in the REV is mainly determined by the fracture aperture distribution. Brooks and Corey (1964), van Genuchten (1980) and Guarracino (2006) have used this capillary equilibrium as the basis for developing mathematical expressions for water content curves and for developing relations between saturation and relative hydraulic conductivity.

The volume of water v contained in a single fracture of aperture b at pressure head h can be expressed as (Figure 1):

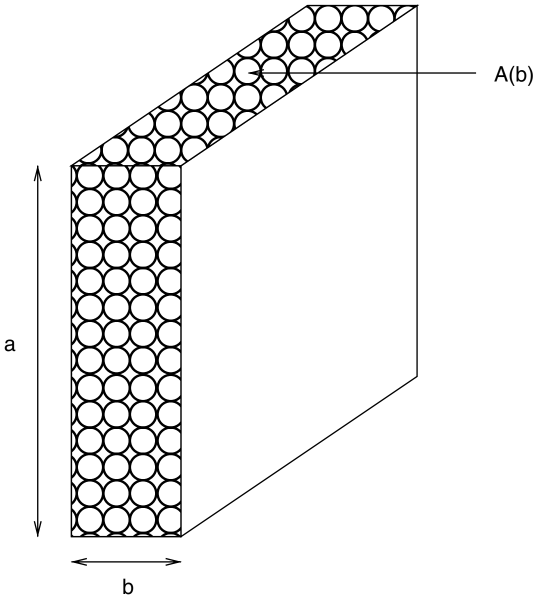

Figure 1. Schematic illustration of a single fracture

$$v(b, h) = \theta(h, b)aA(b) \tag{1}$$

where $\theta(h, b)$ is the water content in the fracture and $A(b)$ the horizontal area of the fracture. Then, the volume of water V contained in the fracture system of the REV is given by:

$$\begin{aligned} V(h) &= \int_{b_1}^{b_2} v(h, b)N(b)db \\ &= \int_{b_1}^{b_2} \theta(h, b)aA(b)N(b)db, \end{aligned} \tag{2}$$

where $N(b)db$ is the number of fractures in the aperture range b to $b + db$.

The expression for water volume when the REV is completely saturated ($h = 0$) is:

$$V(0) = \int_{b_1}^{b_2} \theta_s(b)aA(b)N(b)db, \tag{3}$$

where $\theta_s(b)$ is the maximum water content in individual fractures. When the REV is at residual saturation ($h = \infty$) the water volume becomes:

$$V(\infty) = \int_{b_1}^{b_2} \theta_r(b)aA(b)N(b)db \tag{4}$$

where $\theta_r(b)$ is the residual water content in fractures of aperture b.

From Equations (2) to (4) it is possible to express the effective saturation of the fractured medium S_{FM} as follows:

$$\begin{aligned} S_{FM}(h) &= \frac{V(h) - V(\infty)}{V(0) - V(\infty)} \\ &= \frac{\int_{b_1}^{b_2} S(h, b)A(b)N(b)db}{\int_{b_1}^{b_2} A(b)N(b)db} \end{aligned} \tag{5}$$

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where $S(h,b) = [\theta(h,b) - \theta_r(b)]/[\theta_s(b) - \theta_r(b)]$ is the effective saturation in fractures of aperture b.

Equation (5) can be used to generate effective saturation curves of fractured rocks. To obtain such curves, models for the effective saturation in individual fractures $S(h,b)$, the number of fractures $N(b)db$ within the range b to $b + db$ and the fracture area $A(b)$ are required. Note that closed-form expressions of S_{FM} can only be obtained when the integrals in (5) have closed-form solutions.

Let us begin by deriving an expression for the area of fractures in term of the fracture aperture. According to experimental evidence (Walsh *et al.*, 1991; Hatton *et al.*, 1994) the fracture aperture is related with its length by the following fractal expression:

$$b = c\, L^d \qquad (6)$$

where c is an empirical constant and d is the fractal dimension for the fracture aperture. Then, the fracture area can be calculated as the product of aperture b and length L:

$$A(b) = bL = c^{-1/d} b^{1+1/d} \qquad (7)$$

It is also assumed that the total number of fractures in the aperture range b to $b + db$ obeys a fractal law (Tyler and Wheatcraft, 1990; Renshaw, 2000; Yu *et al.*, 2003):

$$N(b)db = CDb^{-D-1}db \qquad (8)$$

where C is a constant and D is the fractal dimension for the number of fractures.

In this study, a rough walled fracture is conceptualized as a two-dimensional porous medium of thickness b. Then, the effective saturation inside a fracture of aperture b can be described by the well-known van Genuchten–Mualem model (van Genuchten, 1980):

$$S(b,h) = [1 + (\alpha(b)h)^n]^{1/n-1} \qquad (9)$$

where $\alpha(b)$ and n are model parameters. The parameter $\alpha(b)$ is usually estimated as the absolute value of the inverse of air entry pressure or bubble pressure. For the particular case of a single fracture this parameter can be approximated by (Altman *et al.*, 1996):

$$\alpha(b) = \frac{\rho_w g}{2\sigma\cos\varphi} b \qquad (10)$$

where g is the acceleration of gravity, ρ_w water density, σ is surface tension and φ is the contact angle between liquid and solid phases. The coefficient n is an empirical fitting parameter which is assumed to be independent of the fracture aperture.

Using (7), (8) and (9) in (5) we obtain a particular form of the incomplete beta function. In the most general case, no closed-form expression can be obtained for the effective saturation S_{FM}. However, it is easily shown that for the particular case of $n = 1/d - D + 1$ the following closed-form analytical expression is obtained:

$$S_{FM}(h) = \frac{[1 + (\alpha_2 h)^n]^{1/n} - [1 + (\alpha_1 h)^n]^{1/n}}{\frac{1}{n}[(\alpha_2 h)^n - (\alpha_1 h)^n]} \qquad (11)$$

where $\alpha_1 = \frac{\rho_w g}{2\sigma\cos\varphi} b_1$ and $\alpha_2 = \frac{\rho_w g}{2\sigma\cos\varphi} b_2$. Parameters α_1 and α_2 have physical meaning and can be associated with the reciprocal of air entry pressure values in fractures of minimum aperture (b_1) and maximum aperture (b_2), respectively. Moreover, the empirical fitting parameter n of van Genuchten model is related to the pattern of the fracture network, which is characterized by the fractal dimensions of the fracture aperture (d) and the number of fractures (D).

Note that if $\alpha_2 \to \alpha_1$ expression (11) becomes

$$S_{FM}(h) = [1 + (\alpha_1 h)^n]^{1/n-1} \qquad (12)$$

which is identical to the effective saturation of van Genuchten model (9). This result can be interpreted as follows. When $\alpha_2 = \alpha_1$, the fractured porous medium has only fractures of aperture b_1 and the effective saturation inside fractures is $S(h) = [1 + (\alpha(b_1)h)^n]^{1/n-1}$. Due to the rock matrix is assumed to be impervious, the effective saturation of the REV (S_{FM}) is equivalent to the effective saturation in individual fractures.

RELATIVE HYDRAULIC CONDUCTIVITY

Common approaches to derive hydraulic conductivity curves rely on Mualem or Burdine models (Burdine, 1953; Mualem, 1976). These models predict the relative hydraulic conductivity from the knowledge of the water content relation. In the Burdine model pores are represented by a group of parallel capillary tubes with different radii while in Mualem's model pore geometry is more complex. For the particular case of describing water flow in fractured rocks the simple Burdine model seems to be the more consistent one (Kwicklis and Healey, 1993; Liu and Bodvarsson 2001; Guarracino, 2006).

Based on the Burdine model, Brooks and Corey (1964) derived a simple closed form expression to predict relative hydraulic conductivity (K_r) in terms of effective saturation (S). The Brooks–Corey relation can be expressed by

$$K_r(S) = S^{3+2/\lambda} \qquad (13)$$

where λ is a dimensionless index of pore size distribution. Parameter λ can be related to the van Genuchten parameter n by the following equation (van Genuchten, 1980):

$$\lambda = n - 1 \qquad (14)$$

Recently, Liu and Bodvarsson (2001) evaluated the accuracy of Brooks–Corey relation in predicting the relative hydraulic conductivity in unsaturated fractured rocks. In their study, equation (13) is compared with constitutive relations simulated from two-dimensional fracture networks. To improve the accuracy of (13) they proposed a new relation by modifying the tortuosity factor of Burdine's model. The Liu–Bodvarsson relation is given by:

$$K_{rFM}(S_{FM}) = S_{FM}^{3-2S_{FM}^{3/4}+2/(n-1)} \qquad (15)$$

where K_{rFM} refers to the relative hydraulic conductivity of fractured rocks.

In the present study, the proposed constitutive model for fractured hard rocks is represented by the combination of the effective saturation curve (11) and the relative hydraulic conductivity relation (15) derived by Liu and Bodvarsson. Note that the proposed constitutive model has only three independent parameters: α_1, α_2 and n. Parameters α_1 and α_2 can be identified with the reciprocal of air entry pressure values in the fractures of minimum and maximum apertures, respectively, and n is a shape parameter of the classical van Genuchten model.

COMPARISON WITH LIU AND BODVARSSON CONSTITUTIVE RELATIONS

In the present section, effective saturation (11) and relative hydraulic conductivity (15) are compared with the numerical experiment performed by Liu and Bodvarsson (2001). In their work the fracture network is considered to be a fracture continuum where each fracture is conceptualized as a two-dimensional porous medium with constitutive relations represented by the van Genuchten model. For a number of different uniform capillary pressures at the REV boundaries, the corresponding values of effective saturation and relative hydraulic conductivity are obtained by numerical approximation of Richards' equation in a random fracture network. The fracture network consists of five groups of fractures with different average apertures. The computational procedure designed by Liu and Bodvarsson is similar to the laboratory procedure to determine constitutive relations for porous media.

The proposed model has closed-form analytical expressions with three independent parameters α_1, α_2 and n. Model parameters are estimated by fitting the proposed effective saturation curve (11) to the simulated values by Liu and Bodvarsson using an exhaustive search method. The resultant parameter values are $\alpha_1 = 1{\cdot}18 \times 10^{-3}$, $\alpha_2 = 2{\cdot}17 \times 10^{-2}$ and $n = 1{\cdot}66$. The fit between the proposed curve and the simulated values by Liu and Bodvarsson is very good and is shown in Figure 2.

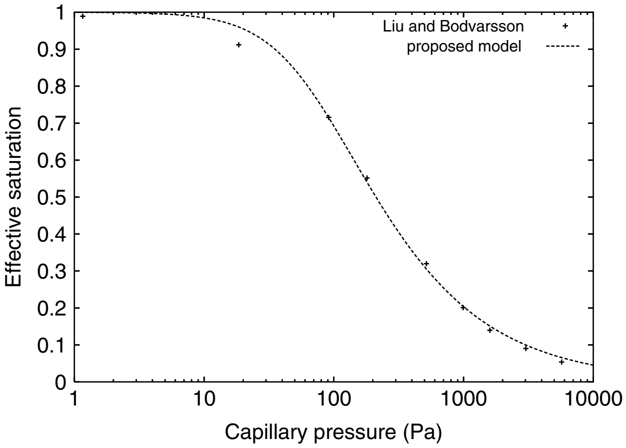

Figure 2. Comparison of the proposed model with the simulated effective saturation of Liu and Bodvarsson (2001)

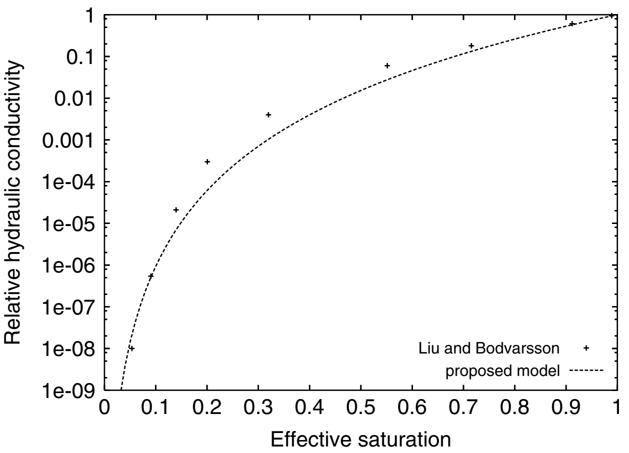

Figure 3. Comparison of the proposed model with the simulated relative hydraulic conductivity of Liu and Bodvarsson (2001)

The relative hydraulic conductivity is predicted using (15) with the value of n obtained from the fitting of effective saturation. Predicted and simulated values obtained by Liu and Bodvarsson are shown in Figure 3. The proposed model fairly good predicts the simulated values over eight orders of magnitude for the whole range of effective saturation values. Then, it can be concluded that the constitutive relations for fractured rocks obtained by Liu and Bodvarsson using numerical simulation techniques can be represented by the analytical expressions (11) and (15) of the proposed model.

CONCLUSIONS

A constitutive model for unsaturated flow in fractured hard rocks has been presented. The conceptual model for effective saturation is based on the representation of fractures by equivalent two-dimensional porous media. It is found that the use of van Genuchten model in conjunction with fractal laws to describe aperture and number of fractures in a REV allows one to obtain a closed-form equation for effective saturation. The combination of this relation and the relative hydraulic conductivity expression proposed by Liu and Bodvarsson (2001) provides a constitutive model specifically designed for water flow in fractured rocks. The constitutive model has analytical expressions that are easy to evaluate with only three independent parameters, which may be obtained by fitting the proposed effective saturation curve to experimental data. Two of the model parameters have physical meaning and can be identified with the reciprocal of the air entry pressure values in the fractures of minimum and maximum apertures. The proposed analytical expressions for effective saturation and hydraulic conductivity can represent the constitutive relations for fractured rocks obtained by Liu and Bodvarsson (2001) using numerical simulation techniques. This study is an effort to understand and characterize unsaturated flow in fractured rocks. The comparison between model results and experimental curves will define the practical usefulness of the proposed model. However, field data for constitutive relations of a fracture

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network are still scarce and unreliable (Liu and Bodvarsson, 2001; Tuller and Or, 2002).

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