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NUMERICAL SIMULATION OF CONSTITUTIVE RELATIONS FOR UNSATURATED FLOW IN FRACTURED POROUS MEDIA

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Summary. In this study we determine constitutive relations (relations between saturation, hydraulic conductivity and pressure head) for unsaturated fractured rocks using a computational procedure that mimics the laboratory technique of measurement. Isotropic three-dimensional rock samples with random vertical and horizontal fractures are computationally constructed. Each fracture is conceptualized as a thick plate of porous medium whose hydraulic properties are described by the well-known van Genuchten model. The procedure used to obtain simulated values of saturation and relative hydraulic conductivity is based on the numerical solution of the steady-state unsaturated flow equation in a three-dimensional domain. A constant value of pressure head (effective pressure head) is prescribed at the top and bottom boundaries and non flow conditions are imposed at side boundaries of the synthetic rock sample. The unsaturated flow equation is solved on a regular mesh of one million elements using a hybridized mixed finite element method. For the prescribed value of pressure head the corresponding values of water saturation and hydraulic conductivity are numerically computed. Then, by selecting different values of pressure head as boundary conditions a complete set of constitutive relations can be defined from the simulation results. The simulated relations are fitted using two recently proposed closed-form analytical expressions for unsaturated fractured rocks. A numerical test designed for fractured basalt shows that both analytical models can match reasonably well the simulated relations.

1 INTRODUCTION

Modeling water flow in unsaturated fractured porous media is of interest to many research areas such as groundwater hydrology, soil science and environmental engineering. Most studies describing water movement through unsaturated porous media are based on the highly non-linear Richards' equation (continuum approach). To solve this equation constitutive relations of effective saturation versus pressure head and relative hydraulic conductivity versus pressure head (or effective saturation) are required. Direct measurements of constitutive relations for fractured rocks are particularly difficult to obtain and experimental data are virtually non existent[1]. A useful alternative to direct measurement is the use of numerical procedures that mimic the laboratory tests usually used to determine constitutive relations for soil samples[2,3].

In the present study constitutive relations for fractured rocks are obtained by numerical simulations of three-dimensional steady-state unsaturated flow in synthetic rock samples. To construct a sample of fractured rock we consider a rock matrix of low permeability with a set of random fractures. Fractures usually contain grains of one or more infilling minerals and for this reason they are conceptualized as classical two-dimensional porous media of high permeability. Water flow through the rock sample is simulated by solving the steady state unsaturated flow equation with the same prescribed values of pressure head at the top and bottom boundaries and no flow conditions at side boundaries. Because the effective pressure head gradient is zero in the vertical direction, the average vertical flow should be, according to Darcy's law, the same as the hydraulic conductivity of the fractured rock sample for the prescribed value of pressure head. For a number of different pressure head values at the boundaries, the corresponding values of effective water saturation and relative hydraulic conductivity can be obtained using numerical approximations. The unsaturated flow equation is solved using a hybridized mixed finite element method which gives a simultaneous approximation to pressure head and water flow. The proposed computational procedure allows to obtain pseudo-experimental constitutive relations that are compared with two analytical expressions of constitutive models recently proposed by Liu and Bodvarsson[3] and Guarracino[4]. Based on numerical simulations, Liu and Bodvarsson propose the use of the saturation curve of van Genuchten model[5] combined with a modified hydraulic conductivity curve of Brooks-Corey model[6] as a constitutive model for fractured rocks. Guarracino derives a saturation curve using fractal concepts and predicts the hydraulic conductivity using the Burdine model[7]. The ability of these models to capture the hydraulic properties of fractured rocks is evaluated by comparing analytical and simulated relations. A numerical test for fractured basalt shows that both models can match the simulated saturation relation reasonably well. A better fit to simulated values of hydraulic conductivity is obtained with the fractal model.

2 FRACTURED ROCK SAMPLE

In this section we describe the computational procedure used to generate three-dimensional samples of fractured rocks. The rock matrix is assumed to have a low permeability and fractures are conceptualized as thick plates of porous media of high permeability. The fracture pattern is composed of three sets of fractures which are mutually orthogonal with random spatial distributions. Similar network patterns have been used by Smith and Schwartz[8] and Liu and Bodvarsson[3] to investigate water flow in two-dimensional fractured rocks.

To construct the fracture network a group of random points is generated using a uniform distribution. For each randomly generated point, a square fracture of length L and aperture b is generated using the following fractal law[9]:

$$b = cL^d \qquad (1)$$

where d is the fractal dimension and c is an empirical constant. In the present study we determine constitutive relations in a cubic sample of 10 cm side. For the sake of simplicity fractures are assumed to be parallel to *xy*, *yz* and *xz* planes. Figure 1 shows a realization of a rock sample generated with the following parameters: $b = 0.1$ cm, $d = 1.13$ and $c = 0.05$.

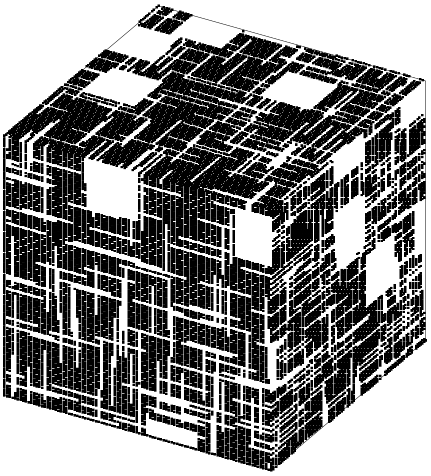

Figure 1: Computationally generated fractured rock sample.

Following Pruess and Tsang[10], Kwicklis and Healey[2], and Liu and Bodvarsson[3] we conceptualize individual rough-walled fracture as two-dimensional porous media with constitutive relations represented by the well-known van Genuchten model[5]:

$$\theta(h) = (\theta_s - \theta_r)\left[1+|\alpha h|^n\right]^{-m} + \theta_r \qquad k(h) = k_s\left[1+|\alpha h|^n\right]^{-m/2}\left\{1-\left[1-\left(1+|\alpha h|^n\right)^{-1}\right]^m\right\}^2 \qquad (2)$$

where θ is the water content; h the pressure head; θ_s and θ_r the saturated and residual water contents, respectively; α, n and m empirical fitting parameters with $m = 1\text{-}1/n$; k the hydraulic conductivity and k_s the saturated hydraulic conductivity. The hydraulic properties of the rock matrix are also described using the van Genuchten model.

3 NUMERICAL PROCEDURE

3.1 Differential problem

The use of numerical simulation to determine effective constitutive relations for unsaturated flow has been reported by a number of researchers[3,11,12]. This methodology is applicable to the particular case of fractured rocks when the rock is densely fractured or when the fractured network and rock matrix allow sufficient interaction to establish a local equilibrium.

The numerical procedure is based on the assumption that the pressure head distribution in the rock sample is constant. This constant value is assumed to be the effective pressure head of the rock sample. To establish an approximately constant value of pressure head we prescribe the same value of pressure head at the top and bottom boundaries and no flow conditions at side boundaries. The water saturation and the hydraulic conductivity values associated to the effective pressure head are estimated by numerical simulation of unsaturated water flow in the rock sample. Then, by establishing different values of effective pressure head we can obtain pseudo-experimental relations of both water saturation and hydraulic conductivity of the fractured rock.

The unsaturated water flow through the rock sample under steady state condition is assumed to obey the following differential problem:

$$\begin{aligned} &\nabla\cdot\mathbf{q}(h)=0, \quad \mathbf{x}\in\Omega \\ &\mathbf{q}(h)=k(h)\nabla(h+z), \quad \mathbf{x}\in\Omega \\ &h(\mathbf{x})=h_e, \quad \mathbf{x}\in\Gamma_T\bigcup\Gamma_B \\ &\mathbf{q}(h)=0, \quad \mathbf{x}\in\Gamma_L \end{aligned} \tag{3}$$

where $\mathbf{q}(h)$ is the water flow; $\mathbf{x}=(x,y,z)$; Ω the computational domain (a cube of size a); Γ_T, Γ_B and Γ_L are the top, bottom and lateral boundaries, respectively; h_e the effective pressure.

3.2 Numerical resolution

The differential problem (3) is solved using a hybridized mixed finite element method which gives a simultaneous approximation to pressure head and water flow[13]. The water flow equation is linearized using a Picard iteration scheme. The use of a mixed finite element method for approximation of the flow equation is especially suitable for two main reasons: it conserves the mass locally and can handle large discontinuities in hydraulic conductivities. The mixed method was implemented for the lowest-order of the Raviart-Thomas-Nedelec space[14,15] on a regular mesh composed of cubic elements. The corresponding degrees of freedom are the values of the pressure head at the center of the cubic element and the values of the normal component of the water flow at the center of each side of the cube. For each Picard iteration, the resulting linear system of algebraic equations is solved using a successive over-relaxation method (SOR)[16].

3.3 Effective saturation and hydraulic conductivity

The effective saturation S_e of the rock sample is computed from the following definition:

$$S_e(h_e)=\frac{\int_\Omega\left[\theta(h)-\theta_r\right]d\Omega}{\int_\Omega\left[\theta_s-\theta_r\right]d\Omega} \tag{4}$$

where the integrals are solved using a quadrature rule and the numerical solution of (3).

The estimation of hydraulic conductivity is based on the assumption that the effective gradient of the pressure head in the rock sample is zero. We have prescribed the same pressure head value (h_e) at the top and bottom boundaries to obtain an approximately constant pressure head distribution. Then, according to Darcy's law, the averaged vertical flux through a horizontal cross–section is equal to the hydraulic conductivity K of the rock sample:

$$K(h_e) = \frac{\int_\Gamma q(h)\, d\Gamma}{\int_\Gamma d\Gamma} \tag{5}$$

where Γ is a horizontal cross–section (the bottom boundary Γ_B, for example). The saturated hydraulic conductivity K_s is obtained when an effective pressure head equal to zero is established in the rock sample. For the sake of simplicity, numerical results will be expressed in terms of the relative hydraulic conductivity which is defined as follows: $K_r(h_e) = K(h_e)/K_s$.

4 SIMULATED CONSTITUTIVE RELATIONS

The described numerical procedure is used to compute constitutive relations for a fractured basalt. The rock sample is assumed to be a cube of 10 cm side with the fracture pattern shown in Figure 1. For hydrological characterization of the rock matrix we use the van Genuchten parameters calibrated by Unger et al.[17] for basalts at the Box Canyon Site (Idaho). We also assume that the hydraulic properties of fractures can be described by the van Genuchten parameters obtained by Carsel and Parrish[18] for a porous medium of loamy sand texture. The van Genuchten parameters of matrix and fractures are listed in Table 1.

	θ_r	θ_s	α [1/cm]	n	k_s [cm/d]
Fractures	0.057	0.41	0.124	2.28	350.2
Matriz	0.10	0.20	0.00489	1.33	0.281

Table 1 : van Genuchten parameters for rock matrix and fractures

The differential problem (3) is solved on a regular mesh of one million of elements where each element is a cube of 1mm side. The simulations are performed for 12 different values of effective pressure head h_e at the top and bottom boundaries. The corresponding values of S_e and K_r are computed using equations (4) and (5). Figure 2 shows the simulated values of S_e versus h_e and K_r in terms of S_e. We have also included in the figure the van Genuchten curves for both matrix and fractures.

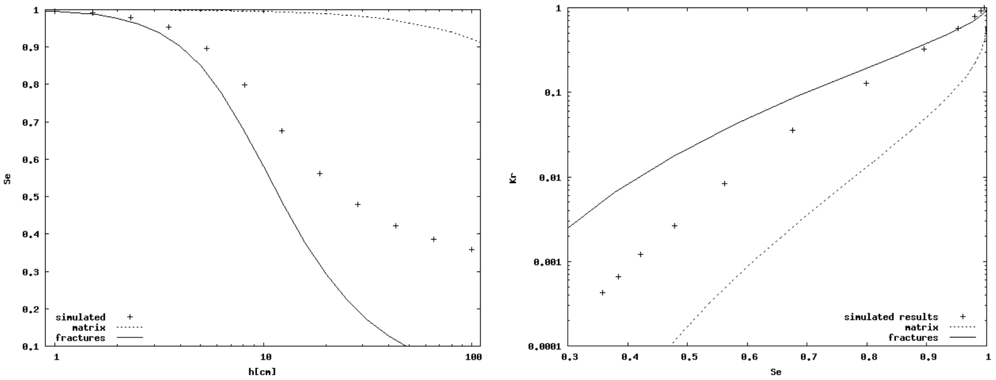

Figure 2: Simulated effective saturation and relative hydraulic conductivity relations.

Note that for small values of h_e (saturation values close to 1) both the simulated values of S_e and K_r are similar to the van Genuchten curves of the fractures. This behavior suggests that near fully saturated conditions the water flow in the rock sample is mainly determined by the hydraulic properties of fractures.

The simulated constitutive relations shown in Figures 2 are used to evaluate two analytical expressions for fractured rocks recently proposed by Liu and Bodvarsson[3] and Guarracino[4]. The procedure used to evaluate the constitutive models consists of two steps. First, the simulated effective saturation relations are fitted with the analytical curves using an exhaustive search method[19]. Second, the fitted parameters obtained for the saturation curve are used to predict the relative hydraulic conductivity curve. This procedure is standard in most practical applications where the hydraulic conductivity is estimated from the measured saturation relations.

The constitutive model proposed by Liu and Bodvarsson[3] is given by the following expressions:

$$S_e = \left[1 + |\alpha h|^n\right]^{-m} \qquad K_r = S_e^{\,3-2S_e^{3/4}+2/(n+1)} \tag{6}$$

where S_e is the van Genuchten effective saturation curve and K_r a modified Brooks-Corey relative hydraulic conductivity curve.

The fractal constitutive model derived by Guarracino[4] reads as follows:

$$S_e = \begin{cases} 1, & h < h_{\min} \\ \dfrac{h^{D-2} - h_{\max}^{D-2}}{h_{\min}^{D-2} - h_{\max}^{D-2}}, & h_{\min} \le h \le h_{\max} \\ 0, & h_{\max} < h \end{cases} \qquad K_r = S_e^{\,2}\, \frac{\left[S_e \left[\left(\dfrac{h_{\min}}{h_{\max}} \right)^{D-2} - 1 \right] + 1 \right]^{\frac{D-4}{D-2}}}{\left(\dfrac{h_{\min}}{h_{\max}} \right)^{D-4} - 1} \tag{7}$$

where D is the fractal dimension of the fracture network, and $h_{\min}$ and $h_{\max}$ are model parameters associated with lower and upper cut-off values for pressure head.

Figure 3 shows the fits of Liu-Bodvarsson and fractal models to the simulated effective saturation relations. The fitted parameters of the two models are: $\alpha = 1.3325$ cm^{-1}, $n = 1.4616$, $D = 1.65$, $h_{\min} = 3.97$ cm and $h_{\max} = 10^{14}$ cm. It can be observed that both models fit fairly well the simulated relations for the whole range of effective pressure head.

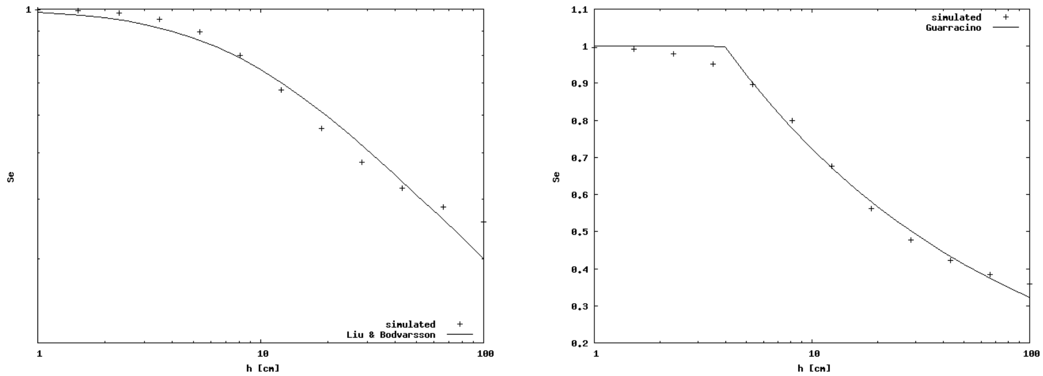

Figure 3: Fit of analytical curves proposed by Liu-Bodvarsson[3] and Guarracino[4] to simulated effective saturation

The predicted values of relative hydraulic conductivity obtained with the model parameters listed above are shown in Figures 4. The Liu-Bodvarsson model overestimates K_r for the whole range of effective saturation. The fractal model can adequately predict K_r for high and intermediate saturations but underestimates the simulated values for small saturations.

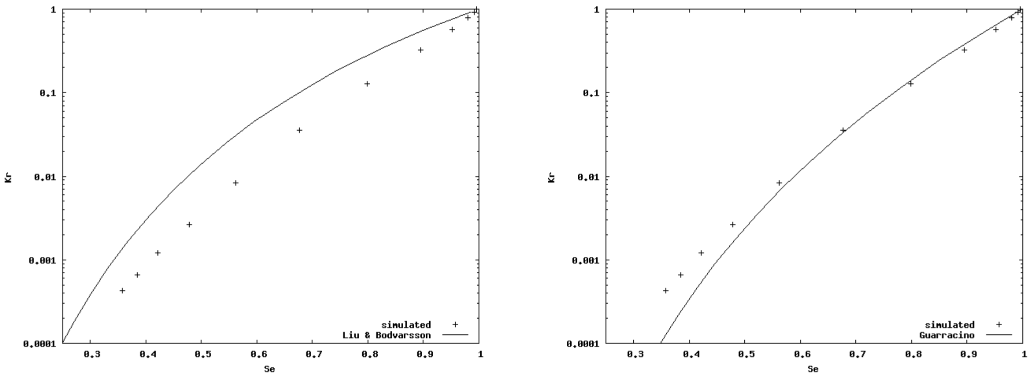

Figure 4: Comparison between simulated relative hydraulic conductivity and predicted values obtained with the analytical models proposed by Liu-Bodvarsson[3] and Guarracino[4]

4 CONCLUSIONS

A numerical procedure that mimics the laboratory experiments used to obtain constitutive relations for porous media has been presented. The steady-state unsaturated flow equation was solved in a three-dimensional domain using a hybridized mixed finite element method. A numerical experiment was performed to simulated constitutive relations for a fractured basalt sample. The simulated curves of effective saturation and relative hydraulic conductivity were fitted using analytical models proposed by Liu and Bodvarsson[3] and Guarracino[4]. From the numerical experiment it is found that the two constitutive models are valid for describing effective saturation relations. However the predicted values of relative hydraulic conductivity obtained with these models are different. The Liu-Bodvarsson model overestimates simulated values for the whole range of water saturation while the Guarracino model underestimates simulated values for small saturation values. The proposed numerical procedure is a valid alternative for characterizing hydraulic properties of fractured rocks when no measured data is available.

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