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A fractal constitutive model for unsaturated flow in fractured hard rocks

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Abstract

A physical conceptual model for water retention in self-similar fractured hard rocks is presented. The geometric pattern of the fracture network is described using a classical fractal object known as the Sierpinski carpet. Assuming this type of geometry, a relatively simple closed-form expression for the water content is obtained. All model parameters can be calculated from the density of the main fractures, the maximum and minimum values of the fracture aperture, and the residual water content. The resulting water content expression is then used to estimate the unsaturated hydraulic conductivity of the fractured medium based upon the well-known model of Burdine. It is found that for large enough ranges of fracture apertures the new constitutive model converges to the empirical Brooks–Corey model.

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1. Introduction

Modeling groundwater flow in unsaturated fractured rocks has received considerable attention in the last two decades. One of the main reasons for focussing on the study of water flow in this type of media is the search for potential safe permanent storage facilities for geological disposal of high-level nuclear wastes. Deep disposal in crystalline rocks is considered to be an effective mean of isolating radioactive wastes from the biosphere. However, groundwater migration could contribute to the return of radionuclides to the surface of the Earth. Thus, simulation of groundwater flow in fractured hard rocks provides a useful tool to establish long-term safety of potential disposal sites.

Most numerical simulations of unsaturated flow in fractured rocks are based on the continuum approach (e.g. Finsterle, 2000). In its simplest form, the fractured 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 constitutive models which largely determine the accuracy of the numerical results. However, such models are virtually nonexistent for fractured hard rocks which

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explains why classical models originally developed for sedimentary rocks are often used (Liu and Bodvarsson, 2001).

The proposed conceptual constitutive model is based on the assumption that the fracture pattern is self-similar. Self-similar scaling is a typical property of fractal objects and it has been observed in fracture networks by several authors. Berkowitz and Hadad (1997) have analyzed natural fractured trace maps representing a wide variety of scales, geological settings and lithologies, and they found that fracture networks display fractal and multifractal properties. Obuko and Aki (1987) reported that the density of different sized fault segments within the San Andreas fault zone is fractal. Barton and Zoback (1992) found that the distributions of fracture aperture and fracture spacing are self-similar over a well-defined range of apertures in the Cajon Pass scientific drill hole. It has also been observed that microfracturing in rocks and fragmentation produced by weathering, explosions, and impacts often satisfy a fractal distribution condition over a wide range of scales (Tchalenko, 1970; Turcotte, 1986).

The mentioned empirical evidence motivates the use of fractal geometry concepts to describe selfsimilar fracture networks in hard rock formations. The paradigm used for the fracture pattern is the Sierpinski carpet, which is a fractal object that contains a selfsimilar geometric pattern of pores. There is not empirical evidence that support the use of this specific fractal to describe a fractured rock. However, the Sierpinski carpet was employed by Tyler and Wheatcraft (1990) to simulate porous media and to relate its fractal dimension to the empirical parameters of the Brooks-Corey constitutive model (1964). A Sierpinski space, an extension of Sierpinski carpet, was also employed to characterize the spatial distribution of a drainage network in the Gardon basin, France (Moussa, 1997).

In this study the water content relation of the fractured media is directly derived from the porosity of the Sierpinski carpet using appropriate cut-off values for the self-similar pattern. The relative hydraulic conductivity is obtained from the water content relation using the Burdine model (Burdine, 1953). It is important to remark that for small enough fracture apertures the proposed relations converge to Brooks–Corey expressions. Similar results were

reported by Tyler and Wheatcraft but in their work the water retention distribution is obtained using an approximation of the pore number distribution of the Sierpinski carpet.

The expressions of the proposed constitutive model are closed-form and easy to evaluate. Another important feature is that all model parameters are completely determined from the density of the main fractures, the maximum and minimum fracture apertures, and the residual water content.

2. Construction of a self-similar fracture network

In this section the basic concepts to describe a twodimensional network of fractures using the Sierpinski carpet are introduced. The Sierpinski carpet is a planar figure in which successively smaller pieces are cut out of the plane to produce a pattern of 'holes' which is self-similar at all scales. In our case, the 'holes' of the carpet will be associated with the fractures.

The Sierpinski carpet can easily be generated using a recursion algorithm. To construct a fracture network we consider a square of size a. The first recursion level consists of subdividing the original square into b_1^2 squares of size $d_1 = a/b_1$. In order to simplify the analysis, only vertical and horizontal fractures will be generated by removing l_1 squares of size d_1 according to a desired geometric pattern. Thus the fracture aperture is determined by d_1 . The selected pattern of fractures must be repeated in each recursion level in order to obtain a self-similar pattern at scales lower than the initial size of the carpet a. In the second recursion level the remaining $b_1^2 - l_1$ squares are newly subdivided in b_1 squares of size $d_2 = a/b_1^2$. In each square of size d_1 , l_1 subsquares of size d_2 are removed according to the initial pattern of fractures. This procedure can be carried out as many times as desired and if the recursion is repeated to infinity the resulting self-similar pattern is filled everywhere with 'holes'.

For an arbitrary value of b the number of squares of size d needed to cover the fractures of apertures equal to or larger than d is given by l. Thus the number of squares to cover the solid phase is b^2 -l. The last number has a power-law scaling with the scale of measurement b of the form (Mandelbrot, 1983)

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Fig. 1. Three levels of recursion of the Sierpinski carpet for parallel fractures.



Fig. 2. Three levels of recursion of the Sierpinski carpet for orthogonal fractures.

 $b^D = b^2 - l \tag{1}$

where $D \in (1,2)$ is the fractal dimension of the Sierpinski carpet.

Fig. 1 shows the first 3 levels of recursion for a network of parallel fractures using the following parameters: a=1, $b_1=5$ and $l_1=5$. Fig. 2 illustrates the case of an orthogonal fracture network obtained assuming a=1, $b_1=5$ and $l_1=9$. The fractal dimension D of both carpets are 1.86 and 1.72, respectively.

3. Water content relation

To derive the water content relation we consider as representative elementary volume (REV) a cube of volume a^3 (see Fig. 3). The pores of the REV are vertical fractures of aperture *d*. The horizontal distribution of the fracture network is assumed to be self-similar and to be described by a Sierpinski carpet as explained in the previous section.

The porosity ϕ of the REV is given by

$$\phi = \frac{\text{volume of porous}}{\text{volume of REV}} = \frac{a^3 l/b^2}{a^3} = \frac{l}{b^2}.$$
 (2)

According to (1) and using d=a/b, porosity can be expressed in terms of the fracture aperture d as:

$$\phi(d) = 1 - \left(\frac{a}{d}\right)^{D-2}.$$
(3)

Expression (3) represents the porosity of a medium with self-similar fractures of apertures greater than *d*.



Fig. 3. Representative elementary volume (REV) of the fractured medium.

It is important to remark that due to D < 2 the porosity approximates to unity as d goes to zero. This porosity value is physically meaningless for representing a 'true' fractured rock and a lower cut-off value for d must be considered. This lower cut-off will be associated with the smallest aperture d_{\min} detected on the REV and thus the porosity of the fractured medium will be $\phi(d_{\min})$.

Suppose now that the REV is initially fully saturated and is dewatered by a tension force. If all fractures of apertures greater than d are drained by a tension h_d then the water content θ is given by

$$\theta(h_d) = \phi(d_{\min}) - \phi(d) + \theta_r \tag{4}$$

where θ_r represents the water held as films on the fracture walls which can not be drained by the tension h_d . If we assume that the fractures drain at capillary pressure then

$$h_d = \frac{2\sigma\cos(\beta)}{\rho g d} \tag{5}$$

where σ is the surface tension of the water, β the contact angle, ρ water density, and g gravity acceleration. It is important to remark that capillary pressure is not uniform in the fracture network (Kwicklis and Healey, 1993) and then h_d is considered to be the 'effective' tension within the REV (Liu and Bodvarsson, 2001).

Finally, substituting (3) and (5) in (4) the desired expression for water content is

$$\theta(h) = \begin{cases} \theta_{s} & h < h_{\min} \\ (\theta_{s} - \theta_{r}) \frac{h^{D-2} - h_{\max}^{D-2}}{h_{\min}^{D-2} - h_{\max}^{D-2}} + \theta_{r} & h_{\min} \le h \le h_{\max} \\ \theta_{r} & h > h_{\max} \end{cases}$$
(6)

where

$$h_{\min} = \frac{2\sigma \cos(\beta)}{\rho g d_{\max}} \quad h_{\max} = \frac{2\sigma \cos(\beta)}{\rho g d_{\min}},$$

$$\theta_s = \left(\frac{a\rho g}{2\sigma \cos(\beta)}\right)^{D-2} (h_{\min}^{D-2} - h_{\max}^{D-2}) + \theta_r$$
(7)

with d_{max} the maximum fracture aperture and θ_s the saturated water content.

4. Fractal dimension D

The expression of the fractal dimension D of a Sierpinski carpet can be computed rearranging (1)

$$D = \frac{\log(b^2 - l)}{\log(b)}.$$
(8)

Using formula (8) it is possible to compute the fractal dimension of the carpets shown in Figs. 1 and 2. However, it is more useful to express D in terms of the physical parameters of the fracture network. Assuming that the fracture network is formed by two families of parallel fractures which mutually cross each other at an angle of 90 degrees, we can compute the number of squares of size d_{max} necessary to cover the area of the main network as

$$l = a^2 \left[\frac{1}{d_{\max}} (n_x + n_y) - n_x n_y \right]$$
(9)

where n_x and n_y are the fracture densities (number of fractures per unit length) in x and y directions, respectively. Hence, substituting (9) in (8) yields the following expression for the fractal dimension:

$$D = \frac{\log\left(\frac{a^2}{d_{\max}^2}\left[1 - d_{\max}(n_x + n_y) + d_{\max}^2 n_x n_y\right]\right)}{\log\left(\frac{a}{d_{\max}}\right)}.$$
(10)



Fig. 4. Dependence of the fractal dimension with maximum fracture aperture.



Fig. 5. Dependence of the fractal dimension with fracture density.

Fig. 4 shows the dependence of fractal dimension D with the maximum fracture aperture d_{max} assuming $n_x = n_y = n = 0.5$ fractures per cm and a = 100 cm. Fractal dimension goes to 2 for small values of d_{max} but falls sharply to 1 for the highest admissible values. The dependence of D with fracture density n when $d_{\text{max}} = 0.1$ cm is shown in Fig. 5. Both curves show similar behavior indicating that values of D near 2 correspond to lightly fractured media (low density and small apertures) and values near 1 to highly fractured media (high density and large apertures).

5. Relative hydraulic conductivity

The two most widely applied models for predicting relative hydraulic conductivity from the knowledge of the water content relation are the models of Burdine (1953) and Mualem (1976). These models differ significantly in their approaches towards pore interaction terms. In the Burdine model pores are represented with a group of parallel capillary tubes with different radii while in the Mualem model pore geometry is more complex. For the particular case of flow in fractured hard rock the simple Burdine model seems to be the more consistent (Liu and Bodvarsson, 2001; Kwicklis and Healey, 1993) and will be adopted to predict relative hydraulic conductivity. The expression of the model given by Burdine is

$$K_r(\theta) = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^2 \frac{\int\limits_{\theta_r}^{\theta} h^{-2}(\mu) \,\mathrm{d}\mu}{\int\limits_{\theta_r}^{\theta_s} h^{-2}(\mu) \,\mathrm{d}\mu}.$$
 (11)

Introducing (6) in (11) we obtain the following closed form for $K_r(h)$:

$$K_{r}(h) = \begin{cases} 1 & h < h_{\min} \\ \left(\frac{h^{D-2} - h_{\max}^{D-2}}{h_{\min}^{D-2} - h_{\max}^{D-2}}\right)^{2} \frac{h^{D-4} - h_{\max}^{D-4}}{h_{\min}^{D-4} - h_{\max}^{D-4}} & h_{\min} \le h \le h_{\max} \\ 0 & h > h_{\max} \end{cases}$$
(12)

Expressions (6) and (12) represent the proposed constitutive model for self-similar fractured hard rocks. Note that all model parameters are determined by geometric parameters of the network n_x , n_y , d_{\min} , d_{\max} , and residual water content θ_r .

The novel constitutive model has some similarities with the well-known Brooks–Corey model, which is

$$\theta(h) = \begin{cases} \theta_s & h < 1/\alpha \\ (\theta_s - \theta_r)(\alpha h)^{-\gamma} + \theta_r & h \ge 1/\alpha \end{cases}$$
(13)

$$K_r(h) = \begin{cases} 1 & h < 1/\alpha \\ (\alpha h)^{-(3\gamma+2)} & h \ge 1/\alpha \end{cases}$$
(14)

where α is the reciprocal of air entry pressure and γ is a model parameter related to pore size distribution. Water content relation (13) is an empirical expression while relative hydraulic conductivity (14) is obtained using the water content relation in the Burdine model.

For large enough ranges of fracture apertures, that is $d_{\min} \ll d_{\max}$, the term h_{\max}^{D-2} can be considered negligible and for this particular case the expressions (6) and (12) are identical to the ones proposed by Brooks and Corey ((13) and (14)). The relation between parameters of both models are $\alpha = 1/h_{\min}$ and $\gamma = 2$ -D.

Comparisons of the proposed and the Brooks– Corey models for three different ranges of fracture apertures are depicted in Fig. 6. The assumed



Fig. 6. Comparison between the Brooks–Corey model and the new relations for different ranges of fracture apertures.

fracture network parameters are $n_x = n_y = 4$ f/cm, $d_{\text{max}} = 10^{-1}$ cm and $d_{\text{min}} = 10^{-3}$, 10^{-5} , 10^{-7} cm, being the ranges of fracture apertures of 2, 4 and 6 orders of magnitude, respectively. According to Fig. 6, the Brooks–Corey model seems to be adequate to describe the hydraulic properties of fractured rocks for large ranges of fracture apertures and low values of pressure head.

6. Parametric analysis

In this section we analyze the influence of the two main model parameters: the fracture density and the maximum aperture. The geometric parameters and physical constants used for the analysis are a=100 cm, $g=980.665 \text{ cm/s}^2$, $\sigma=72.75 \text{ dy/cm}$ (20 °C), $\rho=0.998 \text{ gr/cm}^3$ (20 °C), $\beta=0$ and $\theta_r=10^{-6}$. For

| | <i>n</i> (f/cm) | d_{\min} (cm) | d_{\max} (cm) | h_{\min} (cm) | h_{\max} (cm) | D | θ_s |
|------------------------|----------------------|------------------------|------------------------|-----------------|--|------------------|------------------|
| Network 1 Network 2 | $5 5 \times 10^{-1}$ | 10^{-5} 10^{-5} | 10^{-1} 10^{-1} | 2.63 2.63 | 2.63×10^{5} 2.63×10^{5} | 1.7793 1.9851 | 0.2106 0.1154 |
| Network 3 | 5×10^{-2} | 10^{-5} | 10^{-1} | 2.63 | 2.63×10^{5} | 1.9985 | 0.0131 |

Table 1 Network and model parameters for the analysis of fracture density

the sake of simplicity we consider the same value *n* for fracture density in both direction $(n=n_x=n_y)$.

In order to analyze the influence of the fracture density we consider three fracture networks with different values of n. The geometric parameters of the fracture networks and the computed model parameters are listed in Table 1. The water content and relative hydraulic conductivity curves are shown in Figs. 7 and 8, respectively. As expected, the maximum values of water content decrease with the number of fractures while the relative hydraulic conductivity shows a negligible dependence with the parameter n.

Table 2 lists the parameters of the fracture networks used for the parametric analysis of the maximum fracture aperture d_{max} . Fig. 9 shows that the effects of d_{max} on the water content curves are similar to the ones of parameter *n*. However, the relative hydraulic conductivity curves are strongly influenced by the parameter d_{max} . As shown in Fig. 10, the smaller the maximum fracture aperture, the greater the values of the relative hydraulic conductivity.



Fig. 7. Water content curves of the fracture networks listed in Table 1.

7. Model validation

In this section the proposed model is compared with constitutive relations simulated from twodimensional fracture networks by Liu and Bodvarsson (2001). In their work the network is considered to be a fracture continuum where each fracture is conceptualized as a two-dimensional porous media with constitutive relations represented by the van Genuchten model (1980). For a number of different uniform capillary pressures at the REV boundaries, the corresponding values of effective saturation and relative hydraulic conductivity are obtained for a randomly fracture network. This computational procedure is similar to laboratory procedure to determine constitutive relations to porous media.

The simulated constitutive relations were fitted with the following equations

$$S_{\rm e} = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[1 + (\alpha h)^n\right]^{1/n - 1} \tag{15}$$

$$K_r = S_e^{3-2S_e^{3/4} + 2/(n-1)}$$
(16)



Fig. 8. Relative hydraulic conductivity curves of the fracture networks listed in Table 1.

| | <i>n</i> (f/cm) | d_{\min} (cm) | d_{\max} (cm) | h_{\min} (cm) | h_{\max} (cm) | D | θ_s |
|-------------------------------------|--|-------------------------------------|--|---|--|----------------------------|----------------------------|
| Network 1 Network 2 Network 3 | 5×10^{-1} 5×10^{-1} 5×10^{-1} | $\frac{10^{-5}}{10^{-5}}$ 10^{-5} | $ \begin{array}{r} 1.0 \\ 10^{-1} \\ 10^{-2} \end{array} $ | 2.63×10^{-1} 2.63×10^{0} 2.63×10^{1} | 2.63×10^{5} 2.63×10^{5} 2.63×10^{5} | 1.6990 1.9851 1.9989 | 0.2422 0.1154 0.0074 |

 Table 2

 Network and model parameters for the analysis of maximum fracture aperture

where S_e is the effective saturation, and α and n are empirical parameters. Eq. (15) is the van Genuchten water retention curve and Eq. (16) is a modified Brooks–Corey relative hydraulic conductivity relation.

The comparison between the simulated effective saturation obtained by Liu and Bodvarsson and the



Fig. 9. Water content curves of the fracture networks listed in Table 2.



Fig. 10. Relative hydraulic conductivity curves of the fracture networks listed in Table 2.

curves predicted by Eqs. (6) and (15) is shown in Fig. 11. The proposed model fairly good predicts the simulated values except for high saturations. The resultant parameters are D=1.503, $h_{\min}=0.5$ cm and $h_{\max}=50$ cm.

In order to compare simulated and predicted values of the relative hydraulic conductivity the Eq. (12) is expressed in terms of effective saturation:

$$K_{r} = S_{e}^{2} \frac{\left[S_{e}\left(\left(\frac{h_{\min}}{h_{\max}}\right)^{D-2} - 1\right) + 1\right]^{(D-4)/(D-2)} - 1}{\left(\frac{h_{\min}}{h_{\max}}\right)^{D-4} - 1}.$$
(17)

Fig. 12 shows the simulated K_r values and the curves predicted by Eqs. (16) and (17) using the parameters determined from Fig. 11. The fit to the simulated values is reasonably good and it can be improved by modifying the tortuosity factor in the Burdine model (Eq. (11)) as explained in Liu and Bodvarsson (2001).



Fig. 11. Fit of the proposed model to the simulated effective saturation and the Liu–Bodvarsson model.



Fig. 12. Fit of the proposed model to the simulated relative hydraulic conductivity and the Liu–Bodvarsson model.

8. Conclusions

A physically based constitutive model for unsaturated flow in fractal fractured hard rocks has been presented. The expressions of water content and relative hydraulic conductivity curves have analytical closed-forms and all parameters can be completely determined by the geometry of the main fracture network and the residual water content. The proposed model match reasonably well the simulated constitutive relations obtained by Liu and Bodvarsson (2001) and for large enough ranges of fracture apertures it converges to the empirical Brooks–Corey model.

A parametric analysis indicates that water content strongly depends on fracture density and aperture, while the relative hydraulic conductivity is mainly influenced by the maximum fracture aperture. Strongly fractured rocks have a fractal dimension close to one, while that of weakly fracture formations approaches a value of two.

The proposed constitutive model is an effort to understand and characterize unsaturated flow in fractured hard rocks. The utility of the model to describe water flow in real fractured formations has yet to be proven by comparison with experimental data.

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