Hydro-mechanical analysis of fractured media using discontinuous deformation analysis

Choo, Ling Qian

2017

Choo, L. Q. (2017). Hydro-mechanical analysis of fractured media using discontinuous deformation analysis. Doctoral thesis, Nanyang Technological University, Singapore.

<http://hdl.handle.net/10356/69936>

<https://doi.org/10.32657/10356/69936>

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

**HYDRO-MECHANICAL ANALYSIS OF
FRACTURED MEDIA USING DISCONTINUOUS
DEFORMATION ANALYSIS**

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**SCHOOL OF CIVIL AND ENVIRONMENTAL
ENGINEERING**

2017

HYDRO-MECHANICAL ANALYSIS OF FRACTURED MEDIA USING DISCONTINUOUS DEFORMATION ANALYSIS

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A thesis submitted to the Nanyang Technological University
in partial fulfilment of the requirement for the degree of
Doctor of Philosophy

2017

ACKNOWLEDGEMENTS

First and foremost, I would like to express my sincere gratitude towards my supervisor, Assoc. Prof. Zhao Zhiye whose persistent guidance, motivation, and knowledge have contributed profoundly to my research journey. I have benefited immensely from his constructive advice and mentorship. It is indeed a great pleasure to be one of Prof Zhao's students.

I would also like to thank the members of my thesis review committee for their time and dedication spent in reviewing and evaluating my thesis. My sincere thanks also goes to Nanyang Technological University for the financial support, and all the members of the DDA research group, especially Dr. Tian Qian and Dr. Chen Huimei, for their guidance and assistance.

Last but not least, I would like to thank my family – my parents Mr. Choo Eng Siew and Mdm. Wong Kwan Cheung, my husband Mr. Yeap Leong Hooi, and my sisters Ms. Choo Yi Qian and Ms. Choo Seow Qian. Their continued support, understanding and care have contributed to the timely completion of this thesis.

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ABSTRACT

It is well-established that pore pressure built up in discontinuities has a profound effect on the mechanical behaviors of the jointed rock masses. The discontinuous deformation analysis (DDA) is a discontinuum theory which can account for the interactions between pore pressure and rock mechanics. It is also a numerical method or computer program commonly applied to hydro-geomechanical modeling. Research and development of DDA hydro-mechanical model has been thriving over the last two decades. The main objective of this research study is to further contribute to those efforts. Specifically, the following works have been conducted to achieve this objective: (i) a seepage analysis extension is proposed to the DDA method for the modeling of seepage flow within jointed rock masses; (ii) to improve the computational efficiency of the extension in simulating quasi-static hydro-mechanical problems, a new solution scheme featuring a constant hydraulic aperture is introduced; (iii) a stochastic flow modeling extension is proposed to the DDA method for the simulation of heterogeneous hydraulic conductivity and aperture fields; (iv) a hydraulic crack initiation-propagation extension complete with a coupled hydro-mechanical analysis algorithm is introduced to the hybrid DDA-FEM model for the simulation of hydraulic fracturing problems. To investigate the reliability, efficiency and limitation of the proposed DDA extensions, a series of numerical examples are presented and discussed. The capability of the new DDA extensions in modeling realistic engineering problems are also verified through meaningful case studies.

LIST OF PUBLICATIONS

Journal Paper

1. Choo, L. Q., Zhao, Z., Chen, H., & Tian, Q. (2016). Hydraulic fracturing modeling using the discontinuous deformation analysis (DDA) method. *Computers and Geotechnics*, 76, 12-22. doi:<http://dx.doi.org/10.1016/j.compgeo.2016.02.011>
2. Choo, L. Q., Zhao, Z. Y., Chen, H. M. (Under review). Modelling the stochastic flow behaviours of geological formations using the discontinuous deformation analysis method. *Engineering Geology*.
3. Chen, H. M., Zhao, Z. Y., Choo, L. Q., & Sun, J. P. (2016). Rock Cavern Stability Analysis Under Different Hydro-Geological Conditions Using the Coupled Hydro-Mechanical Model. *Rock Mechanics and Rock Engineering*, 49(2), 555-572. doi:10.1007/s00603-015-0748-4

Conference Paper

1. Choo, L. Q., Zhao, Z. Y., Chen, H. M. (2014). *Hydro-Mechanical Analysis of Fluid Flow through Heterogeneous Conductivity Fields by Discontinuous Deformation Analysis*. Paper presented at the 14th World Conference of Associated research Centers for the Urban Underground Space, South Korea, Seoul.
2. Chen, H. M., Zhao, Z. Y., Choo, L. Q., & Sun, J. P. (2013). Stability analysis of rock caverns under different in-situ stress using the DDA based hydro-mechanical coupled model *Frontiers of Discontinuous Numerical Methods and Practical Simulations in Engineering and Disaster Prevention* (pp. 237-242): CRC Press.

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Chapter 1. Introduction

1.1 Chapter overview

The flow of this introductory chapter is as illustrated in Figure 1.1. Firstly, Section 1.2 highlights the significance of rock mechanics and discusses the role of numerical methods in approaching a rock engineering problem. In Section 1.3, the importance of coupled hydro-mechanical modeling is identified. The feasibility and efficiency of various commonly used numerical methods in capturing the hydro-mechanical behaviors of fractured rock masses are also compared. Section 1.4 highlights the advantages and limitations of the discontinuous deformation analysis (DDA) method in hydro-geomechanical modeling. Research works performed in the current study to overcome these limitations are outlined in Section 1.5. Lastly, Section 1.6 provides the flow through which the research works are presented in the current thesis.

Research Background	The role of DDA	Research overview
<ul style="list-style-type: none">• Numerical modeling of geological problems• Modeling of hydro-mechanical behaviours	<ul style="list-style-type: none">• Hydro-mechanical modeling using DDA• Limitations of DDA hydro-mechanical models	<ul style="list-style-type: none">• Objectives• Scope• Organization

Figure 1.1 An outline of Chapter 1

1.2 Numerical modeling of geological problems

Rock mechanics is classified as a branch of mechanics concerning the mechanical behaviors of rock and rock masses in geological formations (National Research Council 1966, U.S. National Committee for Rock Mechanics 1981). Understanding the fundamental behaviors of rock masses is essential in the design and construction of rock engineering projects such as tunnels, caverns, dams, and underground storage facilities. Examples of rock mechanics applications in rock engineering projects include: (i) stability evaluation of excavations and the surrounding structures, (ii) feasibility studies of construction plans and (iii) forecast and mitigation of geologic hazards such as landslide and rock falls at a construction site (Hoek and Brown 1980).

As a natural geological material, rock masses are characterized by complex DIANE (i.e. discontinuous, inhomogeneous, anisotropic and non-elastic) features (Harrison et al. 2002). A rock mass is also a fractured, porous medium containing fluids or gas in part of the fractures and cavities. To add to these complexities, the force field of a geological setting is constantly changing due to the Earth's crustal motions resulted from the gravity field and the plate tectonic activities such as earthquakes, volcanisms, and mantle convection underneath the earth crust (Condie 2013). All these features of rock masses contribute to considerable nonlinearities in their mechanical behaviors, thus closed-form mathematical solutions hardly exist for rock engineering problems. It follows that numerical models emerge as an important tool to assess the mechanics of rock engineering structures (Jing and Stephansson 2007).

To date, numerical modeling, serving as an ersatz form of laboratory and field studies, has evolved into an essential element of engineering design and analysis (Starfield and Cundall 1988). Through numerical simulations, the mechanical behaviors and failure conditions of a geological structure can be reasonably predicted, and the analysis outputs could assist in the devising of suitable solutions for a geological problem. According to Jing and Stephansson (2007), a numerical model does not have to be extensive or over-refined, but it has to be adequate to define the problem and serve its engineering purposes. Hence, the foremost challenge of numerical

modeling lies in understanding the problem at hand and developing a suitable model to represent the problem.

1.3 Modeling the hydro-mechanical behaviors of geological formations

An important feature of rock masses is that they contain discontinuities such as faults, joints, bedding planes, foliations and blasting-induced cracks between intact rock matrixes. Discontinuities with irregular dimensions and orientations partition a rock mass into numerous rock matrixes of varying configurations and physical properties. Pressurized fluid is frequently present in these discontinuities, thus affecting the force field of the fractured rock mass, and contributing to its non-linear mechanical behaviors (Jaeger et al. 2009, Noorian Bidgoli and Jing 2014). To study the constitutive relation between fluid flow and rock motion is a challenging task due to these material nonlinearities. The challenge is especially acute for large-scale problems involving a complicated discontinuity network. Besides, the need to include the time effect in a hydro-geomechanical study adds to this difficulty (Jing and Stephansson 2007). From the outset, two distinct and inter-related problems need to be solved: (i) the fluid flow across the problem domain, and (ii) the mechanical responses of rock matrixes towards fluid flow.

For most geological settings, numerical modeling is frequently the only means to assess the complex hydro-mechanical processes due to the following reasons. First, site measurements are time-consuming, expensive and difficult to carry out (Starfield and Cundall 1988). Secondly, small-scale laboratory studies are often not adequate to represent large-scale hydrogeological conditions. Paradoxically, it is hard to monitor a large-scale site or laboratory study over an extended time span. On the other hand, closed-form analytical solutions hardly exist for hydro-geological problems involving a complex discontinuity system (Jing and Stephansson 2007). To account for these uncertainty-laden problems, numerical modeling appears to be the last resort.

As far as rock engineering design is concerned, an effective hydro-geomechanical model should be capable of: (i) characterizing the permeability of a geological formation, (ii) predicting the mechanical stability of a rock engineering facility, and (iii) forecasting fluid flow rate, velocities and the corresponding structural deformations over different time scales (David and Le Ravalec-Dupin 2007). To cater the needs of varying material behavioral and continuity assumptions, different numerical methods have been developed. There are two main categories of numerical methods for hydro-geomechanical modeling, namely the continuum and the discontinuum methods. A brief review of the respective methods is presented in the following sections.

1.3.1 Hydro-mechanical modeling using the continuum methods

The most commonly applied continuum methods are the finite element method (FEM), finite difference method (FDM), and the boundary element method (BEM) (Jing 2003). In these approaches, problem domains are assumed to be continuous throughout the mechanical deformation, fluid flow and other physical processes occurring within a pre-defined time span. The simulation of fractured rock behaviors using the framework of continuum method is made possible in the 1960s, when Goodman (1976) introduced a special linkage element to the FEM model. These linkage elements are assigned with zero to small thickness, and are inserted at the interfaces between normal elements. The change in the thickness of the linkage elements enables deformation mechanisms such as separation, slip and rotations of rock blocks to be simulated. However, to ensure the displacement compatibility of the continuous system, large-scale displacement and complete detachment of individual element are not allowed. Moreover, since the solution scheme involves complicated calculation steps such as high-order matrix inversion, adding excessive linkage elements may render the problem ill-posed and cause severe computational instability (Jing and Stephansson 2007).

When modeling a discontinuous system such as a fractured rock mass using the continuum methods, the underlying assumption is that the rock mass behaves as an

equivalent continuum at a macroscopic scale. This “macroscopic scale” must be at least the size of a critical threshold called the REV (representative elementary volume). For this assumed continua, equivalent material properties need to be derived through a homogenization process, to represent the constitutive behaviors of the rock matrixes and fractures across the REV. Herein, the REV defines the minimum volume over which the constitutive properties can be defined to yield representative parameters to a discontinuous system. Continuum methods such as the FEM can only be applied to a discontinuous problem if such representative volume and parameters can be established over the discontinua (Jamtveit and Yardley 2012). However, for rock mass containing highly complex discontinuities, the homogenization process may be overly time consuming and the REV may not exist (Jing and Stephansson 2007).

The limitations highlighted in the preceding paragraphs imply that the continuum-based methods are not suitable for the simulation of problems involving many fractures and large deformations. Modeling a fractured rock mass of these natures using a continuum approach may lead to numerical instability or computational inefficiency. Even with the introduction of special algorithms to treat the discontinuities, rock fracture behaviors and fracturing mechanisms still cannot be handled efficiently by the continuum approaches (Cundall 2001).

1.3.2 Hydro-mechanical modeling using the discontinuum methods

Problems concerning the mechanical behaviors of fractured rock masses are best simulated using the discontinuum framework of analysis such as the distinct element methods and discontinuous deformation analysis (DDA) method (Cundall 2001, Jing 2003). The discontinuum methods, also known as the discrete element methods (DEM), treat a fractured rock mass as an assemblage of discrete blocks. Each block can move or rotate independently, detach from the neighboring blocks or form new contacts with other blocks. This provides a more straightforward and realistic representation of a fractured rock mass compared to the continuum model. In general,

the solution scheme of the DEM comprises the following distinctive components that distinguish it from the continuum methods (Jing and Stephansson 2007).

1. A problem domain discretization algorithm to identify the physical details of blocks (i.e. the block configurations, arrangement and connectivity) within the problem domain based on a pre-defined discontinuity system.
2. A mathematic algorithm that accounts for the kinematics mechanisms of individual blocks.
3. A contact detection and updating algorithm.

Numerous in-house programming codes and commercial software for discontinuous modeling have been developed over the past few decades, with the most widely used for geotechnical modeling being UDEC, 3DEC, DDA and PFC (Lu 2003). These discontinuum approaches are capable of modeling geotechnical problems concerning fluid flow, with one common limitation: the maximum number of particles in a simulation model and the duration of simulation is often limited by the computational power and memory (Zhao et al. 2012). Nevertheless, DEM have proven to be an effective tool for: (i) the hydro-mechanical modeling of rock engineering structures containing a large number of discontinuities (Kim et al. 1999, Chen 2013, Chen et al. 2015b); (ii) the modeling of stress-fluid flow interactions in near-field problems (Jing et al. 1996); and (iii) the establishment of REV and equivalent hydro-mechanical properties for fractured rock models (Jing et al. 1996, Min and Jing 2003, Min et al. 2004).

Assembly of discrete blocks in a discontinuum model resembles the topology of an actual rock mass, hence enabling a hydro-geomechanical problem to be modeled directly with the use of simple constitutive equations (Cundall 2001). Even though the DEM are more computationally expensive than their continuum-based counterparts such as the FEM – mainly due to the intensive contact analyses required for the discrete blocks – the general belief is that the expeditious development in the

computational technology will make the speed gap between the two approaches less significant over the years (Cundall 2001, Khan 2010).

1.4 DDA and Hydro-mechanical modeling

The discontinuous deformation analysis (DDA) method originated by Shi and Goodman (1985) and further developed by Shi (1988) is an implicit DEM commonly used in rock mechanical modeling. Contrary to the explicit DEM which relies on the block relaxation method and the minimization of out-of-balance force/ moment technique to account for the block motions, DDA adopts an implicit time marching scheme which involves the assembly and solving of a global equilibrium matrix to model block kinematics and deformations. The advantages associated with the implicit scheme over the explicit solution includes: larger time step may be used, large-scale block deformation and movement are allowed within each time step, and the equilibrium condition of the discrete block system is automatically guaranteed at each time step.

Compared to other discontinuum approaches such as the distinct element method, DDA is a relatively new approach for discontinuum mechanics analysis. Many extensions and improvements have been proposed to the DDA code over the last few decades, contributing to the advancement of the code in terms of efficiency and functionality. Major efforts to implement and enhance the hydro-mechanical modeling function in DDA can be found in Kim et al. (1999), Jing et al. (2001), Rouainia et al. (2006a), and Koyama et al. (2011). Key contributions of these literatures to the DDA code development will be reviewed in the following chapter.

Although the concept of coupling the DDA with fluid flow has been proposed for decades and numerous enhancements have been introduced ever since, there are still many areas that need to be further improved or developed. For example, the uniform hydrogeological property fields assumed in the DDA model is over-idealized and unrealistic. A homogeneous aperture or hydraulic conductivity field does not exist in reality. In addition, an equivalent parameter is only valid if the REV can be

established over a problem domain, and its value should be carefully determined through a complicated homogenization process (Ababou et al. 1994, Renard and De Marsily 1997, Lewandowska and Laurent 2001, Szymkiewicz 2005). A more straightforward approach to represent a heterogeneous property field is by using the stochastic model. The stochastic model is a useful way of predicting the variation of a hydraulic property in porous media (Bakr et al. 1978b, Neuman 1982, Gelhar 1986, Neuman 1988). It treats the uncertainties in the parametric distribution with a probabilistic technique. Using a stochastic model to simulate the flow conditions of an aquifer is not new in the discipline of hydrology engineering, but this approach has yet to be introduced to most geological modeling codes including the DDA.

Another aspect of the DDA method which is in need of further development is the hydraulic fracturing modeling function. The applications of DDA in simulating hydraulic fracturing mechanisms were demonstrated in Ben et al. (2012), Ben et al. (2013a), and Jiao et al. (2015). These studies proposed the assignation of strong bonds between discrete blocks to simulate an intact rock mass. The breakage of any of these bonds upon the satisfaction of a pre-defined fracture criterion signifies crack formation. Such approach allows the crack initiation and propagation processes to be simulated directly using the DDA method. However, for the pseudo-continuous model to exhibit a practical degree of deformability, the usage of a large number of DDA blocks is inevitable. This became a major drawback of this approach as it gives rise to intensive contact analyses and high computational cost.

1.5 Thesis objective and scope

The main objective of this thesis is to extend and improve the DDA hydro-mechanical model in rock engineering applications. Specifically, the following works have been conducted to achieve the stated objective.

- Recent developments of DDA concerning the hydro-mechanical modeling are reviewed.

- A seepage analysis extension is proposed to the DDA method. The formulation and workflow of the proposed extension are meticulously explained.
- A new solution scheme termed the semi-coupled scheme is introduced to save computational cost. The new scheme adopts a slightly different framework from the coupled and the non-coupled schemes which are commonly applied to the DDA hydro-mechanical analyses.
- A stochastic flow modeling extension is proposed to the DDA method to enable the simulation of heterogeneous hydraulic conductivity and aperture fields. With this, the effects of stochastic flow conditions on rock mechanics can be considered in the DDA hydro-mechanical analysis.
- A hydraulic crack initiation-propagation extension complete with a coupled hydro-mechanical analysis algorithm is introduced to a hybrid DDA-FEM model for the simulation of hydraulic fracturing problems.
- Meaningful numerical studies are performed to verify the capability of each proposed DDA extension in modeling realistic engineering problems. For instance, a wellbore model is utilized to simulate hydraulic fracturing mechanisms in rock engineering structure, while a brick tunnel model is adopted to assess the influences of stochastic flow conditions on different hydro-structural behaviors.

1.6 Thesis organization

This thesis consists of six chapters. The thesis structure is summarized in Figure 1.2 and the highlights of each chapter are presented below.

This introductory chapter provides the theoretical background, objectives and scope of the current research study, and outlines the sequence through which the research works are presented in this thesis.

In Chapter 2, firstly, the basic concepts and theories concerning the DDA hydro-mechanical modeling are reviewed. Then, a review on the recent developments of DDA hydro-mechanical models is provided.

Chapter 3 presents the DDA seepage analysis extension employed in the current study, and discusses different solution schemes commonly adopted in the DDA hydraulic analyses. A slightly different approach, which requires less computational time for each hydraulic analysis iteration, is proposed.

Next, a stochastic flow model is introduced to simulate the heterogeneous hydraulic conductivity and aperture profiles of a flow domain. The theoretical groundings and the mathematical formulations of the stochastic model are provided in Chapter 4. Numerical examples are also presented to verify the capability of the proposed stochastic model in generating plausible stochastic fields, and to investigate how a heterogeneous flow condition may affect the hydro-mechanical behaviors of porous and fractured media.

In Chapter 5, a hydraulic crack initiation-propagation extension is introduced to a hybrid DDA-FEM model for the simulation of hydraulic fracturing problems. A practical numerical study is presented alongside the theoretical background and workflow of the modeling algorithm to substantiate the proposed DDA-based hydraulic fracturing model.

The thesis ends with Chapter 6 which summarizes the contents of the previous chapters, discusses the engineering applications of the current research, and identifies research limitations as well as possible areas of future research.

Figure 1.2 An overview of thesis structure

Chapter 2. A review of DDA hydro-mechanical models

2.1 Chapter overview

The purpose of this chapter is to provide an overview to the theoretical framework, formulation and development of the DDA method. As shown in Figure 2.1, the chapter is divided into two main parts. Firstly, in Section 2.2, the mathematical formulations of the DDA displacement and contact models are introduced. The workflow of the DDA kinematics analysis is also explained.

Efforts to extend the DDA method for hydro-geomechanical analysis have been fruitful in recent years. Major studies concerning this research area are explored in Section 2.3. Comparisons are made between various hydro-geomechanical modeling techniques introduced to the DDA method over the last decade. New developments, findings and applications of the DDA hydro-mechanical models are also discussed.

Figure 2.1 An outline of Chapter 2

2.2 Modeling blocky rock masses using DDA

The DDA method was first introduced in Shi and Goodman (1985) as a back-analysis algorithm to determine a best fit to the deformed configuration of a block system from the empirical displacement and deformation data. The work was later developed into a complete deformation analysis algorithm for blocky systems (Shi and Goodman 1988).

The DDA is similar to the distinct element methods (DEM) such as the UDEC (Itasca Consulting Group 2014) in terms of block-fracture system configuration and treatment of inter-block contacts. However, the solution strategies adopted by the two methods are fundamentally different. The DEM solves the local equations of motion using an explicit time marching scheme and no matrix solver is needed. On the contrary, the implicit solution scheme adopted by the DDA model requires the assembly and solving of a large-scale matrix analogous to the global equilibrium equation of the blocky system. First, the energy minimization principle is used to derive the equations of motion for individual blocks. The local equations of motion are subsequently assembled into the global matrix. The deformation variables in the global matrix are the basic unknowns to be solved in each time step.

The theoretical framework of the DDA method can be found in a number of literatures (Shi and Goodman 1985, Shi and Goodman 1988, Jing 1998, Jing and Stephansson 2007). The following section outlines the key aspects of the DDA formulation, which includes the DDA displacement function and contact model, as well as the workflow of the DDA kinematics analysis.

2.2.1 Displacement function in the DDA method

The deformation of each individual block in a DDA model is represented by six deformation variables: $u_0, v_0, r_0, \varepsilon_x, \varepsilon_y, \gamma_{xy}$, where u_0, v_0 indicate the translational movement of the block in the x - and the y -directions, $\varepsilon_x, \varepsilon_y$ indicate the normal strain

in the respective directions, r_0 denotes the rigid body rotation of the block, and γ_{xy} refers to the corresponding shear strain.

According to the complete first-order displacement approximation, the displacements (u, v) of any arbitrary point (x, y) in a block takes the following form

$$\begin{aligned} u &= a_1 + a_2x + a_3y \\ v &= b_1 + b_2x + b_3y \end{aligned} \quad (2.1)$$

Likewise, the displacement, (u_0, v_0) of the block centroid, (x_0, y_0) takes the following form

$$\begin{aligned} u_0 &= a_1 + a_2x_0 + a_3y_0 \\ v_0 &= b_1 + b_2x_0 + b_3y_0 \end{aligned} \quad (2.2)$$

Subtracting Equation (2.2) from (2.1) gives rise to the following equations

$$\begin{aligned} u &= a_2(x - x_0) + a_3(y - y_0) + u_0 \\ v &= b_2(x - x_0) + b_3(y - y_0) + v_0 \end{aligned} \quad (2.3)$$

It is convenient to express coefficients a_2 , a_3 , b_2 and b_3 in terms of the deformation variables. Based on the infinitesimal strain and rotation tensors

$$\varepsilon_x = \frac{\partial u}{\partial x} = a_2$$

$$\varepsilon_y = \frac{\partial v}{\partial y} = b_3$$

$$\frac{1}{2}\gamma_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) = \frac{1}{2}(a_3 + b_2)$$

$$r_0 = \frac{1}{2}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) = \frac{1}{2}(b_2 - a_3) \quad (2.4)$$

Solving the last two equations for a_3 and b_2 leads to the following

$$b_2 = \frac{1}{2}\gamma_{xy} + r_0$$

$$a_3 = \frac{1}{2}\gamma_{xy} - r_0 \quad (2.5)$$

Substituting Equations (2.4) and (2.5) into (2.3) yields

$$u = \varepsilon_x(x - x_0) + \left(\frac{1}{2}\gamma_{xy} - r_0\right)(y - y_0) + u_0$$

$$v = \left(\frac{1}{2}\gamma_{xy} + r_0\right)(x - x_0) + \varepsilon_y(y - y_0) + v_0 \quad (2.6)$$

The displacement functions can also be expressed in the matrix form as

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 & 0 & -(y - y_0) & (x - x_0) & 0 & (y - y_0)/2 \\ 0 & 1 & (x - x_0) & 0 & (y - y_0) & (x - x_0)/2 \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \\ r_0 \\ \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{pmatrix} \quad (2.7)$$

or simply

$$\begin{pmatrix} u \\ v \end{pmatrix} = [T_i][d_i] \quad (2.8)$$

where $[T_i]$ is the transformation matrix of any block i in the blocky system and $[d_i]$ is the deformation matrix comprising the six deformation variables. Considering every block has a constant stress and strain field, Equation (2.7) can be used to determine the displacements (u, v) of any arbitrary point (x, y) within each block, provided that the strains and the centric displacements of the block are known.

2.2.2 Global equilibrium equation in the DDA method

The formulation of the global equilibrium equation in DDA is similar to that of the FEM. For any block i in a blocky system, the total potential energy Π_i is equal to

$$\Pi_i = \mathbf{U} + \mathbf{V} = \frac{1}{2} \{\varepsilon_i\}^T \{\sigma_i\} dA_i - \{f_i\}^T \{d_i\} \quad (2.9)$$

in which the first term, $\mathbf{U}$ represents the elastic strain energy (assuming linear elasticity) of block i while the second term, $\mathbf{V}$ represents the total works done by the external forces on block i . Notations $\{\varepsilon_i\}$, $\{\sigma_i\}$, $\{f_i\}$ and $\{d_i\}$ in the equation respectively denote the strain, stress, load and deformation vectors of block i , while dA_i indicates the block size.

The derivatives of the potential energy of block i with respect to its six deformation variables, d_{ri} (where $r = 1, 2, \dots, 6$) can be expressed as

$$\frac{\partial \Pi_i}{\partial d_{ri}} = [k_{ii}] \{d_i\} - \{f_i\} \quad (2.10)$$

Based on the principle of potential energy minimization, a mechanical system shall deform or displace to a position corresponding to the minimum total potential energy. Hence

$$\frac{\partial \Pi_i}{\partial d_{ri}} = 0 \rightarrow [k_{ii}] \{d_i\} = \{f_i\} \quad (2.11)$$

The stiffness submatrix, $[k_{ii}]$ is 6×6 in size while both $\{d_i\}$ and $\{f_i\}$ are 6×1 vectors. For a system consisting of N blocks, the global equilibrium matrix takes the following form

$$\begin{bmatrix} k_{11} & k_{12} & k_{13} & \cdots & k_{1N} \\ k_{21} & k_{22} & k_{23} & \cdots & k_{2N} \\ k_{31} & k_{32} & k_{33} & \cdots & k_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k_{N1} & k_{N2} & k_{N3} & \cdots & k_{NN} \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_N \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_N \end{Bmatrix} \quad (2.12)$$

or simply

$$[\mathbf{K}]\{\mathbf{d}\} = \{\mathbf{f}\} \quad (2.13)$$

The off-diagonal submatrices, k_{ij} in Equation (2.12) represents the contributing submatrices of contacts between blocks i and j , while the diagonal submatrices k_{ii} represents the combination of inertia term, elastic stiffness and contact stiffness matrices (if the block is in-contact with any other block) of block i .

The global stiffness matrix $[\mathbf{K}]$ in Equation (2.13) is $6N \times 6N$ in size, while the global displacement and load vectors, $\{\mathbf{d}\}$ and $\{\mathbf{f}\}$ are $6N \times 1$ in size. The total number of displacement variables to be solved is equal to the sum of the degree of freedom of all blocks, $6N$.

The total potential energy in Equation (2.9) encompasses all the potential energies in block i , such as those resulted by the elastic stresses, initial stresses, inertia force, point loading, line loading and area loading. The derivatives of these individual potential energies with respect to the deformation variables are derived, and the corresponding stiffness and load submatrices are formed separately, before being added to Equation (2.12). To derive k_{ij} , k_{ii} and f_i from a potential energy Π_{qi} , the following differentiation equations apply.

For k_{ii} ,

$$\frac{\partial^2 \Pi_{qi}}{\partial d_{ri} \partial d_{si}} \rightarrow k_{ii} \quad (2.14)$$

where d_{ri} and d_{si} are the six deformation variables of block i , and $r, s = 1, 2, 3, \dots, 6$. The derivative k_{ii} leads to a 6 x 6 submatrix which is added to k_{ii} in the global stiffness matrix $[\mathbf{K}]$.

For k_{ij} ,

$$\frac{\partial^2 \Pi_{qi}}{\partial d_{ri} \partial d_{sj}} \rightarrow k_{ij} \quad (2.15)$$

where d_{ri} and d_{sj} are the six deformation variables of blocks i and j , and $r, s = 1, 2, 3, \dots, 6$. The derivative k_{ij} forms a 6 x 6 submatrix which is added to k_{ij} in the global stiffness matrix $[\mathbf{K}]$.

For f_i ,

$$\frac{\partial \Pi_{qi}}{\partial d_{ri}} \rightarrow f_i \quad (2.16)$$

where $r = 1, 2, 3, \dots, 6$ and d_{ri} represents the six deformation variables of block i . The derivative f_i forms a 6 x 1 submatrix which is added to the global load vector $\{\mathbf{f}\}$ in the global equilibrium equation.

2.2.3 Contact detection and definition in DDA

For a discrete block system consisting of more than one block, there must exist a contact analysis algorithm to account for the inter-block contacts. A contact model is a distinctive component of the discrete element methods that distinguishes them from the continuous methods such as the FEM.

In DDA, whether two blocks will come into contact in the subsequent time step is judged by the minimum distance between the blocks during the current time step. The minimum distance n_{ij} between any point in block i and a random point in block j can be expressed as

$$\eta_{ij} = \min\left\{ \begin{array}{l} \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}, \\ \text{either } \forall (x_1, y_1) \in V_i, \quad \forall (x_2, y_2) \in \partial B_j, \\ \text{or } \quad \forall (x_2, y_2) \in V_j, \quad \forall (x_1, y_1) \in \partial B_i \end{array} \right\} \quad (2.17)$$

where ∂B_i and ∂B_j are the boundary segments of blocks i and j , while V_i and V_j are the vertices of the respective blocks. It is impossible for blocks i and j to meet if η_{ij} is greater than two times the maximum displacement, ρ of the points in all blocks, or

$$\eta_{ij} > 2\rho \quad (2.18)$$

where

$$\rho = \max\left\{ \sqrt{u(x, y)^2 + v(x, y)^2}, \quad \forall (x, y) \in B_r, \quad r = 1, 2, \dots, N \right\} \quad (2.19)$$

As illustrated in Figure 2.2, DDA classifies the block contacts into three groups: vertex-to-vertex contacts, edge-to-vertex contacts and edge-to-edge contacts. The first two groups of contacts can be represented by point-line crossing inequalities, while an edge-of-edge contact can be considered as a combination of two edge-to-vertex contacts.

Figure 2.2 Three types of contact in DDA

2.2.4 Block system kinematics in DDA

Two constraints must be complied when contacts are involved: (i) No penetration is allowed between the parts of blocks that are in contact, and (ii) No tension force is introduced to any open contact. In DDA, these constraints are reinforced by the penalty method and the sliding between the block interfaces is controlled by the Coulomb's friction law.

As illustrated in Figure 2.3, the block system kinematics analysis in DDA comprises an “open-close” iteration. First, the derivatives of individual potential energies are computed, assembled into the load or stiffness submatrices, and added to the global equilibrium equation. The global equation is then solved for the displacement variables and the solutions obtained are checked for compliance with the no-penetration, no-tension rules. In the case of noncompliance, constraints at the contact will be adjusted, and the stiffness and force submatrices will be established or removed accordingly. A new set of solutions are then yielded from the modified global equation, and the compliance check and constraint adjustment processes are repeated.

Figure 2.3 Workflow of block kinematics analysis in DDA

Equation (2.12) needs to be solved again and again within every time step, causing the block joints to open and close in the process, hence the name “open-close” iteration. The converging condition of the “open-close” iteration is that the contact status of all block joints remains unchanged over two successive iterations, and the no-penetration (at close contacts), no-tension (at open contacts) constraints are complied. Once convergence is achieved, the same block kinematics analysis cycle is repeated for the next simulation time step. The analysis continues until the final time step is reached.

2.3 Recent development of DDA hydro-mechanical models

DDA is a numerical method widely applied in rock engineering analysis. Over the last few decades, many extensions and improvements have been proposed to the DDA code, contributing to the advancement of the code in terms of efficiency and functionality. Major efforts to introduce and enhance the DDA hydro-mechanical model are documented in Kim et al. (1999), Jing et al. (2001), Rouainia et al. (2006a), and Koyama et al. (2011). Key contributions and findings of these and some other literatures are summarized in Figure 2.4, and are reviewed in the following sections.

2.3.1 The modeling of steady flow through jointed rock masses

Two of the most important pioneering works concerning the DDA hydro-mechanical modeling are Kim et al. (1999) and Jing et al. (2001). These studies form the basis of DDA hydro-mechanical model, and contribute profoundly to the succeeding works in the pertinent areas.

Figure 2.4 Recent development of DDA hydro-mechanical models

.Kim et al. (1999) was probably the first to extend the DDA method for hydro-mechanical modeling. *Kim-model* consists of three major components: (i) a subroutine for seepage analysis, (ii) a subroutine to transform the hydraulic variables into loading terms, and (iii) a mechanical analysis algorithm to analyze joint deformations. The three components interact with one another in a staggered manner, i.e. the outputs of one process are used as the input parameters of the others. For example, through the mechanical analysis, joint details such as aperture, joint length and orientation are determined. Based on these variables, the fluid transmissivity of the joint is calculated and the piezometric heads at the corresponding joint intersections are computed by means of seepage analysis. The piezometric heads are

then being converted into point loads. Joint deformations resulted by these point loads are evaluated through the subsequent mechanical analysis.

In a later study, Jing et al. (2001) introduced a generalized, closed-form expression for the nodal load vector corresponding to fluid-induced block deformations. With these closed-form expressions, the hydraulic heads obtained from a seepage analysis can be converted into loading terms directly. To further simplify the process of hydro-mechanical analysis, Jing et al. (2001) has implemented the cubic law, an expression which relates the joint aperture and length obtained from the mechanical analysis to the joint transmissivity, in the seepage analysis algorithm.

Compared to *Kim*-model, *Jing*-model has a higher computational efficiency – due to the application of many simplified expressions, but less flexibility – as it is bound by the assumptions inherent from these simplifications. For example, only steady, laminar and well-established flow is considered by *Jing*-model, and the friction between flowing water and fracture wall is routinely ignored in the seepage analysis. In contrast, *Kim*-model can simulate both steady laminar and turbulent flows, as well as the effect of relative friction to fluid flow. Nevertheless, *Jing*-model has received considerable attention from the DDA community since its introduction, mainly due to its straightforward formulation and low-complexity solution scheme. Over the past decade, many DDA extensions pertaining to hydro-mechanical analysis (Ben et al. 2012, Chen et al. 2013, Jiao et al. 2014, Chen et al. 2015a, Choo et al. 2016) were developed based on the *Jing*-model.

2.3.2 Laminar versus turbulent flow modeling

The hydro-mechanical model introduced by Kim et al. (1999) allows both laminar and turbulent flows, in either parallel or non-parallel form, to be simulated. Different flow laws are introduced to the model to account for the varying flow conditions. According to *Kim*-model, analyzing the fluid flow in a single fracture consists of the following steps. First, the Reynolds number of the flow and the relative roughness of

the fracture walls are calculated. From there, the type of flow involved is ascertained, and the hydraulic properties, such as the hydraulic conductivity and the degree of non-linearity between the average velocity and the hydraulic gradient, are determined. Based on these parameters, a steady flow analysis is then performed to determine the piezometric heads at every joint intersection and flow rates across all block joints.

To validate the proposed hydro-mechanical model, Kim et al. (1999) reproduced a laboratory work of Grenoble (1988) and compared the simulation outputs, in terms of hydraulic head, with the laboratory measurements. There is a good agreement between the two results. However, probably due to the limitation of laboratory data available for comparison, the impacts of turbulent flow and fluid-block interaction were not considered in the verification example.

2.3.3 Modeling of unconfined aquifers

Unconfined aquifer is very common in rock formations. Theoretically, an aquifer is classified as unconfined if it is intersected by a phreatic surface which may fluctuate according to the atmospheric pressure. In numerical modeling, the location of the phreatic surface is usually determined through the residual flow method (Desai 1976) or the variable conductivity method (Bathe and Khoshgoftaar 1979). An unconfined flow model based on the latter was proposed to the DDA method in Jing et al. (2001). The model adopts an iterative technique to assess the elevation of the phreatic surface. In each iterative cycle, the piezometric heads across the problem domain is computed. Then, the phreatic surface is determined by comparing the vertical coordinate, z_i of a joint intersection i to its piezometric head, h_i . The point is envisaged as above the water table if $h_i < z_i$, below the water table if $h_i > z_i$, and coincides the water table if $h_i = z_i$. By connecting all the points with $h_i = z_i$ (including the interpolated points), and ensuring that the condition $\partial h / \partial n = 0$ (i.e. no flow across the phreatic surface in the normal direction) is satisfied, the location of the phreatic surface can be established. In the case where $\partial h / \partial n > 0$, a corrective flow rate vector, estimated from the excessive flow volume, is added to the flow rate vector. Based on the corrected

flow rate vector, new hydraulic heads are computed and the phreatic surface is updated accordingly. The procedure of updating the flow rate vector and the phreatic surface is repeated until the difference between two successive outputs is smaller than a pre-defined tolerance margin.

The capability of *Jing*-model in defining the phreatic surface of an unconfined aquifer is demonstrated through a numerical example. However, the simulation results are not verified against laboratory or analytical solutions due to the lack of corresponding empirical data.

2.3.4 Modeling of inter-matrixes flows

When modeling the hydro-mechanical behaviors of rock formations, the effect of fluid flux across rock matrixes is frequently ignored due to its insignificance. However, some researchers have argued that matrix flows may alter the pressure distribution profile and affect the mechanical behaviors of a rock structure (Rouainia et al. 2001, Rouainia et al. 2006b). The common practice of ignoring the matrix flows is claimed to have been preventing these phenomena to be addressed. Henceforth, a hydro-geomechanical model which can account for both inter- and intra-matrix flows was proposed to the DDA method by Rouainia et al. (2006a).

Rouaini- model is a combination of two simulation environments: a continuum-based finite element (FE) model for flow analysis, and a discontinuum-based DDA model for block kinematic analysis. The interface works as follows. First, a DDA model, consisting of a finite number of discrete blocks, is established. Then, in a separate modeling environment, a problem domain is discretized into fine triangular mesh to simulate the fluid flow across the blocky system. The outputs of the fluid flow analysis (i.e. the hydraulic heads and the pore pressures of each element) are transferred to the DDA model for block kinematic analysis. In return, the outputs of the kinematic analysis (i.e. the updated aperture of each joint segment) are transferred to the finite element model. Before the subsequent flow analysis, the hydraulic

conductivity of each triangular element in the FE model is updated based on the new aperture profile, according to an area-weighted average method.

Throughout the simulation process, the configuration and the position of the DDA blocks may vary, but those of the finite element model remains fixed. To ensure that the variation of hydraulic pressure along each rock joint can be captured in adequate detail, it is important to adopt an FE mesh which is much refined than the aperture at areas corresponding to the block joints in the overlaying flow model. However, increasing the number of finite elements in the flow model may amplify the computational cost of flow analysis. Therefore, a balance needs to be struck between accuracy and efficiency when deciding the mesh size.

A major drawback of the *Rouainia*-model compared to the pipe network models (Kim et al. 1999, Jing et al. 2001) is that it adopts a more complicated, memory-intensive solution scheme. Nevertheless, the model prevails the other models with its ability to simulate the intra-matrix flow.

2.3.5 Modeling the hydro-mechanical behaviors of granular materials

The conventional DDA hydro-mechanical model (Kim et al. 1999, Jing et al. 2001) considers a problem domain to be an assemblage of polygonal blocks separated by water-permeable joints. Such representation may not be suitable for geological settings with rough, granular texture and high porosity such as Quartzite, Gneiss, sand stone and soil. To extend the DDA hydro-mechanical model for granular media such as these, a particulate method is introduced in Koyama et al. (2011).

As illustrated in Figure 2.5, there are mainly two approaches to model a fluid flow process with the DDA model. In the first approach, each block joint is regarded as a member of a pipe network. Fluid flow is solved based on the pipe geometry and connectivity, and the resultant pore pressure contributes to the load vector of the surrounding blocks directly (Kim et al. 1999, Jing et al. 2001). In the second approach, fluid flow is solved using a separate FEM model and the resultant pore pressure is

interpolated to the underlying DDA model for block kinematic analysis (Rouainia et al. 2001, Rouainia et al. 2006b). *Koyama*-model concerns the latter with disc-shaped rigid blocks.

Figure 2.5 The pipe network method and the coupling DDA-FEM method for fluid flow modeling

Koyama-model considers energy contributions from four main physical processes: gravitation, inertia reaction, fluid flow and contact mechanism. A special contact model to account for the interaction between disc-shaped particles, as well as between particles and wall elements were derived. Mathematical expressions of fluid pressure and fluid-induced potential energy acting on a disc-shaped particle were also introduced. Darcy's law and the mass conservation theory were applied in the seepage analysis, based on the following assumptions: (i) the flow is Darcian and laminar, (ii) the flowing fluid is viscous and incompressible, and (iii) fluid flows in a saturated condition, i.e. any gap between particles is fully occupied by the fluid. Pore pressure distribution obtained from the seepage analysis is transferred from the FEM model to the DDA for mechanical analysis. Subsequently, the inter-particle distances obtained from the mechanical analysis are interpolated to the FEM model for apertures and

hydraulic pressures update. Such coupling process is repeated until the final simulation time step.

It is worth highlighting that the seepage flow within a porous or granular medium can also be modeled through a pipe network method, as demonstrated in Xu et al. (2014). *Xu*-model is conceptually similar to the conventional pipe network models for fractured media (Kim et al. 1999, Jing et al. 2001), except in two aspects. First, the conventional model considers each block joint as a pipe and constructs the pipe network system according to the positions of the block joints in the problem domain, while *Xu*-model discretizes the problem domain with triangular mesh, and considers each mesh line as a member of the pipe network system. Secondly, the hydraulic conductivity of each pipe in the conventional model is derived from the properties of the respective joint; while that in the *Xu*-model is derived from the properties of the surrounding mesh elements, using an area-weighted average method.

Xu-model does not consider the mechanical aspect of the seepage problems. In this context, *Koyama*-model prevails *Xu*-model as it provides a means to investigate the particles movement, as well as the interaction between particles movement and fluid flow. Such interaction is important in geotechnical engineering, especially in the studies of soil liquefaction, quicksand and slope stability problems. Another advantage of the *Koyama*-model is that, as only disc-shaped rigid block is considered in the problem domain, the elastic deformation of individual particles can be ignored, hence simplifying the calculation and reducing the hefty computational cost associated with the coupling FEM-DDA solver.

2.3.6 Modeling the effect of sequential loading/ Unloading

The stability of an underground excavation is frequently related to factors such as the nature and force field of the rock mass, the water table at the construction site, and the excavation sequence adopted (Széchy 1966, Kim et al. 1999, Chen et al. 2013). To enhance the feasibility of DDA in modeling the stability of underground openings

under different excavation stages, Kim et al. (1999) introduced a simple algorithm to simulate the loading/unloading processes during underground excavations. The algorithm consists of the following steps. First, before an excavation, the in-situ stresses in all rock blocks are computed. The stress distribution is updated after every excavation step, and the revised stress distribution is taken as the initial stress condition at the next excavation step. This stress updating process is repeated until the last excavation step.

The proposed sequential loading/unloading algorithm enables an excavation process to be simulated in a progressive manner using the DDA model. With this, the constitutive relations between excavation sequence, seepage flow and the excavation stability can be established and the viability of different excavation methods can be assessed, hence improving the practical application of DDA in underground constructions.

2.3.7 Modeling the stability of breakwaters

A breakwater is a structure constructed along a shoreline to protect the shore from wave and current attacks. The stability of a breakwater design is often evaluated using empirical formulae (Hudson 1958, Van der Meer 1987) or the distinct element methods (DEM) (Cannoo et al. 2008, Latham et al. 2009). Each of these approaches has its pros and cons. The empirical method provides a straightforward prediction on whether a breakwater will displace. However, the approach does not take into account factors such as the contact forces between blocks and the nonlinear wave-structure interactions. On the other hand, the DEM-based breakwater models enable these factors to be considered in the simulation, but it requires an artificial damping term to control the numerical stability (Jing and Stephansson 2007).

Kaidi et al. (2012) endeavored to overcome the abovementioned limitations by introducing a DDA-based breakwater model. The new breakwater model adopts a solution scheme which is similar to that presented in Rouainia et al. (2006b) and Koyama et al. (2011), where the fluid flow is simulated with the finite element

method while the block kinematics with the DDA method. However, instead of using two separate models to represent the continuous fluid system and the discontinuous block system, then superimposing the outputs of the two models to account for the hydro-geomechanical interactions, Kaidi et al. (2012) combined both the fluid and block systems under a single modeling environment.

First, a problem domain consisting of discrete, sparsely-spaced polygonal blocks is established to represent the breakwater structure. Then, the void spaces between the breakwater blocks are discretized into six-noded triangular elements to represent the fluid domain. By using the two-dimensional vertical Navier–Stokes equation, the fluid pressure at the three corner nodes, and the flow velocity at all six nodal points of each triangular element are solved. The fluid pressures are then converted into structural loads acting on the DDA blocks, before added to the DDA global equilibrium equation. By solving the global equation, changes in the block positions can be determined. Accordingly, the geometry of the triangular elements are revised, and the fluid velocities and pressures are updated.

Kaidi-model helps to develop a new understanding of the wave-breakwater interaction. A simulation case presented in the study indicates that the shape of the backwaters plays an important role in determining the backwaters stability. Irregularity in the block shape results in complex, twisted flow path, which facilitates the dissipation of wave energy. Numerical findings as these are useful for breakwater design and performance evaluations.

2.3.8 Hydraulic fracturing modeling

Hydraulic fracturing has recently risen as one of the important aspects of DDA hydro-mechanical modeling. Ben et al. (2012) was probably the first to simulate the hydraulic fracturing process using the DDA model. In *Ben*-model, high bonding strength is assigned between DDA blocks to simulate an intact rock mass. A fracture is said to form when the normal or shear stress in the joint exceeds the pre-defined thresholds. Pore pressure is transmitted through the inter-connected fractures, hence

fracture tends to extend from the fracture tip once it is initiated. A geometrically simplified numerical example was presented in the study to illustrate the proposed hydraulic fracturing model. The study is later extended to problems involving both pre-existing and new fractures (Ben et al. 2013b). However, only simple numerical examples were demonstrated and no validation case was presented by the authors.

Recently, Jiao et al. (2014) introduced a hydraulic fracturing model based on the same pseudo-continuum concept using the framework of DDA. Sophisticatedly discretized problem domains were adopted in most numerical examples presented in the study to improve models deformability and promote the realism of the fracture configuration. The simulation results obtained from these numerical examples were verified against experimental and analytical solutions.

The appeal of both *Ben*- and *Jiao*- models lies in their ease of implementation as no extensive modifications to the original DDA code were needed to realize the simulation of the hydraulic fracturing mechanisms. Nevertheless, for a DDA model to work as a pseudo-continuous body with a practical degree of deformability, a large number of DDA blocks are often needed, hence contributing to a high total contact surface, and a compute-intensive contact analysis.

Chapter 3. Modeling the hydro-mechanical behavior of fractured media using DDA

3.1 Introduction

Chapter 3 provides an overview of the DDA seepage analysis extension employed in the current study. The flow of this chapter is as outlined in Figure 3.1. First, in Section 3.2, the theoretical concepts and mathematical equations pertaining to the hydro-mechanical behaviors of fractured media are reviewed. In section 3.3, a DDA seepage analysis extension is introduced. The formulation and the workflow of the proposed DDA extension are also explained. Three validation cases are then presented to verify the accuracy of the extension. In Section 3.4, a new solution scheme is introduced as an alternative to the coupled and the non-coupled schemes conventionally applied to the numerical hydro-mechanical analyses. The reliability and efficiency of the new solution scheme is verified through a numerical example. Lastly, in Section 3.5, conclusions are drawn based on the works presented in the current chapter.

Figure 3.1 An outline of Chapter 3

The terms ‘fracture’ and ‘joint’ are used interchangeably in the current chapter to refer to any discontinuity separating an otherwise intact block. The following assumptions are applied to the DDA hydro-mechanical analysis model presented in the following sections: (i) only Newtonian fluid is considered; (ii) fluid flow in the fractures obey the continuity equation; (iii) all DDA blocks consist of isotropic material and behave linear-elastically; (iv) large displacement and rearrangement of blocks do not occur; (v) all fractures, except those located along an impermeable boundary are assumed to be fluid-permeable along the fracture plane.

3.2 Modeling fluid flow through a single fracture

In this section, the theoretical framework concerning the physics of fluid flow is presented. The objective is to review the theoretical concepts based upon which the two-dimensional, hydro-mechanical model adopted in the current study is formulated.

3.2.1 Darcy’s law

The governing equations for subsurface flow are based on two fundamental principles: Darcy’s law and the mass conservation principle. In the case of fluid flow through a single fracture, Darcy's law states that the seepage velocity, v_i , along the fracture is directly proportional to the product of the hydraulic gradient between the inlet and the outlet, $\frac{dh}{dx_i}$, and the fluid conductivity, K_i where

$$v_i = -K_i \frac{dh}{dx_i} \quad (3.1)$$

in which $\frac{dh}{dx_i}$ represents the difference in the piezometric heads, h , per unit flow distance, x_i . Subscript i in the expression denotes the plane, in terms of Cartesian axes, along which the flow is directed, i.e. x_1, x_2 refers to x, y planes respectively. The

negative sign in the equation implies that the flow occurs in the direction of head loss, or towards the end with the lower h .

The piezometric head, h , consists of two components, namely the pressure head, $\frac{P}{\rho g}$, and the elevation head, y , as shown in the following equation

$$h = \frac{P}{\rho g} + y \quad (3.2)$$

where P denotes the pore pressure, while ρ and g denote the fluid density and the gravity acceleration respectively.

3.2.2 The continuity equation and the mass conservation principle

In the case of an incompressible fluid flowing through a saturated fracture, the mass conservation principle requires the total mass of fluid retained in a unit element located at any point within the fracture to be consistent with time. That is to say, all processes contributable to fluid mass change, such as the fluid inflow, outflow, storage release, source contribution or sink extraction, must take place at well-coordinated rates so that the fluid volume retained in a unit element does not vary with time.

Figure 3.2 shows a schematic representation of a two-dimensional unit element with side lengths of Δx and Δy . Notations $(\rho v_x)_x$ and $(\rho v_y)_y$ in the diagram represent the fluid influx, while $(\rho v_x)_{x+\Delta x}$ and $(\rho v_y)_{y+\Delta y}$ represent the fluid outflux that occur along the x - and the y -axes. Notation $\mathbf{r}(x, y, t)$ indicates the change in fluid mass induced by the spatial and time effects.

Figure 3.2 Fluid flow processes in a unit element

The total fluid mass retained in the control volume at any one time, t is equal to

$$\frac{\partial \rho}{\partial t} \Delta x \cdot \Delta y \quad (3.3)$$

Should the flow be in a transient state, an additional term would be needed to account for the rate of fluid being released from local storage as a result of head change. The mass of the fluid being released from a control volume per unit decrease of hydraulic head is commonly referred to as the storage coefficient, $\mathbf{S}$, where

$$\mathbf{S} = -\frac{\rho \Delta V}{(\Delta x \Delta y) \Delta h} \quad (3.4)$$

The negative sign in the equation signifies a decrease in the hydraulic head, h , and ΔV denotes the amount of fluid being released from the unit element. Rearranging Equation (3.4) gives rise to the storage term – the additional term to characterize a transient state flow

$$\frac{\rho \Delta V}{\Delta t} = -\mathbf{S} \frac{\Delta h}{\Delta t} (\Delta x \Delta y) \quad (3.5)$$

where Δh denotes the change in the hydraulic head within a specific time interval, Δt .

Combining the fluid influx and outflux, the source/sink term and the storage term into an equilibrium equation leads to

$$\begin{aligned} \frac{\partial \rho}{\partial t} \Delta x \Delta y = & \left[(\rho v_x)_x \Delta y + (\rho v_y)_y \Delta x \right] - \left[(\rho v_x)_{x+\Delta x} \Delta y + (\rho v_y)_{y+\Delta y} \Delta x \right] \\ & - S \frac{\Delta h}{\Delta t} (\Delta x \Delta y) + r(x, y, t) \Delta x \Delta y \end{aligned} \quad (3.6)$$

Dividing Equation (3.6) by the unit area $\Delta x \Delta y$, and assuming the unit element and the time interval to be infinitesimally small in size bring about the following continuity equation

$$\frac{\partial \rho}{\partial t} = \left[\frac{\partial (\rho v_x)}{\partial x} + \frac{\partial (\rho v_y)}{\partial y} \right] - S \frac{\Delta h}{\Delta t} + r(x, y, t) \quad (3.7)$$

The density of an incompressible fluid does not vary with time, hence the density variation term, $\frac{\partial \rho}{\partial t}$, can be eliminated. Then, by expressing the fluid velocities in the form of Darcy's law, the following equilibrium equation is yielded

$$\left[\frac{\partial}{\partial x} K_x \frac{\partial h}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial h}{\partial y} \right] - S \frac{\Delta h}{\Delta t} + r(x, y, t) = 0 \quad (3.8)$$

Or, for a fracture of aperture e

$$\left[\frac{\partial}{\partial x} T_x \frac{\partial h}{\partial x} + \frac{\partial}{\partial y} T_y \frac{\partial h}{\partial y} \right] - S \frac{\Delta h}{\Delta t} + r(x, y, t) = 0 \quad (3.9)$$

where (i) $S = \frac{s}{\rho}$, a dimensionless parameter commonly referred to as the storativity; (ii) $r = \frac{r}{\rho}$, indicating the source/sink term; and (iii) $T_i = K_i \cdot e$, indicating the one-dimensional fluid transmissivities.

3.2.3 The Navier-Stokes equations and the momentum conservation law

According to the momentum conservation law, the total force acting on a fluid mass is equal to the momentum change in the direction of the force, as given below

$$\frac{d m \vec{v}}{d t} = \sum F \quad (3.10)$$

where m , $\vec{v}$ and t denote the fluid mass, the velocity vector, and the time interval during which the momentum change occurs, respectively.

For an infinitesimal unit element of size $dx \cdot dy$, and uniform density ρ , the momentum change can be expressed as

$$\frac{d m v_i}{d t} = \rho \left\{ \frac{\partial v_i}{\partial t} + v_x \frac{\partial v_i}{\partial x} + v_y \frac{\partial v_i}{\partial y} \right\} dx dy \quad (3.11)$$

where subscript i indicates the plane of the momentum change. For a two-dimensional model, $i = 1, 2$ and $x_1, x_2 =$ the x - and y -Cartesian planes. The linear term at the RHS of Equation (3.11) refers to the momentum change with respect to time, while the two non-linear terms refer to the convective acceleration, i.e. acceleration associated with the spatial effects.

On the other hand, “ $\sum F$ ” in Equation (3.10) represents the sum of the forces to be imposed on the volumetric mass (i.e. the body force), and on the surface (i.e. the surface force) of the control element in order to produce the momentum change given in Equation (3.11). The three forces taken into consideration by the current study are the gravity force, F_g , and the pressure and viscosity-induced forces, F_p and F_v , as shown in the following expression

$$\begin{aligned}
\sum F_i &= \text{Body Force} + \text{Surface Force} \\
&= F_g + (F_p + F_v) \\
&= \rho b_i - \left(\frac{\partial P}{\partial x_i} + \sum_j \mu \frac{\partial^2 v_i}{\partial x_j \partial x_j} \right) \quad (3.12)
\end{aligned}$$

where subscripts $i, j = 1, 2$, indicating the x - and the y -Cartesian planes, b_i denotes the acceleration corresponding to the body force, P denotes the pore pressure, μ denotes the fluid dynamic viscosity, and v_i denotes the fluid velocity in the i direction.

Substituting Equations (3.11) and (3.12) into (3.10) for $i, j = 1, 2$, and dividing both sides of the equations by a uniform fluid density, ρ , yield the Navier-Stokes (N-S) equations

$$\begin{aligned}
\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} &= b_x - \frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} \right) \\
\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} &= b_y - \frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} \right)
\end{aligned} \quad (3.13)$$

in which ν denotes the fluid kinematic viscosity where $\nu = \frac{\mu}{\rho}$.

3.3 The hydro-mechanical analysis algorithm

In this section, the derivation of the cubic law – an expression that relates the fluid transmissivity to the aperture, fluid viscosity and density – is presented, as well as the derivation of other flow equations applied in the proposed seepage analysis algorithm.

3.3.1 Derivation of flow equations

In the proposed seepage analysis algorithm, a simplified form of the N-S equations is employed to compute the hydraulic head distribution. Table 3.1 summarizes the assumptions applied in the derivation of the simplified flow equations. Figure 3.3 illustrates the conceptual model of an idealized fracture. In the proposed model, the flow velocity across a fracture is assumed to be uniform, and equals to the mean velocity derived from the theoretical parabolic fluid velocity profile shown in Figure 3.3.

Table 3.1 Assumptions applied in the derivation of simplified flow equations

Assumptions regarding the fracture model	Assumptions regarding the seepage flow
1a) Smooth fracture surface, zero friction between fluid and the fracture walls 1b) Fracture walls are impervious to fluid flow in the normal direction	2a) Only incompressible fluid is considered 2b) Flow only occurs in the direction parallel to the fracture's plane 2c) Only steady and laminar flow is considered 2d) The flow is uniform, i.e. the flow velocity and direction at any two points within a fracture are the same

Figure 3.3 Parabolic distribution of flow velocity within an idealized fracture

Equation (3.14) shows the full N-S equations, with the terms to be eliminated contained in square boxes. Matching the reference number printed on the top right corner of each box to the statement in Table 3.1 reveals the assumption that leads to the elimination of the respective terms. For example, assumption 2c leads to the elimination of the first term in the first equation.

$$\begin{aligned}
\rho \left[\boxed{\frac{\partial v_x^{2c}}{\partial t}} + \boxed{v_x \frac{\partial v_x^{2d}}{\partial x}} + \boxed{v_y \frac{\partial v_x^{2d}}{\partial y}} \right] \\
= b_x - g \frac{\partial h}{\partial x} + \nu \left(\boxed{\frac{\partial^2 v_x^{2d}}{\partial x^2}} + \frac{\partial^2 v_x}{\partial y^2} \right) \\
\rho \left[\boxed{\frac{\partial v_y^{2b,2c}}{\partial t}} + \boxed{v_x \frac{\partial v_y^{2b}}{\partial x}} + \boxed{v_y \frac{\partial v_y^{2b}}{\partial y}} \right] \\
= b_y - g \frac{\partial h}{\partial x} + \nu \left(\boxed{\frac{\partial^2 v_y^{2b}}{\partial x^2}} + \boxed{\frac{\partial^2 v_y^{2b}}{\partial y^2}} \right)
\end{aligned} \tag{3.14}$$

After the elimination process, the two equations are simplified to

$$\nu \frac{\partial^2 v_x}{\partial y^2} = -b_x + g \frac{\partial h}{\partial x} = g \frac{\partial (h - b_x x)}{\partial x} \tag{3.15}$$

$$-b_y + g \frac{\partial h}{\partial y} = 0 \tag{3.16}$$

Assuming that gravity is the only body force acting on the fluid, then in Equation (3.16), $b_y = 0$. Since $g \neq 0$, it is construed that

$$\frac{\partial h}{\partial y} = 0 \tag{3.17}$$

On the other hand, solving Equation (3.15) with respect to v_x leads to

$$v_x = \frac{g}{2\nu} \frac{\partial(h - b_x x)}{\partial x} y^2 + c_1 y + c_2 \quad (3.18)$$

where c_1 and c_2 are unknown constants.

The theoretical parabolic profile of fluid velocity (refer to Figure 3.3) yields the following boundary conditions

$$v_x = 0|_{y=\pm\frac{e}{2}} \quad (3.19)$$

Applying these boundary conditions to Equation (3.18) results in

$$\begin{aligned} c_1 &= 0 \\ c_2 &= -\frac{g}{2\nu} \frac{\partial(h - b_x x)}{\partial x} \frac{e^2}{4} \end{aligned} \quad (3.20)$$

Substituting Equations (3.20) into Equation (3.18) leads to

$$v_x = \frac{g}{2\nu} \frac{\partial(h - b_x x)}{\partial x} \left[y^2 - \left(\frac{e}{2} \right)^2 \right] \quad (3.21)$$

Subsequently, the mean velocity, $\overline{v_x}$, and the flow rate, q_x , can be derived, where

$$\overline{v_x} = \frac{1}{e} \int_{-e/2}^{e/2} v_x dy = -\frac{ge^2}{12\nu} \frac{\partial(h - b_x x)}{\partial x} \quad (3.22)$$

$$q_x = e\overline{v_x} = -\frac{ge^3}{12\nu} \frac{\partial(h - b_x x)}{\partial x} \quad (3.23)$$

Taking $x = 0$ as the reference plane, then q_x at the reference plane can be simplified to

$$q_x = -T_x \frac{\partial h}{\partial x} \quad (3.24)$$

in which T_x denotes the fluid transmissivity – a parameter governed by the gravity acceleration, g , the aperture, e , and the fluid kinematic viscosity, ν , where

$$T_x = \frac{ge^3}{12\nu} \quad (3.25)$$

Equation (3.25) is also known as the cubic law. Dividing T_x by e leads to the hydraulic conductivity, K_x

$$K_x = \frac{T_x}{e} = \frac{ge^2}{12\nu} \quad (3.26)$$

Substituting Equations (3.17) and (3.26) into the continuity equation (Equation (3.9)) yields the following simplified flow equation

$$\frac{ge^3}{12\nu} \left[\frac{\partial^2 h}{\partial x^2} \right] - S \frac{\Delta h}{\Delta t} + \frac{r}{\rho} = 0 \quad (3.27)$$

Considering a case where a joint intersection, j , is connected to m number of different joints, Equation (3.27) can be expanded to

$$\begin{aligned} & \frac{ge_{j1}^3}{12\nu L_{j1}^2} (h_1 - h_j) + \frac{ge_{j2}^3}{12\nu L_{j2}^2} (h_2 - h_j) + \dots + \frac{ge_{jm}^3}{12\nu L_{jm}^2} (h_m - h_j) - S \frac{\Delta h}{\Delta t} + \frac{r_j}{\rho} \\ & = 0 \end{aligned} \quad (3.28)$$

where h_1 , e_{j1} and L_{j1} refer to the hydraulic head at nodal point 1, the aperture, and the distance between nodal points j and 1, respectively. The same applies to similar expressions of different subscripts, i.e. h_2 , e_{j2} , L_{j2} refer to the hydraulic head at nodal point 2, the aperture, and the distance between nodal points j and 2, and so forth.

To solve for h_j , a finite differential-based equation is derived from Equation (3.28). The derivation procedure and the final equation are shown in the following

$$\begin{aligned}
\frac{gh_j}{12\nu} \left(\frac{e_{j1}^3}{L_{j1}^2} + \frac{e_{j2}^3}{L_{j2}^2} + \dots + \frac{e_{jm}^3}{L_{jm}^2} \right) &= h_1 \left(\frac{ge_{j1}^3}{12\nu L_{j1}^2} \right) + h_2 \left(\frac{ge_{j2}^3}{12\nu L_{j2}^2} \right) + \dots \\
&\quad + h_m \left(\frac{ge_{jm}^3}{12\nu L_{jm}^2} \right) + S \frac{\Delta h}{\Delta t} + r_j \\
\frac{gh_j}{12\nu} \left(\sum_{n=1}^m \frac{e_{jn}^3}{L_{jn}^2} \right) &= \left(\sum_{n=1}^m h_i \frac{ge_{jn}^3}{12\nu L_{jn}^2} \right) + S \frac{\Delta h}{\Delta t} + r_j \\
h_j &= \frac{\left(\sum_{n=1}^m h_i \frac{ge_{jn}^3}{12\nu L_{jn}^2} \right) + S \frac{\Delta h}{\Delta t} + r_j}{\frac{g}{12\nu} \sum_{n=1}^m \frac{e_{jn}^3}{L_{jn}^2}} \tag{3.29}
\end{aligned}$$

In which $n=1, 2, 3, \dots, m$, and L_{jn} , the length of a seepage line can be determined by

$$L_{jn} = \sqrt{(x_j - x_n)^2 + (y_j - y_n)^2} \tag{3.30}$$

where x_j, x_n denote the x -coordinates, while y_j, y_n denote the y -coordinates of node j and n . To determine the equivalent aperture size, e_{jn} of a parallel or wedge-shaped fracture, the following equation is applied (Iwai 1976)

$$e_{jn} = e_m \left[\frac{16r_e^2}{(1 + r_e)^4} \right]^{1/3} \tag{3.31}$$

where e_m is the arithmetic mean of e_j and e_n , while r_e denotes the ratio of e_j to e_n . Note that $e_{jn} = e_m$ in the case of a parallel fracture.

Figure 3.4 Schematic diagram illustrating the application of Equation (3.29)

For a flow system consisting of several seepage nodes, the computation of h_j proceeds from one seepage node to the next. The values obtained as h_j in any of the preceding computational steps would be used as h_n in the computation of h_j of the following nodes. The iterative process of solving the h_j is repeated until: (i) a convergent solution is achieved in the case of a steady-state flow analysis; or (ii) the hydraulic head of the last node is solved in the case of a transient-state flow analysis.

3.3.2 Formulation of hydro-mechanical analysis algorithm in DDA

This section explains the workflow of the proposed hydro-mechanical analysis algorithm and how the algorithm is formulated. An outline of the workflow is given in Figure 3.5. First, the seepage network within a numerical model is configured based on the blocks arrangement, after which the pre-defined hydraulic boundary conditions are assigned to the pre-specified locations in the model. Then, the computation of hydraulic head or pore pressure distribution begins, followed by the updates of the block positions and the apertures before proceeding to the subsequent time step.

Configuration of seepage network

The first step towards formulating a hydro-mechanical analysis extension to the DDA model is to establish a mathematical algorithm to configure the seepage network

within discontinuous models. A seepage network defines the fluid flow paths in a problem domain. The two basic components of a seepage network are the seepage node and the seepage line. A seepage node connects to at least one other seepage node in the network via a seepage line. A seepage node is either an existing block vertex, or an additional node introduced to a DDA block at the point-of-contact with another block. In the proposed algorithm, additional seepage nodes are introduced to the DDA model in an automatic manner according to the blocks arrangement, before a hydro-mechanical analysis begins. Figure 3.6 shows a typical DDA seepage model consisting of five distinct blocks. The apertures depicted in the figure are exaggerated to illustrate the relationships between block vertexes, rock joints, seepage nodes and seepage lines.

Figure 3.5 Workflow of the proposed hydro-mechanical analysis algorithm

After the seepage nodes have been configured, seepage lines are introduced. Each seepage line connects two seepage nodes, along a block joint or a joint segment. By denoting a seepage node as j and other seepage nodes connected to node j through different seepage lines as n , the hydraulic heads at node j can be solved using Equation (3.29).

Figure 3.6 A DDA seepage-block model

Definition of hydraulic boundary conditions

The hydraulic boundary conditions of the seepage nodes are defined after the seepage network has been configured. Three types of the hydraulic boundary conditions are considered in the current study, namely:

- 1) Fixed hydraulic head or fixed pore pressure boundary: the hydraulic head or pore pressure of a seepage node assigned with this boundary condition is kept constant for a specific duration, or throughout an analysis. Fixed hydraulic head boundary is prescribed for cases where water level can be measured or inferred, for example in a reservoir model. Fixed pore pressure boundary are commonly prescribed along seepage faces, where water pressure equals to the atmospheric pressure.
- 2) Boundary with variable hydraulic head or pore pressure: the hydraulic head or pore pressure of a seepage node assigned with this boundary condition varies with time at a pre-defined rate. The pressure change in a wellbore can be modeled with this type of boundary condition.
- 3) No-flow boundary: Fluid cannot flow across a no-flow boundary. A natural example of no-flow boundary is groundwater divides. When computing the hydraulic head of a no-flow seepage node, fictitious seepage nodes and lines

will be introduced to the specific node to simulate the backflow effect. Figure 3.7 illustrates the concept of the fictitious seepage network assumed at a no-flow boundary. When applying Equation (3.29) to the illustrated no-flow seepage node, use $m=4$. The lengths and the apertures of the fictitious seepage lines are as defined in the illustration.

Figure 3.7 Fictitious seepage nodes introduced at seepage node located on a no-flow boundary

Computation of nodal hydraulic heads and pore pressures

The seepage analysis begins from seepage nodes with known hydraulic heads. For example, the seepage nodes assigned with fixed hydraulic head or fixed pore pressure, or those assigned with variable head or variable pore pressure.

For a seepage node i assigned with a known hydraulic pressure, P_i , the following equation is applied to convert the hydraulic pressure into nodal hydraulic head, h_i

$$h_i = \frac{P_i}{\rho g} + y_i \quad (3.32)$$

For a seepage node i assigned with hydraulic head or pressure which varies at a pre-defined rate, $\dot{r}$, h_i at a specific time, t , is equal to

$$h_i = \dot{r} \times t \quad (3.33)$$

The hydraulic heads of all other types of seepage node are determined by Equation (3.29). In summary, the computation of hydraulic heads is carried out in the following order during a seepage analysis: (i) seepage nodes with known hydraulic heads or pressures; (ii) seepage nodes directly connected to (i); (iii) seepage nodes directly connected to (ii); and so forth until the hydraulic heads of all seepage nodes are solved.

Mechanical analysis and the update of apertures

Consider Node a (x_a, y_a) and Node b (x_b, y_b) as two seepage nodes of a rigid block where $y_a > y_b$, and h_a, h_b denote the hydraulic head of the two nodes. Below are three possible combinations of h_a, h_b, y_a and y_b :

Case 1: the water table is located above Nodes a and b , i.e. $h_a > y_a$ and $h_b > y_b$.

Case 2: the water table is located below Nodes a and b , i.e. $h_a < y_a$ and $h_b < y_b$.

Case 3: the water table is located between Nodes a and b , i.e. $h_a < y_a$ and $h_b > y_b$.

Different water table height-nodal elevation combinations lead to different hydraulic pressure distribution profiles, as illustrated in Figure 3.8. In Case 1, the hydrostatic pressure increases gradually from Node a to b , while in Case 2, no hydrostatic pressure is present along joint $a-b$. In Case 3, the hydrostatic pressure decreases gradually from Node b to c , where Node c is the intersection point between the water table and joint $a-b$. The coordinates of Node c (x_c, y_c) are given by the following equations

$$x_c = x_a + \frac{(h_a - y_a) \times (x_b - x_a)}{(y_b - y_a) - (h_b - h_a)} \quad (3.34)$$

$$y_c = y_a + \frac{(y_b - y_a) \times (x_c - x_a)}{(x_b - x_a)} \quad (3.35)$$

Figure 3.8 Hydraulic pressure profiles for different water table height-nodal elevation combinations

Nodal hydraulic pressure, P_i , at Nodes *a*, *b*, and *c* can be determined from Equation (3.32), by assigning $i=a, b$ or c and $h_a = h_b = 0$ for Case 2, and $h_a = 0$ for Case 3. To convert the hydraulic pressures into nodal forces, the following equations are applied

$$\dot{F}_i = \frac{L_{ij}}{2} \left[P_i + \frac{1}{3}(P_j - P_i) \right] \quad (3.36)$$

$$\dot{F}_j = \frac{L_{ij}}{2} \left[P_i + \frac{2}{3}(P_j - P_i) \right] \quad (3.37)$$

where j denotes the subsequent node on a block ($j=i+1$), and L_{ij} denotes the distance between nodes i and j . Next, to resolve the nodal forces into the horizontal and the vertical components, F_{ix} and F_{iy} , the following equations are introduced

$$\begin{aligned}\overset{+}{\rightarrow} F_{ix} &= t_1 \dot{F}_i \\ +\uparrow F_{iy} &= -t_2 \dot{F}_i\end{aligned}\tag{3.38}$$

$$\begin{aligned}\overset{+}{\rightarrow} F_{jx} &= t_1 \dot{F}_j \\ +\uparrow F_{jy} &= -t_2 \dot{F}_j\end{aligned}\tag{3.39}$$

where

$$\begin{aligned}t_1 &= \frac{y_i - y_j}{L_{ij}} \\ t_2 &= \frac{x_i - x_j}{L_{ij}}\end{aligned}\tag{3.40}$$

As indicated by notations $\overset{+}{\rightarrow}$ and $+\uparrow$ in Equations (3.38) and (3.39), positive value of F_x and F_y represent a rightward, and an upward force respectively, while any nodal force acting in a direction opposite to these is negative in value.

Subsequently, each pair of the force components F_{ix}, F_{iy} are converted into the general forces, before being added to the load vector of the DDA global equilibrium matrix, as indicated by the following equation

$$[T_i]^T \begin{bmatrix} F_{ix} \\ F_{iy} \end{bmatrix} \xrightarrow{\text{added to}} [F_k]_{6 \times 1}\tag{3.41}$$

in which

$$[T_i]^T = \begin{bmatrix} 1 & 0 & -(y_i - y_0) & (x_i - x_0) & 0 & \frac{(y_i - y_0)}{2} \\ 0 & 1 & (x_i - x_0) & 0 & (y_i - y_0) & \frac{(x_i - x_0)}{2} \end{bmatrix}^T \quad (3.42)$$

$[F_k]$ in Equation (3.41) represents the 6x1 submatrix positioned at the k^{th} row of the global load vector, and it defines the loading conditions of the k^{th} block in the system (Note: block k is where node i is located). The gravity center of Block k is denoted by (x_0, y_0) .

After the DDA contact and mechanical analyses, and before the subsequent hydraulic analysis, the aperture of all seepage lines are updated in accordance with the new locations of the block vertexes. The workflow of the DDA hydro-mechanical analysis algorithm employed in the current study is summarized in Figure 3.9.

3.3.3 Validation cases

In the following section, three case studies are presented to verify the accuracy of the proposed DDA hydro-mechanical analysis algorithm. The case studies compare the outputs of the proposed algorithm with those of the other numerical method, and with the existing laboratory data.

DDA vs UDEC steady flow analyses results

Three steady-state seepage problems were solved using the DDA and UDEC, the Universal Distinct Element Code (Itasca 2011). The objective is to compare the results obtained from the two methods, in order to verify the accuracy of the former.

Figure 3.9 The workflow of DDA hydro-mechanical analysis

Three numerical models, each consisting of 66, 65, and 60 blocks, were employed to model the steady-state flow problems. Figures 3.10 to 3.12 shows the block arrangement in each model and Table 3.2 summarizes the analysis parameters applied in the seepage analyses. Each block in the three models was 1 m x 1 m in size, and was separated from any adjacent block by a constant, uniform aperture measuring 10^{-4} m. The side and the bottom boundaries of the three models were restrained from normal displacements and the effect of blocks' self-weight was ignored during the seepage analysis.

Table 3.2 Analysis parameters applied to Models 1 to 3

<u>Analysis Parameters</u>	<u>Input Values</u>
Time step size	1 s
Hydraulic aperture of joints	0.1 mm
Kinematic viscosity of fluid, ν	$10^{-6} \text{ m}^2/\text{s}$
Fluid density, ρ	1000 kg/m ³
Hydraulic conductivity of joints	8.333 mm/s
Source/sink term	0
Storage term	0

In terms of hydraulic boundary conditions, for Model 1, except the top boundary was assigned with linearly distributed hydraulic head, the other boundaries were impervious. For model 2, the left and the right boundaries were assigned with a fixed hydraulic pressure, while the top and the bottom boundaries were impervious. For model 3, the left boundary and a point at the bottom boundary were assigned with a fixed hydraulic pressure, while the rest of the model's boundary were impervious.

The following details regarding the three simulation models are given in Figures 3.10 to 3.12: (i) the hydraulic boundary conditions, (ii) the hydraulic heads obtained from the DDA method (indicated by the numbers prefixed with D), (iii) the hydraulic heads obtained from the UDEC method (indicated by the numbers prefixed with U), and (iv) the percentage of difference between the two solutions (indicated by the numbers in parentheses).

Model 1

Figure 3.10 Case 1: the simulated hydraulic heads at steady state

Model 2

Figure 3.11 Case 2: the simulated hydraulic heads at steady state

Model 3

Figure 3.12 Case 3: the simulated hydraulic heads at steady state

As can be seen from Figures 3.10 to 3.12, the DDA solutions are in good agreement with the UDEC results. In the three simulation cases, only 5% of the nodes shows different readings, and the largest percentage of difference is merely 0.01%.

Laboratory data vs DDA simulation results

The following numerical example is based on a laboratory experiment presented in Gao (1994). Figure 3.13 outlines the setting of the experiment. The test model comprised 28 rigid concrete blocks. The block arrangement resulted in two perpendicular sets of fracture. All fractures has a uniform aperture of 400 μm , and are separated from each other by a uniform spacing of 20 mm. The side and the bottom boundaries of the model were restrained from normal displacement, and the effect of self-weight was not considered in the seepage analysis. In terms of the hydraulic boundary conditions, the model's left-hand side boundary was assigned with a constant water head of 2.9 m, while a point at the lower right corner of the model was assigned with a constant velocity of 5 cm/s. The rest of the boundaries were assumed to be impervious.

Figure 3.13 The outline of the laboratory experiment (Gao 1994)

By adopting the same model details and analysis parameters, the aforementioned laboratory test was simulated using the proposed DDA seepage analysis extension. As shown in Figure 3.14, the simulated hydraulic heads along the model's bottom boundary are fairly consistent with the measured data obtained from the experiment.

Figure 3.14 A comparison between the measured and the simulated hydraulic heads

DDA vs UDEC transient flow analyses results

To verify the accuracy of the time function in the proposed DDA seepage analysis algorithm, a transient-state seepage problem was simulated using the DDA and the UDEC methods. As shown in Figure 3.15, the numerical model consists of 48 discrete blocks, each measuring 20 mm x 20 mm. A uniform, constant aperture of 400 μm was assumed along all block joints. The model boundaries were mechanically fixed to restrict lateral movements of the boundary blocks. No other mechanical loading was considered and the effect of block self-weight was ignored in the seepage analysis.

At time step zero ($t=0$), all nodal points in the simulation model were assigned with a uniform hydraulic head of 0.2 m. From $t=1$ onwards, a well with a constant influx

rate of 0.001 m/s was introduced to Node A. Except the hydraulic head along the four boundaries were maintained at 0.2 m throughout the seepage analysis, the hydraulic heads of all other nodes varied with time as the result of the fluid withdrawal at Node A.

Figure 3.15 The outline of the numerical model

Figure 3.16 shows the simulated hydraulic heads of Nodes 1 to 4 as a function of time. It can be seen that the DDA results are reasonably close to the UDEC solutions in terms of the amplitude of oscillation, and the number of time steps required to achieve a steady-state flow. This indicates that the time function is appropriately modeled in the proposed seepage analysis algorithm.

a)

b)

c)

d)

Figure 3.16 The resultant hydraulic heads at nodes 1 through 4, obtained from both the proposed DDA flow algorithm, and the UDEC transient flow analysis

3.4 The semi-coupled solution scheme for hydro-mechanical analysis

Figures 3.17 a) and b) outline the general workflow of a coupled, and an uncoupled solution schemes, following the nomenclature of Wang (2000). There are fundamental differences between the two schemes in the way they model a seepage problem. The coupled solution scheme comprises two major subroutines: (i) a subroutine for the seepage analysis; and (ii) a subroutine for the coupling mechanical analysis. The approach employed by the uncoupled solution scheme is relatively simple as it does not comprise a hydraulic analysis subroutine. Instead, pore pressure is assigned to the pre-defined fluid-block interface directly before every mechanical analysis (Wang 2000, Cappa 2005).

The absence of the hydraulic analysis function in the uncoupled scheme makes it a more efficient approach compared to the coupled scheme. However, without the hydraulic analysis, fluid mechanics cannot be modeled. Hence, the uncoupled scheme is only suitable for problems where the hydraulic pressure and boundary can be pre-specified, and would not vary over time. It is shown in an existing study (Jiang et al. 2012) that simulating a seepage problem via an uncoupled solution scheme tends to underestimate the overall block displacements, and the influence extent of a water injection point. For better accuracy, a seepage analysis should take into account: (i) the fluid dynamics, (ii) the block mechanics, and (iii) the interaction between the two processes. In this context, the coupled scheme is more suitable than the uncoupled scheme for seepage modeling, even though its computational cost is comparatively higher.

Figure 3.17 The outline of the a) coupled, b) uncoupled and c) semi-coupled solution schemes

To reduce the computational cost of the coupled solution scheme, a semi-coupled solution scheme is proposed in this section. As can be seen from Figure 3.17 c), the workflow of the semi-coupled solution scheme is identical to that of the coupled solution scheme. The only difference between the two solution schemes is that, under the coupled scheme, the hydraulic aperture is updated at the beginning of every time step, while under the semi-coupled scheme, the hydraulic aperture is kept constant throughout a hydro-mechanical analysis. In other words, the semi-coupled solution scheme distinguishes the hydraulic aperture, i.e. the size of a water pathway, from the mechanical aperture, i.e. the actual size of a rock joint. Further elaboration on the subject of mechanical and hydraulic apertures can be found in Renshaw (1995). According to the semi-coupled scheme, the change in the mechanical aperture does not affect the size of the water pathways. Figure 3.18 depicts the concept of hydraulic and mechanical apertures adopted in the semi-coupled solution scheme, while Table 3.3 shows the relationships between the two apertures under different solution schemes.

Figure 3.18 The concept of hydraulic and mechanical apertures assumed in a semi-coupled solution scheme

Table 3.3 The concept of hydraulic and mechanical apertures in the three solution schemes

Solution schemes	Mechanical aperture (m.a.)	Hydraulic aperture (h.a.)
Coupled	Determined from vertex location	$h.a. = m.a.$
Uncoupled		Not applicable
Semi-coupled		Fixed at a specific value

3.4.1 An overview of the simulation model

A case study is outlined in the following section to verify the applicability and reliability of the proposed semi-coupled solution scheme. First, a seepage problem is solved via the coupled and the semi-coupled solution schemes. Then, the computational speed and the simulation results of the two approaches are compared and evaluated.

Figure 3.19 and Table 3.4 show the configuration of the brick tunnel model and the DDA parameters employed in the current case study. The model is 4.071 m x 4.060 m in size, and consisting of 1215 discrete blocks. Each full block in the tunnel model measuring 220 mm x 71 mm, corresponding to the size of a typical clay brick-mortar

unit. The point of origin (0, 0) is set at the bottom left of the model, with the positive direction of the x - and y -axes pointing to the right, and top respectively. A circular tunnel opening is located at the center of the model. The tunnel is 1.030 m in diameter, and the centroid is positioned at coordinates (2035.5, 2030.0).

At the beginning of the simulation, an initial stress of $\sigma_{yy}=2.2$ MPa was assigned to the model's left and right boundaries, while $\sigma_{xx}=4.4$ MPa was assigned to the model's top and bottom boundaries. After the whole system had reached equilibrium, the simulation of water injection began and the following displacement boundary conditions were introduced: the left and the right boundaries were restrained from horizontal displacement, the top boundary was restrained from vertical displacement, and the bottom boundary was fixed.

Figure 3.19 The configuration of the brick tunnel model

Table 3.4 DDA analysis parameters used in the brick tunnel model

<u>Analysis Parameters</u>	<u>Input value</u>
Total number of time steps	10, 000
Upper limit of time interval	1s per time step
Assumed maximum displacement ratio	0.0009
Block density (kg/m ²)	1800
Young's modulus (GPa)	3
Poisson's ratio	0.3
Joint stiffness (GPa)	30
Storage term (m/s)	0
Source/ Sink term	0.02
Minimum hydraulic aperture (mm)	0.1
Number of seepage nodes	2140
Number of seepage joints	3736

Throughout the analysis, a constant hydraulic aperture of 0.1 mm was assumed for models subjected to the semi-coupled solution scheme. For models subjected to the fully coupled scheme, a variable hydraulic aperture with an initial size of 0.1 mm was assumed for all block joints.

The pore pressure in the tunnel opening varied with time, in the following order:

1. $100 \leq t \leq t_a$: Pore pressure increases at a steady rate of r_f .
2. $t_a < t \leq t_b$: Pore pressure decreases to P_f , at a steady rate of r_f .
3. $t_b < t \leq 10000$: Pore pressure is maintained at P_f .

where t_a denotes the time when fluid injection stops and the peak pore pressure, P_{peak} is achieved, r_f denotes the rate of fluid pressurization, P_f denotes the final pore pressure maintained at the tunnel wall, and t_b represents the time when P_f is first achieved. As shown in Table 3.5, four different combinations of t_a - r_f - P_f were simulated. Comparisons were made between the coupled and the semi-coupled solution schemes in terms of: (i) the computational efficiency, (ii) the simulated pore

pressures at specific time steps, (iii) the simulated block displacements as a function of time, and (iv) the maximum simulated block displacements.

Table 3.5 Details of the simulation models

Model	Solution scheme	Case	t_a	r_f	P_f (MPa)
1	Coupled	1c	850	10	5
	Semi-coupled	1s			
2	Coupled	2c	850	50	5
	Semi-coupled	2s			
3	Coupled	3c	2000	10	10
	Semi-coupled	3s			
4	Coupled	4c	2000	50	10
	Semi-coupled	4s			

3.4.2 Computational efficiency

At the beginning of the numerical simulation, it was assumed that all block joints have a uniform hydraulic aperture of 0.1 mm. The coupled scheme updates the hydraulic aperture at all subsequent time steps. On the other hand, the semi-coupled scheme omits the aperture updating process by assuming a constant hydraulic aperture throughout the analysis.

Table 3.6 compares of efficiency between the coupled and the semi-coupled solution schemes. It is shown that the semi-coupled scheme requires 40% less CPU time than the coupled scheme to complete one run of the seepage analysis. In other words, the omission of the aperture updating process (which includes the computation of aperture change and the update of seepage joints' transmissivity) has improved the computational efficiency of the hydro-mechanical model by 40% in the current example.

Table 3.6 A comparison of efficiency between the coupled and the semi-couple solution schemes

CPU time consumed in seepage analysis (ms per time step)		Efficiency improvement $\frac{(A-B)}{A} \times 100\%$
Coupled (A)	Semi-coupled (B)	40%
5	3	

3.4.3 Resultant pore pressure at specific time steps

Figure 3.20 shows the pore pressure profiles of Models 1 to 4, at time steps 2000 and 10000. The pore pressure profiles are taken at the mid-length, along the y-axis of the respective simulation models. For ease of comparison, the following details are excluded from the pore pressure profiles: (i) the pore pressure variation of the top half of the model, which is virtually identical to that of the bottom half due to the model's symmetry; and (ii) the pore pressure around the tunnel opening, which is equal to P_{peak} at time step 2000, and P_f at time step 10000 for all models.

From Figure 3.20, it can be seen that for nodal points near the tunnel opening, the pore pressures predicted by the semi-coupled scheme are always slightly higher than those predicted by the coupled scheme. The aperture-time relations adopted by the two solution schemes could explain this observation. Theoretically, the aperture of the seepage joints in the vicinity of the tunnel will enlarge with increasing hydraulic pressure applied at the tunnel wall (Indraratna and Wang 1996). While the coupled solution scheme takes into account this pressure-aperture interaction, the semi-coupled solution scheme does not. Consequently, the apertures near of the water source assumed by the semi-coupled scheme are lower, and the pore pressure are higher than those predicted by the coupled scheme.

In general, the pore pressures predicted by the semi-coupled scheme appears to be identical to those predicted by the coupled scheme – especially for nodal points located away from the water source. The closeness between the pore pressures predicted by the two schemes indicates that most block joints did not experience significant aperture change for 10000 s of simulated time, and under the influence of different r_f , P_{peak} and P_f .

3.4.4 Block displacements as a function of time

For each model, the displacement profiles of six measurement points, predicted by both the coupled and semi-coupled solution schemes, were recorded and analyzed. The locations of the six measurement points are given in Figure 3.19. Figures 3.21 and 3.22 show the displacement profiles of measurement point No.1, for the vertical and the horizontal directions. In general, the instantaneous displacements predicted by the semi-coupled scheme are in good agreement with those predicted by the coupled scheme, and the displacement profiles obtained from both solution schemes are identical in terms of the variation trend.

Table 3.7 summarizes the average difference in (i) the maximum horizontal displacements, (ii) the maximum vertical displacements, (iii) the final horizontal displacements, and (iv) the final vertical displacements of the six measurement points, predicted by the coupled and the semi-coupled schemes. The maximum difference between these displacement parameters predicted by the two scheme is less than 6%.

Figure 3.20 Pore pressure at nodal points located along $x=2035\pm5$ mm, Models 1 to

Figure 3.21 Vertical displacement as a function of time for measurement point 1, Models 1 to 4

Figure 3.22 Horizontal displacement as a function of time for measurement point 1, Models 1 to 4

Table 3.7 Average difference in the displacements of six measurement points

Model	Solution scheme	Difference in maximum displacement (%)		Different in final Displacement (%)	
		U_x	U_y	U_x	U_y
1	Coupled	5.91	1.01	5.92	1.01
	Semi-coupled				
2	Coupled	2.29	0.14	2.27	0.14
	Semi-coupled				
3	Coupled	4.81	0.45	4.81	0.45
	Semi-coupled				
4	Coupled	1.02	0.23	1.03	0.23
	Semi-coupled				

3.4.5 Concluding remarks for case study

A semi-coupled solution scheme is proposed in this section to provide a lower computational cost alternative to the coupled solution scheme which is conventionally applied to the DDA seepage analysis. The only difference between the two solution schemes is that, while the coupled scheme updates the hydraulic aperture at the beginning of every time step, the semi-coupled scheme omits this aperture updating process to save computational time.

A case study is presented to verify the reliability of the proposed semi-coupled solution scheme. First, a brick tunnel model was simulated using the semi-coupled and the coupled solution schemes, then the results obtained from the two schemes were compared and evaluated. The following findings were noted from the case study: (i) by omitting the aperture updating process, the computational time engaged in one run of the seepage analysis can be reduced considerably; (ii) the pore pressures and block displacements predicted by the semi-coupled and the coupled schemes for 10000 time steps are identical.

In view of these simulation results, the semi-coupled solution scheme appears to be a reliable alternative to the coupled scheme for quasi-static problems that do not involve large-scale block displacements or significant aperture change.

3.5 Chapter summary

In this chapter, the background of the hydro-mechanical analysis algorithm employed in the current study is established. The formulation and the workflow of the algorithm are also explained. A number of simulation cases, of which the analysis results are consistent with existing theories, are also presented to verify the reliability of the proposed hydro-mechanical analysis algorithm.

The conventional coupled hydro-mechanical model assumes the hydraulic aperture to be a variable that needs to be updated in every time step. In an effort to improve the computational efficiency of the conventional model, the current study showed that the CPU time consumed in a seepage analysis could be noticeably reduced if the hydraulic aperture is treated as a constant, rather than a variable throughout the analysis. This finding lead to the introduction of a new solution scheme featuring a constant hydraulic aperture, which is termed the “semi-coupled” scheme.

In general, fluid flow and joint deformation are considered as a coupled process and are commonly simulated by a coupled hydro-mechanical model. However, at very low injection rate or under high effective pressure, the fluid pressure in joint is unable to counter the confining stress and cause meaningful change to the hydraulic aperture. In such cases, the semi-coupled solution scheme may be adopted to promote computational speed.

Chapter 4. A conceptual model for the simulation of stochastic flow behaviors using DDA

4.1 Introduction

Today, most numerical methods are still relying on the equivalent continuum model to simulate the flow condition of a geological formation. Such an approach can be unrealistic and may lead to misleading predictions of the hydro-geomechanical behaviors. The objective of the current chapter is to introduce a stochastic flow model to the discontinuous deformation analysis (DDA) method. The appeal of the approach lies in its simplicity and realism. It predicts the variations of a hydraulic conductivity field or an aperture profile using a probabilistic framework, and utilizes such predictions in the DDA hydro-mechanical analysis.

The organization of chapter 4¹ is as summarized in Figure 4.1. First, the importance of the stochastic modeling approach is discussed and various stochastic modeling techniques are reviewed in Section 4.2. Section 4.3 provides a comprehensive overview to the framework of the proposed stochastic flow model. In Section 4.4 to 4.7, four numerical cases are presented to demonstrate the capability of the proposed method in modeling stochastic hydraulic conductivity and aperture distributions. The compatibility of the generated stochastic fields and the DDA hydro-mechanical model is also verified through the numerical studies. Lastly, in Section 4.8, a summary of the works presented in the current chapter is provided.

This chapter is based on the following manuscripts of the author:

1. Choo, L. Q., Zhao, Z. Y., Chen, H. M. (Under review). Choo, L. Q., Zhao, Z. Y., Chen, H. M. (Under review). Modelling the stochastic flow behaviours of geological formations using the discontinuous deformation analysis method. *Engineering Geology*.
2. Choo, L. Q., Zhao, Z. Y., Chen, H. M. (2014). *Hydro-Mechanical Analysis of Fluid Flow through Heterogeneous Conductivity Fields by Discontinuous Deformation Analysis*. Paper presented at the 14th World Conference of Associated research Centers for the Urban Underground Space, South Korea, Seoul.

Figure 4.1 An outline of Chapter 4

4.2 Theoretical groundings for stochastic hydro-geological modeling

Material and joint property distributions in rock structures are non-uniform and irregular in spatial variation (Neuman 1982, Molz et al. 2004). Diversified grain size, erratic mineral dispersion in rock blocks, and the existence of discontinuities within a rock structure are some of the major factors contributive to the stochastic property distributions (Al-Faqi 2000, Eaton 2006). As a consequence of these irregularities in material and joint properties, hydraulic properties such as the porosity, aperture and hydraulic conductivity vary spatially in a complex, random manner (Neuman 1997).

Numerous field and laboratory studies have been conducted to assess the hydraulic property distribution in different aquifers. Field observations show significant spatial variability in the geological flow conditions at various scales. For instance, the hydraulic conductivity distribution in a vertical cross-section of Columbus Air Force Base, USA is highly heterogeneous in terms of large-scale variation (Adams and Gelhar 1992). Borden site in Canada, despite being widely accepted as a homogeneous, equivalent porous media, has a comparatively dispersed hydraulic conductivity distribution at a scale of 5×10^{-7} to 2×10^{-4} m/s (Sudicky 1986, Allen-King et al. 2003, Eaton 2006). The hydraulic conductivities of the igneous granite at Bukit Timah, Singapore, though insignificantly small in values, exhibit a

considerable dispersion ranging between 10^{-11} and 10^{-6} m/s, at the depth of 20 to 150 m below the ground surface (Zhao 1998). Even in the case of a single fracture, a considerable amount of laboratory studies have proven that fluid does not spread through a fracture evenly as presumed by the equivalent continuum model, but rather, fluid flows through a limited number of water-bearing channels with highly variable permeability (Tsang and Tsang 1987, Moreno et al. 1988, Cacas et al. 1990).

The non-uniform flow condition within a geological formation and the intricacy associated with it challenge the validity of the equivalent continuum approach commonly applied in numerical simulations. Assuming a single conductivity value for an entire geological model has found to be unrealistic and contributive to misleading simulation results (Theis 1967, Smith 1981, Elfeiki 2000). Furthermore, representative parameters such as the effective hydraulic conductivity and the equivalent aperture derived from small-scale field or experimental data cannot adequately reflect a large-scale flow condition in most geological settings (Sanchez-Vila et al. 2006, Berg and Illman 2013). In view of these concerns, a groundwater flow problem is best simulated using a nondeterministic framework of analysis such as a stochastic approach (Freeze 1975, Neuman 1982, Molz et al. 2004). Contrary to the equivalent continuum model which relies on a representative parameter and the representative element volume (REV) concept to account for a hydraulic property, the stochastic approach expresses a hydraulic property as a stochastic, autocorrelated system derived from pre-defined statistical descriptions.

In the past few decades, numerous stochastic flow models have been proposed to simulate the parametric variation of various hydro-geological properties. One of the most influential methods is the Nearest Neighbor Model (NNM) introduced by Smith and Freeze (1975), based on the works of Whittle (1954), and further developed by Baker (1984). NNM is capable of generating unique, stochastic and spatially autocorrelated conductivity fields based on simple input parameters. The definition of the REV is not required in NNM, hence making it less complicated to be programmed for applications to various numerical models. In terms of usefulness, the capability and efficiency of NNM in generating plausible stochastic hydraulic

conductivity fields have been recognized in several literatures (Smith and Freeze 1979b, Baker 1984, Hopmans et al. 1988).

In a later study conducted by Moreno et al. (1988), a stochastic model is introduced to predict the aperture variation in a single fracture. The two-dimensional model is identical to the NNM model, except it simulates the aperture profile and assumes an exponential auto-covariance relation between the predicted data, while the NNM simulates the stochastic hydraulic conductivity field and assumes a first-order autocorrelation function. A comparison between a simulated aperture profile (Moreno et al. 1988), and an actual fracture profile presented in Pyrak et al. (1985), shows an acceptable degree of resemblance.

Even though DDA is widely accepted as a suitable method for hydro-geological simulations, works related to the stochastic flow modeling are still very limited at the current stage. A framework for stochastic flow simulations using the DDA model has not been presented in detail. Motivated by this gap and the challenges associated with determining a uniform value that can rationally represent the flow condition of a simulation domain, a stochastic flow model is proposed in this chapter as an extension to the DDA method. Figure 4.2 outlines the general procedures involved in the simulation of a hydro-geological problem using the proposed stochastic flow model. First, a pool of random variables is generated from a set of pre-defined statistical descriptions. The random variables will then be assigned as the input parameters to a DDA model to characterize the heterogeneous flow conditions. Consequently, the influences of the random input parameters on the hydraulic heads, pore pressures, flow rates and block displacements can be evaluated through the DDA hydro-mechanical analysis.

Figure 4.2 Procedure of simulating a hydro-geological problem using the proposed stochastic flow model

4.3 Modeling a stochastic hydraulic property distribution

The proposed stochastic flow model requires a flow domain to be discretized into a finite number of cells, all with equalized side lengths. Each cell is to be assigned with a random variable. The generation of the random variables is straightforward. First, a large number of random values are generated by a random number generator seeded with distinctive runtime values. The random values will then be converted into standard Gaussian variables. For a flow domain consisting of n rows and m columns of discretized cells, p (where $p = n \times m$) number of Gaussian variables would be required. Two conversion methods are introduced in the proposed stochastic flow model and the system will randomly select either method to perform each conversion. The random variable generation-conversion process consists of the following steps.

Method 1: by using the Central limit theorem (Yang and Robinson 1986):

1. Define p , the number of random variables, Z to be generated.
2. Assume a continuous uniform distribution $U(0,1)$ for Z , hence mean $\mu=0.5$, standard deviation $\sigma = 1/\sqrt{12}$, and the z -score is equivalent to

$$Z = \frac{\bar{X} - 1/2}{1/\sqrt{12n}}$$

in which $\bar{X}$ is the mean of n random numbers $X_1, X_2, X_3, \dots, X_n$.

3. For simplicity, use $n=12$. Hence,

$$Z = 12\bar{X} - 6 = \sum_{i=1}^{12} X_i - 6$$

4. Generate 12 independent random numbers $X_1, X_2, X_3, \dots, X_{12}$.
5. Compute Z_j where $j = 1, 2, 3, \dots, p$.
6. Return to Step 4 if $j < p$, else end the process.

Method 2: by using the Polar method (Sheldon 2002):

1. Define p , the number of random variables, Z to be generated.
2. Generate two random numbers V_1 and V_2 from a continuous uniform distribution $U(0,1)$.
3. Let $U_1 = 2V_1 - 1$ and $U_2 = 2V_2 - 1$. Hence U_1 and $U_2 \in U(-1,1)$. Compute S where $S = U_1^2 + U_2^2$.
4. If $0 \leq S \leq 1$, proceed to the next step, else go back to step 2.
5. Compute Z_1, Z_2 where

$$Z_1 = \sqrt{\frac{-2\ln S}{S}} U_1$$

$$Z_2 = \sqrt{\frac{-2\ln S}{S}} U_2$$

6. Repeat Step 2 through 5 until p number of random variables are obtained.

After the random variables are generated, converted and distributed to the discretized cells, the autocorrelation process begins. The autocorrelation function employed by the proposed stochastic flow model is formulated based on the first-order autoregressive function (Smith and Freeze 1979b). During the autocorrelation process, the value of the random variable in each cell is re-adjusted according to the value of the random variables in the neighboring cells. Denoting the uncorrelated random variable as ε and its autocorrelated form as Y , the autoregressive relation between the random variables can be expressed as

$$Y_{i,j} = \alpha_x/r_x(Y_{i-1,j} + Y_{i+1,j}) + \alpha_z/r_z(Y_{i,j-1} + Y_{i,j+1}) + \eta\varepsilon_{i,j} \quad (4.1)$$

where subscript $i=1, 2, 3, \dots, c$ denotes the column number and subscript $j=1, 2, 3, \dots, r$ denotes the row numbers of a specific cell. Notations α_x and α_z in the equation represent the autoregressive parameters for the horizontal and vertical directions, while r_x and r_z denote the number of cells connected to cells i, j in the respective directions. Notation η is a factor related to σ_Y by

$$\eta = \sigma_Y \left[\frac{\alpha_x^2 \rho(2,0)}{8} + \frac{\alpha_z^2 \rho(0,2)}{8} + \frac{\alpha_x^2}{8} + \frac{\alpha_z^2}{8} - \alpha_x^2 \rho(1,0) - \alpha_z^2 \rho(0,1) + \frac{\alpha_x \alpha_z \rho(1,1)}{2} + 1 \right]^{\frac{1}{2}} \quad (4.2)$$

in which ρ denotes the correlation coefficient

$$\rho(a,b) = \frac{\sum_{i=1}^{m-a} \sum_{j=1}^{n-b} (Y_{i,j} - \mu_Y)(Y_{i+a,j+b} - \mu_Y)}{\sum_{i=1}^m \sum_{j=1}^n (Y_{i,j} - \mu_Y)^2} \quad (4.3)$$

where a , b represent the lag number in the x - and z -directions respectively. On the other hand, the autoregressive parameter, α for each direction can be estimated by

$$\alpha = 16(16 + \pi\Delta/r_0)^{-1} \quad (4.4)$$

where Δ denotes the size of the discretized cell, and r_0 represents the correlation distance (Bakr et al. 1978a) or integral scale (Smith and Freeze 1979b). r_0 is assumed to be equal to the area beneath graph $\rho(r)$ plotted against r before the graph first crosses the horizontal axis, or simply

$$r_0 = \int_0^m \rho(r) dr \quad (4.5)$$

where m is the first intersection point between graph $\rho(r)$ and line $\rho(r)=0$.

The first order autoregressive relation between the discretized cells is illustrated in Figure 4.3. For a system consisting of p cells, Equation (4.1) can be expressed in the matrix form as

$$[Y] = [W][Y] + \eta[\varepsilon]$$

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_p \end{bmatrix} = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,p} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,p} \\ w_{3,1} & w_{3,2} & \cdots & w_{3,p} \\ \vdots & \vdots & \ddots & \vdots \\ w_{p,1} & w_{p,2} & w_{p,3} & w_{p,p} \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_p \end{bmatrix} + \eta \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \\ \varepsilon_p \end{bmatrix} \quad (4.6)$$

in which $w_{k,l}$ denotes a weighted spatial lag operator, where subscript k and l are the cell numbers. Note that $w_{k,l}$ is equal to $-\alpha_x/r_x$ if cells k and l are continuous in the

horizontal direction, and $w_{k,l} = \alpha_z/r_z$ if the continuity is in the vertical direction. In all other cases $w_{k,l}$ is equal to 0.

Figure 4.3 The first order autoregressive relation between discretized cells

As illustrated in Figure 4.4, it is necessary to assume a larger domain for discretization, i.e. to ensure that the discretized cells are extended beyond the model boundaries, so as to avoid the truncation effect at the model boundary. This way, the need to correlate the values in the near-boundary cells can be eliminated (Hopmans et al. 1988).

Figure 4.4 Relationships between DDA model and the discretized cells for stochastic simulation

Note that our objective is to find a solution for the $[Y]$ matrix that simultaneously satisfies: (i) the pre-determined mean, μ_Y and standard deviation, σ_Y and, (ii) the autoregressive function as defined by Equation (4.6). In order to avoid the challenges and inefficiency associated with inversing and storing of large matrices, an iterative approach is adopted to determine a solution that fulfills the two criteria. In addition, since η is related to the correlation coefficients, of which the values can only be determined when all elements of $[Y]$ matrix are in place, another iterative process is required to predict η with respect to $[Y]$ by using Equation (4.2), and re-adjust $[Y]$ according to the new η . A two-fold convergent solution is considered to have achieved when the difference in the values of $[Y]$ (obtained from the first iterative process) and η (obtained from the second iterative process) between any two successive trials is lower than a certain threshold value, respectively.

The aforementioned autocorrelation process yields normally distributed, convergent Y values with a zero mean and a pre-defined standard deviation σ_Y , i.e. $Y_i \in N(0, \sigma_Y)$. Adding μ_Y to each element of $[Y]$ gives rise to $Y_i \in N(\mu_Y, \sigma_Y)$. To simulate a lognormally distributed property $\hat{Y}$, it is assumed that $Y = \ln \hat{Y}$. Hence, by inversing the natural logarithm function $Y, \hat{Y}_i \in LN(\mu_{\hat{Y}}, \sigma_{\hat{Y}})$ can be obtained. The relationships between $\mu_{\hat{Y}}, \sigma_{\hat{Y}}$ and μ_Y, σ_Y are such that

$$\begin{aligned}\sigma_Y &= \sqrt{\ln\left(\frac{\sigma_{\hat{Y}}^2}{\mu_{\hat{Y}}^2} + 1\right)} \\ \mu_Y &= \ln(\mu_{\hat{Y}}) - \frac{\sigma_Y^2}{2}\end{aligned}\tag{4.7}$$

The last step of the stochastic flow modeling is to allocate non-conductive zone to the stochastic field. The algorithm works as follows. First, the random variables are arranged in a descending order. A threshold value is then determined based on the pre-defined percentage of non-conductive zone, P_o . At the end of the stochastic field generation, assignment and correlation processes, cells with random variables below the threshold value will be identified as non-conductive. During the DDA hydraulic analysis, the non-conductive area is assigned with a near-zero hydraulic conductivity and a near-zero aperture.

Consistent to the finding of existing laboratory studies, the proposed stochastic flow model assumes the hydraulic conductivity of a flow domain to be lognormally distributed (Freeze 1975, Smith and Freeze 1979b, Neuman 1982, Sudicky 1986), while the aperture profile to follow either a normal (Law 1944, Smith 1981, Neuman 1982, Hakami 1995, Hakami and Larsson 1996), or a log-normal distribution function (Moreno et al. 1988, Cacas et al. 1990). Figure 4.5 summarizes the procedure involved in the generation of a stochastic hydraulic conductivity field, which consists of the following nine major steps.

STEP 1: Prompt user to provide the eight input parameters:

- r_n : total number of realizations to be generated,
- n, m : row and column numbers of the discretized cells,
- μ_k, σ_k : mean and standard deviation of the hydraulic conductivity K ,
- α_x, α_z : autoregressive factors for the horizontal and vertical directions,
- P_o : percentage of non-conductive cells.

- STEP 2:** Discretize the flow domain into p cells ($p=n \times m$).
- STEP 3:** Generate and distribute the p numbers of Gaussian variables ε_i to each cell. Construct $[\varepsilon]_{p \times 1}$ arrays accordingly.
- STEP 4:** Construct $[W]_{p \times p}$, the correlation arrays according to α_x , α_z and the cell positions.
- STEP 5:** Solve $[Y]_{p \times 1}$ in Equation (4.6) (Iteration 1), and update η in accordance to the new $[Y]$ (Iteration 2).
- STEP 6:** Re-adjust $[Y]$. Return to STEP 5 if the difference between two successive $[Y]$ or η values is higher than the respective thresholds. Otherwise, proceed to the next step.
- STEP 7:** Add μ_Y to each Y_i to yield $Y_i \in N(\mu_Y, \sigma_Y)$
- STEP 8:** Inverse Y_i to yield $K_i \in LN(\mu_K, \sigma_K)$
- STEP 9:** Identify the non-conductive cells and re-assign each one with $K_i \approx 0$. Repeat steps 3-8 until “ r_n ” number of realizations are obtained.

Figure 4.5 Stochastic generation process of hydraulic conductivity field

Note that a similar procedure applies to the generation of stochastic apertures, e_i . To simulate a lognormally distributed aperture field, simply consider $K_i = e_i$. To generate a normally distributed apertures, consider $Y_i = e_i$ and skip the 8th step in the algorithm. For an identical set of input parameters, an infinite succession of unique, stochastic fields can be generated. In the nomenclature of the Monte Carlo approach, each representation of a stochastic field is termed as a realization. The simulation results of each realization can be collected, summarized and statistically evaluated to estimate the flow condition of an aquifer, to investigate the effect of heterogeneity on the output variables (e.g. hydraulic heads and pore pressures) and to predict the effective conductivity for a heterogeneous flow domain (Smith and Freeze 1979b, Dagan 1982, Gómez - Hernández and Gorelick 1989).

4.4 Simulation of stochastic hydraulic conductivity fields

Consider a flow domain with a stochastic hydraulic conductivity field of which the statistical descriptions are known. To predict the spatial variability of the hydraulic conductivity across the flow domain, Monte Carlo technique can be adopted. First, multiple realizations, each fulfils the predefined statistical descriptions is stochastically generated and assigned to the flow domain. Then, with the help of DDA seepage analysis extension, the fluid transport process within the flow domain is computed. For each realization one gets a set of space-dependent output variables. The ensemble of output variables obtained from all realizations can be statistically analyzed thus reflecting the variation range of the simulation results.

A numerical example is presented in the following section to demonstrate the aforementioned stochastic flow modeling process. Figure 4.6 shows a DDA model consisting of 400 discrete blocks. Each block is characterized by a unique hydraulic conductivity. The statistical descriptions of the stochastic conductivity field are summarized in Table 4.1.

Figure 4.6 Two-dimensional DDA model for stochastic flow analysis

Table 4.1 Input parameters applied the generation of stochastic conductivity field

<u>Analysis Parameters</u>	<u>Input Values</u>
Number of columns, m	20
Number of rows, n	20
Number of realizations, r_n	50
Mean, μ_K (m/s)	4.58
Standard deviation, σ_K (m/s)	2.79
Autoregressive factor in the x direction, a_x	0.5
Autoregressive factor in the z direction, a_z	0.4

4.4.1 The statistically generated hydraulic conductivity fields

A total of 50 Monte Carlo realizations were produced through the process outlined in Figure 4.5. At the end of the generation process, each DDA block is assigned with a lognormally distributed, spatially autocorrelated conductivity variable, K_i . Figure 4.7 shows 25 of the 50 realizations produced. The average mean and standard deviation obtained from the 50 random fields are 4.33 m/s and 2.23 m/s respectively, which are fairly close to the pre-defined values: 4.58 m/s and 2.79 m/s. A plot of the probability density functions of K for different number of realizations, as illustrated in Figure 4.8, shows that K always comply with the theoretical lognormal distribution (Freeze 1975, Smith and Freeze 1979b, Neuman 1982, Sudicky 1986). These observations imply the capability of the proposed algorithm in generating conductivity fields that fulfill the pre-defined statistical descriptions.

The dispersion of a stochastic dataset is often evaluated through autocorrelation plots (Freeze 1975, Smith and Freeze 1979a, Smith and Freeze 1979b, Hopmans et al. 1988). Figure 4.9 shows the mean autocorrelation plots for $\ln K$ in the x - and z -directions. The autocorrelation function, which decay exponentially in both cases, corroborate the first order dependence relation (Smith and Freeze 1979b). On the other hand, Figure 4.10 depicts how r_n affects the mean autocorrelation function in the z -direction. Consistent to the finding in previous studies (Smith 1978, Smith and Freeze 1979a), it is shown that a greater number of realization yielded a mean autocorrelation function that closely approximates its theoretical form. These observations indicate that the first order dependence relation is appropriately expressed in the proposed stochastic model.

Figure 4.7 Stochastically generated hydraulic conductivity fields

Figure 4.8 Probability density functions of K for 10, 25 and 50 realizations

Figure 4.9 Autocorrelation function of $\ln K$ in the x - and z -directions

Figure 4.10 Autocorrelation function in the z direction for different number of realizations

The variation trend of a stochastic field is commonly evaluated through variograms. For ease of interpretation, a theoretical variogram is often fitted to an empirical variogram (Gringarten and Deutsch 2001). Taking realization No. 41 for example, the omni-directional variogram of $\ln K$, fitted by an exponential model, and the anisotropic variograms for the four directions, are given in Figures 4.11 (a) and 4.12 (a) respectively. Figures 4.11 (b) and 4.12 (b) shows the corresponding variograms constructed based on field measurements of $\ln K$ at the Columbus Air Force Base in Mississippi (Rehfeldt et al. 1992). The resemblance of the key features of Figures 4.11 (a), 4.12 (a) with those of Figures 4.11 (b), 4.12 (b) implies the realism of covariance structure adopted in the proposed model.

Figure 4.11 The omni-directional variogram of (a) a generated stochastic field^A and (b) an actual conductivity field^B

^A Generated using GeoR (Ribeiro Jr and Diggle 2009),

^B Adapted from Rehfeldt et al. (1992)

Figure 4.12 Anisotropic variograms of (a) a generated stochastic field^A and (b) an actual conductivity field^B

^A Generated using GeoR (Ribeiro Jr and Diggle 2009),

^B Adapted from Rehfeldt et al. (1992)

4.4.2 DDA hydraulic analysis and statistical evaluation of the analysis results

The following hydraulic boundary conditions were introduced to the DDA model prior to the hydraulic analysis: the top and the bottom boundaries were impervious, the left boundary was assigned with a constant hydraulic head of 0 m, and the right boundary was assigned with a constant hydraulic head of 100 m. To determine the hydraulic head of each block, the following equation is applied

$$H_i = \frac{\sum_{j=1}^q \frac{K_{ij} H_j}{L_{ij}^2}}{\sum_{j=1}^q \frac{K_{ij}}{L_{ij}^2}} \quad (4.8)$$

where K_{ij} and L_{ij} denote the hydraulic conductivity and the flow distance between two adjacent blocks i and j , while H_i , H_j denote the hydraulic head of the respective blocks. Figure 4.13 shows the hydraulic head distributions across the DDA model with hydraulic conductivity profiles as shown in Figure 4.7. As all models share the same boundary conditions and material properties, the differences between the head distribution profiles are solely due to any disparity in the hydraulic conductivity fields.

The hydraulic boundary conditions assumed in the current example induces a continuous flow across the model, from the left boundary to the right. Theoretically, the hydraulic head, H would increase linearly with increasing flow distance, x in the case of a uniform conductivity field. This linear relationship between H and x is depicted by the line graph in Figure 4.14. In the same figure, a box-and-whisker plot is presented to depict the H - x relationships acquired from the 50 generated stochastic fields. Presenting the two graphs in a same figure allow a direct comparison between the stochastic model solutions and the deterministic one. Besides, information such as the mean, median, quartiles, the minimum and the maximum resultant heads presented in the box-and-whisker plot provides the range, variation, dispersion and skewness of the hydraulic heads estimated from the stochastic model.

Comparing the stochastic solution to the deterministic solution, the following observations are noted: (i) moving towards the middle of the model, the stochastic solutions show increasingly significant dispersions from the mean values; (ii) the midspread (indicated by the size of the interquartile range) of the stochastic solution differs from the deterministic solution by ± 0.97 -32.93%; (iii) the total range of H (indicated by the distance between the maximum and the minimum H) of the stochastic solution differs from the deterministic solution by ± 4.02 -66.19%.

Figure 4.13 Hydraulic head distributions of the corresponding conductivity fields

Figure 4.14 Resultant hydraulic heads obtained from the stochastic flow model

Table 4.2 shows the percentage of difference between the results acquired from the first 25 realizations, and those acquired from all the 50 realizations. As can be seen, increasing the total number of realization, r_n from 25 to 50 results in less than 5% of difference in the values of quartiles, minimum and maximum H . Hence, it can be inferred that that any further increment in r_n would not have a substantial effect on the distribution of resultant heads.

Table 4.2 Percentage differences between the resultant hydraulic heads obtained from 25 and 50 realizations

$x(m)$	Average difference (%)			
	First Quartile	Third Quartile	Minimum H	Maximum H
0-5	3.14	3.90	0	4.86
6-10	4.71	2.22	5.13	0
11-15	1.88	0.71	1.73	0.74
16-20	0.06	0.37	3.00	0

Figure 4.15 shows how the standard deviation of the resultant hydraulic head, σ_H varies with the flow distance, x for different numbers of realization, r_n . It is apparent that lower r_n leads to a more erratic fluctuation in σ_H . At $r_n=50$, the graph became reasonably close to the theoretical parabolic shape (Freeze 1975, Smith and Freeze 1979a, Smith and Freeze 1979b). We can hence conclude that 50 realizations are adequate for the simulation of the current hydraulic problem.

Figure 4.15 The influence of total realization number on the standard deviation of resultant hydraulic heads

The following conclusions can be drawn based on the simulation results of the present numerical case:

1. The proposed stochastic flow model is capable of generating stochastic conductivity fields that closely approximate the pre-defined statistical descriptions and the theoretical correlation structure.
2. Simulation results obtained from multiple Monte Carlo realizations can be used to predict the distribution range and the variation structure of the output variables.
3. The output variables obtained from the stochastic model are visibly different from that obtained from the equivalent continuum model. The percentage of

difference varies as a function of distance from the nearest fixed head boundary. In the current numerical case, the maximum difference between the two solutions is 66.2%.

4.5 Simulating the aperture distributions of a natural fracture

The capability of the proposed stochastic flow model in simulating the aperture distribution of a natural fracture is verified through the following numerical example. The measurement data to be simulated was presented in Hakami and Larsson (1996). A laboratory technique, consisting of the following steps, was proposed in the study to measure the void geometry of a natural fracture. First, the fracture under study is injected with fluorescent epoxy resin before the fracture-containing specimen is cut into smaller segments. Then, with the aid of a stereo-microscope and an image analysis system, the aperture profile of each segment is analyzed. A fractured rock specimen was employed by the study to demonstrate the application of the proposed technique. The specimen, a 190 mm diameter and 410 mm long medium-grained granite core sample, was divided into eight segments as depicted in Figure 4.16. The fracture under study was located subparallel to the core axis of the specimen. The statistical descriptions of the apertures in each subarea, as estimated by the image analysis system are given in Table 4.3. The number of data point being assessed, p , the data mean, μ_Y and the standard deviation, σ_Y of the measured apertures were used as the inputs in the generation of the stochastic aperture profiles. It was assumed that each subarea consists of $\sqrt{p}$ rows and $\sqrt{p}$ columns of equalized cells, and contains apertures that follow a normal distribution.

Figure 4.16 Schematic diagrams illustrating the core sample and the eight sub-segments

Table 4.3 Statistical descriptions of the apertures in subarea A to H

Subarea	Number of data points	Mean aperture, μm	Standard deviation, μm	Median, μm		
				Measured	Predicted	% difference
A	5836	365	133	366	365	0.27
B	5825	307	133	317	306	3.47
C	3525	380	151	373	370	0.80
D	3840	349	145	338	340	0.59
E	3220	384	157	358	370	3.35
F	3468	358	150	331	360	8.76
G	2423	379	207	336	346	2.98
H	1679	360	231	321	340	5.92

The procedure involved in the generation of a stochastic aperture profile is similar to that adopted in the generation of a stochastic conductivity field. First, p number of Gaussian variables, ε_i are generated and distributed to the discretized cells. Next, the variable in each cell is spatially correlated to the variables in the surrounding cells using a first-order autoregressive function. The outputs of the correlation process is then added by μ_Y to yield normally distributed Y values with predefined mean, μ_Y and standard deviation, σ_Y . Lastly, the stochastic dataset is subjected to a statistical evaluation during which unsuitable entry will be discarded. For subarea A, the evaluation process consists of the following steps.

1. Compute the overall percentage of the following aperture ranges
 - a. <200 mm
 - b. 200-500 mm
 - c. >500 mm
2. If any of the following filtering conditions is satisfied, discard the present entry and repeat Steps 1 and 2.
 - a. the overall percentage of aperture <200 mm is more than 12%
 - b. the overall percentage of aperture 200-500 mm is less than 20%
 - c. the overall percentage of aperture >500 mm is more than 12%
3. If none of the filtering conditions is satisfied, accept the present entry as a suitable realization.

The above filtering conditions were established in accordance with the distribution of the measured data. For the other subareas, similar evaluation process with varying filtering conditions was applied to screen out the unsuitable dataset. In each case, the stochastic field generation process ended when a total of 20 suitable realizations were obtained.

Also acquired from the image analysis system were the probability density functions (p.d.f.) of the measured apertures in each of the eight subareas, as indicated by the solid lines in Figure 4.17. For comparison purposes, the p.d.f. of the simulated data are plotted as dashed lines in the same figure. It can be seen that the p.d.f. of the simulated data, averaged from the 20 realizations, are reasonably close to those of the measured data in terms of shape, skewness, peak positions and peak frequency. In addition, the medians computed from the simulated data are fairly agreeable to that of the measured data, as shown in Table 4.3. The average difference in median for subareas A-H is merely 3.27 %.

The results highlighted in the Figure 4.17 and Table 4.3 indicate that (i) the proposed stochastic flow model is capable of producing aperture profiles that fulfill the pre-defined statistical descriptions; (ii) measured data can be easily incorporated in the stochastic field generation process. From a different perspective, these results also imply that the accuracy and realism of a generated stochastic field is closely related to the amount of measured data available.

Figure 4.17 The probability density functions of the measured and simulated apertures

4.6 Modeling the stochastic aperture profile of a fractured medium

A numerical model is outlined in this section to simulate the aperture profile of a heterogeneous fracture, and to estimate the hydraulic heads and fluid flow rates across the fracture. Similar to the previous example, the fracture plane was partitioned into numerous cells, each of which was assigned with a unique aperture. The difference between the two examples is that, while the aperture is assumed to be normally distributed in the previous case, the current example models the aperture profile as a lognormal distribution function. The procedure of generating a stochastic aperture profile is as described in the previous section, with one additional, final step: by assuming $Y_i = \ln e_i$, inverse the natural logarithm function to obtain e_i , the lognormally distributed apertures. In this example, the two-dimensional stochastic field was discretized into 20 x 20 discretized cells, i.e. $p = 400$.

4.6.1 Predicting the spatial correlation structure of aperture profile

Figure 4.18 shows 20 aperture profiles generated from the input parameters given in Table 4.4. The magnitude of these input parameters are consistent to the aperture data presented in Moreno et al. (1988). Each row of the generated aperture profiles in Figure 4.18 differs from the other rows in terms of the magnitude of the autoregressive factor α . Aperture profiles A1-A4 correspond to an autoregressive factor of 0.2, while aperture profiles B1-B4, C1-C4, D1-D4, and E1-E4 correspond to an autoregressive factor of 0.3, 0.4, 0.5 and 0.6, respectively.

Figure 4.18 Stochastically generated aperture profiles with different autoregressive factor, α

Table 4.4 Input parameters for the generation of stochastic aperture profiles

<u>Analysis Parameters</u>	<u>Input Values</u>
Number of columns, m	20
Number of rows, n	20
Number of realizations, r_n	50
Mean, μ_e (μm)	1.7
Standard deviation, σ_e (μm)	0.43
Percentage of non-conductive cells, P_o	50

For comparison purposes, eight number of stochastic aperture profiles generated with identical input parameters by using a different numerical code, COVAR (El-Kadi 1986) are presented in Figure 4.19. Aperture profiles X1 to X4 correspond to an autoregressive factor, α of 0.3, while Y1 to Y4 correspond to $\alpha = 0.6$. The theoretical framework account for these stochastic aperture profiles can be found in Moreno et al. (1988). Comparing Figures 4.18 and 4.19, the variation trend of the aperture fields with identical α appears to be similar. It is apparent that lower α results in a more scattered stochastic field, and the spatial correlation of the apertures increases as α increases. The closeness between the two sets of results in terms of the variation trend implies that the correlation function is appropriately expressed in the proposed stochastic flow model.

Figure 4.19 Stochastic aperture profiles with $\mu = 1.7$, $\sigma = 0.43$ and α as defined in the diagram, generated using numerical code COVAR (Adapted from Moreno et al. (1988))

4.6.2 Simulation of non-conductive apertures

In reality, majority of the joints in a fractured medium is not water-conductive (Cacas et al. 1990) and the fluid flow paths may only makes up less than 20% of the fracture area (Moreno et al. 1988). Geological properties such as the aperture size, joint surface roughness, joint orientation, and the presence of infill, in association with fluid properties such as the density and the viscosity of the flowing liquid, may collectively affect the conductivity of a rock fracture. To produce a more realistic hydro-geological model, the proposed approach allows users to specify the percentage of non-conductive aperture, P_o within a problem domain. The algorithm works as follows. First, the generated apertures are arranged in a descending order. Then, based on the distribution of the apertures and the pre-defined P_o , a threshold aperture, e_t is determined. At the end of the stochastic field generation and correlation processes, cells with aperture size below e_t will be identified as non-conductive apertures and be assigned with $e_i \approx 0$.

Figure 4.20 shows the aperture profiles produced when the stochastic field D4 in Figure 4.18 is subjected to different P_o . D4A to D4F each corresponds to a P_o of 0, 10%, 20%, 30%, 40%, and 50%. A scanning electron micrograph of a natural fracture surface is presented in Figure 4.21. The image, which was first published in Pyrak-Nolte et al. (1987), indicates the non-conductive apertures in the fracture sample by white shading, and the conductive apertures by black shading. It is apparent that a substantial portion of the fracture surface is non-conductive. A comparison between Figure 4.21 and the generated aperture profile D4F shows a considerable degree of resemblance in terms of the non-conductive aperture distribution across the fracture. This observation brings about two major implications. First, the ability of the proposed stochastic model to simulate non-conductive apertures could be useful in promoting the realism of a generated aperture profile. Secondly, it is possible to predict the aperture variation in a natural fracture using the proposed stochastic flow model in conjunction with the Monte Carlo method.

Figure 4.20 Aperture profiles with varying non-conductive zone percentage

Figure 4.21 A scanning electron micrograph of a natural fracture surface
(Reprinted from Moreno et al. (1988))

4.6.3 DDA hydraulic analysis using the stochastic aperture profiles

Fluid flow through a heterogeneous fracture can be evaluated with the seepage analysis extension in DDA. To calculate the hydraulic pressure of a cell i , the following equation is applied

$$P_i = \frac{\sum_{j=1}^q \frac{e_{ij}^3 P_j}{12\mu L_{ij}^2}}{\sum_{j=1}^q \frac{e_{ij}^3}{12\mu L_{ij}^2}} \quad (4.9)$$

where $j = 1, 2, 3, \dots, q$, denoting the cells connected to i and μ denotes the kinematic viscosity of the flowing fluid. Notations e_{ij} and L_{ij} represent the equivalent aperture and the flow distance between cells i and j , while P_i, P_j denote the hydraulic pressures of the respective cells. To evaluate the flow rate, q_{ij} between cells i and j , the following equation is applied

$$q_{ij} = \frac{e_{ij}^3}{12\mu} \frac{P_i - P_j}{L_{ij}} \quad (4.10)$$

Equations (4.9) and (4.10) yield the pore pressure of a cell, and the volumetric flow rate between the centroids of two adjacent cells. Before the flow analysis, the following hydraulic boundary conditions were introduced to the simulation model: a constant hydraulic pressure of 10 Pa and 0 Pa were assigned to the left and the right boundaries, while no-flow condition was imposed at the upper and the lower boundaries.

Figure 4.22 shows the hydraulic pressure distributions obtained from aperture profiles D4A-D4F. Theoretically, the presence of non-conductive apertures limits the fracture surface accessible for fluid flow, thus obstructing the pore pressure distribution across the model. This phenomenon is well reflected by the simulated pore pressure profiles, where models with higher percentage of non-conductive apertures are associated with higher numbers of high- and low-pressure cells, and lower numbers of intermediate-pressure cells.

Figure 4.22 Hydraulic pressure distributions corresponding to the aperture profiles shown in Figure 4.20

The corresponding flow rate distributions are given in Figure 4.23. Consistent with the findings of an existing study (Moreno et al. 1988), it is shown that the variation range of the flow rates is far more dispersed than the variation range of the apertures. The flow rates vary over several orders of magnitude due to the cubic relations assumed between the aperture and the flow rate. When the percentage of non-conductive joints increased, the phenomenon of preferential flow paths, i.e. fluid channeling through a limiting number of joints that carries large volumetric flow rates, become increasingly obvious (Moreno et al. 1988, Berkowitz 2002).

Figure 4.23 Fluid flow rates corresponding to the aperture profiles shown in Figure 4.20

The results presented in Figures 4.22 and 4.23 shows the effects of flow channeling on pore pressure distribution and fluid flow rates. The proposed stochastic flow model enables a non-uniform flow condition such as these to be simulated and analyzed effortlessly. However, it should be noted that the reliability of the outputs depends closely on the quality of the inputs. For an accurate simulation result, the statistical parameters used in the generation of stochastic fields such as the autoregressive

factor, α and the percentage of non-conductive zone, P_0 , should closely reflect the actual flow conditions of the problem domain being studied.

4.7 Modeling a sewerage tunnel using the stochastic flow model

The influences of different aperture fields on the fluid flow conditions across a heterogeneous fracture are discussed in the previous section. In the following numerical example, the stochastic modeling concept is applied to a brick tunnel model to investigate the influences of aperture field heterogeneity on the hydro-mechanical behaviors of a jointed rock mass.

Figure 4.24 and Table 4.5 shows the configuration of the tunnel model, and the DDA parameters employed in the hydro-mechanical analysis. The model is 4.071 m in width, 4.060 m in height and consisting of 1215 discrete blocks. Each complete block measured 220 mm x 71 mm, corresponding to the size of a typical brick-mortar unit. A circular tunnel opening of diameter 1.030 m is located at the center of the model.

A confining stress of $\sigma_{yy}=2.2$ MPa was assigned to the model's left and right boundaries, while $\sigma_{xx}=4.4$ MPa was assigned to the top and the bottom boundaries. After the whole system had reached equilibrium, the simulation of water injection began and the following displacement boundary conditions were introduced: the left and the right boundaries were restrained from horizontal displacement, the upper boundary was restrained from vertical displacement and the bottom boundary was fixed.

Figure 4.24 The configuration of the brick tunnel model

Table 4.5 DDA analysis parameters for the brick tunnel model

<u>Analysis Parameters</u>	<u>Input values</u>
Total number of time step	1200
Upper limit of time interval	1s per time step
Assumed maximum displacement ratio	0.0009
Block density (kg/m ²)	1800
Young's modulus (GPa)	3
Poisson's ratio	0.3
Joint stiffness (GPa)	30
Storage term (m/s)	0
Source/ Sink term	0.02
Minimum hydraulic aperture (mm)	0.1
Number of seepage nodes	2140
Number of seepage joints	3736

4.7.1 The stochastically generated aperture distributions

The brick joints in the tunnel model were characterized by five different aperture profiles: F0, F1, F2, F3 and F4. The statistical descriptions of each aperture profile are given in Table 4.6. F0 corresponds to a homogeneous model with an equivalent aperture of 0.1 mm. F1 and F2 differ from F0 in terms of the standard deviation, while F3 and F4 differ from F1 and F2 in terms of the percentage of non-conductive joints in the model.

Table 4.6 Statistical descriptions of aperture profiles F0 to F4

Aperture profiles	Mean, μ_e (mm)	Standard deviation, σ_e (mm)	Percentage of non-conductive joints, P_0 (%)
F0	0.1	0	0
F1	0.1	0.01	0
F2	0.1	0.033	0
F3	0.1	0.01	50
F4	0.1	0.033	50

Figure 4.25 shows the stochastically generated aperture profiles F1 – F4. To assign each of these aperture details to the tunnel model, the following procedure was applied. First, the model is divided into 20 x 20 cells, each measuring 203.55 mm x 203 mm. Each cell i is assigned with a normally distributed and spatially correlated random variable, e_i . e_i represents the aperture size of all brick joints located within cell i . For any joint located within two different cells j and k , the following formula is applied to determine the equivalent aperture, e_i from e_j and e_k (Iwai 1976)

$$e_i = e_m \left[\frac{16r_e^2}{(1 + r_e)^4} \right]^{1/3} \quad (4.11)$$

where e_m denotes the arithmetic mean of e_j and e_k , and r_e denotes the ratio of e_j to e_k .

The non-conductive apertures in F3 and F4 were simulated through the procedure highlighted in Section 4.6.2. To avoid the division-by-zero error during the subsequent hydraulic analysis, the current example assigned $e_i = 0.0001$ mm, instead of $e_i = 0$ to the non-conductive apertures.

Figure 4.25 Stochastically generated aperture profiles F1 to F4

4.7.2 DDA hydro-mechanical analysis

During the first 850 analysis time steps, hydraulic pressure was assigned to the tunnel wall at a steady increment rate of 50 kPa/s to simulate water injection. At the following time steps, the pressurization rate decreased at -50 kPa/s to simulate water discharge. The distribution of hydraulic pressure through the inter-connected brick joints is calculated by the following continuity equation

$$P_i = \frac{\sum_{j=1}^q \frac{e_{ij}^3 P_j}{12\mu L_{ij}^2}}{\sum_{j=1}^q \frac{e_{ij}^3}{12\mu L_{ij}^2}} \quad (4.12)$$

in which $j=1.2.3,\dots,q$, indicating the total number of nodes connected to a node i and μ denotes the kinematic viscosity of the flowing fluid. Notations e_{ij} , L_{ij} denote the equivalent aperture and the flow distance between nodes i and j , while P_i , P_j denote the hydraulic pressures at the respective nodes.

The hydraulic pressures are then converted to the normal forces through the following equations

$$\dot{F}_i = \frac{L_{ij}}{2} \left[P_i + \frac{1}{3}(P_j - P_i) \right] \quad (4.13)$$

$$\dot{F}_j = \frac{L_{ij}}{2} \left[P_i + \frac{2}{3}(P_j - P_i) \right] \quad (4.14)$$

Subsequently, the normal forces are resolved into the vertical and horizontal vectors as follows

$$F_{ix} = \frac{y_i - y_j}{L_{ij}} \dot{F}_i$$

$$F_{iy} = \frac{x_i - x_j}{L_{ij}} \dot{F}_i$$

$$F_{jx} = \frac{y_i - y_j}{L_{ij}} \dot{F}_j$$

$$F_{jy} = -\frac{x_i - x_j}{L_{ij}} \dot{F}_j \quad (4.15)$$

where $(x_i, y_i), (x_j, y_j)$ are the Cartesian coordinates of nodes i and j . Next, each pair of force vectors F_{ix}, F_{iy} are converted into the general forces before being added to load vector in the DDA global equilibrium matrix. Assuming node i is located at the k^{th} block of the blocky system, and $[F_k]$ denotes the 6 x 1 submatrix positioned at the k^{th} row of the load vector, then F_{ix}, F_{iy} are added to $[F_k]$ after being converted to the general force as follow.

$$\begin{bmatrix} 1 & 0 & -(y_i - y_0) & (x_i - x_0) & 0 & \frac{(y_i - y_0)}{2} \\ 0 & 1 & (x_i - x_0) & 0 & (y_i - y_0) & \frac{(x_i - x_0)}{2} \end{bmatrix}^T \begin{bmatrix} F_{ix} \\ F_{iy} \end{bmatrix} \xrightarrow{\text{added to}} [F_k] \quad (4.16)$$

where x_0, y_0 denote the gravity center of block k . The displacement variables in the global equilibrium matrix are then solved through the open-close iterations in DDA. Lastly, the aperture of each brick joint is updated according to the nodal displacements of the corresponding blocks, and the new aperture is applied in Equation (4.12) for the computation of nodal pore pressure at the subsequent time step.

Figure 4.26 shows the simulated pore pressure distributions corresponding to the five aperture profiles at time step 1200 (equivalent to approximately 1000 s of simulated time). It is apparent that different aperture profiles result in different pore pressure variations within the model. Pore pressure distributed rather uniformly in model F0 due to the homogeneous flow condition assumed. Aperture profiles F1 and F2, each corresponding to a variation range of 0.13 mm and 0.21 mm, display a more dispersed pore pressure distribution compared to F0. In the case of aperture profiles F3 and F4, pore pressure seems to accumulate at certain parts of the two models because the fluid flow was restricted by the presence of non-conductive joints.

Figure 4.26 Pore pressure distributions corresponding to different aperture profiles, obtained at time step 1200

Different pore pressure distributions stimulate varying degrees of block displacement. Figure 4.27 shows the vertical and horizontal displacements of blocks 1 and 2 as a function of time and Table 4.7 summarizes the final displacement of the respective blocks in all simulation cases. The location of the two blocks in the tunnel model are shown in Figure 4.24. From the displacement plots, it can be seen that the displacement profiles of F1 closely resemble those of F0. On the contrary, the displacement profiles of F2 show significant deviation from those of F0 and F1. This is because while F1 of $\sigma=0.01$ mm has an almost homogeneous aperture distribution, F2 of $\sigma=0.033$ mm features a comparatively dispersive aperture distribution. Due to these differences, the block displacements corresponding to F2 are more erratic compared to those corresponding to F0 and F1. In the case of F3 and F4, the displacement profiles of block 1 and 2 are generally low in magnitude. This finding can be explained by analyzing pattern of pore pressure distribution around the two blocks. As both blocks 1 and 2 are located within the minimal pore pressure zone of models F3 and F4, the flow-induced joint stress exerted on the two blocks are less significant. Hence, the displacement of these blocks in the respective models are low in magnitude.

Table 4.7 The maximum displacements of blocks 1 and 2

Aperture profiles	y - displacement (mm)		x - displacement (mm)	
	Block 1	Block 2	Block 1	Block 2
F0	6.33	9.26	8.09	9.67
F1	6.39	8.97	7.56	9.12
F2	9.71	11.8	10.2	12.2
F3	5.04	6.02	6.17	7.68
F4	5.8	5.61	5.94	5.92

Figure 4.27 Displacement profiles of blocks 1 and 2 as a function of simulation time

The simulation results highlighted in Figures 4.26 and 4.27 bring about the following implications. First, the hydro-mechanical behaviors predicted by using different aperture profiles can be appreciably divergent. Hence, simulating a heterogeneous hydraulic property using a homogeneous model may lead to inaccurate and unrealistic analysis results. It is also worth noting that the computational efficiency of the stochastic flow model is comparable to that of the homogeneous model. The additional CPU time consumed in the generation of a 20 x 20 autocorrelated aperture profile with $\mu=0.1$ mm, $\sigma=0.033$ mm and $\alpha=0.5$ is approximately 15 ms.

4.8 Chapter summary

Hydraulic aperture and fluid conductivity are some of the most diverse properties in Earth Science. The spatial variability of the two parameters within an aquifer are often too intricate to measure and model in detail. A way out of this dilemma is by generating an ensemble of possible realizations to represent the uncertainty in the stochastic property distribution. The stochastic concept has been receiving considerable attention since its introduction a few decades ago, but has yet to be incorporated in most hydro-geological modeling approaches. Instead, most numerical methods including the DDA are still relying on the arguable equivalent continuum model in hydrogeological simulations.

In this Chapter, a stochastic flow model is introduced to the DDA method to predict the spatial variability of two important hydraulic parameters – the hydraulic conductivity and the aperture. The framework for the proposed stochastic flow model is presented in a comprehensive manner. Through a series of numerical examples, the ability of the proposed model in simulating various stochastic flow conditions is also verified. There is a good agreement between the generated stochastic fields and the existing stochastic modeling theories. Furthermore, the influences of flow heterogeneity on the hydro-mechanical behaviors of a geological model can be evaluated with the DDA method easily. On account of its feasibility and effectiveness, the proposed stochastic flow model appears to be a reliable alternative to the equivalent continuum model conventionally applied in the DDA hydro-mechanical modeling.

Chapter 5. Hydraulic fracturing modeling using hybrid DDA

5.1 Introduction

Recent attempts to couple DDA blocks with finite element meshes have been regarded as fruitful. By discretizing a DDA block into triangular finite elements, the stress distribution within the DDA block is refined and the block deformability is improved. The hybrid model is proven to be a more efficient approach compared to the uncoupled DDA model in modeling fracturing mechanisms. In this Chapter, a hydraulic crack initiation-propagation extension complete with a coupled hydro-mechanical analysis algorithm is introduced to the hybrid DDA model for the simulation of hydraulic fracturing problems.

Figure 5.1 illustrates the flow of chapter 5². In Section 5.2, the existing DDA hydraulic fracturing models is reviewed, and the research motivation is discussed. Section 5.3 provides the theoretical framework of the hybrid DDA model, followed by a detailed introduction of the proposed HF analysis algorithm in Section 5.4. Verification examples presented in Sections 5.5 and 5.6 show the capability of the proposed algorithm in performing hydro-mechanical analysis on fractured media. In Section 5.7, a wellbore numerical example is presented to investigate the effect of time step size, fracturing fluid viscosity and injection rate on the crack initiation and model breakdown pressures. Finally, in Section 5.8, conclusions are drawn based on the functionalities and limitations of the proposed DDA-based HF analysis algorithm.

² This chapter is based on the following publication from the author:

Choo, L. Q., Zhao, Z., Chen, H., & Tian, Q. (2016). Hydraulic fracturing modeling using the discontinuous deformation analysis (DDA) method. *Computers and Geotechnics*, 76, 12-22. doi:<http://dx.doi.org/10.1016/j.compgeo.2016.02.011>

Theoretical groundings	The proposed hydraulic fracturing model	Numerical cases
<ul style="list-style-type: none"> • A review of DDA Hydraulic fracturing models • Hybrid DDA model: background and advantages 	<ul style="list-style-type: none"> • Discretization of DDA blocks • Displacement function • Fracture criterions • The solution scheme 	<ul style="list-style-type: none"> • Modeling of inter-connected fractures • Modeling of a planar crack • Modeling of a wellbore example

Figure 5.1 An outline of Chapter 5

5.2 Theoretical groundings for DDA hydraulic fracturing analysis

Hydraulic fracturing (HF), the process by which pressurized fluid is used to induce the initiation and propagation of fractures within rock matrices, plays an important role in stimulating oil and natural gas production in low-permeability reservoirs (Kerr 2010, Vengosh et al. 2013). To maximize production rates and minimize drilling costs, there is a need to understand the mechanics of the hydraulic fracturing process so that information such as the crack initiation pressure, the extensiveness of the induced fracture network and the size of the opening resulting from different fracturing fluids can be reasonably predicted (Rani et al. 2015).

Discontinuous deformation analysis (DDA), an implicit version of the discrete element method (DEM), has been recently used by several researchers in the simulation of HF problems (Ben et al. 2013b, Ben et al. 2013a, Jiao et al. 2015). Contrary to continuous numerical approaches such as the finite element method (FEM) where the problem domain is assumed to be a continuum, a DEM model consists of discrete blocks or particles. Fractures are represented by broken bonds between neighboring particles and are supposed to develop automatically without remeshing (Jing and Stephansson 2007). This feature of the DEM allows pre-existing discontinuities such as cracks, joints, faults and beddings to be modeled easily.

Problems involving the concurrent formation and elongation of multiple fractures can also be simulated without difficulty (Lee and Jeon 2011).

One of the earliest attempts to couple DDA with HF simulation was made by Ben et al. (2013a). The model assigns strong bonds along the adjacent interface between discrete blocks to simulate an intact rock mass. The breakage of any of these bonds upon the satisfaction of a pre-defined fracture criterion signifies crack formation. Numerical cases involving pre-existing and new fractures were presented in a later study (Ben et al. 2013b). However, only simple, conceptual HF models consisting of equalized square blocks were demonstrated and no validation case was presented by the authors. A recent DDA HF model introduced by Jiao et al. (2014) adopts a similar formulation, but with a more sophisticatedly discretized problem domain to promote the realism of the fracture configuration. Several experimental studies were presented in the study to verify the reliability and effectiveness of the proposed model. In a general sense, the appeal of these DDA HF models lies in their ease of implementation as no extensive modification to the original DDA code were needed to realize the simulation of the HF mechanisms. Nevertheless, for these models to work as a pseudo-continuous body with varying stress field and a practical degree of deformability, a large number of blocks are needed, thus leading to a computationally prohibitive contact analysis.

Even though the DDA has been widely accepted as a suitable discrete method for the simulation of jointed rock structure, it does have two major drawbacks: (i) an extensive contact analysis is needed between the discrete blocks; (ii) the conventional DDA with constant strains has a relatively poor accuracy in stress evaluation. Those two drawbacks are great hindrances to HF simulations. A hybrid model between the DDA and the finite element methods can minimize the significance of these limitations (Shyu 1993, Bao 2010, Tian 2014). By introducing the finite element mesh to most parts of the problem domain, much fewer DDA blocks are needed. With this, the concerns regarding high computational cost caused by increased contact pairs can be eliminated as only the block boundaries of the hybrid model are subjected to the contact analysis. Considering each mesh line as a possible crack path, an intra-block fracturing process can be simulated directly without the need of re-meshing.

Moreover, by coupling the finite element mesh into DDA blocks, the stress distribution within each block is refined and the block deformability is improved. On the other hand, the key advantage of the hybrid DDA model over other continuum-based methods such as the FEM, hybrid FEM-FVM and hybrid BEM-FEM methods is that, the hybrid DDA model inherited the well-constituted block kinematics algorithm from the DDA. In the continuum-based model, the displacement compatibility between elements is maintained by keeping constant element-node connectivity topology and consistent orders of the trial function between the neighboring elements (Jing 2003). In addition to this inter-element displacement function, the DDA contact function is also incorporated in the hybrid DDA-FEM method to model the inter-block connections. This allows the motion and interaction between discrete blocks to be taken into account during the modeling of a fracturing process. In other words, both inter- or intra-block discontinuities can be simulated simultaneously and easily with the hybrid DDA-FEM model.

As it embraces the advantages of both the FEM and the DDA methods, the hybrid model has proven to be an efficient tool in simulating the crack propagation processes (Bao 2010, Tian 2014). In view of that, it would be beneficial if the existing crack propagation analysis algorithm in the hybrid DDA model can be further developed for HF analyses. The key differences between simulating an HF problem and other fracturing problems are: (i) in an HF model, pore pressure exists within fractures, in addition to the confining stresses applied on the model's boundaries; (ii) a fluid flow analysis algorithm needs to be established to determine the pore pressure at all fluid-passable nodes; (iii) a coupling mechanical analysis is also needed for the computation of nodal displacements resulting from the pore pressure. Focusing on these differences, a new DDA extension is introduced in this chapter for the simulation of HF problems. The proposed extension, which comprises a hydraulic crack initiation-propagation algorithm and a coupled hydro-mechanical analysis function, is presented in the following sections.

5.3 Block fracturing analysis using the hybrid DDA model

5.3.1 Discretization of DDA blocks

Figure 5.2 illustrates the relationships between DDA blocks, triangular finite elements, virtual joints and rock joint in a hybrid DDA model. A hybrid model consists of polygonal blocks discretized by a triangular finite element mesh. There is no restriction on the shape of the block as any polygon can be discretized into triangular elements. The nodal displacements of these triangular elements are the basic unknowns to be solved within each time step. The grid lines separating the triangular elements are referred to as virtual joints, and the boundary lines marginating each discrete block are called rock joints. The separation of a joint when a pre-defined fracture criterion is met signifies the formation of a crack either within a block (in the case of a virtual joint) or along the block boundaries (in the case of a rock joint).

Figure 5.2 A typical hybrid DDA model consisting of two blocks discretized by triangular elements

5.3.2 Displacement functions

The displacement functions for the nodal variable-based, hybrid DDA model presented in this section are similar to that of the classic FEM model with a triangular mesh (Zienkiewicz et al. 2013). Figure 5.3 shows a typical triangular element with vertices i, j, m arranged in an anticlockwise order. The displacement (u, v) at any point (x, y) within the triangular element can be defined by two linear polynomials

$$\begin{aligned} u &= \alpha_1 + \alpha_2 x + \alpha_3 y \\ v &= \alpha_4 + \alpha_5 x + \alpha_6 y \end{aligned} \quad (5.1)$$

where parameters $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5$, and α_6 are constants. The displacements at a vertex a (where $a=i, j, m$) can be evaluated as

$$\begin{aligned} u_a &= \alpha_1 + \alpha_2 x_a + \alpha_3 y_a \\ v_a &= \alpha_4 + \alpha_5 x_a + \alpha_6 y_a \end{aligned} \quad (5.2)$$

Figure 5.3 A triangular element and the notations used for the nodal displacements

By rearranging these two sets of simultaneous equations, parameters $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5$, and α_6 can be expressed in terms of the displacement variables (u_a, v_a), and the element displacements (u, v) can be determined by the following equations

$$\begin{aligned} u &= \frac{1}{2\Delta} [(a_i + b_i x + c_i y)u_i + (a_j + b_j x + c_j y)u_j + (a_m + b_m x + c_m y)u_m] \\ v &= \frac{1}{2\Delta} [(a_i + b_i x + c_i y)v_i + (a_j + b_j x + c_j y)v_j + (a_m + b_m x + c_m y)v_m] \end{aligned} \quad (5.3)$$

in which

$$\begin{aligned} a_i &= x_j y_m - x_m y_j \\ b_i &= y_j - y_m \\ c_i &= x_m - x_j \end{aligned} \quad (5.4)$$

Following a cyclic permutation of the subscripts in the $i-j-m$ sequence, similar expressions can be obtained for the other coefficients.

Equations (5.3) can also be expressed in the standard matrix form as

$$\mathbf{u} = \begin{Bmatrix} u \\ v \end{Bmatrix} = N \mathbf{a} = \begin{bmatrix} N_i & 0 & N_j & 0 & N_m & 0 \\ 0 & N_i & 0 & N_j & 0 & N_m \end{bmatrix} \begin{Bmatrix} u_i \\ v_i \\ u_j \\ v_j \\ u_m \\ v_m \end{Bmatrix} \quad (5.5)$$

where

$$N_a = \frac{a_a + b_a x + c_a y}{2\Delta} \quad (5.6)$$

in which $a=i, j, m$, and Δ represents the surface area of the triangular element ijm .

The aforementioned linear displacement function guarantees the continuity of the displacement along the common edge between any two adjacent elements.

On the other hand, the total strain at any point within the element can be expressed as

$$\varepsilon = \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = S\mathbf{u} = SN\mathbf{a} = B\mathbf{a} \quad (5.7)$$

where

$$B = SN = \begin{bmatrix} \frac{\partial N_i}{\partial x} & 0 & \frac{\partial N_j}{\partial x} & 0 & \frac{\partial N_m}{\partial x} & 0 \\ 0 & \frac{\partial N_i}{\partial y} & 0 & \frac{\partial N_j}{\partial y} & 0 & \frac{\partial N_m}{\partial y} \\ \frac{\partial N_i}{\partial x} & \frac{\partial N_i}{\partial y} & \frac{\partial N_j}{\partial x} & \frac{\partial N_j}{\partial y} & \frac{\partial N_m}{\partial x} & \frac{\partial N_m}{\partial y} \end{bmatrix} \quad (5.8)$$

or, simply,

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = \frac{1}{2\Delta} \begin{bmatrix} b_i & 0 & b_j & 0 & b_m & 0 \\ 0 & c_i & 0 & c_j & 0 & c_m \\ c_i & b_i & c_j & b_j & c_m & b_m \end{bmatrix} \begin{Bmatrix} u_i \\ v_i \\ u_j \\ v_j \\ u_m \\ v_m \end{Bmatrix} \quad (5.9)$$

5.3.3 Simultaneous equations

A hybrid DDA model consists of distinct blocks, each made up of triangular elements connected at common nodes. Assuming there are n nodes in a block system, the global equilibrium equations take the following form

$$\begin{bmatrix} k_{11} & k_{12} & k_{13} & \dots & k_{1n} \\ k_{21} & k_{22} & k_{23} & \dots & k_{2n} \\ k_{31} & k_{32} & k_{33} & \ddots & k_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k_{n1} & k_{n2} & k_{n3} & \dots & k_{nn} \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_n \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_n \end{Bmatrix} \quad (5.10)$$

Each element k_{ij} in the coefficient matrix is a 2x2 submatrix. Both d_i and f_i are 2x1 submatrices, where d_i represents the deformation variables $\{u_i, v_i\}^T$ of node i and f_i represents the corresponding equivalent nodal forces $\{f_{ix}, f_{iy}\}^T$.

The coefficient and load submatrices are established through the minimization of potential energy resulting from elastic strains, boundary displacement constraints, bolting connections, external and internal loadings in the form of point or distributed load, frictional force, inertia force and contact force (Bao 2010, Tian 2014). The submatrices for each of these mechanisms are to be computed separately and added to the global equations in accordance with the node index. It is worth noting that the contact submatrix that accounts for the contact mechanism between boundary nodes is a unique component of the hybrid DDA model that distinguishes it from the FEM model. If the whole problem domain contains only one block, then the system equations are identical to those of the FEM.

5.3.4 Fracture criteria

In the hybrid DDA model, joint opening is initiated by either a tensile or shear stress. According to the maximum tensile strength criterion, when the normal stress in a joint, σ_n exceeds a pre-determined threshold value of the tensile strength σ_t , a tensile failure occurs.

In the tangential direction, the Mohr-Coulomb criterion applies

$$\tau = c + \sigma_n \tan \phi \quad (5.11)$$

where τ , c and ϕ are the maximum shear strength, cohesion and internal friction angle of the intact rock. A shear failure is said to occur if the shear stress in a joint exceeds τ .

5.4 Hydraulic fracturing analysis in the hybrid DDA model

Figure 5.4 shows the procedure involved in solving an HF problem by using the proposed DDA extension. The shaded boxes in the flowchart indicate processes relating to HF analysis, which include the computations of: (i) fluid pressure distribution within the existing fracture network, (ii) nodal displacements induced by the fluid pressure, and (iii) fracture extension due to mechanical deformation at the fracture tip. The procedure is derived from a staggered solution scheme whereby the hydraulic and the mechanical equations are solved separately, and the output variables are transferred between the functions to achieve a convergent solution within each time step (Minkoff et al. 2003).

The proposed HF model is subjected to the following assumptions: (i) all blocks consist of isotropic material and behave linear-elastically; (ii) fracture can only propagate along the real joints (i.e. the rock joints and virtual joints illustrated in Figure 5.2); (iii) fluid flow in fracture obeys the continuity equation; (iv) fracturing fluid obeys the cubic law and is incompressible; (v) all joints and nodes linked to the fluid injection point through inter-connected fractures are fluid-passable.

5.4.1 Fundamental equations used in hydro-mechanical analysis

A numerical coupled hydro-mechanical analysis comprises the iterative process of determining the fluid pressure distribution within the fluid-passable joints, the update

of the load submatrices in accordance with the fluid pressure exerted on the joints, and the computation of the nodal displacements induced by the fluid pressure.

The equations used for hydraulic analysis in the proposed HF model are formulated based on the mass conservation law. Consider a case where an incompressible fluid flows across a joint intersection. The principle of mass conservation requires the mass of fluid retained within a unit element to be equal to the fluid influx minus the outflux and the source/sink contribution, plus the storage release. Assuming that the unit element is of infinitesimally small volume, this equilibrium condition can be expressed by the following continuity equation (Jing and Stephansson 2007)

$$\frac{\partial q_i}{\partial x_i} = \frac{r}{\rho}(x_i, t) - S_r \left(\frac{\Delta h_t}{\Delta t} \right) = 0 \quad (5.12)$$

where q_i and x_i represent the flow rate and flow distance in the i direction, ρ denotes the fluid density, and $r(x_i, t)$ represents the source/sink term. The storage term is denoted by $-S_r \left(\frac{\Delta h_t}{\Delta t} \right)$, in which S_r represents a joint's storativity, and Δh_t represents the head difference within a specific time interval, Δt .

Figure 5.4 Procedure of solving an HF problem by using the hybrid DDA model

Note that $q_i = v_i e_i$, where v_i and e_i denote the flow velocity and the aperture width. The relationship between v_i and the change in the hydraulic head, h_i along x_i , as defined by Darcy's law is

$$v_i = -k_i \frac{\partial h_i}{\partial x_i} \quad (5.13)$$

while the relationship between the hydraulic conductivity, k_i and the aperture width, e_i , as assumed by the cubic law is

$$k_i = \frac{g e_i^2}{12 \nu} \quad (5.14)$$

where g is the gravitational acceleration and ν represents the fluid kinematic viscosity.

Substituting Equations (5.13) and (5.14) into Equation (5.12) leads to

$$\frac{\partial}{\partial x_i} \left(\frac{g e_i^3}{12 \nu} \frac{\partial h_i}{\partial x_i} \right) - S_r \left(\frac{\Delta h_t}{\Delta t} \right) + \frac{r}{\rho} (x_i, t) = 0 \quad (5.15)$$

Consider the case where a joint intersection j is connected to n number of nodes i as illustrated by Figure 5.5, Equation (5.15) can then be written as

$$\sum_{i=1}^n \frac{\partial}{\partial x_{ij}} \left(\frac{g e_{ij}^3}{12 \nu} \frac{\partial h_j - h_i}{\partial x_{ij}} \right) - S_r \left(\frac{\Delta h_t}{\Delta t} \right) + \frac{r}{\rho} (x_i, t) = 0 \quad (5.16)$$

where x_{ij} denotes the distance from node i to node j and e_{ij} denotes the hydraulic aperture of joint $i - j$.

Figure 5.5 A hybrid DDA rock model and its constituent blocks, meshes and fractures

An iterative approach is adopted to determine h_j . Subsequently, h_j is converted into the pore pressure p_j as follows

$$p_j = \rho g (h_j - y_j) \quad (5.17)$$

where y_j denotes the elevation of node j relative to an arbitrary datum. The hydraulic pressure is assumed to be distributed linearly along the water-block interface. Hence, the nodal force, f_j resulting from the pore pressure can be expressed as

$$f_j = \frac{x_{ij}}{2} \left(\frac{2}{3} p_i + \frac{1}{3} p_j \right) \quad (5.18)$$

where subscripts i and j denote any two nodes located on the same side of an element, while p_i and p_j denote the pressures at the respective nodes. As depicted in Figure 5.6, the nodal forces will then be resolved into the horizontal and vertical vectors and

added to the free term at the right-hand side of Equation (5.10) according to the node index.

Figure 5.6 The conversion of the hydraulic head into the point loading

After the global mechanical analysis is conducted and the locations of all element vertices are updated, a new aperture, e_{ij} will be computed for every joint segment using the wedge-shaped aperture formula (Huitt 1956, Iwai 1976)

$$e_{ij} = e_m \left[\frac{16r_e^2}{(1+r)^4} \right]^{\frac{1}{3}} \quad (5.19)$$

where

$$e_m = \text{mean aperture} = \frac{1}{2} (e_i + e_j)$$

$$r_e = \frac{e_i}{e_j}$$

e_i, e_j : aperture sizes at the two ends of a joint.

The updated aperture will be applied in Equation (5.16) at the subsequent time step to calculate the nodal hydraulic head.

5.5 Modeling the hydraulic head distribution within a fracture network

Typically, a numerical seepage analysis consists of the following steps: (i) identification of the seepage network, (ii) definition of the hydraulic boundary conditions and, (iii) computation of the hydraulic head distribution. The aim of the following numerical example is to perform a seepage analysis on a fractured model using the proposed DDA extension.

Figure 5.7 shows a 200 mm x 200 mm rock model consisting of four DDA blocks and 274 triangular mesh elements. The model contains an inter-connected fracture network with a constant, uniform aperture of 0.0001 m and by-segment lengths as listed in Table 5.1. The fracture walls in the model are impervious in the normal direction and the fluid in the fracture is viscous and incompressible. The seepage flow that occurs along the fracture axis is assumed to be laminar, steady and uniform.

Figure 5.7 A discretized rock model containing an inter-connected fracture system. Smaller diagram on the right indicates the fracture system and block boundaries

As shown in Table 5.1, nodes 12 and 20 are impermeable, dead-end nodes. At time step zero ($t=0$), the hydraulic head at all nodes were fixed at 100 Pa. The hydraulic heads at nodes 1, 17 and 22 were then changed to 0 Pa, 140 Pa and 110 Pa, respectively at the subsequent time step. By neglecting the storage and source/sink terms, the updated hydraulic heads at all other nodes as a result of the change were solved by Equations (5.16) using an iterative approach.

Table 5.1 Boundary conditions at specific nodes and the by-segment fracture lengths

Node No.	Boundary Condition		
1	Fixed hydraulic head (0 m)		
12	Impermeable node		
17	Fixed hydraulic head (140 m)		
20	Impermeable node		
22	Fixed hydraulic head (110 m)		
Flow path	Length (m)	Flow path	Length (m)
1-2	0.022361	8-13	0.023575
2-3	0.022361	9-10	0.025
3-4	0.022361	10-11	0.025
4-5	0.022361	11-12	0.025
5-6	0.026877	13-14	0.023561
5-18	0.022361	14-15	0.023575
5-21	0.038079	15-16	0.025
6-7	0.023561	16-17	0.067181
6-18	0.023575	18-19	0.029155
7-8	0.003616	18-21	0.029155
7-13	0.03334	19-20	0.029155
8-9	0.025	21-22	0.029155

The simulation results are summarized in Table 5.2. It can be seen that the flow rate varies from node to node to satisfy the pre-defined hydraulic boundary conditions. The negligible percentage of error at each node indicates that the solution fulfills the mass conservation theorem. These results have verified the accuracy of the proposed DDA extension in calculating hydraulic head distribution within a fracture network.

Table 5.2 Nodal hydraulic heads and percentages of unbalanced flow

Node No.	Hydraulic head (m)	Unbalanced flow rate (m/s)	Total flow rate (m/s)	Percentage of error* (%)
2	17.4023	1.6667E-08	0.05801	0
3	34.8046	-1.6667E-08	0.05801	0
4	52.2069	0	0.05801	0
5	69.6092	-1.4324E-06	0.05801	0.002
6	76.0907	6.5914E-06	0.01496	0.044
7	80.9138	-7.8294E-06	0.01447	0.054
8	83.3256	0	0.00723	0
9	83.3256	0	0	-
10	83.3256	0	0	-
11	83.3256	0	0	-
12	83.3256	0	0	-
13	85.7374	7.8144E-06	0	0.054
14	90.5604	-7.7994E-06	0.01447	0.054
15	95.3840	2.5850E-06	0.01447	0.018
16	100.8103	8.9079E-07	0.01447	0.006
18	76.2530	6.4710E-08	0.01447	0
19	76.2530	0	0.02263	0
20	76.2530	0	0	0
21	87.7959	1.6903E-09	0.04354	0

$$* \text{ Percentage of error} = \frac{\text{Unbalanced flow rate}}{\text{Total flow rate}} \times 100 \%$$

The appeal of using the hybrid DDA model to solve an HF problem lies in its efficiency. First, the introduction of the finite element meshes reduces the number of blocks required in a problem domain significantly, hence making the hybrid DDA model a more efficient approach compared to the conventional DDA model. Furthermore, refining the finite element mesh in a hybrid DDA model would not compromise its computational speed to the same extent as increasing the block number in a conventional DDA model does, as only the boundary nodes will be scanned during the search of the seepage network.

5.6 Modeling the mechanical response of a planar crack subjected to hydraulic pressure

After the hydraulic heads and pressures at all fluid-passable nodes are obtained, the next step is to convert these values into point loadings. Then, the resultant nodal displacements are computed by considering all other applied loadings and constraints assigned to the model. Finally, new apertures are determined based on the updated joint locations.

A planar crack model consisting of 1828 elements is employed to simulate this pore pressure-aperture interaction. As shown in Figure 5.8, the model is 46.08 m in width and 46.08 m in height. The block matrix has a Young's modulus of $E = 40$ GPa and a Poisson's ratio of $\nu = 0.22$. A 21.6 m long fracture is located centrally along the mid-span of the model. An initial stress state of $\sigma_{xx} = -30$ MPa and $\sigma_{yy} = -15$ MPa was assigned on the model's boundaries, and a uniform hydraulic pressure of $p = 20$ MPa was applied along the fracture.

Figure 5.8 A planar crack subjected to confining pressures

5.6.1 Validation of the pore pressure-aperture relation

For verification purposes, the mechanical response obtained from the hybrid DDA model was compared to the analytical solution and UDEC results (Itasca 2011). The analytical solution for the fracture opening is given by (Charlez 1997, Itasca 2011)

$$w = \frac{|\sigma_{yy} + p|}{E} \frac{4(1 - \nu^2)}{\sqrt{a^2 - x^2}} \quad (5.20)$$

where w denotes the fracture opening, a denotes half of the fracture length and x represents the distance from the fracture mid-length.

As depicted in Figure 5.9, fracture openings predicted by the hybrid DDA model show remarkable agreement with both the analytical and the UDEC solutions. The average percentage of difference between the results obtained from the hybrid DDA model and the other two methods is less than 1 percent.

Figure 5.9 A comparison between the fracture openings obtained from the analytical solution, DDA and UDEC analysis results (Itasca, 2011)

5.6.2 Computational efficiency of the hybrid DDA

A similar planar plate model was employed to compare the efficiency of the hybrid DDA model to that of the conventional DDA. The conventional model used in this comparison shares the same configuration and analysis parameters as the hybrid model shown in Figure 5.8, and was discretized into the same details of blocks as that of the elements in the hybrid model. Springs of a very high stiffness are placed at the blocks' interface (except along the planar crack) in the conventional model to ensure displacement compatibility.

The numerical analyses were conducted as follows. First, both the hybrid and the conventional models were subjected to boundary stresses of $\sigma_{xx} = -30$ MPa and $\sigma_{yy} = -15$ MPa. Hydraulic pressure was then introduced to the respective planar cracks at a constant increment rate of 100kPa per simulation time step. As given in Table 5.3, two different time step sizes were applied in the hydro-mechanical analyses and comparison was made in terms of the total CPU time required to achieve a specific simulated time.

Table 5.3 The computational efficiency of the hybrid DDA model in comparison to the conventional DDA

Time step size (10^{-6} s)	Type of DDA model	Total time step	Total simulated time (10^{-6} s)	CPU time (ms)
1	Conventional	1000	1000	97107
	Hybrid	1000	1000	48579
10	Conventional	100	1000	8149
	Hybrid	100	1000	3521

It is apparent that the hybrid model consumed less CPU time than the conventional model in both cases, mainly due to the substantial reduction in the total contact surface and the total degree of freedom. These results bring out the following implications: (i) the introduction of the FEM mesh into DDA block has improved the computational efficiency of the DDA model in simulating a continuous or fractured domain; (ii) in view of this improved computational efficiency, the hybrid model is more suitable than the conventional DDA model in modeling HF problems where the number of real fractures is markedly less than the number of block joints.

5.7 Modeling the hydraulic fracturing process in a borehole model

Consider a borehole model assigned with an anisotropic stress field. Once the fracturing process is initiated by the fluid pressure acting on the borehole wall, the injection fluid starts to fill the newly-opened joint. This penetration process of the fracturing fluid causes a progressive increase in the pore pressure along the joints. When the pressure in any joint exceeds the pre-determined threshold value, the existing crack propagates and the fluid-passable path is extended.

By using the proposed DDA extension, the aforementioned crack opening and propagation processes were simulated. The effects of time step size, fracturing fluid viscosity and injection rate on the fracture profile, crack initiation and model breakdown pressures were also investigated through a series of case studies.

Summarized in Table 5.4 are the details of the six selected simulation cases. An equivalent time step size of 2×10^{-3} s was used in these cases. Fracturing fluid was injected into the borehole at various virtual pressures ranging between 0.5 MPa/s and 1.5 MPa/s. Cases 1, 3 and 5 utilized a low-viscosity (0.1 mPa s) fracturing fluid, while a high-viscosity (20 mPa s) fracturing fluid was used in Cases 2, 4 and 6. The simulation results were evaluated in terms of the crack initiation and model breakdown pressures – the former being the fluid pressure in the borehole when the first crack is formed and the latter refers to the pressure at which the model is broken into halves.

Table 5.4 A summary of the HF simulation cases

Case	Fluid viscosity (mPa s)	Injection rate (MPa/ s)	<u>Crack initiation</u>		<u>Model breakdown</u>	
			Time step	Hydraulic pressure (MPa)	Time step	Hydraulic pressure (MPa)
1	0.1	0.5	32523	32.404	32587	32.465
2	20	0.5	32523	32.404	32593	32.471
3	0.1	1.00	16483	32.724	16525	32.808
4	20	1.00	16483	32.724	16528	32.814
5	0.1	1.50	11063	32.826	11093	32.916
6	20	1.50	11063	32.826	11101	32.940

Figure 5.10 illustrates the configuration of the rock specimen being simulated. The specimen is 200 mm x 200 mm in size, with a borehole of diameter 20 mm located at the center. The corresponding numerical model is made up of 1510 triangular elements connected by virtual joints. Confining pressures of 10 MPa and 5 MPa were applied along the x- and the y-axes, respectively. After the whole system has reached equilibrium, the following displacement boundary conditions were introduced: the top boundary was restrained from vertical movement, the left and right boundaries were restrained from horizontal movement, while the bottom boundary was fixed.

Figure 5.10 Rock model used for hydraulic fracturing simulation.

5.7.1 Calibration

By referring to the macroscopic parameters of Lac du Bonnet (LdB) granite, uniaxial compression and Brazilian tests were simulated to calibrate the microscopic properties of the rock model. Table 5.5 summarizes the values of Young's modulus, bond strength and friction angle assigned to the model when the outputs corroborated the experimental and simulation results presented in previous studies (Falls et al. 1992, Al - Busaidi et al. 2005). These calibration results were used as the input parameters for our borehole model.

Table 5.5 The micro and macro analysis parameters

Micro parameters			
Young's Modulus, MPa 65			
Bond normal strength, MPa 15.8			
Cohesion, GPa 1.1			
Friction angle ϕ 26.57°			
Macro parameters	DDA simulation results	PFC simulation results (Al - Busaidi et al. 2005)	Experimental results (Falls et al. 1992, Al - Busaidi et al. 2005)
Unconfined peak strength σ_c , MPa	215	192	200
Brazilian tensile strength σ_t , MPa	12	32.9	9.3
Young's modulus, GPa	69	68	69

5.7.2 Selection of time step size

In DDA, the time step size can be taken as the time interval between two successive mechanical analyses. The selection of a proper time step size is crucial as it may affect the accuracy of the simulation outputs. For instance, during a hydro-mechanical analysis, different time step sizes give rise to different flow volumes within each time step, thus inducing different magnitudes of block displacement. Subsequently, the fluid transmissivity of a rock joint may differ over several orders of magnitude due to the cubic relations assumed between the aperture and the fluid transmissivity. Different fluid transmissivities will in turn, affect the flow volume in the following time step, and so forth. To decide the time step size for the current example, a series of trial cases were carried out to inspect the results consistency with different time step selections.

Figure 5.11 displays the simulated crack initiation pressure for different fluid injection rates as a function of time step size. The plot indicates that for each fluid

injection rate, there exists a minimum threshold time step. The crack initiation pressure becomes fairly consistent when the time step size is larger than the minimum threshold. This minimum threshold is case-specific and may be affected by factors such as the model's configuration and the value of the other input parameters. In this particular example, the minimum threshold values are approximately 0.0016 s, 0.002 s and 0.0025 s for fluid injection rates of 1.5, 2 and 2.5 MPa/s respectively.

Figure 5.11 Crack initiation pressure for different fluid injection rates as a function of time step size. Triangular markings labeled 1, 2 and 3 indicate the “minimum threshold” time step for injection rates 1.5, 2 and 2.5 MPa/s respectively

While these results imply favor to the selection of a large time step size, there is, however another limiting condition to consider. In DDA, the use of a large time step size may trigger a recursion process during which the time step size will be reduced so as to ensure the satisfaction of the small strain assumption, and to promote contact convergence. This recursion process increases the solution time considerably (Khan et al. 2010, Tian 2014).

More studies need to be carried out to research the time step size selection in DDA. Considering both accuracy and efficiency, we suggest the use of time step sizes larger than the minimum threshold by not more than 50% or 0.001 s, whichever is smaller.

5.7.3 Results and discussion

Fracture mechanisms

The fracturing mechanism that took place in each model comprises a few common steps. First, tiny cracks start to form at the two opposite sides of the borehole when the pressure around the borehole exceeds the joints' strength. Then, the cracks propagate in the direction parallel to that of the maximum principal stress. Eventually, when the cracks extend to the model's boundaries, the model is broken into halves. From Figure 5.13, it can be seen that the failure profiles of all six models are similar, even though they are each subjected to different time step sizes, fluid viscosities and injection rates. The orientation of these crack paths are consistent with the observations reported in corresponding experimental studies (Ishida et al. 2004, Stanchits et al. 2012, Chang et al. 2016). This implies that the confining stress is appropriately expressed in the hybrid DDA models.

Figure 5.12 The orientation of fracture propagation obtained from a laboratory experiment (Chang et al. 2016)

Figure 5.13 Fracture profile for simulation models

Influence of fluid injection rate

The relationship between the fluid injection rate and the crack initiation pressures is captured in Figure 5.14 and Table 5.4. The simulation result, which associates a higher fluid injection rate to an increased crack initiation pressure, corroborates the

findings of existing experimental studies (Zoback et al. 1977, Haimson and Zhao 1991, Zhao 1995). Similar to the experimental findings (Haimson and Zhao 1991), the difference between the simulated crack initiation pressures induced by a fluid injection rate of 0.6 MPa/s, and that induced by a fluid injection rate of 1 MPa/s is less than 0.5 MPa, and the difference is less significant between higher fluid injection rates.

A possible explanation to the positive correlation between the fluid injection rate and the crack initiation pressure is that, a rise in the injection rate induces a drop in the infiltration volume due to the storage effect (Lhomme 2005). When the drop becomes dominant, fluid pressure and joint stresses around the borehole region becomes lower compared to cases assigned with a comparatively slower injection rate. Consequently, more time would be needed for the first fractures to form within the model. Another explanation is that a slower seepage rate promotes a more viscous flow (Lhomme 2005), which stimulates a subsidence in the elements' effective stress, and an increment in the joint stress. As joint stress escalates, a lower crack initiation pressure entails (Schmitt and Zoback 1993, Shimizu et al. 2011).

Figure 5.14 The simulated values for crack initiation pressure as a function of time

Influence of fluid viscosity

Figure 5.15 compares the distribution of pressure at regions around the borehole in the case of low-viscosity fracturing fluid (Case 5) and that of high-viscosity fracturing fluids (Cases 6) at two different time steps. The two models show significant differences in terms of fracture length and high-pressure zone coverage, at both time steps. A deduction for these observations is that the high penetration power of the low-viscosity fluid used in Case 5 allows the fluid to flow through the interconnected pores easily, hence giving rise to a wider high-pressure zone around the borehole region. The increased surface of high-pressure zone facilitates fracture propagation and subsequently, leads to a lower model breakdown pressure. Consistent with this inference, Cases 1, 3 and 5 of low-viscosity fluid are associated with comparatively lower breakdown pressures than the cases assigned with a high-viscosity fracturing fluid, as shown in Table 5.4. Similar finding regarding the fluid viscosity-model breakdown pressure relation was presented in several existing experimental studies (Zoback et al. 1977, Ishida et al. 2004, Stanchits et al. 2012). Furthermore, the fact that the fractures generated in cases using low-viscosity fluid are wavier compared to cases using high-viscosity fluid (refer to Figure 5.13) is also consistent with experimental observations (Ishida et al. 2004).

Figure 5.15 A difference in stress profiles in models using low and high-viscosity fracturing fluid, at two different borehole pressures

5.8 Chapter summary

The objective of Chapter 5 is to introduce an efficient simulation tool for hydraulic fracturing (HF) problems, using the framework of a hybrid DDA-FEM model. In the hybrid model, DDA blocks are discretized by FEM meshes to refine the stress distribution within each block, so as to improve the block deformability. Compared to the conventional DDA model, the hybrid model is proven to have a higher computational efficiency as the number blocks involved in the contact analysis can be substantially reduced.

The efficiency and accuracy of the hybrid model in simulating hydraulic fracturing problems are verified through a series of numerical case studies in this chapter. In addition, by employing a borehole model, the influence of time step size, fluid injection rate and fracturing fluid viscosity on the crack initiation and model breakdown pressures are investigated. Key findings are summarized as follows: (i) fractures extend in the direction parallel to that of the maximum compressive principal stress; (ii) slower fluid injection rate leads to lower crack initiation pressures; (iii) fracturing fluid of a lower viscosity results in lower model breakdown pressures; and (iv) different choices of the time step size in the analysis may affect the result accuracy and computational efficiency.

Although the scope of the current study is limited to modeling intra-block HF processes, by taking into account the inter-block contact mechanisms and fracture-joint interactions, it is possible to extend the current DDA model to HF problems involving more than one DDA block.

Chapter 6. Summary, conclusions and recommendations

6.1 Chapter overview

The flow of this closing chapter is as illustrated in Figure 6.1. Firstly, Section 6.2 summarizes the contributions and limitations of the research works presented in each chapter. Then, in Section 6.3, conclusions are drawn based on the implications and findings of the current study. Finally, thematic areas that can be further pursued to extend and improve the current DDA hydro-mechanical models are highlighted in Section 6.4.

Summary	Conclusions	Recommendations for future work
<ul style="list-style-type: none">• Research objectives• Contributions• Limitations	<ul style="list-style-type: none">• Implications of proposed models• Findings from numerical studies	<ul style="list-style-type: none">• works related to stochastic flow modeling• works related to hydraulic fracturing model

Figure 6.1 An outline of Chapter 6

6.2 Summary

It is well established that pore pressure built up in discontinuities inexorably affect the mechanical responses of jointed rock masses to loadings. The discontinuous deformation analysis (DDA) is a discontinuum theory which can account for such constitutive relations between fluid-filled discontinuities and rock blocks. It is also a numerical method or computer program commonly applied to hydro-geomechanical modeling. Research and development on DDA hydro-mechanical model has been thriving over the last two decades. The main objective of this research study is to

further contribute to those efforts. In the following, key contributions and limitations of the current research are summarized.

6.2.1 Chapter 3: Modeling the hydro-mechanical behavior of fractured media using DDA

In this chapter, a DDA hydro-mechanical model is introduced. The theoretical background and the workflow of the proposed model are provided. A number of simulation cases, of which the analysis results appear to be consistent with existing theories, are also presented to verify the reliability of the proposed algorithm.

In the same chapter, a new solution scheme termed the “semi-coupled scheme” is introduced to the DDA hydro-mechanical model. The semi-coupled scheme distinguishes the hydraulic aperture, i.e. the size of a water pathway, from the mechanical aperture, i.e. the physical distance between two adjacent blocks. According to the new scheme, the former is assumed to remain constant throughout the entire simulation. With this, the need to update the hydraulic aperture at every time step is eliminated, and hence a considerable decrease in the cost of seepage analysis can be expected. However, this constant-aperture assumption (and so is the semi-coupled scheme) is only valid for quasi-static problems that do not involve large-scale block displacements.

6.2.2 Chapter 4: A conceptual model for the simulation of stochastic flow behaviors using DDA

The objective of this chapter is to introduce a stochastic flow model to assess the spatial variability of two important hydraulic parameters, i.e. the hydraulic conductivity and the aperture. The appeal of the model lies in its simplicity and realism. It predicts the variations of a hydraulic conductivity field or an aperture profile using the Monte-Carlo method.

There are two ways to apply the generated stochastic aperture/ hydraulic conductivity field. The first way is to select the most realistic and representative realization based

on experience and available measured data, and to utilize such predictions in the DDA hydro-mechanical analysis. The second way is to subject all realizations to the DDA hydro-mechanical analysis, and statistically analyze the ensemble of results to compute the mean, the variance, the covariance or the probability density function to evaluate the uncertainty in the expected result.

A major limitation of the proposed stochastic flow model is that, a large number of realizations are often required to minimize the output uncertainty, thus leading to a high computational cost. Furthermore, there is not always clear which number of realizations is necessary for the convergence of the method. Another drawback is that, additional field data such as log-conductivity at a specific grid, even if available, cannot be explicitly taken into account in the stochastic field generation process. Nevertheless, compared to other stochastic flow modeling approaches, the proposed model is less restricted by the availability of field information and is easier to be coded into a computer program. Through a series of numerical studies, the ability of the current model in simulating different stochastic flow conditions is verified. There is a good agreement between the generated stochastic fields and the existing stochastic modeling theories.

6.2.3 Chapter 5: Hydraulic fracturing modeling using hybrid DDA

The objective of this chapter is to introduce an efficient simulation tool for hydraulic fracturing (HF) problems, using the framework of a hybrid DDA model. In the hybrid model, DDA blocks are discretized by FEM meshes to refine the stress distribution within each block and to improve block deformability. The capability of the proposed model in simulating hydraulic fracturing mechanisms is demonstrated through a series of numerical examples, and the simulation results appear to be consistent with the laboratory observations reported in existing studies. It is also noted that the current hybrid HF model prevails the conventional DDA HF model in terms of computational efficiency.

The performance of the hybrid DDA-FEM method is highly sensitive to the choice of the input parameters. Before solving any numerical case, large amount of time

needs to be spent to determine the suitable set of input parameters to be used. Even an experienced user needs to spend a lot of time in trial-and-error to obtain the most suitable parameters. Furthermore, the analysis time increases tremendously with any increase in the model's complexity as more time need to be spent in the crack updating process and the contact analysis iterations. For complex fracture problems, the hybrid DDA-FEM model does not exhibit better computational efficiency compared to the conventional DDA model.

6.3 Conclusions

The following conclusions can be drawn based on the implications and findings of the current research study.

- When solving a quasi-static problem using the DDA hydro-mechanical model, it may not be necessary to update the hydraulic aperture during every time step. Depending on the problem magnitude and nature, the benefits of a fully coupled solution scheme may not justify the high computational cost that comes along.
- The hydro-mechanical behaviors predicted by using different hydraulic conductivity fields or aperture profiles are divergent. Hence, simulating a heterogeneous hydraulic property using an assumed homogeneous model can lead to inaccurate and unrealistic analysis results.
- The ability of the proposed stochastic model to simulate non-conductive apertures could be useful in promoting the realism of a generated aperture profile.
- When the percentage of non-conductive joints increased, the phenomenon of preferential flow paths, i.e. fluid channeling through a limiting number of joints that carries large volumetric flow rates, becomes increasingly obvious.

- The discretization of DDA blocks with finite element meshes reduces the intensity of block-block contact significantly, hence inducing the number of open-close iterations to decrease and the computational speed to increase during the contact analysis.
- In view of the improved computational efficiency, the hybrid DDA-FEM model is more suitable than the conventional DDA model in modeling hydraulic fracturing problems.
- The simulation results of a wellbore model subjected to fluid pressure around the opening, and confining stresses along the model's boundaries, bring about the following implications: (i) hydraulic fractures tend to initiate at the wellbore wall and extend in the direction parallel to that of the maximum compressive principal stress; (ii) slower fluid injection rate leads to lower crack initiation pressures; (iii) fracturing fluid of a lower viscosity results in lower model breakdown pressures; and (iv) different choices of the time step size may affect the result accuracy and computational efficiency.

6.4 Recommendations for future works

Listed below are some of the thematic areas where further research can be pursued.

- The stochastic flow model proposed in Chapter 4 enables a heterogeneous flow condition to be considered in DDA hydro-mechanical analysis. A number of numerical studies have been carried out to verify the capability of the proposed model in generating plausible and realistic stochastic hydraulic conductivity fields and aperture profiles. However, corresponding empirical data that can be used for comparison and validation are extremely limited. To further validate the proposed model and to contribute to the existing stochastic modeling theories, more field or laboratory studies in this area are highly recommended.

- The proposed stochastic flow model is unconditional, i.e. additional field data such as log-conductivity at a specific grid cannot be explicitly taken into account during the generation of a stochastic field. Supplementary information as such can only be applied to the model through a time-consuming filtering process, as demonstrated in Section 4.5. To overcome this limitation, works should continue towards developing an efficient method to generate stochastic fields conditional on all available data.
- The hydraulic fracturing model introduced in Chapter 5 shows that the introduction of the FEM mesh into DDA block has improved the computational efficiency of the DDA model in simulating hydraulic fracturing problems. To further develop the proposed model, it is worthwhile to take into account the scale effect and material non-linearity in the solution scheme. In addition, towards a more realistic fracture mechanics modeling, factors such as fracture dimensions and stress intensity at the fracture tip need to be considered in the fracture propagation criterion.
- It is shown in a numerical example that the choice of time step size has a significant effect on the efficiency and accuracy of the hybrid DDA-FEM model. It is also noted that the range of suitable time step size varies on a case-by-case basis. Preliminary study to investigate how an analysis parameter affects the range of valid time step size, and how the simulation output varies when different time step sizes are chosen, is presented in Chapter 5. To gain further insight into this subject, a more in-depth study on the relations between time step size, other analysis parameters, and the simulation outputs should be carried out. Works should continue along this line towards developing a comprehensive guideline for time step size selection.

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