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Studies on coupled hydromechanical effects in single fractures

A contribution to DECOVALEX II Task 3 'Constitutive relationships of rock joints'

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In STUK this study was supervised by **Esko Eloranta**

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Keywords: hydraulic simulations, fractured rock, Monte Carlo methods, spent fuel disposal

ABSTRACT

This report addresses the question of hydromechanical coupling in single fractures by looking at the internal heterogeneity of the fractures.

In the first study, heterogeneity of flow paths inside fractures subject to normal stress is investigated. It considers a laboratory investigation where, using a triaxial loading chamber, the flow conditions through a natural fracture are monitored while the normal stress is increased in a step-wise manner. Simultaneously the mechanical displacement is measured. Fracture surfaces are characterized using optical laser-profilometry. This data is used to characterize the fracture aperture distributions. Based on this data the heterogeneous transmissivity distributions for the numerical model are determined, assuming cubic law to be valid locally. Due to the measurement accuracy of the laser profilometry, the transmissivities are best assigned only with an accuracy corresponding to given aperture intervals rather than the exact aperture values recorded. The effect of varying stress is simulated by moving the fracture surfaces with respect to each other, thus altering the aperture-contact distribution inside the fracture. An agreement between the measured and the modeled data was achieved to some extent. However, the transmissivity distributions yielding the best results were at some locations highly discontinuous, with narrow channels governing the flow. Then the system becomes very sensitive to the transmissivity properties at such locations and the measurement accuracy of the aperture data becomes crucial.

The second study addresses the question of effect of stress on fracture transmissivity from the point of view that eventually—in field scale applications—large data bases relating hydraulic behavior to mechanical behavior will be needed. A procedure is suggested to obtain statistical distributions of hydraulic and transport apertures based on information on fracture surface roughness profiles. Preliminary results for implementing the approach are also given. The so-called Joint Roughness Coefficient classification is related to fractal dimension after the procedure by Seidel and Haberfield (1995) and a large number of roughness profile realizations are generated for each JRC-class. These surfaces are then placed together to form actual fractures. The pairing of the surfaces is made by placing two surfaces with similar statistical properties together. By doing this to a large number of surface pairs, aperture distributions for the different JRC classes are generated. The obtained aperture distributions provide an interesting basis for comparison to the few actual aperture measurements that exist today. The comparison shows that the values generated are within the range of the measured data, but too large a number of contact points is generated. Therefore, before the initiation of the flow simulations and 'mechanical experiments' where the surfaces will be moved with respect to each other to simulate the shear behavior, inclusion of the 'degree of matedness' criterion into the generation routine is proposed.

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Avainsanat: hydrauliset simuloinnit, rakoillut kallio, Monte Carlo -menetelmät, käytetyn ydinpolttoaineen loppusijoitus

TIIVISTELMÄ

Tässä tutkimuksessa tarkastellaan kalliorakojen virtausta hydromekaanisten kytkentöjen näkökulmasta.

Työn ensimmäinen osa käsittelee raon sisäisten virtausreittien muuttumista rakoon kohdistuvan normaalijännityksen funktiona. Tutkimus käsittelee kolmiaksiaali-koetta, jossa raon läpi tapahtuvaa virtausta monitoroidaan samalla kun rakoon kohdistuvaa normaalijännitystä asteittain kasvatetaan. Samanaikaisesti mitataan raon sulkeutumista kuvaavaa mekaanista siirtymää. Laserprofilometrillä mitattujen rakopintatopografiatiedostojen avulla luodaan vastaavat rakojen avaumajakaumat. Näiden perusteella luodaan raon sisäinen heterogeeninen vedenjohtokykyjakauma olettaen virtauksen paikallisesti noudattavan ns. kuutiolakia. Laserprofilometrin mittaustarkkuuden rajoitusten vuoksi avaumajakaumaa tarkastellaan 50 µm avauma-intervalleissa eikä tarkkojen, suoraan mittauksesta saatujen numeroarvojen avulla. Normaalijännityksen vaikutusta simuloidaan siirtämällä luotuja rakopintoja suhteessa toisiinsa, jolloin raon sisäinen avauma- ja vedenjohtokykyjakauma samalla muuttuvat. Virtauskenttä mallinnetaan kussakin jännitystilanteessa käyttäen reunaehtoina kyseisessä tilanteessa mitattuja virtaama- ja painearvoja.

Näin suoritettu simulointisarja tuottaa kalibroinnin jälkeen mittausaineiston kanssa osittain yhteensopivan tuloksen. Yhteensopivuus ei kuitenkaan ulotu kaikkiin normaalijännitystilanteisiin. Parhaan yhteensopivuuden tuottavassa avaumajakaumassa virtaama tapahtuu muutamassa kapeassa kanavassa. Tällöin tulos on hyvin herkkä kyseisen kohdan avaumalle, ja rakojen pinnankarkeuden mittaustarkkuus tulee keskeiseksi tekijäksi.

Tutkimuksen toinen osa käsittelee rakojen hydromekaanista käyttäytymistä todennäköisyyspohjaisesti. Kenttämittakavaan tutkimuksissa keskeiseksi kysymykseksi muodostuu rakojen suuri heterogeenisyys, johon jännitystilan muutokset vaikuttavat niinikään vaihtelevasti. Näissä tutkimuksissa tarvitaankin laajoja aineistoja rakojen mekaanisen ja hydraulisen vuorovaikutusten välisestä riippuvuudesta. Tätä taustaa ajatellen tutkimuksen toisessa osassa esitetään lähestymistapa rakojen hydraulisia ja kulkeutumisominaisuuksia kuvaavien parametrijakaumien todennäköisyyspohjaiseksi määrittelemiseksi, lähtökohtana tieto rakojen pinnankarkeusarvoista. Lähestymistavassa kalliomekaanista, ns. JRC-luokittelua vastaavat rakojen pinnankarkeusprofiilit kuvataan fraktaalidimension avulla. Kullekin JRC-luokalle – jota kutakin vastaa eri fraktaalidimension arvo – generoidaan suuri määrä raon pinnankarkeusprofiileja. Näiden rakopintojen avulla muodostetaan kutakin JRC-luokkaa vastaavat rakojen avaumajakaumat. Avaumat muodostetaan yhdistämällä kerrallaan kaksi saman tilastollisen populaation ja fraktaalidimension (JRC-luokan) eri reaalisaatiota. Tekemällä tämä suurelle joukolle pintapareja saadaan kutakin JRC-luokkaa vastaavat avaumajakaumat. Määritettyjä avaumajakaumia voidaan käyttää Monte Carlo- tyyppisten virtaus- ja kulkeutumissimulointien pohjana, jolloin saadaan arvioitua eri karkeusluokkia vastaavat hydrauliset parametrijakaumat.

Generoituja avaumajakaumia verrattiin kirjallisuudessa esitettyihin vastaaviin mitattuihin esimerkkijakaumiin. Vertailun perusteella generoidut avaumat ovat samaa suuruusluokkaa mitattujen arvojen kanssa. Generointi tuotti kuitenkin mitattuun aineistoon verrattuna liian suuren määrään nolla-avaumia eli kohtia, joissa rakopinnat ovat kosketuksissa tai leikkaavat toisiaan. Tämän vuoksi luonnollinen jatkotutkimus ennen varsinaisia virtaussimulointeja ja rakopintoja toisiinsa nähden siirtämällä tehtäviä 'mekaanisia kokeita' onkin, että generointirutiiniin lisätään rakopintojen yhteensopivuuden astetta mittaava kriteeri.

PREFACE

This report addresses the question of hydromechanical coupling in single fractures by looking at the internal heterogeneity of the fractures as well as their variability in response to varying stress.

The first study (Paper I) Niemi et al. (1997) looks at the issue based on laboratory experiments on a single fracture specimen. Laboratory tests with a tri-axial cell are carried out to test the effect of varying normal stress on the hydraulic behavior of a fracture. Detailed numerical modeling of the flow is carried out by taking into account the internal heterogeneity of the fracture as well as the variation of this heterogeneity in response to the observed increase in normal stress. Surface roughness measurements with laser profilometry are used to derive the initial fracture aperture distributions.

The second study (Paper II) Niemi and Vaittinen (1998) addresses the question of hydromechanical coupling in fractures in a statistical sense. When characterizing the flow and transport in field scale fractured rock, we are dealing with a large number of possible fracture aperture distributions. Such variability is usually best treated by means of statistical analyses and stochastic simulations and distributions of possible values rather than individual exact values are of interest. Therefore a framework is proposed to link rock surface roughness characteristics to their hydraulic and transport characteristics in a statistical sense. A procedure is proposed and preliminary modeling work is presented.

Stockholm November 4th, 1998

Auli Niemi

CONTENTS

PAPER I, Niemi, A.P, Vaittinen, T.A., Vuopio, J. A. and Pöllä, J.P. (1997) ‘Simulation of Heterogeneous Flow in a Natural Fracture under Varying Normal Stress’. Int. J. Rock Mech. & Min. Sci. Vol. 34. No. 3–4, 1997.

PAPER II, Niemi, A. and Vaittinen, T. (1998) ’Generation of fracture surfaces and aperture distributions for Monte Carlo simulations—Contributions for DECOVALEX II Task 3’. Progress Report for Radiation and Nuclear Safety Authority (STUK). Helsinki, Finland. March 1998.

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PAPER I

Simulation of heterogeneous flow in a natural fracture under varying normal stress

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CONTENTS

ABSTRACT

Keywords: Coupled processes, fluid flow, fractures, hydraulic conductivity, laboratory tests, models, numerical analysis, rock core, stress.

The present study considers flow heterogeneity in individual fractures under varying degrees of normal stress. We simulate a laboratory investigation where, using a triaxial loading chamber, the flow conditions through a natural fracture were monitored while the normal stress was increased in a step-wise manner. Simultaneously the mechanical displacement was measured. Fracture surfaces have been characterized using optical laser-profilometry. We use this data as a preliminary basis for determining the fracture aperture distributions. Based on this data the heterogeneous transmissivity distributions for the numerical model are determined, assuming cubic law to be valid locally. The effect of varying stress is simulated by moving the fracture surfaces with respect to each other and thus altering the aperture-contact distribution inside the fracture. An agreement between measured and modeled data was achieved to some extent. However, the transmissivity distributions yielding the best results were at places very discontinuous with narrow channels governing the flow route. The system then becomes very sensitive to the transmissivity properties at the critical locations and the measurement accuracy of the aperture data becomes crucial.

1 INTRODUCTION AND BACKGROUND

For the correct prediction of a possible radionuclide transport from a geological nuclear waste repository, a thorough understanding of the heterogeneous distribution of flow and transport pathways in fractured rock is essential. It is now widely recognized that flow in such rocks takes place in heterogeneous channels very different from the classical parallel-plate fracture model. It is also known that the nature of such heterogeneity changes as a response to varying stress fields, which increase and decrease the areas of contact and tortuosity of the flow paths. Understanding this coupled behavior is important for many environmental and engineering applications where the stress field in the rock is altered for example by underground excavations.

In this work the coupled hydromechanical behavior of an individual natural fracture under varying stress is modeled, by taking into account the flow path heterogeneity inside the fracture. We base our conclusions on hydromechanical laboratory measurements, laser profilometry data and numerical simulation.

Earliest studies for modeling flow in individual fractures assumed the flow to be analogous to laminar flow between two perfectly smooth parallel plates. This leads to the so-called ‘cubic law’, with the intrinsic permeability of the fracture (k) being a function of the aperture (e). In subsequent studies, however, it has been observed that the cubic relation breaks down at smaller apertures, due to surface contacts. Several authors have investigated this effect and proposed corrections to the cubic law (e.g. Tsang and Witherspoon, 1981, Brown, 1987). Application of distributed modeling with geostatistically generated aperture and transmissivity distributions has also been used by several investigators. They have used a locally valid cubic law approach, where transmissivity distribution has been determined with cubic law but by taking into account the local aperture variations (Nordqvist et al., 1992, Moreno et al., 1988, Moreno et al., 1990).

2 HYDROMECHANICAL EXPERIMENT

We are investigating a hydromechanical experiment where the effect of varying normal stress on the fracture flow rate is measured (Püllä et al., 1995). The experiment was done using a triaxial loading chamber. Core samples with single fractures parallel to the sample axis were tested. The core samples were approximately 102 mm in diameter and 100 mm in length. Confining pressure was increased step-wisely and water was injected into the fracture from below at a constant rate of 0.05 cm³/s while the water injection pressure needed to maintain this flow rate was recorded. For each value of the confining pressure the corresponding sample deformation was measured with an extensiometer. Based on this value the fracture closure was determined.

For the present study, one natural fracture was selected to be analyzed further. The fracture was tested twice. A hysteresis effect could be observed in the stress-mechanical closure behavior so that when the first experiment produced a maximum mechanical closure of 70 µm for the maximum normal stress of 16 MPa, the second cycle only produced a closure of 35 µm for the same stress. This hysteresis is believed to be due to the fact that some of the original roughness of the rock is lost during the first cycle. The relevant measurement data for the second test cycle are summarized in Table I. Figure 1 shows the development of the stress v.s. mechanical closure and Figure 2 shows the development of corresponding hydraulic aperture (as determined from cubic law) v.s. mechanical closure for this second test.

Inspection of the stress-closure relation in Figure 1 shows a rather linear and continuous increase in both values. Therefore the experiment has not yet reached the part where further increases of the stress do not close the fracture any more or the closing is at least very slow. Therefore the commonly used Bandis et al. (1983) equation (equation 1, see for example Cook, 1987) does not describe this data well.

Table I. *Data from the second test cycle for the investigated natural fracture (based on the results of test 2311B of Püllä et al., 1995).*

Stress (MPa)	Mechanical closure of the fracture (µm)	Average water injection pressure (MPa) ¹
2	0.0	0.0305
4	4.7	0.0427
6	9.1	0.0544
8	13.4	0.0698
10	18.2	0.0836
12	23.3	0.1010
16	35.6	0.1280

1) Pressure needed to maintain the 0.05 cm³/s injection flow rate

$$\sigma = \frac{DK_i}{\left(1 - \frac{D}{D_m}\right)} \tag{1}$$

where σ = stress
D = volumetric (mechanical) closure of the fracture
K_i = $\partial\sigma/\partial D$ at $\sigma=0$, that is the initial specific stiffness of the fracture
D_m = maximum volumetric closure of the fracture.

The fitting was done, however, and gave an estimate of 500 µm for the maximum closure.

Hydraulic aperture v.s. mechanical closure curve (Figure 2) exhibits an irreducible flow behavior observed also by other investigators (e.g. Pyrak-Nolte et al., 1988, for several examples see Cook, 1987), where at higher values of mechanical closure the hydraulic conductivity does not decrease any more. This means that some isolated large pores are still closing without effect to the connected flow paths. The irreducible effect is not very pronounced and can be observed only for a relatively short pressure range. It is possible, however, that if the experiment would have been continued with higher stresses, a more pronounced effect could be observed. This effect is an indication of the heterogeneous character of the flow paths inside the fracture.

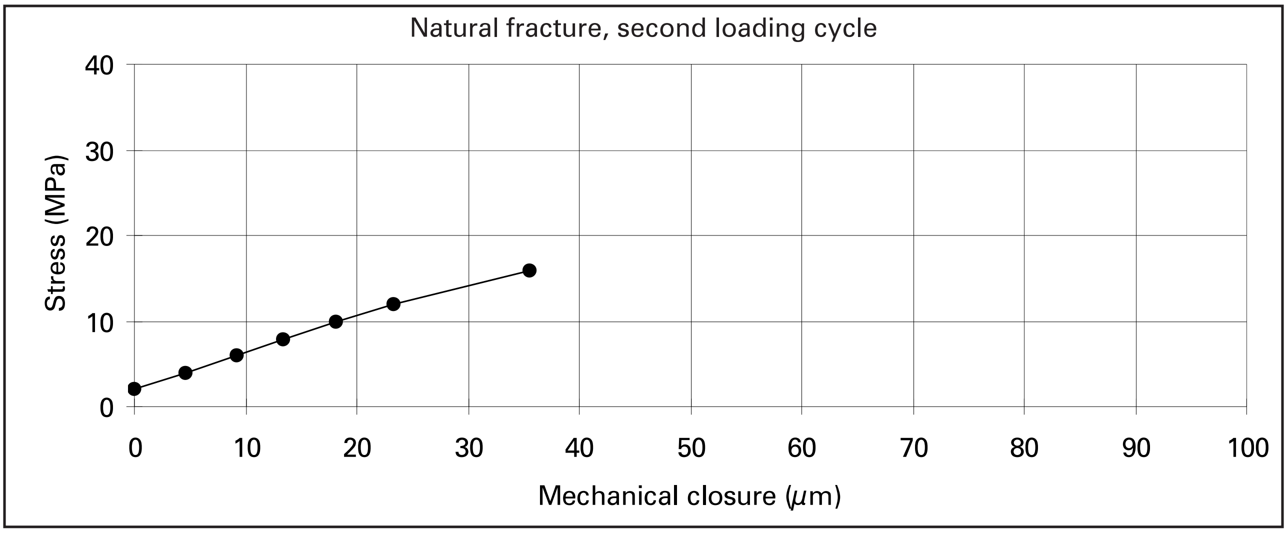

Figure 1. *Development of mechanical closure as a function of stress for the investigated experiment (based on results of Püllä et al., 1995).*

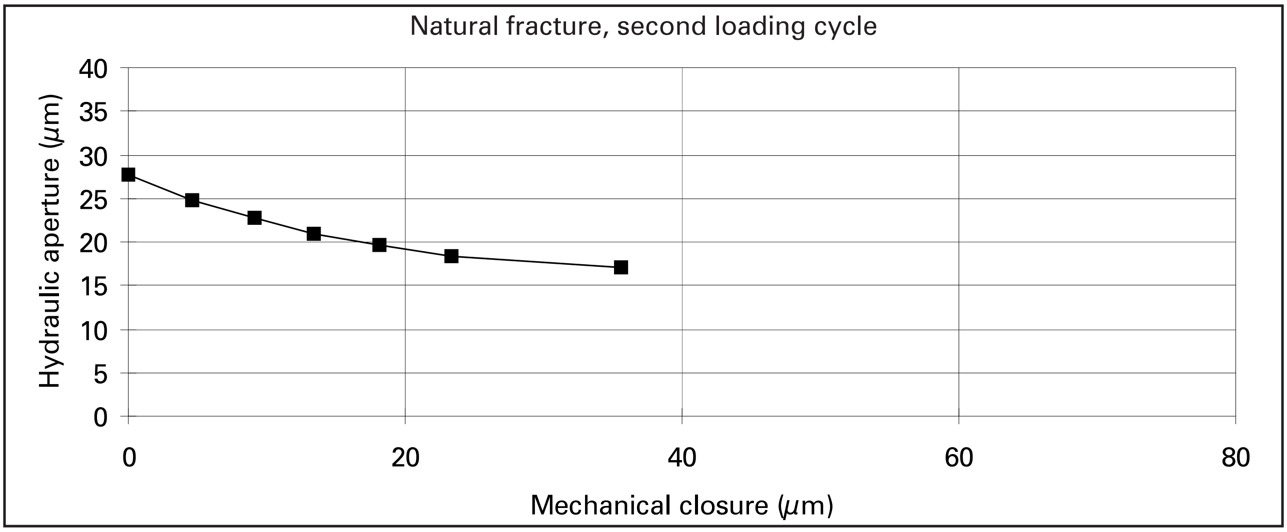

Figure 2. *Development of hydraulic aperture based on cubic law v.s. mechanical aperture for the investigated experiment (based on results of Pöllä et al., 1995).*

3 DATA ON SURFACE ROUGHNESS AND FRACTURE APERTURE CALCULATION

The roughness of the fracture surfaces has been measured by means of laser profilometry. The scan lines across the sample were taken at 1 mm intervals. Along each scan line the distance between individual measurement points was about 0.25 mm. The measurements have been carried out at the Helsinki University of Technology, Laboratory of Fotogrammetry (Mononen et al., 1996) and are described in detail in Vuopio (1997). We use this data as a preliminary basis for determining the heterogeneous aperture distribution.

Based on the profilometry data, the TerraModeler (1995) geographical modeling program was used to generate 3-dimensional models of the rock surfaces. These in turn could be visualized, inspected and moved around with MicroStation (1995) CAD-program**.** This capability will be especially beneficial later on when the more complex effects of shear stress on fracture opening and closure will be modeled. Here the changes in normal stress were modeled by moving the surfaces closer to/farther away from each other. Parts of rock coming into contact with each other were simply assumed to disappear. This is a reasonable preliminary assumption used by other investigators in comparable studies (Brown, 1987, Moreno et al. 1990). For determining the fracture aperture distributions, local distances between the two surfaces were determined and variable transmissivity distributions calculated based on this data.

Example of an aperture-contact distribution with this data is shown in Figure 3a. Discretized transmissivity distribution corresponding to the aperture distribution in Figure 3a is shown in Figure 3b. Inspection of the data shows a clear tendency; the left hand side is much more closed than the right hand side. The samples were scanned twice and the same effect could be observed in both cases. This pronounced effect could also be observed in the simple flow test where water was injected evenly into the fracture from the top while the fracture was held closed without actual pressure and the surfaces wetted in this manner were photographed (Figure 4.).

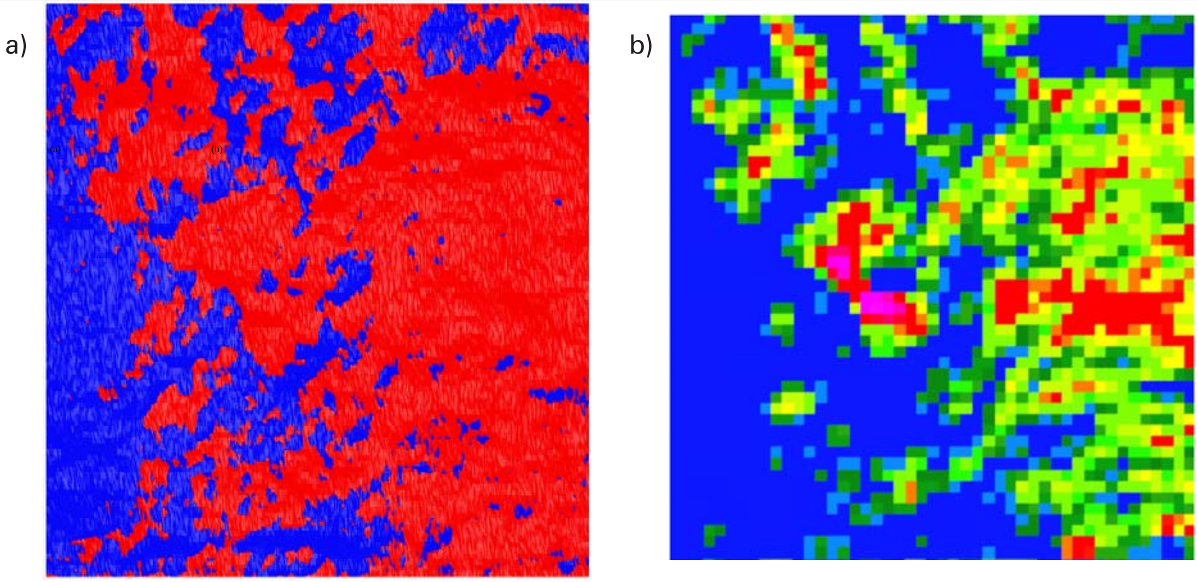

Figure 3. *a) Example distribution of areas of surface contact (blue) and open areas (red) in the fracture and b) the corresponding discretized transmissivity distribution for the finite-element model.*

Figure 4. *Flow wetted fracture surfaces at time t=t1 after an instantaneous water injection input from the upper boundary (dark area is wet).*

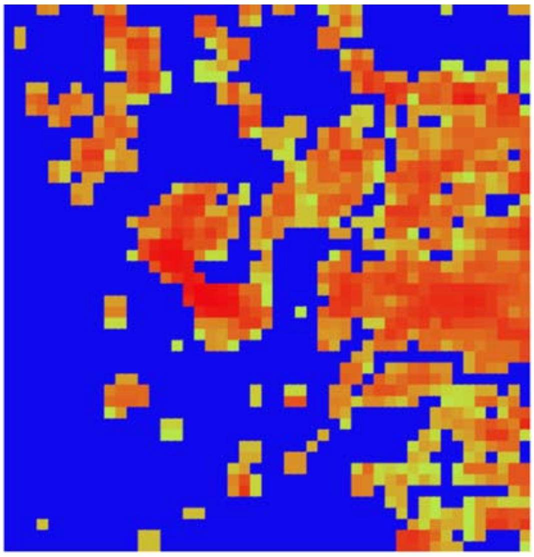

Figure 5. *Transmissivity distribution based on 100 µm aperture intervals, from simulations calibrated to test sequence with 0,043 MPa water injection pressure.*

4 NUMERICAL MODEL

In the numerical simulations the fracture is represented with a two-dimensional model, defined through the locally variable transmissivity distribution. The effect of normal stress is simulated by moving the surfaces vertically closer to each other. The objective of the simulations is to find the distance between the two surfaces that would yield the correct flow rate through the system, for the given pressure boundary condition and for the transmissivity distribution determined based on the fracture aperture distribution at that position.

The boundary conditions were set as follows. At the upper and lower boundaries, specified head boundary conditions corresponding to the pressure conditions during the experiment were used. No flow was allowed to cross the two other sides. In these preliminary modeling studies the average pressures shown in the Table I were used at the injection boundary. The injection flow was actually somewhat transient during each interval in the case of the natural fracture (Pöllä et al., 1995). In spite of this, to be able to observe the effect of heterogeneity separately, the average steady state flow situation was chosen to be modeled first. This would be a logical extension to a simple cubic law approximation.

For the simulations the numerical code CASA (Kuhlmann, 1992) was employed. The code solves the continuity equation for saturated groundwater flow in three dimensions. It uses finite-element solution method, with isoparametric elements and quadratic shape functions. The program is actually designed for the inverse solution of the groundwater flow equation. Here only the direct solution capability is used and the algorithm was chosen for this study because it has previously proven accurate in cases where sharp permeability contrasts from one element to the next occur (Kuhlmann, 1992, Niemi, 1994). As the problem to be solved here is two-dimensional, the equation to be solved here is

$$\frac{\partial}{\partial x}\left[T_x\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[T_y\frac{\partial h}{\partial y}\right]=S\frac{\partial h}{\partial t}+Q \qquad (2)$$

where T_x, T_y are transmissivities, S = storage coefficient and Q = external sinks and sources. In steady state the first term on the right hand side disappears and the only parameter needed is transmissivity as a function of location.

The transmissivity distributions for the model were determined based on the local aperture values assuming cubic law to be locally valid. According to cubic law, fracture transmissivity (T) can be determined based on the fracture aperture (e) through the expression $T = e^3\rho g/12\mu$, where ρ = density of water, g = acceleration due to gravity and μ = dynamic viscosity of water. The transmissivity was determined through this expression for local sections of the fracture plane, the size of these sections being 2 mm × 2 mm.

5 PRELIMINARY RESULTS

As the distance between the two surfaces is not known, simulations were carried out to search for the correct distance. Table II shows results of three simulations where the injection water pressure at the upper boundary was held at 0.043 MPa corresponding to the test interval with second smallest stress value in Table I. The steady state flow rate going through the system was simulated and the distance was varied until an input/output flow rate equal to the measured value 0.05 cm^3/s was achieved. The Table II shows the simulated input/output flow rate, hydraulic aperture calculated based on this flow rate as well as the arithmetic means of the local physical apertures on the 2 mm × 2 mm grid. From the simulated flow values the smallest one was essentially equal to the flow rate used during the measurement. Also the mean mechanical aperture is reasonable and similar to aperture data observed elsewhere. Cox and Wang (1993) report mean apertures (obtained with dyed-fluid technique) of 37 μm for a fracture from Stripa and 42 μm for a fracture from Dixie Valley.

Once an agreement with one injection pressure was achieved, the pressure was increased to a value corresponding to another injection pressure for which data was available. Results could be obtained upto an injection pressure of 0.084 MPa corresponding to a stress of 10 MPa. For this run the fracture was closed relative to the base case with 0.043 MPa by 14 μm which corresponds to the measured difference in mechanical closure between the two cases. The simulated flow rate is shown in the second column of Table III indicating a relatively good agreement with the measured value as well.

The second row in Table III shows results from a comparison study where the effect of the reporting accuracy of the aperture data was considered. In these simulations the problems were kept identical to the previous ones, but the apertures were divided into 100 μm classes and one transmissivity was assigned to all aperture values falling into each class. Thus, all apertures < 50 μm were assigned one transmissivity, apertures between 50–150 μm one transmissivity, apertures between 150–250 μm one value etc. This was done to account for the uncertainties in the measurement accuracy of the laser profilometry. A preliminary calibration measurement was carried out to determine this accuracy experimentally and a mean standard error as high as 50 μm was obtained. This value, however, also included systematic variation in the tested rock surface itself and the actual mean standard error is therefore smaller (Vuopio, 1997 and Mononen, oral communication). The determination of the measurement accuracy exactly still requires further calibration, but based on this preliminary result the error is in any case several tens of microns. Therefore, classifying the data into 100 μm intervals is a more realistic approach than looking at the exact values of the measurements. Inspection of the simulation results in Table III shows that the simulated flow rates are of the same order of magnitude than in the previous case and also very close to the experimental value. In general, not only in the example case shown, the transition from the exact values into transmissivity intervals did not affect the results very much. It did, however, in certain cases improve the numerical performance. Some cases that produced mass balance errors with the 'exact' values did not do so with the interval values. This is evidently due to the smoother nature of the transmissivity field and consequently less sharp permeability contrasts that typically cause numerical errors. In conclusion, use of the interval transmissivities appears the most suitable approach for this type of data.

Figure 5 (page I-8) shows the discretized interval transmissivity distribution for the first simu-

Table II. *Summary of a calibration run; the simulated flow rates, the corresponding hydraulic apertures and mean mechanical apertures for three different fracture surface positions.*

Simulation identifier	Simulated flow rate Q(in) / Q(out) [m^3/s]	Hydraulic aperture from cubic law [μm]	Arithmetic mean of the local apertures [μm]
1	4×10^{-6}	110	90
2	3×10^{-7}	50	50
3	5×10^{-8}	25	35

Table III. *Summary of the simulated flow rates (m^3/s) for two calibrated cases.*

	Case with 4 MPa stress in Table I	Case with 10 MPa stress in Table I
Transmissivities based on recorded aperture values	5×10^{-8}	2×10^{-8}
Transmissivities in 100 μm aperture classes	7×10^{-8}	6×10^{-8}

lation case in Table III. Inspection of the Figure shows that at places the conductive connections are very narrow. Therefore, the flow rate through the system becomes very sensitive to the transmissivity properties at these locations. When the surfaces were brought closer together in the second case shown in Table III, the amount of contacts increased somewhat but the critical connections did not disappear. With even larger closures corresponding to the two highest pressures in Table I, the amount of contacts became so high that no continuous connections from the inflow boundary to the outflow boundary existed any more and no meaningful solution could be obtained for the flow computation.

6 CONCLUSIONS AND FUTURE WORK

We are modeling a laboratory experiment where, using a tri-axial loading chamber, the flow conditions through a fracture were monitored under varying normal stress. Fracture surfaces have been measured using optical laser-profilometry and these data were used as a preliminary basis for determining the fracture aperture distributions. The variable transmissivity distributions for the numerical model were determined by assuming cubic law to be valid locally. Due to the measurement accuracy of the laser profilometry, the transmissivities are best assigned only with an accuracy corresponding to 100 µm aperture intervals. The simulations did yield results comparable to the measured data. However, the calibrated cases in which an agreement was achieved in terms of measured flow parameters and mechanical closure, corresponded to transmissivity distributions where some of the critical conductive connections are very narrow. Then the system becomes very sensitive to the transmissivity properties at the critical locations and the measurement accuracy of the aperture data becomes important. Presently work is underway to investigate alternative methods for aperture and surface roughness characterization in order to validate or update the present experimental aperture distributions. The work is also continued in the area of modeling the fracture flow under shear strain situation. The described modeling tools allow us to physically model the processes relevant to shear stress situation and to look at the changes in flow path heterogeneity given the roughness characteristics of the fracture surfaces.

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Paper II

Generation of fracture surfaces and aperture distributions for Monte Carlo type hydraulic simulations

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CONTENTS

1 INTRODUCTION

When modeling flow and transport in field scale fractured media, the fracture characteristics usually need to be described through their statistical properties. In the largest of scales stochastic continuum and equivalent porous medium approaches may be used, but even then the information on individual fractures—even if homogenized into continuum properties—is introduced in a probabilistic, not in a deterministic sense.

While studies on individual fractures are important for learning about flow processes inside the fractures, in field studies we are interested in the span of possible values to be encountered and how they influence the flow and transport processes. Furthermore, it is of interest to understand how they are affected when the stress conditions influencing the fractures are altered. Therefore, large data bases are needed concerning fracture aperture distributions and the effect of varying stress on these distributions as well as on the subsequent flow and transport behavior.

In this progress report these issues are discussed. First some earlier work concerning the effect of stress on fracture transmissivities is cited after which an outline is suggested as to how to approach the problem in a probabilistic sense. Finally, preliminary work for implementing the approach is reported.

2 BACKGROUND ON EFFECT OF STRESS ON FRACTURE TRANSMISSIVITIES

Several authors have investigated the effect of stress on fracture aperture and subsequently fracture transmissivity. Overview of the topic is given for example in NRC (1996).

The general understanding is that the effects of normal stress are better understood than the effects of shear stress. Under increasing normal stress the typical behavior is like that shown in Figure 1. This has been observed by several authors both for granitic and sedimentary rocks. For example references see Cook (1987) and NRC (1990).

In Figure 1 we can see that the decrease in permeability with increasing stress is first significant due to closing of the fracture and subsequent increase in tortuosity. At later stages the decrease becomes slower approaching an asymptotic irreducible flow rate value, where flow is controlled by a few critical necks while some of the larger isolated voids may still be closing in response to the increasing stress.

Derschowitz et al. (1991) in their modeling work for Stripa granite use an expression relating the fracture transmissivity T (m²/s) to the imposed normal stress σ (Pa)

$$\left(\frac{T}{T_0}\right)=\left(\frac{\sigma}{\sigma_0}\right)^{-\beta} \tag{1}$$

where T_0 and σ_0 are transmissivity and normal stress at a reference stage. According to the authors the values for coefficient β vary between 0.2 and 2 with β=1 representing a reasonable value. They also show the resulting model curves along with experimental data from Stripa granite (Figure 2).

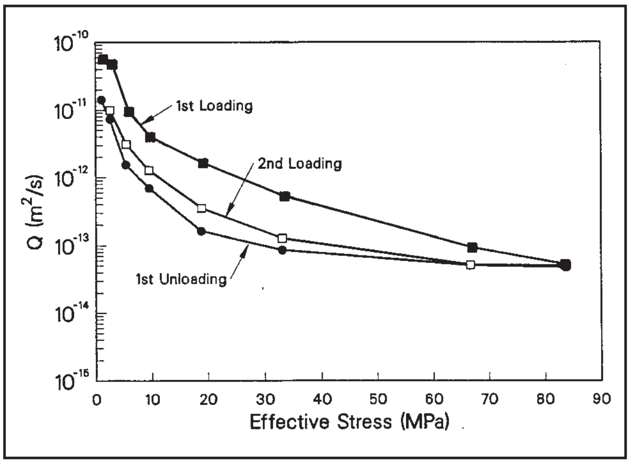

Figure 1. *Flow per unit gradient as a function of effective stress (Myer, 1991 as reported in NRC, 1996).*

Rutqvist (1995) relates the change in fracture transmissivity ΔT to the hydraulic aperture e and applied normal stress according to

$$T=T_i+\Delta T=\frac{\rho g}{12\mu}\left[e_i+f_d\cdot\frac{\sigma'_{ni}}{k_{ni}}\left(1-\frac{\sigma'_{ni}}{\sigma'_n}\right)\right]^3 \tag{2}$$

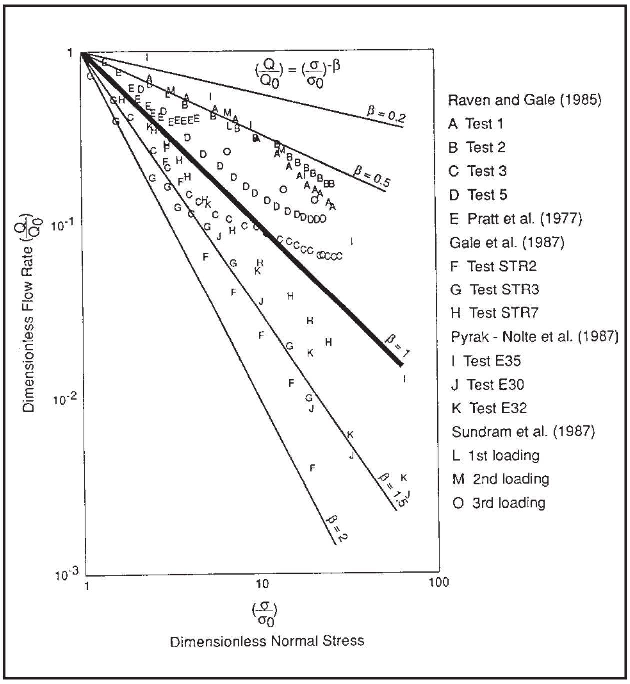

Figure 2. *Effect of stress on flow rate; experimental results and model curves (Derschowitz et al., 1991).*

where ρ = density of water (kg/m^3), g = acceleration due to gravity (m/s^2), μ = dynamic viscosity of water (kg/ms), e_i = initial hydraulic aperture (m), σ'_{ni} = initial effective normal stress (Pa), σ'_n = effective normal stress (Pa), k_{ni} = initial normal stiffness (Pa/m), f_d = correction factor taking into account the fact that decrease in hydraulic aperture due to normal stress is different (usually less i.e. $f_d < 0$) than the decrease in mechanical aperture.

Equation (2) expresses the well known cubic law aperture in terms of normal stress and fracture stiffness. It should be emphasized that the apertures e in equation (2) are not mechanical apertures but hydraulic apertures i.e. functions of flow rate response to applied pressure gradient. The significant fitting parameter in this expression is the term f_d, which will vary from fracture to fracture due to different opening distributions, autocorrelation structures etc.

Witherspoon et al. (1980) and Cook et al. (1990) have modified the cubic law expression to account for decrease in transmissivity due to fracture surface roughness and aperture contacts starting from fracture geometric properties as follows (adapted from NRC, 1996)

$$T = \frac{1}{f}\frac{(1-d)}{(1+d)}\frac{\rho g}{12\mu}b^3 + T_{irr} \qquad (3)$$

where b represents the mechanical aperture and is defined through $b = b_o-(b_m+\xi)$, b_o= maximum closure, b_m = mechanical closure in response to the applied normal stress and ξ = additional change in aperture to ensure conservation of volume, d = percentage of aperture contact area of the total fracture area, f = friction factor to account for tortuosity due to surface roughness even if the apertures are not in contact ($f > 1$) and T_{irr}= transmissivity corresponding to the irreducible flow (e.g. Figure 1.).

Expression (3) attempts to relate the microscopic scale variations in fracture geometry to overall fracture transmissivity. In comparison to equation (2) the apertures are mechanical apertures and the decrease in transmissivity due to increased stress is taken into account in the correction terms outside the cubic proportionality term. If validated by several sets of experimental data, the equation could provide means to relate microscopic variations in fracture apertures to fracture transmissivity and transmissivity changes due to aperture variations. To determine values for the various fitting parameters is of course complicated. In addition, the fitting does not account for anisotropy in aperture structure.

The effect of shear stress on fracture transmissivity is more complicated than the effect of normal stress. Increase in shear stress can result either in increase or decrease of fracture transmissivity. At low normal stress the application of shear stress may cause one fracture surface to ride up the asperities of the other, leading to what is known as dilation (e.g. Tsang, 1990). At the other extreme, at high normal stresses the friction resisting the slipping exceeds the strength of the rock and the asperities may be sheared off. The complex interaction of these processes can cause the fracture transmissivity either to increase or decrease during a shearing process. While some experimental data exists to quantify these effects (see for example Makurat et al., 1990, NRC, 1996), constitutive models are still needed to account for this behavior. In the conclusions of the first phase of DECOVALEX, this was also addressed as one of the key questions to be addressed.

3 PROPOSED STOCHASTIC MODELING PROCEDURE

A stochastic modeling procedure that could be used to model the effect of normal or shear stress on fracture transmissivities in a statistical sense, could consist of the following steps

(1) Generation of fracture surfaces based on general information on their properties. Characterization is done by means of the statistical properties reported in the literature, i.e. probability density functions and spatial correlation characteristics of the surface roughness heights.

(2) Joining of two surfaces (usually two different surface profile realizations with same statistics) to form a fracture and the resulting aperture field. Again, if this is done statistically by generating a number of realizations, a number of aperture realizations will result representing the aperture characteristics arising from those surfaces roughness characteristics.

(3) Generation of numerous fracture realizations with the previously derived aperture statistics and simulation of flow and transport with these aperture distributions with a Monte Carlo-approach. The resulting output statistics will be distributions of hydraulic and transport apertures.

(4) Movement of the surfaces with respect to each other to simulate the effect of stress, as well as repeating the steps (2) and (3) to obtain new distributions for flow and transport apertures. It should be pointed out that to model the shear behavior, a simple geometric model that has been used by investigators for modeling behavior under normal stress is not sufficient, as these do not take into account frictional sliding and aperture breakage (e.g. NRC, 1996).

Some of the key points to consider when carrying out such a procedure are

- selection of representative fracture surface statistics
- proper fitting of the surfaces to generate realistic aperture statistics
- proper selection of the conceptual model for flow

In the following chapters the first two points will be discussed and related modeling work will be presented. For discussion on the selection of the proper model for flow i.e. validity of Navier-Stokes/Stokes, Reynolds and Darcy/‘cubic-law’ approaches, the reader is referred to e.g. Brown (1987) and NRC (1996). In their recent study Mourzenko et al. (1997) use the Stokes equation to simulate the effect of normal stress on fracture flow in some example realizations.

4 GENERATION OF FRACTURE GEOMETRY DISTRIBUTIONS

4.1 Generation of fracture surfaces

Fracture surface profiles are typically measured by means of mechanical or optical profilometers. Numerous different standards exist to characterize the resulting surface roughness. Usually the roughness is described by means of average deviation of local surface heights from the mean and a measure describing their spatial correlation. Mathematically the deviation about the mean is usually described by means of a probability density function and the spatial correlation by means of an autocorrelation or power spectrum function. Since standard deviation of a measured quantity always depends on the scale of the measurement, in this case the step interval of the measurement, the resulting statistics of surface roughness also depend on the resolution of the measurement or analysis method used.

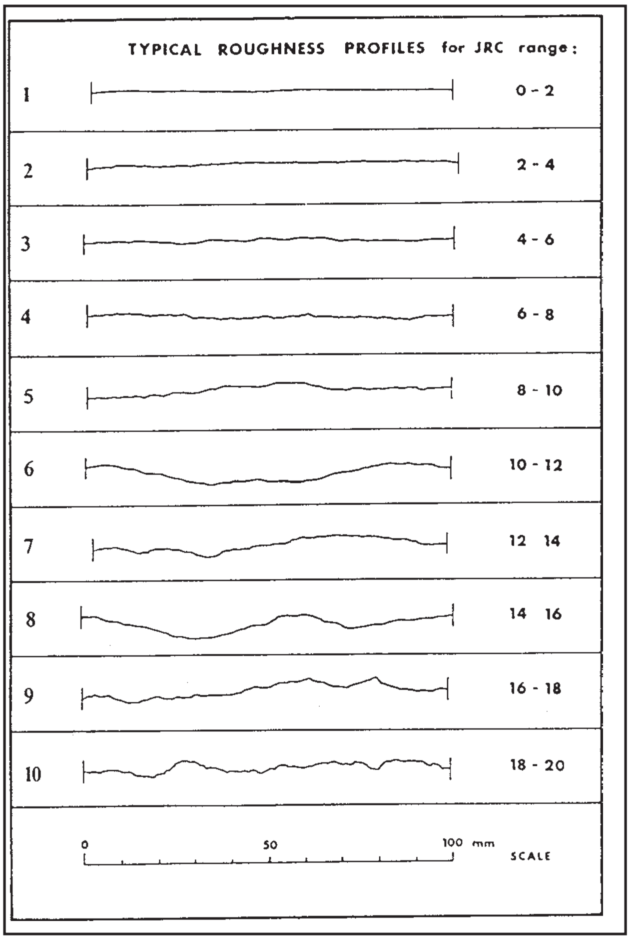

Figure 3. *Typical JRC values for joint samples of different roughness (after Barton and Choubey, 1977).*

Table I. *Estimated fractal dimensions for ISRM standard roughness profiles according to different investigations (after Seidel and Haberfield, 1995; 'current study' referring to their study).*

JRC	Lee et al.	Turk et al.	Current study
0–2	1.000446	1	1.00009
2–4	1.001687	1.0019	1.00054
4–6	1.002805	1.0027	1.00072
6–8	1.003974	1.0049	1.0014
8–10	1.004413	1.0054	1.0018
10–12	1.005641	1.0045	1.004
12–14	1.007109	1.0077	1.0053
14–16	1.008055	1.007	1.0081
16–18	1.009584	1.0104	1.0096
18–20	1.013435	1.017	1.012

Several studies have indicated that natural fractures exhibit surfaces that can be represented by means of fractal dimension D. This can be determined based on the power α of the spectral density function relation. When α is 2…3, like it usually is in case of natural fractures, the fractal dimension D can be estimated from $D = 2.5\text{-}\alpha/2$ (Brown, 1995).

In the present study, for generation of fracture surfaces the method of Seidel and Haberfield (1995) was used. They relate the commonly used fracture roughness measure JRC (Joint Roughness Coefficient of Barton and Choubey, 1977, defined for standard ISMR roughness profiles) to fractal dimension. Figure 3 shows the standardized profiles for different JRC-classes and Table I shows results of different investigators relating fractal dimensions to these profiles.

Furthermore, Seidel and Haberfield (1995) relate the fractal dimension D to the standard deviation of the chord angles s_θ as

$$s_\theta \approx \cos^{-1}(N^{(1-D)/D}) \qquad (4)$$

where N = number of divisions of the profile (number of chords). For the definition of the terms for single chord geometry, see Figure 4a. By introducing a value of D into equation (4) for a JRC-class, the corresponding standard deviation of the chord angles characterizing that JRC-class can be determined.

The generation of the profiles was done by the method of midpoint displacement. In this method, the profile is intersected by successive bi-sections and the chord angle for each bisection is determined from the normal distribution defined by a

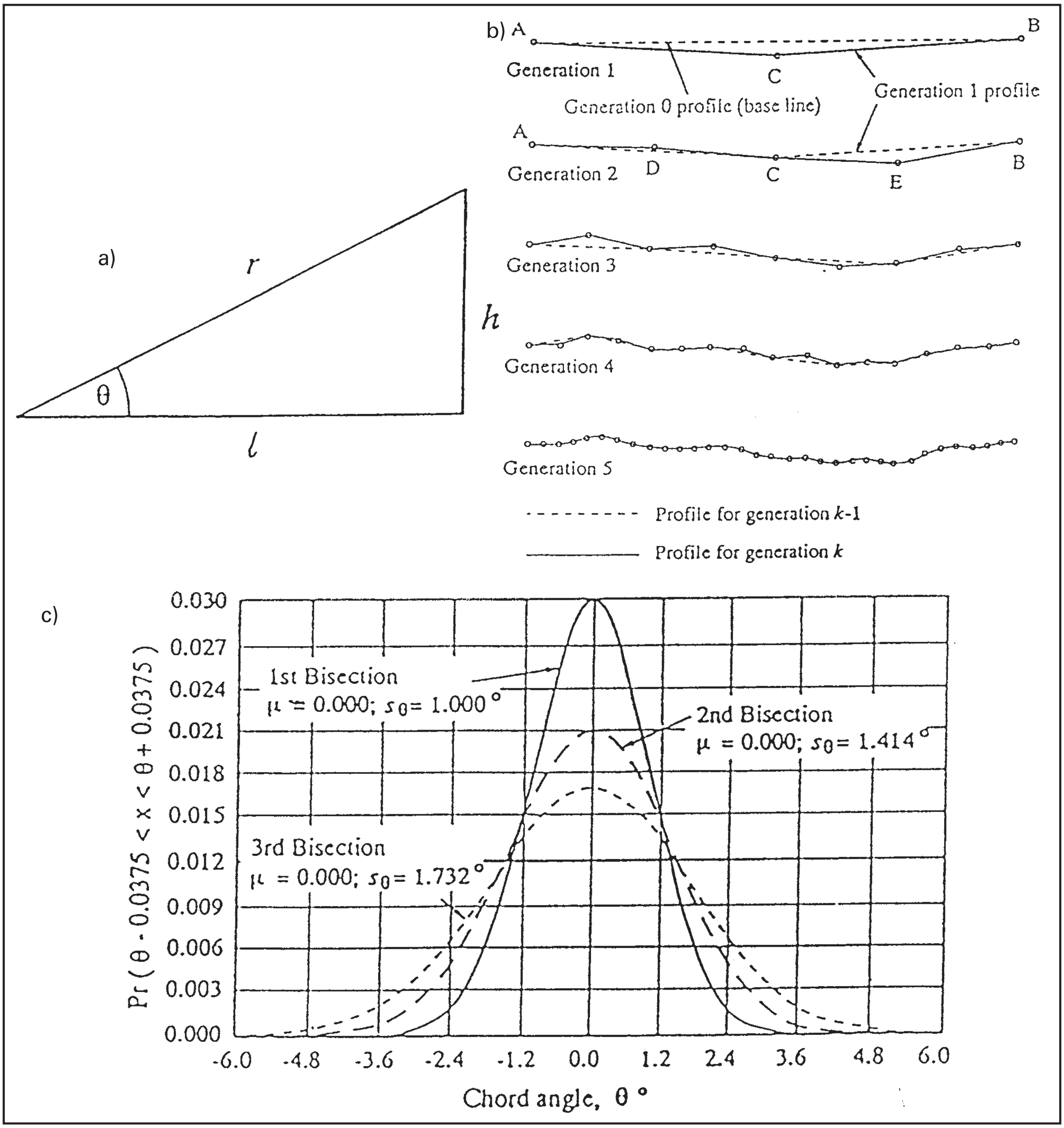

Figure 4. *Generation of the fractal roughness profiles with the method of midpoint displacement a) single chord geometry, b) principle of successive bisections, and c) chord angle distributions for successive bisections (Seidel and Haberfield, 1995).*

zero mean and the previously defined standard deviation ($N(0,s_\theta)$) (Figures 4b and c). Due to the change in total length after each division, the standard deviation is scaled accordingly after each division (Figure 4c) to account for the shortening of intersection to be bisected (see Seidel and Haberfield, 1995 or the review of Vuopio and Pöllä, 1997 for details).

In their study, Seidel and Haberfield (1995) obtained good results with this approach in reproducing the standard JRC roughness profiles. In the present study this approach was adopted and implemented into numerical format i.e. an algorithm was written that could generate roughness profiles according to the previously described outline. Figure 5 shows two sets of generated random realizations, corresponding to different angle standard deviations and therefore different JRC-classes. Comparison of these results to the standard profiles shows a similar general appearance with essentially smooth profiles in the lower roughness classes with increasing roughness with increase in the JRC-class. Comparison of the two different sets of generated realizations shows also some difference between the realizations, as can be expected.

For comparison, variograms were also plotted based on the generated roughness realizations. For generating each variogram ten profiles were always combined in order to make the data sets more representative and the variograms more stable (Figure 6). Inspection of the variograms shows the expected power relation (fractal-like) variogram behavior with higher JRC-classes producing steeper slopes. It should be pointed out that for a truly fractal profile, a variogram sill is

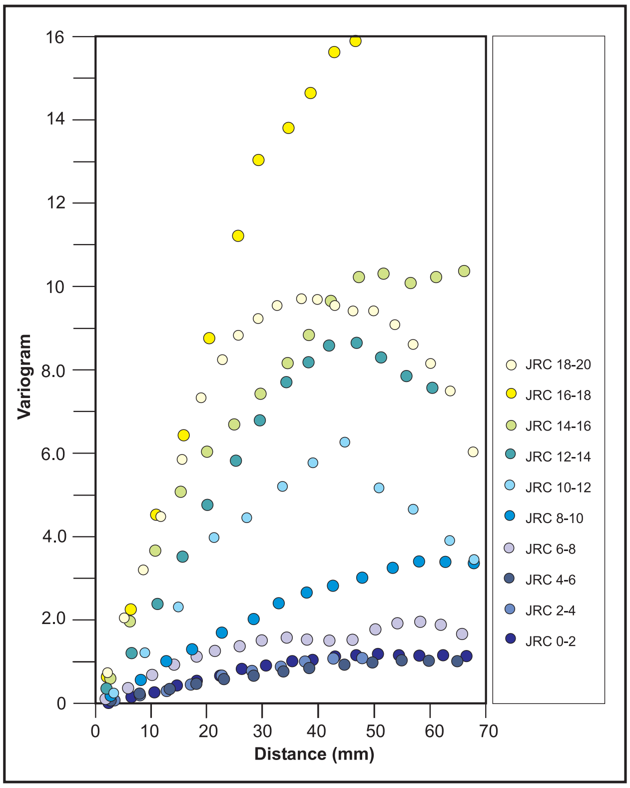

Figure 6. *Variograms of the constructed of the generated profiles (data of 10 profiles of similar roughness characteristics in each variogram).*

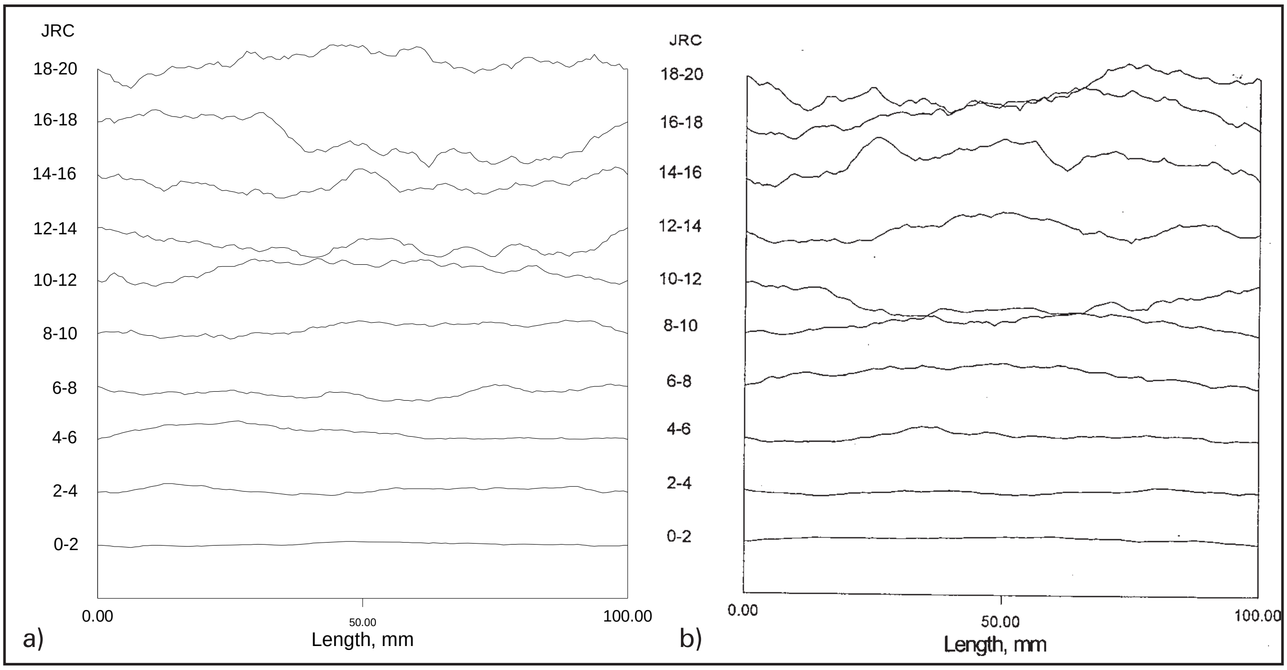

Figure 5. *Two sets of generated random roughness profiles corresponding to different JRC-classes a) realization set 1 and b) realization set 2.*

not produced but the variogram continues to increase (La Pointe, 1997). Inspection of the variograms in Figure shows this behavior. The sudden decrease in some variograms at about 50 mm (about half of the sample length) in some roughness classes may reflect the decrease in the number of observation points, since as a rule of thumb variograms should not be constructed to larger distances than half of the total observation length. It could, however, also be a reflection of the generation method, where the generation was started at the middle of the sample.

The above generation routine produces fracture roughness profiles in one dimension. To generate full two dimensional surfaces, one has to define whether the surfaces exhibit self-similar or self-affine characteristics. The latter means that different fractal scaling is used in X and Y directions. The conversion is made by means of so-called Hurst exponent. The issue is discussed more closely e.g. in La Pointe (1997) and Barton and La Pointe (1995).

4.2 Generation of aperture distributions

Several authors have used the method of placing two fractures of same roughness characteristics (same statistical properties but different realizations) to form a fracture (for example Brown (1987) and Mourzenko et al. (1995, 1997). This is an attractive approach because ample data exists on surface roughness characteristics while only a very limited number exists on fracture apertures. In addition, to be able to model the behavior under shear situation—as is the objective here—the sur-

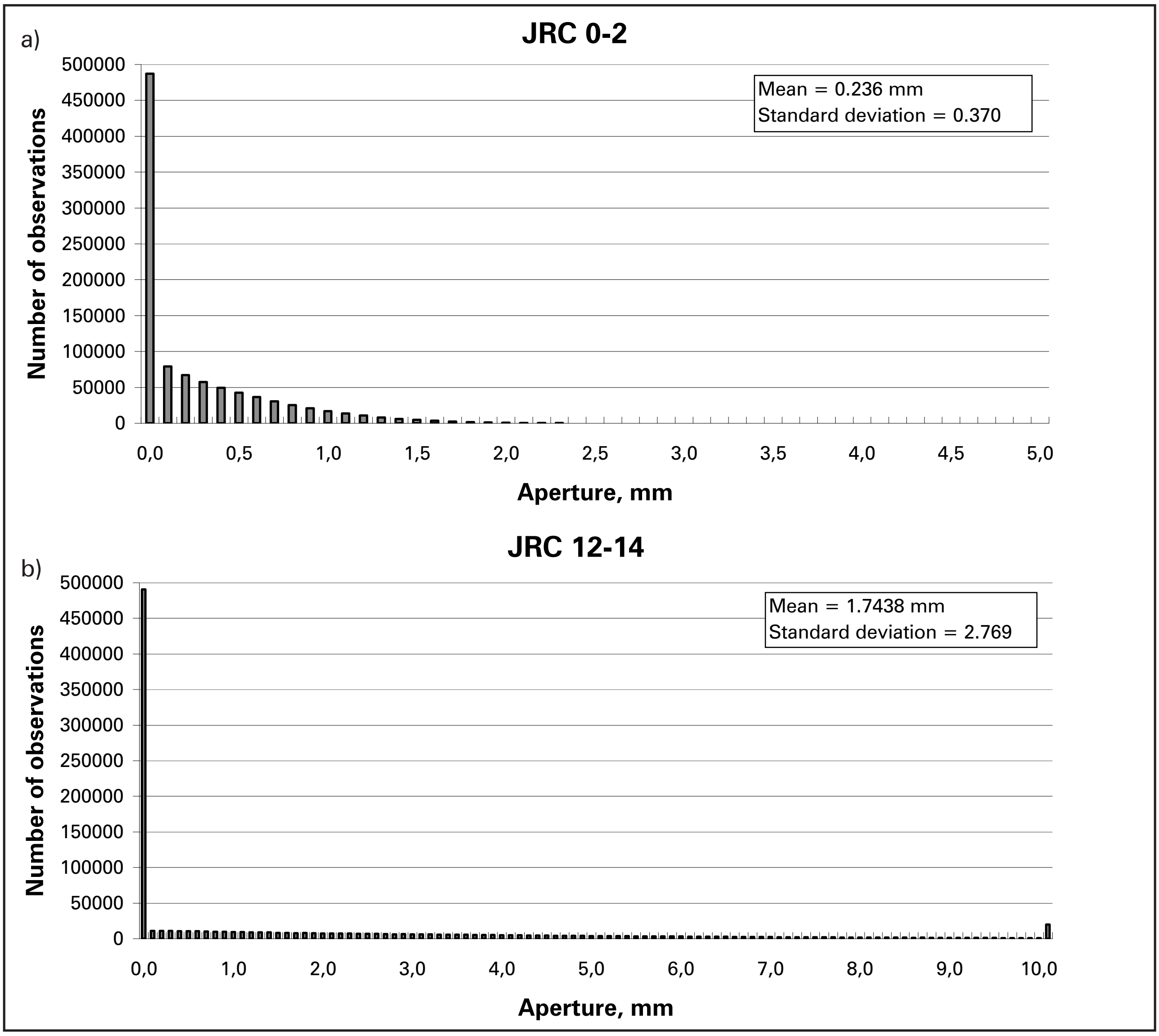

Figure 7. Monte Carlo-based aperture distributions for two different roughness classes a) JRC 0-2 and b) JRC 12–14.

face geometries are needed in any case.

It is of interest to see if the different fracture surface roughness characteristics produce different aperture characteristics. To investigate this, a large number of surface realizations was generated and randomly combined with another surface of the same roughness characteristics (same D and therefore same JRC). For each JRC-class a large number of realizations was generated and the resulting aperture distributions computed. Number of realizations was increased until the aperture statistics converged. Figure 7 shows the resulting aperture distributions for two different roughness classes. The highest column at left corresponds to zero apertures i.e. locations where the surfaces were in contact or overlapping. Comparison of the two figures shows that with smaller surface roughness the resulting stochastic apertures are smaller than in the rougher case. Especially in the smoother case the aperture distribution appears log-normal. For comparison, Figure 8 shows example measurements by Hakami (1995) for two different fractures. The first (Figure 8a) correspondes to a well mated fracture with very little spread in the aperture values, while the other (Figure 8b) is characterized as a minor fault, with generally large apertures but also a large portion of zero-apertures. Hakami tested a number of fractures and these two samples presented the extreme ends of the spectrum. The character of the other fractures tested fell somewhere between these two.

Comparison of the generated values to these measured data shows that the generated values are well within the range of values measured by Hakami. The portion of apertures in contact is, however, clearly larger in the generated data. This is a consequence of the fact that no geological 'history' was yet introduced into the generation. In other words, whenever the randomly mated surfaces crossed each other the aperture was set to zero i.e. as a point of contact. This approach has been often used when generating aperture distributions from opposing surfaces. Based on the

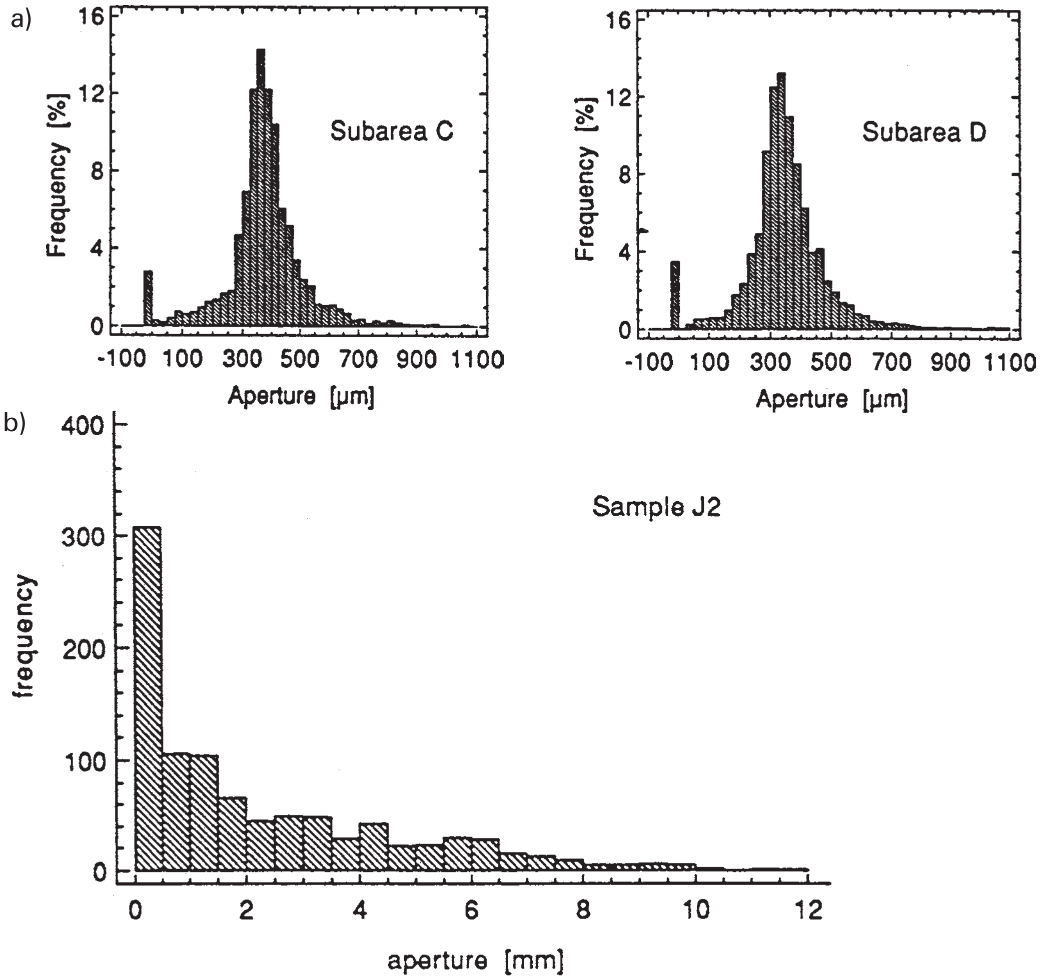

Figure 8. *Measured aperture distributions for a) example sections of a well mated fracture and b) a minor fault with a large variation on aperture (Hakami, 1995).*

results in Figures 7 it seems, however, that a natural next step would be to introduce a ‘degree of matedness’ criterion into the generation routine. The possibility to derive the statistical aperture data from the surface roughness data by means of the so-called mismatch length scale e.g. (Thompson and Brown, 1991) could also be investigated. Also, the approach by Roberds et al. (1990) to derive statistical properties of local apertures from the statistical properties of the opposing fracture surfaces could be investigated for its applicability for the present study.

5 SUMMARY AND CONCLUSIONS

This progress report addresses the question of effect of stress on fracture transmissivity from the point of view that eventually—in field scale applications—large data bases relating hydraulic behavior to mechanical behavior will be needed. A procedure is suggested to obtain statistical distributions of hydraulic and transport apertures based on information on fracture surface roughness profiles. Preliminary results for implementing the approach are also given. The so-called Joint Roughness Coefficient classification is related to fractal dimension after the procedure by Seidel and Haberfield (1995) and a large number of roughness profile realizations are generated for each JRC-class. These surfaces are then placed together to form actual fractures. The pairing of the surfaces is made by placing two surfaces with similar statistical properties (same JRC class and same fractal dimension) together. By doing this to a large number of surface pairs, aperture distributions for the different JRC classes are generated. The obtained aperture distributions provide an interesting basis for comparison to the few actual aperture measurements that exist today. The comparison shows that the values generated are within the range of the measured data, but the number of contact points generated is too large. Therefore, before the initiation of the flow simulations and 'mechanical experiments' where the surfaces will be moved with respect to each other to simulate shear behavior, inclusion of the 'degree of matedness' criterion into the generation routine is proposed.

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