Contact mechanism of a rock fracture subjected to normal loading and its impact on fast closure behavior during initial stage of fluid flow experiment

Bo LI¹⁾, Zhihong Zhao²⁾, Yujing JIANG^{1,3)}, Lanru Jing⁴⁾

¹⁾ School of Engineering, Nagasaki University, Nagasaki 852 8521, Japan

²⁾ Department of Civil Engineering, Tsinghua University, Beijing 100084, China

³⁾ State Key Laboratory of Mining Disaster Prevention and Control Co-founded by Shandong Province and the Ministry of Science and Technology, Shandong University of Science and Technology, Qingdao 266590, China

⁴⁾ Department of Land and Water Resources Engineering, Royal Institute of Technology, Stockholm 100 44, Sweden

Corresponding author:

Bo Li, School of Engineering, Nagasaki University, Nagasaki 852-8521, Japan.

Tel: +81-95-819-2616

Fax: +81-95-819-2627

Email address: libo@nagasaki-u.ac.jp

ABSTRACT:

Fast closure of rock fractures has been commonly observed in the initial stage of fluid flow experiments at environmental temperatures under low or moderate normal stresses. To fully understand the mechanisms that drive this fast closure, the evolution of local stresses acting on contacting asperities on the fracture surfaces prior to fluid flow tests need to be evaluated. In this study we modeled numerically the asperity deformation and failure processes during initial normal loading, by adopting both elastic and elastic-plastic deformation models for the asperities on a real rock fracture with measured surface topography data, and estimated its impact on initial conditions for fluid flow test performed under laboratory conditions. Compared with the previous models that simulate the normal contact of a fracture as the approach of two rigid surfaces without deformations, our models of deformable asperities yielded smaller contact areas and higher stresses on contacting asperities at a given normal stress or normal displacement. The results show that the calculated local stresses were concentrated on the contacts of a few major asperities, resulting in crushing of asperity tips. With these higher contact stresses, however, the predicted closure rates by pressure solution are still several orders of magnitude lower than the experimental measurements at the initial stage of fluid flow test. This indicates that single pressure solution may not likely to be the principal compaction mechanism for this fast closure, and that the damages on contacting

asperities that occur during the initial normal loading stage may play an important role.

Keywords: Rock fracture; Fluid flow experiment; Fast closure; Contact mechanism; Elastic;

Crushing

1. Introduction

In fractured rocks of low/negligible matrix permeability, fractures are the dominate pathways for fluid flow and mass transport. A reliable understanding of fluid flow and transport characteristics of rock fractures under loading is therefore a critical issue in many rock engineering applications, such as underground nuclear waste repositories, CO₂ sequestration and enhanced geothermal systems.

Coupled stress-flow-transport experiments in rock fractures provide direct measurements under laboratory conditions on short-term evolutions of flow rate/differential pressure and effluent mineral mass concentrations etc., under necessary and proper boundary conditions according to the targeted coupled Thermal-hydraulic-Mechanical-chemical (THMC) processes. Additional measurements on fracture surface geometry and inner matrix structure using laser profilometer and X-ray CT measurements before, after or during the experiments are also implemented for independently monitoring process evolution rates and for facilitating numerical modeling. Such experiments have been extensively performed and reported in literature for different rocks, e.g., limestone (Polak et al., 2004; McGuire et al., 2013), novaculite (Polak et al., 2003; Yasuhara et al., 2006a) and granite (Yasuhara et al., 2011). Most of these experiments adopted cylindrical samples, placed in tri-axial pressure cells and heated to different elevated temperatures. Continuous monitoring data of flow rate and

differential fluid pressure (usually either of them was kept constant) was used to understand the evolutions of transmissivity and hydraulic aperture by adopting the cubic law, and the measured effluent mineral mass concentrations were helpful to understand the details of water-rock interaction mechanism. Despite the still limited number of publications for such experiments, the data obtained are important basis for understanding the fundamental behavior of the coupled THMC processes in rock fractures, especially the impact of the stress and deformation/failure of rock fractures on flow and transport processes.

Yasuhara et al. (2003, 2004, 2006b, 2011) used lumped parameter models of solute transport in rock fractures to represent the principal chemical processes on minerals on contacting rough fractures and on free surfaces. These models simplified the dispersedly distributed contacts on rough fracture surfaces as one single representative contact surrounded by an appropriate tributary area, and incorporated the processes of pressure solution at this contact, solute diffusion along a thin film in it, and precipitation/dissolution on void wall surfaces. Given that these models averaged out localized effects on largely dispersed contacts, such simplified models may be only suitable for the cases with homogeneous geometries of contacts and void spaces. Yasuhara et al. (2006b) established a numerical model by employing the Lagrangian–Eulerian method to study the localized evolutions of aperture and solute concentration in a fracture, for arbitrary effective stresses, fluid and rock temperatures, and

fluid flow rates. This model exhibited a much better performance than the lumped parameter models, fitting especially well with the experimental results when elevated temperatures were applied. These models, however, were not able to represent the fast decrease of fracture apertures, i.e., fast closure, that is commonly observed in the initial stages of fluid flow experiments. Yasuhara and Elsworth (2008) attributed these fast closure phenomena to sub-critical crack growth and found that a stress corrosion mediated compaction model was more suitable to accommodate these observations than pressure solution mediated compaction model. Zhang et al. (2011) also compared these two models using FEM analyses, and showed that aperture closure rate induced by stress corrosion was six orders of magnitude higher than that due to pressure solution.

In the models described above, the local stress, σ_a , acting on each contacting asperity, was assumed to be identical and given by

$$\sigma_a = \frac{\sigma_n}{c} \quad (1)$$

where σ_n is the effective confining stress acting over the fracture sample, and c is the contact area ratio (total contact area / nominal area of fracture surface). This assumption only holds true if contacting occurs simultaneously on all contacts, which by default should have the

same height and geometry of asperities in contact, under a normal loading. In reality, even a perfectly mated fracture may not be able to reach such an ideal behavior, since errors of relocation of the two blocks of the sample fracture before testing cannot be avoided. For fracture asperities of different sizes and shapes, during a normal loading process, usually a few number of major asperities of greater sizes and heights come into contact at first, followed by gradual increase of contacts of moderate and then small asperities, accompanied by progressive deformation and/or failure (crushing) of tips of early contacted major asperities, leading to closure increase of a fracture. The evolutions of the stress concentrations and possible mechanical failures on the asperity tips then determine the closure rate, and it may not be realistic to use overall averaged contact area (Eq. (1)) for estimating the apparent effective stress acting on the fracture sample if a few large asperities of unstationarity dominate the mechanical and fluid flow processes.

The mechanics of contacts of asperities on rock fracture surfaces are usually assumed as Hertzian contacts, from which rock fracture deformation under normal loading is derived considering elastic deformation (e.g., Greenwood and Williamson, 1966; Brown and Scholz, 1985; Yoshioka and Scholz, 1989a,b; Yoshioka, 1994a) or both elastic deformation and plastic deformation (e.g., Brown and Scholz, 1986; Yoshioka, 1994b). These studies used statistical parameters (e.g., Gaussian distribution and Gamma distribution) to describe the geometry of

rough surfaces without taking into account the interactions between local asperities, therefore, the distribution of stress on each local contact cannot be properly evaluated. Pyrak-Nolte and Morris (2000) modeled a fracture as two half-spaces separated by a regular lattice of cylindrical asperities with heights determined by the local apertures. This approach considered the interaction of asperities and therefore provided more precise local stress and displacement distributions on fracture surfaces. Ameli et al. (2014) extended the original model of Pyrak-Nolte and Morris (2000) to consider dissolution-induced surface alteration. SEM micrographs of a granite fracture sample captured after a fluid flow experiment (Yasuhara et al., 2011) clearly demonstrated a crushed asperity, providing an evidence for the occurrence of mechanical failures of asperities during initial normal loading of fluid flow tests. On the other hand, how and when these failures/crushing occur during tests still remain unknown. In order to deepen our understanding on this phenomenon, the local stresses acting on early contacting asperities need to be accurately calculated separately first.

In this study, we mainly used a direct quadratic mathematical programming method based on variational principle of minimum total complementary potential energy to examine the local stress and the real contact area distributions in the initial normal loading process prior to the fluid flow test, by using the digitized surfaces of the Arkansas novaculite fracture sample adopted in Yasuhara et al. (2006a). Both elastic and elastic-plastic contact models were

applied, and the hardness of quartz, the major mineral component of the rock, was assumed as the criterion for checking the onset of mechanical failures on asperity tips. In this way, we aimed to obtain a more realistic stress distribution on individual contacting asperities. We compared the calculated distribution of local stresses with the mean stresses adopted in previous studies (e.g., Yasuhara et al., 2006a), and investigated the possible explanations for the fast closure of fractures during the initial stage of the fluid flow experiment concerned.

2. Reappreciation of Fluid Flow Experiment Results Conducted on Arkansas Novaculite

2.1 Tested fracture closure results

Arkansas novaculite was adopted in the fluid flow experiment conducted by Yasuhara et al. (2006a), which is >99.5% quartz with a density, ρ_g , of 2.65 g/cm³. Cylindrical core sample was split to form a single diametric fracture, which was loaded to a net effective stress of 1.38 MPa in a tri-axial pressure cell. Both surfaces of the fracture were profiled with a 3-D laser scanner on a 50 μ m grid in the x, y plane, one of which is shown in Fig. 1. Several major asperities with steep slopes and greater heights were observed on the fracture surface, which could come into contact in the early stage of normal loading and bear more loads during the subsequent loading stages.

The experiment started at a controlled flow rate, Q , of 1.0 mL/min and a temperature, T , of

20 °C, which altered during test, in the range $Q = 1.0 \sim 0.0625$ mL/min and $T = 20 \sim 120$ °C, respectively. Differential pressure between the inlet and outlet of the sample was continuously measured throughout the test, combined with prescribed flow rates, yielding the evolution of equivalent hydraulic aperture of the fracture by using the cubic law, as shown in Fig. 2. A fast and continuous decrease of hydraulic aperture from 18.5 μm to 10.3 μm during the first 858 hr of the test can be observed at temperature of 20 °C. This fast closure may be attributed to a single or the combination of the following mechanisms: (1) pressure solution induced mass dissolution (Yasuhara et al., 2006b); (2) subcritical cracking induced compaction (Yasuhara and Elsworth, 2008; Zhang et al., 2011); and (3) mechanical crushing of contacting asperity tips (Yasuhara et al., 2011).

During a flow test, along with the dissolution of contacting asperities, the total contacting area increases and therefore stresses on individual contacting asperities decrease. The third mechanism mainly takes place during the initial normal loading process, and thus is not the direct reason of the fast closure of fracture during the fluid flow tests in which the normal loading is usually kept constant. However, the crushing/damage of asperity tips induces irreversible changes on the geometry of asperities and produces crushed zones of gouge materials that may have impact on the first two mechanisms. Pressure solution mediated compaction efficiently halts when the stress magnitude on a contact drops below a critical

stress determined by considering the energy balance under applied stress and temperature conditions (Revil, 1999). If contacting asperities are treated as Hertzain contact, which is a commonly accepted and reasonable simplification, kinetics of both sub-critical and mechanical cracking are primarily controlled by the stresses acting on and the shape of the contacting asperities. To identify the predominance of these mechanisms, one therefore needs to quantitatively investigate the local stresses on individual contacts, especially in the initial normal loading stage prior to the fluid flow test.

2.2 Initial normal loading process on the fracture

If the mechanical deformation is assumed to have negligible influence on the geometry of fracture surfaces, the digitized surface topography (Fig. 1) could be used to estimate the inner structures of fractures during normal loading, by simply moving one surface normally towards another and calculate the point-to-point distances between the approaching asperities. The relation between mechanical aperture, h_M , which is the arithmetic average of these point-to-point distances, and contact area ratio, c , which is the number of grids of contact areas in the numerical model with zero distances divided by the total number of grids of the nominal plane of fracture sample, is then obtained. The normal closure of fractures can then be derived by using Bandis' hyperbolic function (Bandis et al., 1983) as:

$$\sigma_n = k_{n0} \left(\frac{u_n}{1 - u_n/u_{nmax}} \right) \quad (2)$$

where k_{n0} is the initial normal stiffness at a prescribed stress state, u_n is the normal displacement and u_{nmax} is the maximum normal displacement, approached asymptotically with increasing normal stress. The basic parameters of k_{n0} and u_{nmax} need to be experimentally evaluated. Since there were no directly measured experimental data of closures in Yasuhara et al. (2006a), we assumed that the maximum fracture closure equals to the approaching distance of the two surfaces starting when the first pair of grids come into contact, continuing until the closure of the last void was reached. Then, the maximum normal displacement, u_{nmax} , was calculated as 554 μm for this fracture, by simulating the approaching of the two digitized surfaces and calculating the distance of each pair of grids.

By substituting measured differential pressure and prescribed flow rate at the start of fluid flow test into the cubic law, an equivalent hydraulic aperture was obtained as 18.5 μm , corresponding to a contact area ratio of 5.0%. Assuming that mechanical aperture was equal to equivalent hydraulic aperture by using the cubic law as in Yasuhara et al. (2006b), the normal displacement from the start of loading (0 MPa) to the loading stress of 1.38 MPa was calculated, by continuously approaching the two surfaces to a mechanical aperture of 18.5 μm .

Substituting this normal displacement $u_n=325 \text{ }\mu\text{m}$, $u_{nmax}=554 \text{ }\mu\text{m}$ and $\sigma_n=1.38 \text{ MPa}$ into Eq. (2) led to $k_{n0}=1.755 \text{ GPa/m}$. The loading-displacement curve can then be drawn as shown in Fig. 3. The parameters of this curve were derived based on the approach of two rigid surfaces without deformation and the contact area was merely the area of geometrical interference between the two surfaces. This model is labeled as rigid model in the rest of this paper.

2.3 Influence of the relation between mechanical and hydraulic apertures

It is well known that the mechanical aperture of a fracture is usually larger than the hydraulic aperture estimated based on parallel-plate model (Olsson and Barton, 2001; Li et al., 2008). The ratio of hydraulic aperture to mechanical aperture h_H/h_M was found strongly related to the ratio σ_{apert}/h_M , where σ_{apert} is the standard deviation of the local mechanical apertures (i.e., local point-to-point distances). Zimmerman and Bodvarsson (1996) proposed an equation relating h_H/h_M to σ_{apert}/h_M and contact area ratio c by using a two-term perturbation estimate in conjunction with a tortuosity correction, written as:

$$h_H^3 \approx h_M^3 \left[1 - 1.5 \frac{\sigma_{apert}^2}{h_M^2} + \dots \right] (1 - 2c) \quad (3)$$

Xiong et al. (2011) conducted coupled shear-flow tests on rock fractures and their

corresponding numerical simulations by solving Navier-Stokes equations. Based on the best-fitted values of the tested and simulated results, they proposed a similar empirical equation for Reynolds number less than 1 as:

$$h_H^3 \approx h_M^3 \left(1 - \frac{\sigma_{apert}}{h_M} \right) \quad (4)$$

For the studied fracture (Fig. 1), h_H was estimated as 18.5 μm and the Reynolds number was very small. We could then continuously make the two fracture surfaces approach and search best-fit values of h_M , σ_{apert} and c that yield a similar value of 18.5 μm for h_H according to Eqs. (3) or (4). These values were found when normal displacement became 321 μm , at which the corresponding c and h_M were calculated as 2.62% and 22.8 μm , respectively. Substituting these values into Eqs. (3) and (4) yielded two values of 18.8 μm and 17.9 μm for h_H , respectively. The difference of the values of normal displacements at the compression stress of 1.38 MPa between the cases considering equivalent value of h_H and h_M and considering reduced value of h_H from h_M is negligible (i.e., 325 μm comparing to 321 μm). However, the differences in c and h_M calculated from the two cases were significantly large at this state, which could have strong influences on the following estimation of flow and chemical reaction processes. For instance, substituting $\sigma_n = 1.38$ MPa, $c = 5.0\%$ and $c = 2.62\%$,

into Eq. (1), we obtain $\sigma_a = 27.6$ MPa and $\sigma_a = 52.7$ MPa, respectively, where one value is nearly two times of the other. Since the rates of pressure solution and sub-critical cracking depend on the stresses acting on contacts, the relation between mechanical aperture and hydraulic aperture is important in the analyses of fluid flow experiment results.

3. Application of 3-D Contact Models on Rock Fractures

Following the pioneer work of Greenwood and Williamson (1966), a large number of statistical models have been developed to account for the contact problems of rough surfaces. Detailed reviews of the theories and applications of these models can be found in Bhushan (1998) and Persson (2006). Neglecting of interactions between contacting asperities and over-simplified assumptions of asperity geometry in these models have restricted their applications in engineering practices, especially for the problems where estimation of local stresses on contact areas is required. By means of the digitized surface geometries, several numerical techniques have been developed to solve contact problems of rough surfaces. One of them uses variational principle, in which, the elastic contact problem is reduced to finding a minimum value of the total complementary potential energy (Bhushan, 1998). This method is convenient to implement and is capable of efficient and accurate calculation of contact stresses. We adopted this method to solve the contact problem of the novaculite rock fracture

concerned in this study during the initial normal loading process prior to the fluid flow test.

3.1 Elastic contact model

Bhushan (1998) presented the details about the mathematical formulation of the variational method. Only basic derivation is summarized below.

A typical contact problem is schematically drawn in Fig. 4. Assuming the novaculite rock as a linear elastic material, the total complementary potential energy, V^* , of the two contacting surfaces of the fracture is given by

$$V^* = \frac{1}{2} \iint_{\Omega} p \bar{u}_z dx dy - \iint_{\Omega} p \bar{u}_z^* dx dy \quad (5)$$

where p is the contact stress, $\bar{u}_z$ is the composite normal surface displacement within contacting area, $\bar{u}_z^*$ is the total prescribed displacement within assumed contact area calculated based on geometrical interference (Fig. 4b). $\bar{u}_z$ results from a normally distributed compressive stress and can be calculated in terms of the infinite half-space solution of Boussinesq's integration,

$$u_z(x, y) = \frac{1}{\pi E^*} \iint_{\Omega} \frac{p(x', y') dx' dy'}{\sqrt{(x - x')^2 + (y - y')^2}} \quad (6)$$

where E is elastic modulus and ν is Poisson's ratio. For novaculite, the values of E and ν are 70 GPa and 0.20, respectively (Yasuhara and Elsworth, 2008). The composite elastic modulus E^* is given by

$$\frac{1}{E^*} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \quad (7)$$

where the subscripts 1 and 2 denote the two contacting bodies, respectively. After discretization, Eq. (6) becomes

$$(\bar{u}_z)_l = \sum_1^M C_{kl} p_k \quad (8)$$

where k and l are the two indices representing the contact stress location and surface displacement location, respectively. M is the total number of initial contact points where the geometrical interference occurs. C_{kl} is the influence coefficient matrix that relates stress to surface displacement. Eq. (5) can then be discretized as,

$$V^* = \frac{1}{2} \sum_{l=1}^M p_l \left(\sum_{k=1}^M C_{kl} p_k \right) - \sum_{i=1}^M p_i \bar{u}_{zi}^* \quad (9)$$

Or in a tensor form

$$\mathbf{V}^*(\mathbf{p}) = \frac{1}{2} \mathbf{p}^T \cdot \mathbf{C} \cdot \mathbf{p} - \mathbf{p}^T \cdot \mathbf{u} \quad (10)$$

$\mathbf{V}^*(\mathbf{p})$ has its minimum if $\mathbf{p}^*$ meets the following condition,

$$\mathbf{p}^* = \mathbf{C}^{-1} \cdot \mathbf{u} \quad (11)$$

The contact stress, p , in the above equation has positive values within contact area and becomes zero in the void space. Therefore, the following Kuhn-Tucker complementary conditions need to be satisfied:

$$p(x, y) \geq 0 \text{ and } g(x, y) = \bar{u}_z + h_0(x, y) - u_n = 0 \text{ (within contact area)} \quad (12a)$$

$$p(x, y) = 0 \text{ and } g(x, y) = \bar{u}_z + h_0(x, y) - u_n > 0 \text{ (out of contact area)} \quad (12b)$$

where $h_0(x, y)$ is the initial local aperture at node (x, y) when the normal load has not been applied, $g(x, y)$ is the surface gap after surface deformation started, and u_n is the rigid-body approach of the two surfaces, equal to the normal displacement.

The computational procedure to find local stress distribution started by solving Eq. (11) to obtain the contact stresses on an initial computational domain (i.e., the geometrical interference area, see Fig. 4a), in which the local contact stresses with minus values were set to zero. The obtained stresses were substituted into Eq. (8) to determine the surface displacement, which was then used to calculate the surface gap over the entire domain. The elements where the gaps were negative were added to the contact area while the ones where the gaps were larger than zero were set as noncontact area. The iteration continued until the complementary conditions Eq. (12) were satisfied for all elements. Gauss-Seidel method was used to effectively solve these equations. The validity of this numerical model has been verified by applying it to a Hertzian contact and checking the computed results with the theoretical results. More details about the computation procedure of this method are presented in Tian and Bhushan (1996). This model was labeled as elastic in the rest of this paper.

3.2 Simplified elastic-plastic contact models

When plastic deformation takes place on a contact of asperities, permanent deformation is

produced, resulting in changes of the geometry of the contacting asperities during each incremental normal loading or normal displacement step. Under the conditions that the plastic deformation is only confined within very small regions in the contacting asperities, and that the change on the geometry of the elastically deformed surface is negligible, the aforementioned equations in Section 3.1 for solving contact stress on elastic contacts still hold.

For the elastic-plastic contacts, the total deformation consists of an elastically deformed part and a plastically deformed part, namely the residual displacement. The residual displacement has to be estimated in terms of the subsurface stress field, plastic stress and plastic strain, based on, for instance, Chiu's method (Chiu, 1977, 1978) that divides subsurface plastic domain into small cubic elements in which the plastic strain is considered constant (e.g., Jacq et al., 2002; Wang and Keer, 2005; Wang, et al., 2010). Although these models have been successfully applied to metals in which failures take place in terms of large plastic deformations, their performance is still questionable when applying to brittle materials like rocks. For brittle materials, the computed plastic deformation in contacting asperities may be represented as the crushing of asperity tips (Brown and Scholz, 1986 and Yasuhara et al., 2011), instead of continuous material plastic flow. The crushing originates from micro-crack initiation and propagation in the subsurface plastic zones of contacting asperities, taking place

instantly after the contact stress reaches a critical value, resulting in permanent changes of asperity geometry.

Since this study aimed to give a first order estimation on the stress and real contact area distributions of a normally loaded rock fracture, and given the fact that the plastic deformation on this fracture was very small due to the low normal stress and high material strength, we assumed that the permanent geometry change induced by micro-cracks underneath the contacts had negligible influence on the total plastic deformation. Therefore, the fracture surface geometry change due to plastic deformation in a normal loading process was considered by continuously removing the crushed asperity tips according to a critical stress.

It is well known that the onset of plastic deformation of a rock material occurs when the normal stress of a contact exceeds its hardness (Brown and Scholz, 1986). Indentation tests on quartz revealed a hardness of $H \approx 10$ GPa at room temperature (Evans, 1984), which can then be used as a critical value for detecting the onset of plastic deformation. For an elastic-perfectly plastic contact, the contact stress will be a constant equal to H after reaching H , leading to an additional restriction condition.

$$0 \leq p(x, y) \leq H \quad (\text{within contact area})$$

Based on Eq. (5), Tian and Bhushan (1996) proposed a simple model taking into account the contribution of energy dissipation induced by plastic deformation to the total complementary potential energy as

$$\begin{aligned}
 V^* &= \frac{1}{2} \iint_{\Omega} p^e \bar{u}_z^e dx dy + \iint_{\Omega} H \Delta u_z^p dx dy - \iint_{\Omega} p \bar{u}_z^* dx dy \\
 &= \frac{1}{2} \iint_{\Omega} p \bar{u}_z dx dy - \iint_{\Omega} p \left(\bar{u}_z^* - \frac{1}{2} \Delta u_z^p \right) dx dy
 \end{aligned}
 \tag{14}$$

where the superscripts e and p denote elastic and plastic deformations, respectively. Then Eq. (11) can be solved following the same procedure for elastic contacts, by using a surface displacement, $\mathbf{u}$, that takes into account the plastic deformation as

$$u_k = \bar{u}_{zk}^* - \frac{1}{2} \Delta u_z^p
 \tag{15}$$

where Δu_z^p is the incremental surface displacement of plastic deformation and is given by

$$\Delta u_z^p = \Delta \bar{u}_z^p \left[1 + \frac{E_1(1 - \nu_2^2)}{E_2(1 - \nu_1^2)} \right]^{-1}
 \tag{16}$$

where $\Delta \bar{u}_z^p$ is the total incremental displacement of contact surfaces in the area where plastic deformation occurs.

In this study, the two surfaces of the fracture had identical values of E and ν , thus $\Delta u_z^p = 1/2 \Delta \bar{u}_z^p$. Then, a fixed amount of $1/4 \Delta \bar{u}_z^p$ was diminished from the heights of the elements where plastic deformations take place at each incremental displacement. This model was labeled as EP1 in the rest of this paper.

If we consider the contact between two asperity tips as a contact between two spheres, the contact pressure, contact area and subsurface stresses in the elastic regime can be solved following the Hertzian theory of elastic contact (Hertz, 1882; Johnson, 1985). The radius of the contact area, a , is given by

$$a^3 = \frac{3FR}{4E^*} \quad (17)$$

where F is the applied load, and R is the effective radius of sphere.

When the mean local stress on a contact reaches the hardness, H , the plastic deformation will occur, at a critical approach distance, Δu_c , given by (Yoshioka, 1994b)

$$\Delta u_c = \left(\frac{3\pi}{4} \right)^2 R \left(\frac{H}{E^*} \right)^2$$

(18)

Substitute Eq. (17) into Eq. (18), a relation between a and Δu_c can be obtained as

$$a = \frac{4\Delta u_c E^*}{3\pi H}$$

(19)

The principal stresses in the subsurface area of contacting spheres can also be calculated based on Hertzian theory of elastic contact. By using these stresses, a maximum shear stress can be found at a depth of $0.45a$, when $\nu = 0.20$, according to either von Mises or Mohr-Coulomb failure criterion. Micro-cracks induced by shear failure may initiate at this depth, gradually propagating towards the surface of contact areas, coalescent with the tensile cracks initiated at the edge of contacting surface, and finally leading to the crushing of the asperity tips above this depth (Shah and Wong, 1997). The consequences of crushing can be observed in the SEM micrographs of fracture surfaces after test in Yasuhara et al. (2011), where some crushed pieces were squeezed out and distributed around a contacting asperity with the tip being flattened. Since a crushed asperity only has limited bearing capacity for normal loading, we proposed a more robust model that once plastic deformation was detected on a surface element, its geometry would be altered by diminishing its height with a magnitude of $1/2 \times 0.45a$, where a was calculated by Eq. (19) with $\Delta u_c = \bar{u}_z$. In reality,

when the loading rate is slow, most pieces of the crushed parts remain in their original positions, and may still bear reduced stresses due to their own residual strength in the subsequent loading process. This conceptual model is therefore a highly simplified one that may exaggerate the asperity height reduction due to crushing of asperity tips. Its main aim is to give an upper bound (completely eliminating possible crushed zones) of the influence of crushing of contacting asperities on the calculated stresses and contact areas. This model is labeled as EP2 in the rest of this paper.

Note that during normal loading-unloading test on rock fractures and the fluid flow test with large flow rates, the contacting asperities may detach each other due to the tensile stress or the dissolution of bridging minerals between asperities. The pull-off force acting on contacts needs to be taken into account in the calculations in these conditions, the mathematical expressions of which could be referred to a few more sophisticated models such as JKR model (Johnson et al., 1971) and DMT model (Derjaguin et al., 1975) in the literature. In this study, we only considered the two surfaces of a fracture approached towards each other continuously to reach a prescribed normal stress (confining stress). During this process, the normal stresses acting on contacts monotonically increased and the pull-off force did not act on these contacts. Therefore, the effect of pull-off force was not included.

3.3 Calculated results of contact stresses and contact areas

The digitized surfaces of the fracture concerned have a length of 88.95 mm and a width of 45.9 mm (Fig. 1), divided by 1779×918 square elements of an identical size of $0.05 \text{ mm} \times 0.05 \text{ mm}$. The position of one surface of the fracture was fixed and the other surface was moved towards the fixed one normally with an incremental normal displacement of $1 \text{ }\mu\text{m}$ at each step, and the local contact stresses and contact areas were calculated in each numerical model using the aforementioned theories. The calculations started when the first pair of surface elements came into contact and continued until the normal displacement reached $300 \text{ }\mu\text{m}$.

The calculated normal stress-normal displacement curves of four models (rigid, elastic, EP1 and EP2) are shown in Fig. 5. The normal displacements of these curves at the compression stress of 1.38 MPa are $217 \text{ }\mu\text{m}$ (elastic), $239 \text{ }\mu\text{m}$ (EP1), $263 \text{ }\mu\text{m}$ (EP2) and $325 \text{ }\mu\text{m}$ (rigid), respectively. Compared with the normal displacement of $321 \text{ }\mu\text{m}$ and mechanical aperture of $22.8 \text{ }\mu\text{m}$ estimated from the relation of mechanical aperture and hydraulic aperture at the compression stress of 1.38 MPa , the elastic and elastic-plastic models provide smaller normal displacements and larger mechanical apertures. These biases may be attributed to the assumptions for the initial state before loading and the strict normal approach of surfaces, and the unavoidable relocation errors of fracture surfaces in the numerical models.

Due to the unevenly distributed stresses on the surfaces, the two surfaces of the models did not always approach towards each other normally without rotation or shear during normal loading, which may cause mismatch of the position in x, y plane between the digitized contacting surfaces and the real contacting surfaces during experiments. Well-designed normal loading apparatus is required in future studies to eliminate these errors. Some fluctuations of EP2 curve are due to the treatment of removing all possible crushed zones at each approaching step.

The curves of the models with surface deformation show larger curvatures and smaller maximum normal displacements than that of the rigid model. Note that the curve of the rigid model was not obtained directly from the normal loading test but was estimated based on a few assumptions described in Section 2.2 that led to a theoretical value of u_{nmax} , using Bandis' law. In reality, these assumptions will result in overestimation of the u_{nmax} to some extents, since several contacts (i.e., at least three) rather than one are required to stabilize the two contacting surfaces at the initial state when loading has not been applied, and some voids may remain open even after being loaded to very high normal stresses, which contribute to the residual transmissivity. Compression test results reported in literature reveal that u_{nmax} is usually smaller than 300 μm (the end-point of normal displacement used in the calculations of this study, see Fig. 5) for fresh and mated rock fractures, regardless of rock types (e.g., Bandis

et al., 1983; Matsuki et al., 2008). Therefore, $u_{nmax} = 554 \mu\text{m}$ used in the rigid model seems to have highly overestimated the real u_{nmax} . The normal stress-normal displacement curves can be easily obtained through laboratory compression tests on rock fractures, implementation of which is strongly recommended for future fluid flow experiments.

The distributions of local contact stress at the compression stress of 1.38 MPa of the elastic and the elastic-plastic models are shown in Fig. 6. In both models, stresses were concentrated on a major asperity centered at a location around $x = 28 \text{ mm}$ and $y = 4 \text{ mm}$. The maximum local stress of the elastic model was as high as 47769 MPa, almost 5 times larger than the hardness, H , of the rock. This result provided significant evidence for the need for considering plastic deformations on the tips of major asperities. Subjected to Eq. (13), the local stresses were restricted by H in the elastic-plastic models. The reduced stresses from the elements where local stresses were larger than H were redistributed on the contacting elements with lower stresses. This redistribution produced a stress distribution on the major (large) asperity with a flattened top where a large number of elements had stresses close to H for EP1 model (see the middle in Fig. 6). For the EP2 model, due to the overestimated reduction of asperity heights at the crushed elements, the local stresses on the major asperity were greatly diminished, comparing with that of the elastic model and EP1 model, and the stresses were more widely distributed on more contacts.

The evolutions of contact area ratios of the four models along with the increase of normal displacement are shown in Fig. 7. The contact area distributions of the rigid model and the elastic model at the normal displacement of 300 μm and 3-D view of a major asperity are shown in Fig. 8. The contact area ratios at the compression stress of 1.38 MPa are 0.009% (elastic), 0.017% (EP1) and 0.030% (EP2), respectively. Due to the elastic deformation of asperities on fracture surfaces, the real contact area in the fracture is smaller than the geometrical interference area (as predicted by the rigid model, see Fig. 4a) at a given normal stress or displacement. Comparisons of the results of elastic and elastic-plastic models with the result of the rigid model support this argument as demonstrated in Fig. 7. The contact area ratio of EP1 is almost identical with that of EP2, which are both larger than that of the elastic model due to the flattening of asperity tips on the plastically deformed contacts. A steep slope can be identified on the major asperity, where contacts mainly took place along the summits of the slope. Sliding along such slopes may be another important contact mode during normal loading process which has not been taken into account in the current study. More sophisticated models that incorporate both the normal and shear contacts on fracture surfaces are therefore required in the future study to give more accurate estimations on contact stress and possible failures.

4. Implications on Compaction Mechanism of Fast Closure of Fractures

The critical stress of a contacting asperity, below which the pressure solution will not occur, is given by (Revil, 1999):

$$\sigma_c = \frac{E_m(1 - T/T_m)}{4V_m} \quad (20)$$

where V_m is the molar volume of the solid material ($2.27 \times 10^{-5} \text{ m}^3\text{mol}^{-1}$ for quartz), E_m and T_m are the heat and temperature of fusion, respectively ($E_m=8.75 \text{ kJmol}^{-1}$ and $T_m=1883 \text{ K}$). The critical stress was then calculated as 79.7 MPa at $T=20 \text{ }^\circ\text{C}$ for quartz. The dissolution mass flux of pressure solution on contacting asperities was given as (Yasuhara et al., 2006b)

$$\frac{dM_{\text{diss}}^{\text{PS}}}{dt} = \frac{3V_m^2(\sigma_a - \sigma_c)k_+\rho_g A_c}{RT} \quad (21)$$

where t is time, k_+ is the dissolution rate constant of the solid ($k_+=3.09 \times 10^{-13} \text{ molm}^{-2}\text{s}^{-1}$ at $20 \text{ }^\circ\text{C}$), A_c is the contact area of contacting asperity ($A_c=\pi a^2$), and R is the gas constant ($R=8.31 \text{ Jmol}^{-1}\text{k}^{-1}$).

The change of asperity height due to pressure solution during each time step is calculated as

$$dh_i = h_i^n - h_i^{n+1} = \frac{dM_{\text{diss}}^{\text{PS}}}{dt} \frac{\Delta t}{\rho_g A_e} \quad (i = 1, 2, \dots, M) \quad (22)$$

where h_i is the aperture and A_e is the area of an element. This equation doesn't include the dissolution and precipitation taking place on free faces since their contributions to the fracture closure are much smaller than the dissolution on contacts. At each time step, the height of every element on one surface where $\sigma_a > \sigma_c$ was reduced by a value of $1/2 dh_i$ to represent the dissolved part. By doing so, the compression stress calculated by Eq. (11) would become less than 1.38 MPa. The two surfaces were then forced to approach at very small incremental displacement until the compression stress restored to 1.38 MPa. Such cycles proceeded until the elapsed time from the beginning of flow test reached 800 hr, and the aperture change during this process was recorded to calculate the closure rate dh/dt .

Substituting the calculated contact ratio of each model at $\sigma_n = 1.38$ MPa into Eq. (1), the mean local contact stresses for the four models were calculated as 27.6 MPa (rigid), 15498.5 MPa (elastic), 7965.5 MPa (EP1) and 4614.0 MPa (EP2), respectively. Only the mean contact stress of the rigid model was below σ_c . Yasuhara et al. (2006b) had to use much modified values of σ_c ($0.1\sigma_c$) and k_+ ($k_+ \times 10^6$ in the lumped parameter model and $k_+ \times 5 \times 10^6$ in the distributed parameter model) to accommodate the fast closure of fracture in the initial stage of experiment, considering pressure solution as the principal compaction mechanism.

In this study, the original values of all parameters were used for calculation without modification, and the obtained relation between closure rate and time is shown in Fig. 9. The calculated closure rates of EP1 and EP2 are almost identical with an order of 10^{-15} m/s, which are several times smaller than that of the elastic model, due to the much greater contact stresses in the elastic model (see Fig. 6) that would result in faster dissolution on contacts. These results demonstrate a significant impact of mechanical models of rough surface contacts, which will lead to different results for subsequent chemical reaction simulations. Although these models yielded roughly 2 orders of magnitude larger closure rates than that of the rigid model (10^{-17} m/s) reported by Yasuhara and Elsworth (2008), the calculated closure rates were still around 4 orders lower than the experimental results (10^{-11} m/s), revealing that the pressure solution alone might unlikely be the principal fast closure mechanism in the initial stage of fluid flow experiments.

Yasuhara and Elsworth (2008) used a stress corrosion model to accommodate the measured fast closure by assuming that the contacting asperities deform proportionally with the crack velocity. This model, however, would result in unrealistically large closure rates for the elements subjected to large contact stresses (e.g., a stress of 2 GPa would result in a closure rate in the order of 10^4 m/s). This model is therefore inapplicable for the calculation of closure rate of the fracture concerned using contact stresses calculated by the contact mechanics

models presented in this study, in which many elements undergone large contact stresses (see Fig. 6). More accurate description on the relation between crack velocity and closure rate is required before the stress corrosion model could be applied to more common cases with contact stresses of different magnitudes involved.

In addition to chemical degradation, mechanical creep may also play an important role in the fast closure phenomenon. To fully understand its contribution, a creep model that takes into account the time-dependent deformational behavior of elastically and/or elastic-plastically deformed contacting asperities is required. Based on the obtained initial local stress distribution and deformation on rough fracture surfaces, a proper creep model could then be easily incorporated into the contact mechanics models to assess the time-dependent deformational behavior of a fracture. Compression creep tests have revealed that quartzite has a magnitude of creep rate with an order of 10^{-10} strain/s, subjected to compressive stresses with orders of 10^7 to 10^8 Pa (Drescher and Handley, 2003). If we consider the main contacting asperities have sizes with orders of 10^{-4} to 10^{-3} m as commonly observed on fracture surfaces (Fig. 8), the stress calculated by the rigid model (27.6 MPa) will lead to a closure rate of the fracture with orders of 10^{-14} to 10^{-13} m/s due to creep. Since the creep rate increases proportionally with increasing compressive stress (Brantut et al., 2013), the elastic and elastic-plastic models that produced stresses 2-3 orders greater than the rigid

model may have a good chance to gain a closure rate that is close to that of the experimental measurement (10^{-11} m/s). However, most creep models in literature were proposed for macroscopic intact rocks, which cannot reflect the creep behavior of microscopic contacting asperities of irregular shapes under wet conditions, especially when crushed zones exist in the contacts. A new creep model is under development starting with the long-term loading tests on single hemispherical rock specimens combined with X-ray CT measurements of cracking processes inside.

As demonstrated in Fig. 6, significantly concentrated stresses were predicted to be distributed on the contacts of a few major asperities. We identified a rectangular area on the fracture surface in a region with the range on x axis from 24 mm to 34 mm and on y axis from 0 mm to 10 mm, serving as the initial contact area during the initial normal loading (see the rectangular defined by dash lines and the 3-D view in Fig. 8). At the compression stress of 1.38 MPa, the mean contact stresses in this rectangular area were 17535.9 MPa (elastic), 8892.7 MPa (EP1) and 4659.7 MPa (EP2), respectively, much larger than the mean contact stresses over the whole fracture sample surfaces.

The results indicate that the term “stress concentration” in the contact problem of rough surfaces have two implications: Firstly, since contact stresses can only occur in the contact areas, the mean stress on contact areas should equal to the normal compression stress divided

by the contact area ratio, c (i.e., Eq. (1)), resulting in a stress concentration from the normal compression stress to the mean stress on the contacts (i.e., mean contact stress). Secondly, among all the contacts, the contacts of major asperities may have higher and more concentrated contact stresses than those on other contacts (i.e., unevenly distributed local contact stresses). The rigid contact model and its mean contact stress as adopted in previous studies, generally overestimated the contact area and underestimated the local contact stresses, especially on the major asperities, thereby resulting in underestimated chemical reaction rates on contacting asperities.

At the compression stress of 1.38 MPa, the ratio of the accumulated contact areas, on which the local stresses are larger than H , to the total contact areas were predicted as 60.1% (elastic), 22.3% (EP1) and 7.8% (EP2), respectively. The results indicate that considerably large portions of the contact areas have reached the critical stress for the onset of plastic deformation. Since the elastic model did not take into account the plastic deformation at all, and EP2 model overestimated the geometry changes caused by plastic deformation, the more realistic plastic deformation was likely to be the one bounded by these two models, e.g., the results of or close to that of the EP1 model. Further studies by carrying out compression tests on rock fractures with measured surfaces before and after tests are required in the future to establish more accurate plastic deformation models.

The evolutions of crushed volumes (zone of plasticity) of asperity tips of the EP1 and EP2 models, calculated by using Eq. (16) and Eq. (19) respectively, are shown in Fig. 10. EP1 model exhibited a smooth and progressive increase of the crushed volume along with the increase of normal displacement. In the EP2 model, the diminished volume of surface geometry was a function of the local stresses at surface elements of the contacting asperities, resulting in undulation in the magnitude of crushed volume at each incremental normal displacement. The accumulated crushed volumes for the models of EP1 and EP2 are $6.4 \times 10^6 \mu\text{m}^3$ and $6.0 \times 10^7 \mu\text{m}^3$ respectively, at the compression stress of 1.38 MPa. In reality, these crushed zones are composed of merely the assemblies of pieces and grains of mineral gouges caused by breakage of asperity tips, with low strength and high deformability, porosity and transmissivity, thus providing abundant specific surface areas for water-rock reactions of transport. If these crushed zones were completely removed during loading, such as in the model EP2, an excessive normal closure of 44 μm (see Fig. 5) was required to reach the compression stress of 1.38 MPa, by comparing the elastic and EP2 models. This process is analogous to the continuous removal of minerals by dissolution and fluid advection, resulting in the increase of contact areas and decrease of aperture under a constant normal stress. Dissolution of the crushed zones is therefore highly possible to be one of the main mechanisms that drive the fast closure of fractures in the initial stage of fluid flow

experiments. More sophisticated models are, however, required to clarify the failure mechanisms of asperity tips during initial normal loading and the subsequent mechanical creep behavior, and their influences on the total fracture closure in future studies.

5. Concluding Remarks

This study investigated the local contact stresses and contact area distributions during initial normal loading process of a rough rock fracture, before fluid flow tests, using 3-D numerical models of four different contact mechanics models, and predicted their influences on the initial fast fracture closures that occur in coupled stress-flow-transport experiments. The elastic contact model of a rough fracture was rigorously derived based on the variational principle. Two simplified elastic-plastic contact models considering contacting asperity geometry changes induced by crushing of asperity tips were developed to represent the influences of plastic deformations. Earlier experiments and models in Yasuhara and Elsworth (2006b) and Yasuhara and Elsworth (2008) were used as the physical and mathematical start points, with focus of investigation on the effects of initial normal loading on the experimentally often observed fast closure of fractures during fluid flow tests. The models developed in the previous literature often assumed the rough fracture surfaces as two rigid surfaces, where the geometrical interference area was adopted as the contact area. The results

thus led to overestimated contact area and underestimated mean stress over real contact areas. In elastic and elastic-plastic models, the results were more consistent with theoretical understanding of contact mechanics of rough surfaces with significant effects of asperity unstationarity caused by dominating effects of a few major asperities, revealing a roughly 2 orders of magnitude larger mean contact stress than that predicted by the rigid model for this study.

On the other hand, with these higher concentrated stresses of deformable asperity models, however, the predicted closure rates of the fracture by pressure solution are still several orders of magnitude lower than the experimental measurements at the initial stage of fluid flow test. This finding indicates that although pressure solution actively takes place on most contacting asperities and it provides well-fitted predictions to the experimental results later than the fast closure stage (Yasuhara et al., 2006a,b), it alone may not likely to be the principal compaction mechanism for this fast closure phenomena.

The calculated results also demonstrate that the local stresses are not evenly distributed but concentrate on the contacts of a few major asperities, when unstationary fracture topography are present. These major asperities have larger heights and slopes compared with the average values of the sample, so that they may come into contact in the early periods of normal loading, and bear most portion of the normal loads acting on the fracture samples. These

concentrated stresses can reach the yielding strength or hardness of the rocks concerned, triggering mechanical failures at the tips of contacting asperities, generating gouge materials, resulting in the increase of contact area and decrease of contact stresses. The calculated results of the elastic-plastic models demonstrated the plastic deformations taking place on the tips of major asperities, which served as a theoretical explanation for the flattened asperity tips observed in SEM images (Brown and Scholz, 1986; Yasuhara et al., 2011). The development of crushed zones on major asperities makes the fracture more deformable, and increases the area of interfaces (cracks) where chemical processes (e.g., dissolution and sub-critical cracking) could take place more actively, thus facilitating subsequent fracture closure. Our models can be further extended to include fluid flow, and to incorporate with more sophisticated compaction and creep models that take into account the mechanical and chemical properties of crushed zones to fully accommodate the fast closure phenomena on rock fractures in the future.

A number of difficulties were encountered during the 3-D numerical modeling of contact of fractures. Significant ones include the assumptions of the initial contact state before loading and the strict normal approaching of opposing potential contact surfaces without rotation or inclination strictly due to unavoidable numerical artifacts, similar to the unavoidable relocation error of contact of rough surfaces during laboratory experiments. For the

continuation of this study, normal loading tests on rock fractures will be designed and conducted on cubic fracture samples confined within rigid loading boxes in order to reduce significantly, if not completely, these errors. Pre- and post- experimental measurements of fracture surfaces combined with CT imaging of the crushed zones on major asperities will be implemented, aiming to quantitatively investigate the failure mechanism on asperities and to help build up more realistic and accurate contact mechanics models of rough rock fractures.

Acknowledgements

This study was partially funded by Grant-in-Aid for Young Scientists (B) (No. 24760690), Japan and National Natural Science Foundation of China (No.51379117). The authors like to thank Dr. Hideaki Yasuhara in Ehime University, Japan for providing the laser scanned surface topography data of the rock fracture sample that was used in this study.

Reference

- Ameli P, Elkhoury JE, Morris JP, Detwiler RL. Fracture permeability alteration due to chemical and mechanical processes: a coupled high-resolution model. *Rock Mech Rock Eng* 2014;47:1563-1573.
- Bandis SC, Lumsden AC, Barton NR. Fundamentals of rock joint deformation. *Int J Rock*

Mech Min Sci Geomech Abstr 1983;20:249-268.

Bhushan B. Contact mechanics of rough surfaces in tribology: multiple asperity contact.

Tribol Lett 1998;4:1-35.

Brantut N, Heap MJ, Meredith PG, Baud P. Time-dependent cracking and brittle creep in crustal rocks: A review. J Struct Geol 2013;52:17-43.

Brown SR, Scholz CH. Closure of random elastic surfaces in contact. J Geophys Res 1985;90:5531-5545.

Brown SR, Scholz CH. The closure of rock joints. J Geophys Res 1986;91:4939-4948.

Chiu YP. On the stress field due to initial strains in a cuboid surrounded by an infinite elastic space. J Appl Mech 1977;44:587-590.

Chiu YP. On the stress field and surface deformation in a half-space with a cuboidal zone in which initial strains are uniform. J Appl Mech 1978;45:302-306.

Derjaguin BV, Muller VM, Toporov YP. Effect of contact deformations on the adhesion of particles. J Colloid Interface Sci 1975;53(2):314-326.

Drescher K, Handley MF. Aspects of time-dependent deformation in hard rock at great depth. J. S. Afr. Inst. Min. Metall 2003;103(5):325-335.

Evans B. The effect of temperature and impurity content on indentation hardness of quartz. J Geophys Res 1984;89:4213-4222.

Hertz H. On the contact of elastic solids. *J Reine und Angewandte Mathematik* 1882;92:156-171.

Greenwood JA, Williamson JBP. Contact of nominally flat surfaces. *Proc R Soc Lond* 1966;A 295:300–319.

Jacq C, Nelias D, Lormand G, Girodin D. Development of a three-dimensional semi-analytical elastic-plastic contact code. *J Tribol* 2002;124:653-667.

Johnson KL. *Contact mechanics*, Cambridge University Press 1985.

Johnson KL, Kendall K, Roberts AD. Surface energy and the contact of elastic solids. *Proc R Soc London* 1971;A324:301-313.

Li B, Jiang Y, Koyama T, Jing L, Tanabashi Y. Experimental study of the hydro-mechanical behavior of rock joints using a parallel-plate model containing contact areas and artificial fractures. *Int J Rock Mech Min Sci* 2008;45:362-375.

Matsuki K, Wang EQ, Giwelli AA, Sakaguchi K. Estimation of closure of a fracture under normal stress based on aperture data. *Int J Rock Mech Min Sci* 2008;45:194-209.

McGuire T, Elsworth D, Karcz Z. Experimental measurements of stress and chemical controls on the evolution of fracture permeability. *Transport Porous Med* 2013;98:15-34.

Olsson R, Barton N. An improved model for hydromechanical coupling during shearing of rock joints. *Int J Rock Mech Min Sci* 2001;38:317-329.

- Persson BNJ. Contact mechanics for randomly rough surfaces. *Sur Sci Rep* 2006;61:201-227.
- Revil A. Pervasive pressure-solution transfer: A poro-visco-plastic model. *Geophys Res Lett* 1999;26:255-258.
- Polak A, Elsworth D, Yasuhara H, Grader AS, Halleck PM. Permeability reduction of a natural fracture under net dissolution by hydrothermal fluids. *Geophys Res Lett* 2003;30:2020.
- Polak A, Elsworth D, Liu J, Grader AS. Spontaneous switching of permeability changes in a limestone fracture with net dissolution. *Water Resour Res* 2004;40:W03502.
- Pyrak-Nolte LJ, Morris JP. Single rock fractures under normal stress: the relation between fracture specific stiffness and fluid flow, *Int J Rock Mech Min Sci* 2000;37:245-262.
- Shah KR, Wong TF. Fracturing at contact surfaces subjected to normal and tangential loads. *Int J Rock Mech Min Sci* 1997;34:727-739.
- Tian X, Bhushan B. A numerical three-dimensional model for the contact of rough surfaces by variational principle. *J Tribol* 1996;118:33-42.
- Wang F, Keer LM. Numerical simulation for three dimensional elastic-plastic contact with hardening behavior. *J Tribol* 2005;127:494-502.
- Wang ZJ, Wang WZ, Hu YZ, Wang H. A numerical elastic-plastic contact model for rough surfaces. *Tribol Trans* 2010;53:224-238.

- Xiong X, Li B, Jiang Y, Koyama T, Zhang C. Experimental and numerical study of the geometrical and hydraulic characteristics of a single rock fracture during shear. *Int J Rock Mech Min Sci* 2011;48:1292-1302.
- Yasuhara H, Elsworth D, Polak A. A mechanistic model for compaction of granular aggregates moderated by pressure solution. *J Geophys Res* 2003;108:2530.
- Yasuhara H, Elsworth D, Polak A. Evolution of permeability in a natural fracture: significant role of pressure solution. *J Geophys Res* 2004;109:B03204.
- Yasuhara H, Polak A, Mitani Y, Grader AS, Halleck PM, Elsworth D. Evolution of fracture permeability through fluid-rock reaction under hydrothermal conditions. *Earth Planet Sci Lett* 2006a;244:186-200.
- Yasuhara H, Elsworth D. A numerical model simulating reactive transport and evolution of fracture permeability. *Int J Numer Anal Meth Geomech* 2006b;30:1039-1062.
- Yasuhara H, Elsworth D. Compaction of a rock fracture moderated by competing roles of stress corrosion and pressure solution. *Pure Appl Geophys* 2008;165:1289-1306.
- Yasuhara H, Kinoshita N, Ohfuji H, Lee DS, Nakashima S, Kishida K. Temporal alteration of fracture permeability in granite under hydrothermal conditions and its interpretation by coupled chemo-mechanical model. *Appl Geochem* 2011;26: 2074-2088.
- Yoshioka N, Scholz CH. Elastic properties of contacting surfaces under normal and shear

loads: Theory. J Geophys Res 1989a;94:17681-17690.

Yoshioka N, Scholz CH. Elastic properties of contacting surfaces under normal and shear

loads: Comparison of theory with experiment. J Geophys Res 1989b;94:17691-17700.

Yoshioka N. Elastic behavior of contacting surfaces under normal loads: A computer

simulation using three-dimensional surface topographies. J Geophys Res 1994a;99:

15549-15560.

Yoshioka N. The role of plastic deformation in normal loading and unloading cycles. J

Geophys Res 1994b;99:15561-15568.

Zimmerman RW, Bodvarsson GS. Hydraulic conductivity of rock fractures. Transport Porous

Med 1996;23:1-30.

Zhang Y, Zhang W, Yang C. FEM analysis for influences of stress corrosion and pressure

solution on THM coupling in dual-porosity rock mass. Sci China Tech Sci 2011;7:

1748-1756.

Fig. 1 View of one surface of the tested fracture in Yasuhara et al. (2006a).

Fig. 2 Evolution of measured hydraulic aperture with time. A fast closure of fracture can be observed at the first 858 hours of test at a constant temperature of 20 °C (Yasuhara et al. 2006a).

Fig. 3 Relation of normal stress and normal displacement based on the rigid model. The effective confining stress applied on the fracture during flow-through test is 1.38 MPa.

Fig. 4 Schematic view of a typical contact of asperities on fracture surfaces. (a) Cross-sectional view of deformation on contacted asperities; (b) deformation of a Hertzian contact.

Fig. 5 Calculated normal stress-normal displacement curves by the models of elastic, EP1, EP2 and rigid.

Fig. 6 3-D local contact stress distributions calculated by the models of elastic (upper), EP1 (middle) and EP2 (bottom) at the compression stress of 1.38 MPa.

Fig. 7 Evolutions of calculated contact area ratios with the increase of normal displacement.

Fig. 8 Distributions of contact areas of the rigid model (upper) and the elastic model (middle) at normal displacement of 300 μm and the 3-D surface view of the major asperity that come into contact at first during normal loading (bottom). The distributions of other two models are close to that of the elastic model. The rectangular in dash line marks the position of the major asperity.

Fig. 9 Comparisons of the closure rate at the first 800 hr of flow test between the measured results (Yasuhara et al., 2006a) and the calculated results of three models. To fit the view, multipliers of 10^{11} and 10^{15} were applied to the values of experimental measurement and calculations, respectively.

Fig. 10 Evolutions of crushed volumes of asperity tips calculated by models EP1 and EP2.