INVESTIGATING THE INFLUENCE OF MECHANICAL ANISOTROPY
ON THE FRACTURING BEHAVIOUR OF BRITTLE CLAY SHALES
WITH APPLICATION TO DEEP GEOLOGICAL REPOSITORIES

by

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Abstract

Investigating the influence of mechanical anisotropy on the fracturing behaviour of brittle clay shales with application to deep geological repositories

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Clay shales are currently being assessed as possible host rock formations for the deep geological disposal of radioactive waste. However, one main concern is that the favourable long-term isolation properties of the intact rock mass could be negatively affected by the formation of an excavation damaged zone (EDZ) around the underground openings. This thesis investigated the deformation and failure process of a clay shale, namely Opalinus Clay, with particular focus on the influence of anisotropy on the short-term response of circular tunnels. To achieve this goal, a hybrid *continuum-discontinuum* numerical approach was used in combination with new field measurements from the Mont Terri underground research laboratory. The response of Opalinus Clay during the excavation of a full-scale emplacement (FE) test tunnel was characterized by geodetic monitoring of wall displacements, radial extensometers and longitudinal inclinometers. The deformation measurements indicated strong directionality induced by the combined effect of *in situ* stress field and presence of bedding planes striking parallel to the tunnel axis, with the most severe deformation occurring in the direction approximately perpendicular to the material layering. Computer simulations were conducted using a newly-extended combined finite-discrete element method (FEM/DEM), a numerical technique which allows the explicit simulation of brittle fracturing and associated seismicity. The numerical experimentation firstly focused on the laboratory-scale analysis of failure processes (e.g., acoustic activity) in brittle rocks, and on the role of strength and modulus anisotropy in the failure behaviour of Opalinus Clay in tension and compression. The fracturing behaviour of unsupported circular excavations in laminated rock masses was then analyzed under different *in situ* stress conditions. Lastly, the modelling methodology was applied to the aforementioned FE tunnel to obtain original insights into the possible EDZ formation process around emplacement tunnels for nuclear waste. The calibrated numerical model suggested delamination along bedding planes and subsequent extensional fracturing as key mechanisms of the damage process poten-
tially leading to buckling and spalling phenomena. Overall, the research findings may have a potential impact on the constructability and support design of an underground repository as well as implications for its long-term safety assessment procedure.
Dedication

This thesis is dedicated to my father Romano Lisjak and in memory of my mother Marina J. Bradley (1960-1990).
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This thesis marks the end of a research period that has been made possible thanks to several generous individuals, whose collaboration and support have been greatly appreciated.

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Preface

This thesis has been prepared as five separate journal articles. The original contributions by the authors are described below.

Chapter 2

Title: Discrete modelling of fracturing processes in discontinuous rock masses
Authors: Lisjak, A., Grasselli, G.
To be submitted to: *Journal of Rock Mechanics and Geotechnical Engineering*

A. Lisjak conducted the literature review and wrote the manuscript. G. Grasselli edited the text and will be the senior responsible author (SRA) of the publication.

Chapter 3

Title: Numerical simulation of acoustic emission in brittle rocks by two-dimensional finite-discrete element analysis
Authors: Lisjak, A., Liu, Q., Zhao, Q., Mahabadi, O.K., Grasselli, G.
Published in: *Geophysical Journal International*

A. Lisjak developed the overall modelling strategy, carried out the FEM/DEM numerical simulations, and interpreted the results. Q. Liu performed the seismic analysis of the synthetic seismograms and interpreted the related results. Q. Zhao investigated the simulated acoustic response using the adjoint method. O.K. Mahabadi developed and calibrated the compression test model on granite. Q. Liu wrote the section of the manuscript relative to the travel-time inversion of acoustic signals and energy scaling analysis, while A. Lisjak wrote the remaining main body of the text. Q. Liu, O.K. Mahabadi, and G. Grasselli edited the text. The senior responsible author (SRA) of the publication was G. Grasselli.

Chapter 4

Title: Numerical modelling of the anisotropic mechanical behaviour of Opalinus Clay at the laboratory-scale using FEM/DEM
Authors: Lisjak, A., Tatone, B.S.A., Grasselli, G., Vietor, T.
Published in: *Rock Mechanics and Rock Engineering*

A. Lisjak developed the modelling strategy, carried out the numerical simulations, and interpreted the results. B.S.A. Tatone generated the discrete fracture networks. The manuscript was written by A. Lisjak and edited by B.S.A. Tatone, G. Grasselli, and T. Vietor. The senior responsible author (SRA) of the publication was G. Grasselli.
Chapter 5

Title: Numerical analysis of failure mechanisms around unsupported circular excavations in clay shales

Authors: Lisjak, A., Grasselli, G., Vietor, T.

Submitted to: International Journal of Rock Mechanics and Mining Sciences

A. Lisjak developed the modelling strategy, carried out the numerical simulations, and interpreted the results. The manuscript was written by A. Lisjak and edited by G. Grasselli and T. Vietor. The senior responsible author (SRA) of the publication was G. Grasselli.

Chapter 6

Title: The excavation of a circular tunnel in a bedded argillaceous rock (Opalinus Clay): short-term rock mass response and numerical analysis using FEM/DEM

Authors: Lisjak, A., Garitte, B., Grasselli, G., Müller, H. R., Vietor, T.

To be submitted to: Tunnelling and Underground Space Technology

The field measurements were processed and interpreted by A. Lisjak partially on the basis of a preliminary analysis carried out by B. Garitte and T. Vietor. H.R. Müller was the project manager of the FE experiment. A. Lisjak developed the modelling strategy, carried out the numerical simulations, and interpreted the results. The manuscript was written by A. Lisjak and edited by B. Garitte, H.R. Müller, and G. Grasselli. The senior responsible author (SRA) of the publication will be G. Grasselli.
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### List of Acronyms

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<th>Full Form</th>
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<tr>
<td>AE</td>
<td>Acoustic Emission</td>
</tr>
<tr>
<td>ANDRA</td>
<td>Agence Nationale pour la gestion des Déchets RA dioactifs (Radioactive Waste Management Organization, France)</td>
</tr>
<tr>
<td>BD</td>
<td>Brazilian Disc</td>
</tr>
<tr>
<td>BGR</td>
<td>Bundesanstalt für Geowissenschaften und Rohstoffe (Federal Institute for Geosciences and Natural Resources, Germany)</td>
</tr>
<tr>
<td>BPM</td>
<td>Bonded Particle Model</td>
</tr>
<tr>
<td>DDA</td>
<td>Discontinuous Deformation Analysis</td>
</tr>
<tr>
<td>DEM</td>
<td>Discrete Element Method</td>
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<td>DFN</td>
<td>Discrete Fracture Network</td>
</tr>
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<td>DGR</td>
<td>Deep Geological Repository</td>
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<tr>
<td>EDZ</td>
<td>Excavation Damaged Zone</td>
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<td>EdZ</td>
<td>Excavation disturbed Zone</td>
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<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
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<td>FE</td>
<td>Full-scale Emplacement</td>
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<tr>
<td>FEM</td>
<td>Finite Element Method</td>
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<tr>
<td>FEM/DEM</td>
<td>Hybrid Finite-Discrete Element Method</td>
</tr>
<tr>
<td>FLAC</td>
<td>Fast Lagrangian Analysis of Continua</td>
</tr>
<tr>
<td>FPZ</td>
<td>Fracture Process Zone</td>
</tr>
<tr>
<td>GRS</td>
<td>Gesellschaft für Anlagen- und Reaktorsicherheit (Global Research for Safety, Germany)</td>
</tr>
<tr>
<td>GUI</td>
<td>Graphical User Interface</td>
</tr>
<tr>
<td>ISRM</td>
<td>International Society for Rock Mechanics</td>
</tr>
<tr>
<td>LDP</td>
<td>Longitudinal Displacement Profile</td>
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<tr>
<td>LEFM</td>
<td>Linear Elastic Fracture Mechanics</td>
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<tr>
<td>Acronym</td>
<td>Description</td>
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<tr>
<td>LUOEX</td>
<td>Large Underground COncept Experiments</td>
</tr>
<tr>
<td>NAGRA</td>
<td>Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (National Cooperative for the Disposal of Radioactive Waste, Switzerland)</td>
</tr>
<tr>
<td>NWMO</td>
<td>Nuclear Waste Management Organization (Canada)</td>
</tr>
<tr>
<td>OPA</td>
<td>Opalinus Clay</td>
</tr>
<tr>
<td>PFC</td>
<td>Particle Flow Code</td>
</tr>
<tr>
<td>SF/HLW</td>
<td>Spent Fuel and vitrified High-Level nuclear Waste</td>
</tr>
<tr>
<td>SJM</td>
<td>Smooth Joint Model</td>
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<tr>
<td>THM</td>
<td>Thermo-Hydro-Mechanical</td>
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<tr>
<td>UCS</td>
<td>Uniaxial Compressive Strength</td>
</tr>
<tr>
<td>UDEC</td>
<td>Universal Distinct Element Code</td>
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<tr>
<td>URL</td>
<td>Underground Research Laboratory</td>
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Chapter 1

Introduction

1.1 Problem scope

Clay shales are currently being assessed as host rocks for the underground disposal of solid radioactive waste. The key characteristics that make these argillaceous rocks suitable for nuclear waste storage include: very low hydraulic conductivity, low diffusion coefficients and good retention capacity for radionuclides, potential for self-sealing of open fractures, and lack of economic value (Blümling et al., 2007). However, one main concern is the formation of an excavation damaged zone (EDZ) around the emplacement tunnels comprising the underground repository. That is, the favourable long-term isolation properties of the intact rock mass could be negatively affected by the disturbance and damage associated with the underground excavations. In particular, a permeability increase of several orders of magnitude may be induced in the EDZ due to the formation of newly-connected porosity in response to rock fracturing (Tsang et al., 2005). Another relevant issue, which affects the short-term construction stage, is the instability and squeezing behaviour of the newly-excavated underground openings. In this context, the design of support measures as well as the choice of excavation method and sequencing are directly affected by the particular geomechanical properties of clay shales, as further described below. An extensive experimental research program is being carried out at the Mont Terri underground rock laboratory (URL) (Thury and Bossart, 1999) on Opalinus Clay, a clay shale formation selected to potentially host a deep geological repository (DGR) for high-level nuclear waste in Switzerland. Since 1996, the international research at the Mont Terri URL has involved fourteen organizations from several countries, including Belgium, Canada, France, Germany, Japan, Spain, Switzerland and the USA, all of which are considering argillaceous formations as potential host rocks for the disposal of nuclear waste.

A large body of experimental evidence suggests that the mechanical behaviour of shales is heavily influenced by a distinctive stiffness and strength anisotropy. This directionality in the mechanical response arises at different spatial scales within the rock due to a number of factors, including the laminated clayey micro-structure, the presence of foliation and bedding planes, and preferably-oriented rock mass features such as joints and tectonic faults. At the laboratory-scale, variation of elastic response, strength characteristics and failure mechanisms with varying angle between the principal stress directions and the specimen layering orientation is typically observed (e.g., McLamore and Gray, 1967;
Niandou et al., 1997). At the field-scale, the stability of underground structures in laminated shales is highly dependent upon the relative orientation between the bedding orientation and the excavation axis. In particular, catastrophic bending and buckling of layers around drifts (Blümling et al., 2007), premature collapse of borehole walls (e.g., Økland and Cook, 1998; Marschall et al., 2006), and ground support and tunnel construction difficulties (e.g., Einstein, 2000; Perras and Diederichs, 2009), have been reported when excavating in the direction parallel to the bedding plane strike.

According to the preliminary design of the Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA), the emplacement tunnels for spent fuel and vitrified high-level nuclear waste (SF/HLW) will be excavated in Opalinus Clay at a depth ranging between 500 and 900 m under flat-lying bedding conditions. Conversely, due to the local stratigraphy at the Mont Terri URL, most of the field studies to date have been mainly focused on the response of excavations aligned with the dip direction of bedding planes inclined at about 30-50° (Fig. 1.1). Although the latter case has been proven less prone to tunnel instabilities, it cannot be considered fully representative of the actual repository conditions, whereby the excavation axis striking parallel to the bedding is expected to play a key-role in controlling the tunnel behaviour.

Numerical simulation is being widely used as a tool to assist in the design of DGRs. To date, the vast majority of numerical models adopted to analyze the stability of openings in layered rocks have been based on continuum mechanics principles using classic shear failure theory for elasto-plastic materials (e.g., Adhikary and Guo, 2002; Jia and Tang, 2008; Riahi and Curran, 2009). With this technique the presence of layers is smeared to produce a fictitious continuous material that exhibits mechanical characteristics that are similar to the original discontinuous medium. However, a number of experimental observations demonstrate that clay shales may fail in a brittle manner under low-confinement conditions such as those characterizing the near-field of the excavation. In particular, rock mechanics tests on Opalinus Clay indicate that the rock failure process, including the stress-strain response, fracture mechanisms and acoustic activity, is typical of that for brittle materials (Naumann et al., 2007; Amann
et al., 2011, 2012). Also, several field observations highlight strongly localized failure patterns in the
form of brittle fracturing, including excavation-parallel extensional cracks (i.e., spalling) (e.g., Bossart
et al., 2002; Yong et al., 2010).

1.2 Approach

This thesis aims at investigating the failure process of Opalinus Clay with particular focus on the influ-
ence of anisotropy on the short-term mechanical response of underground excavations. A combination
of field measurements and numerical tools were used to achieve this goal.

Field measurements from a recently-excavated, full-scale emplacement (FE) test tunnel at the Mont
Terri URL were used to quantitatively characterize the short-term rock mass response. For the first
time, the behaviour of Opalinus Clay was analyzed under \textit{in situ} conditions similar to those of the actual
repository tunnels from both a geometrical (i.e., same tunnel shape and dimensions) and structural geo-
logical (i.e., tunnel oriented parallel to the bedding strike) point of view. The analyzed monitoring data
included measurements of tunnel wall convergences, radial deformations using multi-point extensome-
ters, vertical deflections from longitudinal chain inclinometers, and pore water pressure. In particular, a
detailed analysis of the anisotropic response was possible owing to the adopted geometric layout of the
monitoring system accounting for the bedding orientation.

Numerical simulations were carried out using the combined finite-discrete element method (FEM/DEM)
(Munjiza, 2004; Mahabadi et al., 2012a), a numerical technique which allows modelling the tran-
sition from \textit{continuum} to \textit{discontinuum} by explicitly simulating brittle fracture processes. The numerical
experimentation firstly focused on the laboratory-scale analysis of failure processes (e.g., acoustic ac-
tivity) in brittle rocks, and on the role of strength and stiffness anisotropy on the failure behaviour of
Opalinus Clay in tension and compression. Secondly, the fracturing behaviour of unsupported circular
excavations in laminated rock masses was analyzed under different \textit{in situ} stress conditions. Lastly,
the modelling methodology was applied to the aforementioned FE tunnel excavation to obtain further
insights into the possible EDZ formation process around emplacement tunnels for nuclear waste.

1.3 Research objectives

In this study, the fracturing behaviour of brittle clay shales was investigated. To achieve this goal, the
following research objectives were developed:

1. \textit{Determine under which conditions the acoustic emission (AE) associated with the failure process
of brittle rocks can be numerically captured using FEM/DEM.}

This objective was addressed by developing an algorithm to extract seismic information based on
the monitoring of internal variables in proximity to propagating cracks. The extracted numerical
information was verified by travel-time inversion and energy scaling of cross-analyzed synthetic
seismograms. The technique was then validated by analyzing the AE statistics of a numerical
compression test on a heterogeneous rock sample (Chapter 3).
2. Devise a micro-mechanical modelling procedure to capture the distinct variation of failure mechanism and associated strength response that is typically observed in clay shales as a function of the relative orientation between layering and principal stresses.

This objective was addressed by developing two distinct approaches in the framework of FEM/DEM. A “discrete approach” captured strength anisotropy as an emergent property of a homogeneous, isotropic medium containing a distribution of preferably oriented, finite-sized cracks (Chapter 4). A “smeared” approach captured strength anisotropy by introducing directionality in the cohesive strength parameters of the fracture model (Chapter 5).

3. Test the hypothesis that the mechanical behaviour and failure mechanisms of clay shales are governed by material anisotropy.

This objective was addressed by extending the FEM/DEM code to accommodate the modelling of anisotropy of stiffness and strength. Standard rock mechanics tests on Opalinus Clay were then simulated and the results compared to published experimental results (Chapter 4 and 5).

4. Isolate the impact of material anisotropy on the failure mechanisms and mechanical response around excavations in clay shales.

This objective was addressed by simulating the excavation of an unsupported, circular excavation under isotropic in situ stress conditions. The final fracture pattern was compared with typical damage zones reported in the literature and the evolution of damage analyzed based on the simulation results (Chapter 5).


This objective was addressed by analyzing the monitoring data collected during the recent excavation of the FE tunnel at the Mont Terri URL (Chapter 6). The field measurements were provided by NAGRA and included: tunnel wall convergences, rock mass displacements measured by radial extensometers and longitudinal inclinometers, and pore pressure measurements.

6. Provide a numerical interpretation of the deformation response observed in the field in terms of possible fracturing process.

This objective was addressed by first calibrating the FEM/DEM based on the measured deformation response of the FE tunnel and then analyzing the simulated evolution of damage (Chapter 6).

1.4 Thesis overview

This thesis consists of five articles prepared for peer-reviewed journals. Each chapter contains an introduction and a literature review. Therefore, background materials on numerical modelling of anisotropic materials, details of the FEM/DEM implementation, description of the mechanical behaviour of clay.
shales, and damaged zone around excavations in Opalinus Clay are described throughout Chapters 3 to 6.

Chapter 2 presents a literature review of selected discrete element (DEM) and hybrid finite-discrete element (FEM/DEM) modelling techniques that have recently emerged in the field of rock mechanics as simulation tools for fracturing processes in discontinuous rock masses. Specifically, the DEM computer codes, UDEC and PFC, and the FEM/DEM codes, ELFEN and Y-Geo, are considered. The fundamental principles of each code are illustrated with particular emphasis on the approach specifically adopted to simulate fracture nucleation and propagation and to account for the presence of rock mass discontinuities. Furthermore, a review of application studies focusing on laboratory-scale models of the rock failure process and on the simulation of damage development around underground excavations is provided. Also, a brief overview of continuum-based approaches is given. This chapter will be submitted as a review article to the *Journal of Rock Mechanics and Geotechnical Engineering*.

Chapter 3 numerically investigates the acoustic activity associated with the failure process of brittle rocks. Quasi-dynamic seismic information is extracted from a FEM/DEM model with a newly developed algorithm based on the monitoring of internal variables (e.g., relative displacements and kinetic energy) in proximity to propagating cracks. AE of a wing crack propagation model based on this algorithm are cross-analyzed by travel-time inversion and energy estimation from seismic recordings. The modelling technique is then applied to the simulation of a laboratory compression test on a granite sample. The micro-mechanical parameters of the heterogeneous model are first calibrated to reproduce the macroscopic stress-strain response measured during standard laboratory tests. Subsequently, AE frequency-magnitude statistics, spatial clustering of source locations, and the evolution of AE rate are analyzed. This chapter has been published in the *Geophysical Journal International* (Lisjak et al., 2013b).

Chapter 4 illustrates new developments that have been introduced into FEM/DEM to model layered materials and demonstrates their effectiveness in capturing the short-term mechanical response of Opalinus Clay at the laboratory-scale. In particular, a transversely isotropic elastic constitutive law is implemented to account for the anisotropic elastic modulus, while a procedure to incorporate a distribution of preferentially oriented defects is devised to capture the anisotropic strength (i.e., “discrete” approach). Laboratory results of indirect tensile tests and uniaxial compression tests are used to calibrate the numerical model. Subsequently, the calibrated model is validated by investigating the effect of confinement and the influence of the loading angle with respect to the specimen anisotropy. Simulated fracture patterns are discussed in the context of the theory of brittle rock failure and analyzed with reference to the EDZ formation mechanisms observed at the Mont Terri URL. This chapter has been published in *Rock Mechanics and Rock Engineering* (Lisjak et al., 2013c).

Chapter 5 introduces a new micro-mechanical technique to capture strength anisotropy in FEM/DEM and applies the approach to the simulation of the EDZ around a circular tunnel in horizontally bedded Opalinus Clay. Motivated by the inability of the “discrete” approach (Chapter 4) to correctly capture bedding plane delamination in field-scale models, the new “smeared” approach introduces anisotropy directly into the fracture model by imposing that the cohesive strength of each crack element is a func-
tion of the relative orientation between the crack element itself and the layering orientation. Similar to Chapter 4, the effectiveness of the numerical technique is quantitatively demonstrated by simulating standard rock mechanics tests on Opalinus Clay. Subsequently, the evolution of damage around a circular tunnel is investigated and the simulated fracturing process discussed in the context of the fracture pattern observed at the Mont Terri URL. Furthermore, the influence of in situ stress on resulting EDZ geometry is analyzed together with possible implications for ground support and tunnel constructability. This chapter has been submitted to the International Journal of Rock Mechanics and Mining Sciences.

Chapter 6 firstly details the results of the rock mass monitoring program carried out during the construction of the FE tunnel at the Mont Terri URL, with particular focus on the short-term deformation response. Secondly, the deformation behaviour observed in the field is numerically back-analyzed using both a linear elastic, finite element model with ubiquitous joint analysis and a FEM/DEM simulation. In particular, the FEM/DEM model is first calibrated based on the tunnel wall convergences measured in the field and then used to obtain further insights into the fracturing processes leading to the formation of the EDZ. Finally, the possible effects of varying in situ stress conditions and support stiffness on the final fracture pattern and displacement field are highlighted. This chapter will be submitted to the journal Tunnelling and Underground Space Technology.

Appendix A details the implementation of several newly-developed FEM/DEM algorithms, including (i) a transversely isotropic, linear elastic triangular element, (ii) an in situ stress initialization routine, (iii) a cohesive element with direction-dependent strength parameters and acoustic emission recording, and (iv) an absorbing boundary condition.

Appendix B reports the computational time of selected FEM/DEM models.
Chapter 2

Discrete modelling of fracturing processes in discontinuous rock masses

2.1 Introduction

A large body of experimental research shows that the failure process in brittle rocks under compression is characterized by complicated micro-mechanical processes, including the nucleation, growth and coalescence of microcracks, which lead to strain localization in the form of macroscopic fracturing (Lockner et al., 1991; Benson et al., 2008). The evolution of microcracking, typically associated with the emission of acoustic energy, results in a distinctive non-linear stress-strain response, with macroscopic strain softening commonly observed under low-confinement conditions (Brace et al., 1966; Bieniawski, 1967; Martin, 1997; Eberhardt et al., 1997). Furthermore, unlike other materials (e.g., metals), rocks exhibit a strongly pressure-dependent mechanical behaviour (Jaeger and Cook, 1976). A variation of failure mode, from axial splitting to shear band formation, is indeed often observed for increasing confining pressures (Horii and Nemat-Nasser, 1986). This variation in failure behaviour is reflected in a non-linear failure envelope (Kaiser and Kim, 2008) and in a transition from brittle to ductile post-peak response (Paterson and Wong, 2004). At the rock mass level, the failure process observed during laboratory-scale experiments is further complicated by the presence of discontinuities, such as joints, faults, shear zones, schistosity planes, and bedding planes (Goodman, 1989). Specifically, discontinuities affect the response of the intact rock by reducing its strength and inducing non-linearities and anisotropy in the stress-strain response (Hoek and Brown, 1980a; Hoek et al., 2002). Furthermore, discontinuities add kinematic constraints on the deformation and failure modes of structures in rocks (Hoek et al., 1995; Hoek, 2006) and cause stress and displacement redistributions to sensibly deviate from linear elastic, homogenous conditions (Hammah et al., 2008).

Aside for the intrinsic uncertainties associated with the determination of reliable in situ input parameters, the application of numerical modelling to the analysis of rock engineering problems represents a challenging task owing to the aforementioned features of the rock behaviour. In particular, the progressive degradation of material integrity during the deformation process together with the influence of
pre-existing discontinuities on the rock mass response have represented a major drive for the development of new modelling techniques. In this context, the available numerical approaches are typically classified either as continuum- or discontinuum-based methods (Jing and Hudson, 2002).

The main assumption of continuum-based methods is that the computational domain is treated as a single continuous body. Standard continuum mechanics formulations are based on theories such as plasticity and damage mechanics, which adopt internal variables to capture the influence of history on the evolution of stress and changes at the micro-structural level, respectively (de Borst et al., 2012). Conventionally, the implementation of continuum techniques is based on numerical methods, such as non-linear finite elements (FEM), Lagrangian finite differences (FDM), and boundary elements (BEM), with the incorporation of plasticity-based material models. However, standard strength-based, strain-softening constitutive relationships cannot capture localization of failure as the lack of an internal length scale results in the underlying mathematical problem to become ill-posed (de Borst et al., 1993). Among the main consequences of adopting a standard continuum to simulate strain localization are the fact that, by doing so, localization occurs in a region of zero thickness and consequently an unphysical mesh sensitivity arises. To overcome these shortcomings, the description of the continuum must account either for the viscosity of the material by incorporating a deformation-rate dependency, or for the change in the material micro-structure by enhancing the mathematical formulation with additional terms (de Borst et al., 1993). The latter technique, known as regularization, include non-local (e.g., Bažant and Pijaudier-Cabot, 1988), gradient (e.g., Mühlhaus and Aifantis, 1991), and Cosserat micropolar (e.g., Mühlhaus and Vardoulakis, 1987) models. Alternatively, cohesive crack models have been proposed under the assumption that damage can be represented by a dominant macro-fracture lumping all non-linearities into a discrete line (e.g., Hillerborg et al., 1976; Bažant and Oh, 1983). That is, a fictitious crack concept is employed to represent the effect of a fracture process zone ahead of the crack tip whereby small-scale yielding, micro-cracking or void growth and coalescence are assumed to take place. For the case of heterogeneous rocks, strain localization has also been successfully simulated by damage models with statistically distributed defects. A number of variations of this approach have been developed for numerical schemes such as FEM (Tang, 1997), FDM (Fang and Harrison, 2002b), smooth-particle hydrodynamics (Ma et al., 2011), cellular automaton (Feng et al., 2006), and lattice models (Blair and Cook, 1998).

Within continuum models, two approaches are commonly employed to account for the presence of rock mass discontinuities. If the number of discontinuities is relatively large, homogenization techniques are typically adopted. The most widely used homogenization approach consists of reducing, within a conventional elasto-plastic model, the rock mass deformation modulus and strength parameters to account for the degrading effect induced by the local geological conditions (Hoek et al., 2002; Hoek and Diederichs, 2006). More advanced models can also include transversely isotropic elastic response induced by preferably oriented joints (Amadei, 1996) or failure-induced, plastic anisotropic behaviour (e.g., Mühlhaus, 1993; Dyszlewicz, 2004). However, the classic homogenization approach is typically limited by the fact that slip, rotations and separation as well as size effects induced by discontinuities cannot be explicitly captured (Hammah et al., 2008). Alternatively, if the problem is controlled by a
relatively low number of discrete features, special interface (or joint) elements can be incorporated into the continuum formulation (e.g., Goodman et al., 1968; Ghaboussi et al., 1974; Wilson, 1977; Pande and Sharma, 1979; Beer, 1985). This technique, also known as the combined continuum-interface method (Riahi et al., 2010), can accommodate large displacements, strain and rotations of discrete bodies. However, it is accurate as long as changes in edge-to-edge contacts are negligible throughout the solution (Hammah et al., 2007). That is, owing to the fixed interconnectivity between solid and joints and the lack of an automatic scheme to recognize new contacts, only small displacement/rotations along joints can be correctly captured (Cundall and Hart, 1992).

Discrete (or discontinuous) modelling techniques, commonly referred to as the Discrete Element Method (DEM), treat the material directly as an assembly of separate blocks or particles. According to the original definition proposed by Cundall and Hart (1992), a DEM is any modelling technique that (i) allows finite displacements and rotations of discrete bodies, including complete detachment, and (ii) recognizes new contacts automatically as the simulation progresses. DEMs were originally developed to efficiently treat solids characterized by pre-existing discontinuities having spacing comparable to the scale of interest of the problem under analysis and for which the continuum approach described above might not provide the most appropriate computational framework. These problems included: blocky rock masses, ice plates, masonry structures, and flow of granular materials. DEMs can be further classified according to several criteria regarding, for instance, the type of contact between bodies, the representation of deformability of solid bodies, the methodology for detection and revision of contacts, and the solution procedure for the equations of motion (Jing and Stephansson, 2007). Based on the adopted solution algorithm, DEM implementations are broadly divided into explicit and implicit methods. The most notable implementations of the former group, known also as the Distinct Element Method (Cundall and Strack, 1979a), are arguably represented by the Universal Distinct Element Code (UDEC) (Itasca Consulting Group Inc., 2013b) and the Particle Flow Code (PFC) (Itasca Consulting Group Inc., 2012b). On the other hand, the best known implicit DEM is the Discontinuous Deformation Analysis (DDA) method (Shi and Goodman, 1988). Despite the fact that DEMs were originally developed to model jointed structures and granular materials, the application of DEM was subsequently extended to the case of systems where the mechanical behaviour is controlled by discontinuities that emerge as natural outcome of the deformation process, such as the brittle fracture of rocks. Specifically, the introduction of bonding between discrete elements allowed capturing the formation of new fractures and thus extended the application of DEM to model the transition from continuum to discontinuum.

As observed by Bičanić (2003), the original boundary between continuum and discontinuum techniques has become less clear as several continuum techniques are capable of dealing with emergent discontinuities associated with the brittle fracture process. In particular, the hybrid approach known as the combined finite-discrete element method (FEM/DEM) (Munjiza et al., 1995; Munjiza, 2004) effectively starts from a continuum representation of the domain by finite elements and allow a progressive transition from a continuum to a discontinuum with insertion of new discontinuities.

The scope of this chapter is to provide a summary of selected discrete element and hybrid finite-discrete element modelling techniques that have recently emerged in the field of rock mechanics as
simulation tools for fracturing processes in rocks and rock masses. Specifically, the DEM computer codes, UDEC and PFC, and the FEM/DEM codes, ELFEN (Rockfield Software Ltd., 2004) and Y-Geo (Mahabadi et al., 2012a), were considered. It is noteworthy that the aforementioned codes are not the only ones available to the rock mechanics research community. For instance, the particle-based open-source program YADE (Kozicki and Donzé, 2008, 2009) has found recent application to the 3D modelling of progressive failure in jointed rock masses (Scholtès and Donzé, 2012; Harthong et al., 2012). Also, modified versions of the DDA method, originally developed to model blocky rock masses (e.g., Hatzor and Benary, 1998; Bakun-Mazor et al., 2009; Hatzor et al., 2010), have been employed to simulate fracturing processes in brittle materials (Ke, 1997; Koo and Chern, 1997; Lin et al., 1996; Pearce et al., 2000).

For each code, the fundamental implementation principles are illustrated with particular emphasis on the approach specifically adopted to simulate fracture nucleation and propagation and to account for the presence of rock mass discontinuities. The description of the fundamental principles is accompanied by a brief review of application studies focusing on laboratory-scale models of rock failure process and on the simulation of damage development around underground excavations. Extensive reviews regarding numerical methods in rock mechanics can be found elsewhere (Jing and Hudson, 2002; Jing, 2003). Detailed illustration of fundamentals and application of discrete element method is provided by Jing and Stephansson (2007) and Bobet et al. (2009). Also, a review of modelling techniques for the progressive mechanical breakdown of heterogeneous rocks and associated fluid flow is provided by Yuan and Harrison (2006).

2.2 Distinct element methods (explicit DEM)

The term distinct element method refers to a particular class of DEM that uses an explicit time-domain integration scheme to solve the equations of motion for rigid or deformable discrete bodies with deformable contacts (Cundall and Strack, 1979a). Within the rock engineering community, the best-known codes are the Particle Flow Code (PFC2D/PFC3D) (Itasca Consulting Group Inc., 2012b,c) and the Universal Distinct Element Code (UDEC/3DEC) (Cundall, 1980; Cundall and Hart, 1985; Itasca Consulting Group Inc., 2013b,a), which represent the solid material as an assembly of rigid particles and deformable blocks, respectively.

2.2.1 The Particle Flow Code (PFC)

Fundamental principles

Particle-based models were originally developed to simulate the micromechanical behaviour of non-cohesive media, such as soils and sands (Cundall and Strack, 1979a). With this approach, the granular microstructure of the material is modelled as a statistically generated assembly of rigid circular particles of varying diameter. The contact between particles are typically assigned a normal and shear stiffness as well as friction coefficient. The commercially available code PFC represents an evolution of previ-
ous particle-based codes, namely BALL and TRUBAL (Cundall and Strack, 1979b), whereby cohesive bonds are applied between particles to simulate the behaviour of solid rocks. The resultant model is commonly referred to as the bonded-particle model (BPM) for rock (Potyondy and Cundall, 2004). In a BPM, crack nucleation is simulated through breaking of internal bonds while fracture propagation is obtained by coalescence of multiple bond breakages. Blocks of arbitrary shapes can form as result of the simulated fracturing process and can subsequently interact with each other.

Two types of bonds are typically used in PFC: the contact bond and the parallel bond. In the contact bond model, an elastic spring with constant normal and shear stiffnesses, $k_n$ and $k_s$, acts at the contact points between particles, thus allowing only forces to be transmitted. In the parallel bond model, the moment induced by particle rotation is resisted by a set of elastic springs uniformly distributed over a finite-sized section lying on the contact plane and centered at the contact point (Figure 2.1). This bond model reproduces the physical behaviour of a cement-like substance gluing adjacent particles together.

As further described in the next section, parallel-bonded rock models have been widely used to study fracturing and fragmentation processes in brittle rocks. However, one of the major drawbacks of this type of model is the unrealistically low ratios of the simulated unconfined compressive strength to the indirect tensile strength for synthetic rock specimens (Cho et al., 2007; Kazerani and Zhao, 2010); the straightforward adoption of circular (or spherical) particles cannot fully capture the behaviour of complex-shaped and highly interlocked grain structures that are typical of hard rocks. Furthermore, low emergent friction values are simulated in response to the application of confining pressure. To overcome these limitations a number of enhancements to PFC were proposed. Potyondy and Cundall (2004) showed that by clustering particles together (Fig. 2.2a) more realistic macroscopic friction values can be obtained. Specifically, the intra-cluster bond strength is assigned a different strength value than the bond strength at the cluster boundary. Cho et al. (2007) showed that by applying a clumped-particle geometry...
Intra-cluster bonds; white: inter-cluster bonds) and (b) effect of cluster material using particle clusters: (a) clusters of size 7 and bonds (black: Fig. 11. Introducing complex grain-like shapes into the PFC2D by Mosher et al. [59], who have studied the cracking compressive and tensile strengths of granite is suggested that contributes to the large difference in the break, then damage mechanisms that more closely match the ratio of unconfined compressive strength to indirect tensile strength. (a) Particle clustering (after Potyondy and Cundall (2004), © Elsevier, reproduced with permission). (b) Clustered particles vs. clumped particles (after Cho et al. (2007), redrawn). (c) Flat-joint contact model showing the effective interface geometry (after Potyondy (2012), redrawn).

(Fig. 2.2b) a significant reduction of the aforementioned deficiencies can be obtained, thereby allowing to reproduce correct strength ratios, non-linear behaviour of strength envelope and friction coefficients comparable with laboratory values. More recently, Potyondy (2012) developed a new contact formulation, namely the flat-joint model, aimed at capturing the same effects of a clumped BPM model (or of a grain-based UDEC model as described below) with a computationally more efficient method (Fig. 2.2c). The partial interface damage and continued moment-resisting ability of the flat-jointed model allows to correctly match both the direct tensile and the unconfined compressive strength of a hard rock.

Another issue arising from the particle-based material representation of PFC is the inherent roughness of interface surfaces representing rock discontinuities (Fig. 2.3a). This roughness typically results in an artificial additional strength along frictional or bonded rock joints. This shortcoming was overcome by the development of the smooth-joint contact model (SJM) (Mas Ivars et al., 2008), which allows to simulate a smooth interface regardless of the local particle topology (Fig. 2.3b). The combination of the BPM to capture the behaviour of intact material with the SJM for joint network lead to the development of the so-called synthetic rock mass (Ivars et al., 2011), which aims at numerically predict rock mass properties, including scale effects, anisotropy, and brittleness, that cannot be obtained using empirical methods.

Main advantages of the PFC modelling methodology include the simple mathematical treatment of the problem, whereby complex constitutive relationships are replaced by simple particle contact logic, and the natural predisposition of the approach to account for material heterogeneity. On the other hand, considered the high level of simplification introduced, extensive experimental validation is needed to verify that the method can capture the observed macroscopic behaviour of rock. Moreover, an extensive calibration based on experimentally measured macro-scale properties is required to determine the contact parameters that will predict the observed macro-scale response.
Applications

PFC has been extensively used within the rock mechanics community to numerically investigate the fundamental processes of brittle fracturing in rocks by means of laboratory scale models. Potyondy et al. (1996) first proposed a synthetic PFC model that could reproduce modulus, unconfined compressive stress, and crack initiation stress of the Lac du Bonnet Granite. Extended results were illustrated by Potyondy and Cundall (2004) with the simulation of the stress-strain behaviour during biaxial compression tests for varying confining pressures. Several features of the rock behaviour emerged from the BPM model, including elasticity, fracturing, damage accumulation producing material anisotropy, dilation, post-peak softening and strength increase with confinement. Since PFC simulates quasi-static deformation by solving the equations of motion, elasto-dynamics effects, such as stress wave propagation and cracking-induced acoustic emission (AE), can be explicitly simulated. In this context, Hazzard and Young (2000) developed a technique to dynamically quantify AE in a PFC model. The approach was validated by simulating the seismic $b$ value of a confined test on granite. The aforementioned approach was further improved by introducing moment tensor calculation based on change in contact forces upon particle contact breakage and was applied to the micro-seismic simulation of a mine-by experiment in a crystalline rock (Hazzard and Young, 2002) and of an excavation-induced fault slip event (Hazzard et al., 2002). Three-dimensional simulations of acoustic activity using PFC3D were proposed by Hazzard and Young (2004). Diederichs (2003) used PFC simulations to explore the aspects of grain-scale tensile damage accumulation under both macroscopically tensile and compressive conditions. A BPM was employed as numerical analogue to study the effects of tensile damage and the sensitivity to low confinement in controlling the failure of hard rock masses in proximity of underground excavations. Application of PFC to determining the fracture toughness of synthetic rock-like specimen was illustrated by Moon et al. (2006). Analysis of failure and deformation mechanisms during direct shear loading of rock joints have also been carried to obtained original insights into rock fracture shear behaviour and asperity degradation. Rasouli and Harrison (2010) investigated the relation between Riemannian roughness parameter and shear strength of profiles comprising symmetric triangular asperities sheared at different normal stress levels. Asadi et al. (2012) extended the previous results with consideration of the shear strength and asperity degradation processes of several synthetic profiles including triangular,
Chapter 2. DEM Modelling of Rock Mass Fracturing

sinusoidal and randomly generated profiles. Zhao (2013) simulated single- and multi-gouge particles in a rough fracture segment undergoing shear and investigated the behaviour of gouge particles as function of the applied confinement. Another important mechanism of the failure process in rocks, such as the initiation and propagation of cracks from pre-existing flaws, has been analyzed using BPM. Zhang and Wong (2012b) numerically simulated the cracking process in rock-like material containing a single flaw under uniaxial compression, while Zhang and Wong (2012a) investigated the coalescence behavior for the case of two stepped and coplanar pre-existing open flaws. The effect of confinement on wing crack propagation was studied by Manouchehrian and Marji (2012).

BPMs have been successfully applied to the study of damaged zones around underground openings. The spalling phenomena observed around the Atomic Energy of Canada Limited’s (AECL) mine-by experiment tunnel (Martin et al., 1997) were first simulated by Potyondy (1998). Further analysis of the notch formation process in terms of coalescence of ruptured bonds was provided by Potyondy and Cundall (2004) using a PFC2D model embedded in a continuum finite-difference model (Fig. 2.4a). Hazzard and Young (2002) provided a micro-seismic simulation of the same excavation by comparing the actual seismicity recorded underground with the simulated spatial and temporal distribution of events. The effect of low stiffness spray-on liner of fracture propagation based on in situ conditions of the above mentioned mine-by experiment was numerically studied by Tannant and Wang (2004). Similarly, Potyondy and Cundall (2000) used PFC2D to predict damage formation adjacent to a circular excavation in an anisotropic gneissic tonalite at the Olkiluoto deep geological repository. Fakhimi et al. (2002) showed that a BPM could match failure load, crack pattern, and spalling observed during a biaxial compression test on a sandstone specimen with a circular opening (Fig. 2.4b). Numerical studies on thermally-induced fracturing around openings in granite were carried out by Wanne and Young (2008) and Wanne (2009) for a laboratory-scale heater experiment and the AECL’s Tunnel Sealing Experiment, respectively. Sagong et al. (2011) investigated the influence of the joint angle on the rock fracture and joint sliding behaviors around an opening in a jointed rock model.

2.2.2 The Universal Distinct Element Code (UDEC)

Fundamental principles

In UDEC the computational domain is discretized into blocks using a finite number of intersecting discontinuities. Each block is internally subdivided using a finite difference or a finite volume scheme for calculation of stress, strain and displacements. Model deformability is captured by an explicit, large strain Lagrangian formulation similar to the continuum code FLAC (Itasca Consulting Group Inc., 2012a). The mechanical interaction between blocks is characterized by compliant contacts using a finite stiffness in the normal direction and a tangential stiffness together with a shear strength criterion (e.g., Coulomb-type friction) in the tangential direction to the discontinuity surface. Similarly to PFC, static problems are treated using a dynamic relaxation technique by introducing viscous damping to achieve steady state solutions.

When using the classic formulation of UDEC, rock failure is captured either in terms of plastic
yielding (e.g., Mohr-Coulomb criterion with tension cut-off) of the rock matrix or displacements (i.e., sliding, opening) of the pre-existing discontinuities. That is, new discontinuities cannot be driven within the continuum portion of the model and therefore discrete fracturing through intact rock cannot be simulated. However, Lorig and Cundall (1989) showed that this shortcoming can be overcome by introducing a polygonal block pattern, such as the Voronoi tessellation, to the UDEC capability. As depicted in Fig. 2.5, a physical discontinuity is created when the stress level at the interface between block exceeds a threshold value either in tension or shear. Although new fractures are so propagated, this technique is not based on a fracture mechanics approach. That is, unlike classic LEFM models, fracture toughness and stress intensity factors are not considered. Furthermore, material softening in the fracture process zone, typically captured using cohesive-crack models, is disregarded.

Although polygonal block models are computationally more expensive than particle-based ones, they can provide a more realistic representation of the rock micro-structure (Lemos, 2012). Owing to the full contact between grains and better interlocking offered by the random polygonal shapes, the grain-based UDEC model overcomes some of the limitations of parallel-bonded particle models, as further described below.

**Applications**

Owing to the above mentioned characteristics, grain-based DEM have been employed to study the fracturing behaviour of rocks. Christianson et al. (2006) used a grain-based UDEC model to numerically complement laboratory testing on a lithophysal rock under confined conditions. The mechanical degradation of the same rock type was investigated by Damjanac et al. (2007) using a similar technique. The model was then up-scaled to study the stability of emplacement drifts at Yucca Mountain under mechanical, thermal, and seismic loading as well as time-dependent effects. Using a UDEC-Voronoi
model, Yan (2008) investigated the laboratory-scale step-path failure (e.g., wing cracking and fracture coalescence) in a sample containing pre-existing joints with application to slope stability problems. A similar approach was adopted by Lan et al. (2010) to numerically assess the effect of heterogeneity on the micromechanical extensile behavior during compression loading on Lac du Bonnet Granite and Åspö Diorite. The model directly incorporated several sources of heterogeneity, including microgeometric heterogeneity, grain-scale elastic heterogeneity, and microcontact heterogeneity. A calibration procedure to determine a unique set of micro-parameters for a grain-based UDEC model was developed by Kazerani and Zhao (2010). A series of numerical experiments (i.e., uniaxial/triaxial compression and Brazilian tension) was used to assess the relationship between macro- and micro-parameters. The model was also shown to correctly capture the ratio of compressive to tensile strength of rock samples measured in the laboratory, therefore overcoming some of the original defects of parallel-bonded particle models. Finally, the grain-based UDEC approach was also employed to study the effect of joint persistence on the evolution of damage during direct shear tests (Alzo’ubi, 2012).

Last, it is worth mentioning three approaches that were proposed to capture fracture processes in UDEC as an alternative to the adoption of a polygonal structure. Firstly, based on fracture mechanics considerations, a time-dependent joint cohesion was implemented by Kemeny (2005) to capture the progressive mechanical degradation during the failure of rock bridges along discontinuities. The model was validated using several laboratory-scale examples and then used to investigate the time-dependent degradation of drifts for the storage of nuclear waste at Yucca Mountain. Secondly, Jiang et al. (2009) developed an expanded distinct element method (EDEM) based on UDEC whereby potential cracks with bonding strengths equivalent to the rock matrix are pre-distributed within the model based on the plastic regions and direction of principal stresses obtained from a preliminary elasto-plastic analysis. The approach was applied to the simulation of cracking around a large underground excavation in a blocky rock mass. Lastly, Kazerani et al. (2012) implemented a UDEC model whereby the rock ma-

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**Fig. 2.5.** UDEC modelling of fracture propagation in rock. (a) Normal and shear stiffnesses between blocks. (b) Constitutive behaviour in shear and tension \((i = \{s, n\})\). Figures redrawn after Kazerani and Zhao (2010).
terial is represented as a collection of irregular-sized deformable triangles with cohesive boundaries controlling the material fracture and fragmentation properties. A reasonable agreement was found between numerical simulation and experimental laboratory results of compressive, tensile and shear tests on plaster. As further illustrated in Section 2.3.2, this model share several characteristics of the Y-Geo implementation of the combined finite-discrete element method.

### 2.3 The hybrid finite-discrete element method

In the hybrid continuum-discontinuum technique known as the combined finite-discrete element method (FEM/DEM) the simulation starts with a continuous representation of the solid domain of interest. As the simulation progresses, typically via explicit integration of the equations of motion, new discontinuities are allowed to form upon satisfying some fracture criterion, thus leading to the formation of new discrete bodies. In general, the approach blends FEM techniques with DEM concepts. The latter algorithms include techniques for detecting new contacts and for dealing with the interaction between discrete bodies, while the former techniques are used for the computation of internal forces and for the evaluation of a failure criterion and the creation of new cracks. Hybrid finite-discrete element models should not be confused with coupled continuum-discontinuum approaches (e.g., Pan and Reed, 1991; Billaux et al., 2004) which represent the problem far- and near-fields using continuum-based and DEM techniques, respectively.

In the following sections, the fundamental principles of two common FEM/DEM implementations are briefly illustrated, namely ELFEN (Rockfield Software Ltd., 2004) and Y-Geo (Munjiza, 2004; Mahabadi, 2012), as well as their application to the study of the fracturing behaviour of rocks.

#### 2.3.1 ELFEN

**Fundamental principles**

The continuum formulation of ELFEN is based on an explicit finite element model. Material softening (or hardening) is captured using a non-associative Mohr-Coulomb elasto-plastic model with shear strength parameters, including cohesion, friction angle and dilation, defined as function of the effective plastic strain. The localization of strain is obtained by regularizing the standard description of the continuum with the incorporation of fracture mechanics principles in the equations governing the evolution of state variables (Owen and Feng, 2001; Klerck et al., 2004). In particular, material softening associated with fracturing is captured under the main assumption that the quasi-brittle failure is extensional in nature. As thoroughly described by Klerck (2000), the extensional failure is modelled directly and indirectly for the cases of tensile stress and compressive stress fields, respectively. Under direct tension, several constitutive models can be used such as the Rotating Crack and the Rankine tensile smeared crack. With these models, material strain softening is fully governed by the tensile strength and the specific fracture energy parameters. Under compressive stress fields, a Mohr-Coulomb yield criterion is combined with a fully anisotropic tensile smeared crack model. With this approach, known as the com-
(a) (b) (c)

**Fig. 2.6.** Nodal fracture scheme of ELFEN. (a) Initial state before fracturing, (b) intra-element crack insertion, and (c) inter-element crack insertion. Figure redrawn after Klerck (2000).

*Pressive fracture model*, the extensional inelastic strain associated with the dilation response is explicitly coupled with the tensile strength in the dilation direction. That is, increments of extensional strain are associated with tensile strength degradation in the perpendicular direction.

Upon localization of damage into crack bands and complete dissipation of the fracture energy, a discrete fracture is realized. Hence, the transition from continuous to discontinuous behaviour involves transferring a virtual smeared crack into a physical discontinuity in the finite element mesh (Owen and Feng, 2001). The mesh topology update is based on a nodal fracture scheme with all new fractures developing in tension (i.e., mode I) in the direction orthogonal to the principal stress direction where the tensile strength becomes zero. This procedure is numerically accomplished by first creating a non-local failure map for the whole domain based on the weighted nodal averages of a failure factor, defined as the ratio of the inelastic fracturing strain to the critical fracturing strain. Secondly, a failure direction is determined for each nodal point where the failure factor is greater than one based on the weighted average of the maximum failure strain directions of all elements connected to the node. Finally, a discrete crack is inserted through the failure plane. As depicted in Fig. 2.6, the insertion of a new crack can be accomplished using two different algorithms (Klerck et al., 2004). The *intra-element* insertion drives a new fracture along the crack propagation direction by directly splitting the finite elements. In this case, a local adaptive remeshing may be necessary to achieve an acceptable element topology and avoid highly-skewed sliver elements that could decrease the numerical stability threshold of the integration time step. Conversely, with the *inter-element* insertion, the discrete crack is snapped to the existing element edge most favourably orientated with respect to the failure plane. Following the crack insertion, the damage variables in the adjacent finite elements are set to zero and the contact along the two newly-created surfaces is treated using a contact interaction algorithm (e.g., penalty or Lagrangian multiplier method).
Applications

First applications of ELFEN to modelling rock failure under compressive loads were proposed by Klerck (2000). In particular, the simulation of borehole breakouts indicated that the aforementioned compressive fracture model of ELFEN can describe both the axial splitting typical of brittle materials and the shear failure usually observed in more ductile ones (Fig. 2.7). A study of fracture development around deep tunnels was proposed by Sellers and Klerck (2000) using laboratory-scale models. As observed in the laboratory, the model could reproduce fractures developing sub-parallel to the excavation boundary as well as the confining effect of pre-existing joints on the development of damage. Moreover, the experimentally measured acoustic activity was analyzed using the release of kinetic energy simulated by the model as numerical equivalent. Coggan et al. (2003) described several examples of rock engineering application of ELFEN, including stability analysis of roof beams and pillars in underground excavations and rock slope stability problems. Klerck et al. (2004) proposed a quantitative analysis of compression tests on rocks with direct comparison of the load-displacement response and of the evolution of fracture development with experimental data (Fig. 2.8a). This type of analysis was subsequently extended to three dimensional models aimed at study the influence of the intermediate principal stress on rock fracturing and strength near excavation boundaries (Cai, 2008). The results clearly showed that the generation of tunnel surface parallel fractures and microcracks can be attributed to material heterogeneity and to the existence of relatively high intermediate principal stress as well as zero to low minimum principal stress confinement (Fig. 2.8b). Investigation of failure behaviour of rock specimens under indirect tensile stress conditions were first proposed by Cai and Kaiser (2004) and, more recently, by Cai (2013). The simulation of crack initiation and propagation from a pre-existing flaw highlighted the influence of the flaw frictional resistance on the development of primary and secondary cracks as well as on the failure load. Application of ELFEN to the investigation of damage mechanisms (e.g., surface wear and tensile fracturing) along joint planes under direct shear conditions was illustrated by Karami and Stead (2008). A discrete fracture rock mass model was proposed by Pine et al. (2006) by combining...
an ELFEN model with the fracture geometry generated by a Discrete Fracture Network (DFN) software. The approach was used to obtain insights into the influence of pre-existing joints on the rock mass behaviour in underground pillars, rock slides, and block caving operations (Eberhardt et al., 2004; Pine et al., 2007; Vyazmensky et al., 2010b,a). Yan (2008) numerically analyzed fracture coalescence and rock failure mechanisms in laboratory-scale specimens containing step-path fractures. The study was also extended to the simulation of rock bridge fracture associated with potential toe breakout failure in large open pit slopes. Original application of ELFEN to the investigation of failure behaviour of layered rocks can be found in Stefanizzi (2007) and Stefanizzi et al. (2008).

2.3.2 Y-Geo

Fundamental principles

The continuum representation of Y-Geo is based on the discretization of the modelling domain with three-noded triangular elements together with four-noded cohesive elements embedded between the edges of all adjacent triangle pairs (Fig. 2.9a). The elastic deformation of the bulk material is captured by the constant-strain, linear-elastic triangular elements with impenetrability between elements enforced by a penalty function method (Munjiza and Andrews, 2000). Fracture nucleation within the continuum is simulated by the breakage of the cohesive elements (Munjiza et al., 1999). Since fractures can nucleate only along the boundaries of the triangular elements, arbitrary fracture trajectories can be reproduced within the constraints imposed by the initial mesh topology. Unlike ELFEN, the mesh topology in Y-Geo is never updated during the simulation and re-meshing is not performed. Consequently, a sufficiently small element size should be adopted to reproduce the correct mechanical response (Munjiza and John, 2002).

The constitutive behaviour of crack elements is implemented in terms of relative displacement between opposite triangle edges and incorporates principles of non-linear elastic fracture mechanics (Fig. 2.9b). Material starts to yield, in tension or shear, upon reaching a displacement value corresponding to the peak cohesive strength. The peak strength values are defined in mode I and mode II by a
constant tensile strength, $f_t$, and a shear strength, $f_s$, calculated according to the Mohr-Coulomb criterion, respectively. The complete breakage of the crack element and thus the nucleation of a discrete crack is accomplished after dissipating the material fracture energy release rate, $G_c$. Upon breakage of the cohesive surface, the crack element is removed from the simulation and therefore the model transition from a continuum to discontinuum is locally completed. A Coulomb-type friction is applied along every newly-created fracture. As the simulation progresses, finite displacements and rotations of discrete bodies are allowed and new contacts are automatically recognized.

Given the above modelling assumptions, the Y-Geo implementation of FEM/DEM, rather than ELFEN’s approach, can be considered closer to a fully discrete method. In ELFEN, a real transition from a continuous elasto-plastic medium to a solid with discrete fractures is accomplished by dynamically inserting cracks into the model. Conversely, the material representation of Y-Geo resembles that one of a particle-based DEM with rigid particles and deformable particle bonds replaced by deformable triangles and cohesive elements, respectively.

**Applications**

Early applications of Y-Geo aimed at validating the adopted FEM/DEM implementation in the context of the failure processes typically observed during standard rock mechanics tests on brittle rocks. Mahabadi et al. (2009) investigated the influence of loading rate and sample orientation during a Brazilian test simulation on a layered rock. Mahabadi et al. (2010c) simulated the behaviour of a homogeneous rock sample under biaxial loading conditions. The model captured the main phenomena observed in a triaxial test including localization of failure, fracture initiation and evolution, increase of strength with
confined, and brittle-ductile transition. Mahabadi et al. (2010a) showed good agreement between the experimental results of a high-strain rate Brazilian disc test and Y-Geo simulation results in terms of tensile strength, failure time, and fracture mechanisms. Subsequently, the numerical experimentation with Y-Geo focused on the mechanical behaviour of heterogeneous granitic rocks under different loading conditions. A procedure to incorporate actual micromechanical input parameters of the rock, together with the real distribution of mineral constituents, into a FEM/DEM model was developed by Mahabadi et al. (2012b). Overall, the simulation results showed that by including accurate micromechanical parameters and the intrinsic rock geometric features, such as spatial phase heterogeneity and microcracks, the model can more accurately predict the mechanical response of rock specimen under direct tension (Mahabadi, 2012). Also, heterogeneity was shown to play a key role in controlling the non-linear stress-strain behaviour associated with the damage progress under compressive loading conditions (Fig. 2.10a). Recently, Lisjak et al. (2013b) extended the capabilities of Y-Geo to capture the behaviour of transversely isotropic rocks. The approach was validated by investigating the laboratory-scale fracturing behaviour of a clay shale, namely Opalinus Clay (Fig. 2.10b).

Finally, Rougier et al. (2011) developed a three-dimensional version of the Y-code of Munjiza (2004) and analyzed the effect of energy dissipation during the simulation of Split Hopkinson Pressure Bar Brazilian experiments.
Chapter 3

Numerical simulation of acoustic emission in brittle rocks by two-dimensional finite-discrete element analysis


A link to the published paper can be found at http://dx.doi.org/10.1093/gji/ggt221

Abstract

Stress waves, known as acoustic emissions (AE), are released by localized inelastic deformation events during the progressive failure of brittle rocks. Although several numerical models have been developed to simulate the deformation and damage processes of rocks, such as non-linear stress-strain behaviour and localization of failure, only a limited number have been capable of providing quantitative information regarding the associated seismicity. Moreover, the majority of these studies have adopted a pseudo-static approach based on elastic strain energy dissipation that completely disregards elasto-dynamic effects. This paper describes a new AE modelling technique based on the combined finite-discrete element method (FEM/DEM), a numerical tool that simulates material failure by explicitly considering fracture nucleation and propagation in the modelling domain. Given the explicit time integration scheme of the solver, stress wave propagation and the effect of radiated seismic energy can be directly captured. Quasi-dynamic seismic information is extracted from a FEM/DEM model with a newly developed algorithm based on the monitoring of internal variables (e.g., relative displacements and kinetic energy) in proximity to propagating cracks. The AE of a wing crack propagation model based on this algorithm are
cross-analyzed by travel-time inversion and energy estimation from seismic recordings. Results indicate a good correlation of AE initiation times and locations, and scaling of energies, independently calculated with the two methods. Finally, the modelling technique is validated by simulating a laboratory compression test on a granite sample. The micro-mechanical parameters of the heterogeneous model are first calibrated to reproduce the macroscopic stress-strain response measured during standard laboratory tests. Subsequently, AE frequency-magnitude statistics, spatial clustering of source locations, and the evolution of AE rate are investigated. The distribution of event magnitude tends to decay as power law while the spatial distribution of sources exhibits a fractal character, in agreement with experimental observations. Moreover, the model can capture the decrease of seismic $b$ value associated with the macro-rupture of the rock sample and the transition of AE spatial distribution from diffuse, in the pre-peak stage, to strongly localized at the peak and post-peak stages, as reported in a number of published laboratory studies. In future studies, the validated FEM/DEM-AE modelling technique will be used to obtain further insights into the micro-mechanics of rock failure with potential applications ranging from laboratory-scale microcracking to engineering-scale processes (e.g., excavations within mines, tunnels and caverns, petroleum and geothermal reservoirs) to tectonic earthquakes triggering.

3.1 Introduction

Acoustic emissions (AE) are broadly defined as high-frequency transient elastic waves generated by a sudden release of stored strain energy within a material (Lockner, 1993). In brittle rocks, AE are triggered by localized inelastic deformation events, such as micro-cracking, pore collapsing, and grain boundary slip, that characterize the material deformation and damage process.

In laboratory studies, AE recording has been used in passive geophysical monitoring to investigate the fracturing behaviour of brittle rocks. Unlike traditional integral rock damage indicators, such as non-linear deformation and variation of elastic wave propagation properties, the AE method offers the advantage of detecting individual fracture events. Consequently, AE source location has been employed to experimentally observe the nucleation and growth of cracks and their eventual coalescence into a macroscopic fault (e.g., Lockner et al., 1991; Thompson et al., 2006; Benson et al., 2008). Using the variation of AE properties which occurs in response to the damage evolution, the staged character of the brittle fracturing and the associated characteristic stress threshold values have been analyzed (Eberhardt et al., 1997). Furthermore, the Kaiser effect, the mechanism by which AE are only detected during the first loading to a certain stress state under compression, has been used to assess the amount of damage developed in rocks (e.g., Holcomb et al., 1990). It has also been demonstrated that the seismogenic (i.e., brittle) failure is a self-similar and scale-invariant process over a dimension range that spans several orders of magnitude, from grain-scale cracking to mining-induced seismicity and tectonic earthquakes (Scholz, 1968a; Hanks, 1992). Therefore, the acoustic activity of rock recorded in the laboratory has been considered a small-scale equivalent system for the seismicity of rock masses or in the Earth’s crust.

In the field, AE monitoring was historically introduced as a mine design and rockburst prediction tool (Obert and Duvall, 1957). Subsequently, the method has been employed to characterize the evolu-
tion of the damaged zone around underground excavations (e.g., Young and Maxwell, 1992; Falls and Young, 1998; Pettitt et al., 2002), and, in petroleum and geothermal engineering, to study the fracture zone induced by fluid injection during hydraulic fracturing (e.g., Pearson, 1981; Majer and Doe, 1986; House, 1987).

A great deal of research has focused on developing and validating numerical models that could capture the progressive mechanical breakdown of rocks (see Yuan and Harrison, 2006). However, only a limited number have been capable of providing quantitative output relative to the associated acoustic activity. Moreover, the majority of these studies have been based on a static approach that disregards the radiated seismic energy and the elastic wave propagation, as further explained in Section 3.2. According to Hazzard and Young (2002), two main reasons can be identified for modelling AE in rocks. Firstly, the ability to extract and quantify seismic information from the models, together with the simulated stress-strain behaviour and damage observations, can provide an additional tool to validate the modelling methodology and increase the confidence in the simulation results. Secondly, a successfully validated AE model can be used to investigate the relationships between simulated seismicity, damage and deformation characteristics, and model properties.

In this study, an innovative numerical approach, based on the combined finite-discrete element method (FEM/DEM) (Munjiza, 2004; Mahabadi et al., 2012a), is proposed to simulate AE associated with the brittle failure of rock. It is shown that the seismic information, including AE initiation time, location and energy, obtained from the analysis of FEM/DEM synthetic seismograms can be related to the information extracted by monitoring the motions of AE sources within the model. The 2D modelling technique is validated by simulating the acoustic activity of a granite sample under uniaxial compressive load.

The paper is organized as follows. In Section 3.2, the major studies on AE simulation are briefly reviewed. In particular, differences between material representation types (e.g., *continuum* versus *discontinuum*) and AE modelling approaches (i.e., static versus dynamic) are highlighted. In Section 3.3, the fundamental principles of FEM/DEM are illustrated with special emphasis on the assumptions inherent in the material failure modelling technique. In Section 3.4, the simulation of AE is discussed within the context of FEM/DEM. A new algorithm, developed to extract seismic information by internally monitoring AE sources, is presented (Section 3.4.2). The AE of a wing crack propagation model based on this algorithm are cross-analyzed by travel-time inversion and energy estimation from seismic recordings (Section 3.4.3). Finally, in Section 3.5, the results of a compression test simulation on a heterogeneous rock are presented. The simulated acoustic activity is first analyzed in relation to the macroscopic stress-strain behaviour of the sample. Subsequently, the AE frequency-magnitude statistics, clustering behaviour, and rate evolution are discussed with reference to published experimental results.
3.2 Related studies on AE simulation

Three main modelling methodologies have been adopted to simulate the acoustic activity associated with the failure process of brittle and quasi-brittle materials: (i) continuum damage models, (ii) particle-based discrete element method (DEM) models, and (iii) lattice models. Moreover, a fourth class of models can be identified which focuses exclusively on the emission of acoustic waves from a single crack propagating in an elastic medium.

In continuum damage models, the effect of fracturing on the material mechanical behaviour is smeared over the material volume that contains the potential crack by degrading the corresponding material properties (e.g., strength or stiffness) according to a continuum law. Thus, the dynamics of crack nucleation and growth is not explicitly considered and a mesoscopic description of the failure process is provided. The theoretical premises for the simulation of AE based on elastic damage mechanics were first discussed by Tang et al. (1997) and implemented in a finite-element code known as RFPA (Tang, 1997). Progressive failure of rock and associated non-linear stress-strain behaviour was captured by an elastic-brittle element constitutive law together with a heterogeneous distribution of the rock parameters. In this context, AE was simulated by a static approach: an acoustic event was associated with each damaged element and the corresponding elastic strain energy dissipation was used as analogous of the released seismic energy. The aforementioned model was used to investigate the evolution of seismic energy release during the failure process of heterogeneous rock specimens in compression (Tang and Kaiser, 1998), and to analyze the acoustic activity and the Kaiser effect during a three-point bending test on a concrete beam (Zhu et al., 2010). Following similar principles, a number of other models have been introduced. For instance, Fang and Harrison (2002a) adopted a local degradation model to analyze the brittle fracture of a rock sample under confined compression and to simulate the associated released energy evolution. Similarly, Feng et al. (2006) developed an elasto-plastic cellular automata model to simulate the acoustic activity of brittle rock under uniaxial compression. A slightly different approach was developed by Amitrano et al. (1999) on the basis of a local scalar damage model with tensorial elastic interaction. In this model, the size of the events was assumed proportional to the total number of elements damaged during a single loading step. The approach was shown to be capable of capturing power law distributions of damage events in space and size domains, and subsequently adopted to investigate the relationship between seismic $b$ value and brittle-ductile transition observed during laboratory tests on granitic rocks (Amitrano, 2003). A rheological model accounting for elastic deformation, viscous relaxation, and evolution of damage was introduced by Lyakhovsky et al. (1997), which was then used to simulate long histories of crustal deformation and to study the coupled evolution of earthquakes and faults (Lyakhovsky et al., 2001).

Particle-based DEM models represent the rock material as an assembly of rigid circular or spherical particles that are bonded together at their contact points. Although a relatively simple set of micro-mechanical interaction laws is used, these models can reproduce several typical features of the macroscopic rock behaviour including elasticity, fracturing and damage accumulation (Potyondy and Cundall, 2004). Crack nucleation is simulated through breaking of internal bonds while fracture propagation is obtained by coalescence of multiple bond breakages. Particle-based DEM models simulate quasi-static
deformation by solving the equations of motion. Therefore, elasto-dynamics effects including stress wave propagation and cracking-induced acoustic emission can be explicitly simulated. Hazzard and Young (2000) developed a technique to dynamically quantify AE in a 2D bonded-particle model for rocks. Particle kinetic energy upon bond breakage was monitored and used to directly quantify seismic energy radiated from the source. By clustering multiple bond breakages together in space and time, realistic $b$ values were obtained for a confined compression test simulation on granite. The aforementioned approach was further improved by introducing moment tensor calculation based on change in contact forces upon particle contact breakage, and was applied to the micro-seismic simulation of a mine-by experiment in a crystalline rock (Hazzard and Young, 2002) and of an excavation-induced fault slip event (Hazzard et al., 2002). 3D simulations of acoustic activity using particle-based DEM were proposed by Hazzard and Young (2004) and Invernizzi et al. (2011). While the former represented the direct extension of the 2D method described above, the latter adopted a simplified assumption in evaluating acoustic event size whereby the event magnitude was assumed proportional to the number of broken bonds in a given time interval. Nevertheless, the latter model was able to reproduce the power law distribution of event size and the decrease of $b$ value with increasing applied stress observed during unconfined compression and three-point-bending tests on concrete.

A class of methods directly related to the DEM particle models is represented by the lattice (or network) models. Similar to DEM models, continuum constitutive laws are replaced with a mechanical system of springs or beams. However, unlike DEM models, the particle contact pattern is fixed during the simulation and therefore large displacements and deformation cannot be simulated. Heterogeneous material structure is modelled, for instance, by imposing random failure thresholds on the springs or by removing a fraction of the links. Due to their simple description of elasticity and material micro-structural disorder, lattice models are only used to provide a mesoscopic description of the general statistics of the fracturing process in brittle and quasi-brittle materials (Alava et al., 2006). An example of lattice model based on a scalar damage model was introduced by Zapperi et al. (1997). Using the analogy between mechanical fracture and fusion in a resistor network, the model captured amplitudes and intervals between sequential events distributed according to a power law. The amplitude of events was assumed to be equal to the number of links damaged for a given voltage (i.e., stress) increment. Wang (2000) developed a static lattice model to study the rock failure and earthquake process. In particular, the effect of crack density, represented by pre-existing broken bonds, on the $b$ value was investigated under the assumption of proportionality between event magnitude and potential energy released by a broken bond. Unlike the aforementioned quasi-static approaches, the dynamic model of Minozzi et al. (2003) was used to explicitly analyze the AE waveforms emitted by a propagating crack in a 2D lattice subjected to anti-planar deformation. The acoustic response was related to the internal damage of the sample, and power law distributions of acoustic energy were obtained in agreement with experimental observations.

Finally, it is worth mentioning an additional class of models (e.g., Hirose and Achenbach, 1991; Lysak, 1996; Andreykiv et al., 2001; Bizzarri, 2011) which focuses on the emission of acoustic waves by solving the elasto-dynamic problem associated with the initiation and sub-critical growth of pre-existing
crack-like flaws of idealized shaped (e.g., penny-shaped, disc, ellipse). Based on a continuum fracture mechanics approach, this type of models aims at either quantifying the relationships between crack parameters (e.g., crack area and stress intensity factor) and AE signal (e.g., amplitude and frequency spectrum), or, through the application of self-consistent friction laws, modelling the dynamic rupture of seismogenic faulting processes (e.g., see Bizzarri, 2011, for a review).

In the context of the first three classes of methods described above, the numerical methodology adopted for this study, namely FEM/DEM, uses continuum mechanics principles and DEM techniques to describe the elastic deformation and the material failure process, respectively. Unlike the majority of the approaches described above, the event seismic energy is estimated using a quasi-dynamic technique which explicitly evaluates the kinetic energy in proximity to spontaneously propagating cracks. Given the mesoscopic representation of the fracturing process by means of cohesive elements, the accurate simulation of dynamic crack propagation and associated phenomena (see Freund, 1990) is beyond the scope of this work. Instead, the focus of this paper is on the extraction of quasi-dynamic AE information from a numerical model that aims at capturing the main features of the failure process in brittle rocks (e.g., non-linear stress-strain behaviour, localization of failure).

3.3 Fundamental principles of FEM/DEM

The combined finite/discrete element method (FEM/DEM) is a numerical method pioneered by Munjiza et al. (1995) for the dynamic simulation of multiple interacting deformable bodies. The technique combines DEM algorithms that capture the interaction and fracturing of different solids with continuum mechanics principles that describe the elastic deformation of discrete bodies. For this study, a 2D FEM/DEM code, known as Y-Geo (Mahabadi et al., 2012a), was used. This code represents an extension of the original Y2D code of Munjiza (2004) and is undergoing development at the University of Toronto for geomechanical applications. All models illustrated in the following sections were solved under plane stress conditions.

3.3.1 Governing equations

In FEM/DEM, each solid is discretized as a mesh consisting of nodes and triangular elements. An explicit second-order finite-difference time integration scheme is applied to solve the equations of motion for the discretized system and to update the nodal coordinates at each simulation time step. In general, the governing equations for a FEM/DEM system can be expressed as

$$M \ddot{x} + C \dot{x} = R(x),$$

(3.1)

where $M$ and $C$ are the lumped mass and damping diagonal matrices of the system; $x$ is the vector of nodal displacements; and $R(x)$ is the nodal force vector which includes the contributions from the external loads, $f_l$, the interaction forces acting across discrete bodies, $f_i$, the deformation forces, $f_d$, and the crack bonding forces, $f_c$. Numerical damping is introduced in the governing equation to account for
energy dissipation due to non-linear material behaviour or to model quasi-static phenomena by dynamic relaxation (Munjiza, 2004). The matrix $C$ is equal to

$$ C = \mu I, \quad (3.2) $$

where $\mu$ and $I$ are the damping coefficient and the identity matrix, respectively.

Interaction forces, $f_i$, are calculated either between contacting separated bodies or along internal discontinuities (i.e., pre-existing and newly created fractures). In the normal direction, body impenetrability is enforced using a penalty method (Munjiza and Andrews, 2000), while in the tangential direction, discontinuity frictional behaviour is simulated by a Coulomb-type friction law (Mahabadi et al., 2012a). Deformation forces, $f_e$, are computed on an element-by-element basis under the assumption of isotropic linear elasticity. Crack bonding forces, $f_c$, are used to simulate material failure, as further explained in the next section.

### 3.3.2 Material failure modelling

The progressive failure of rock material is simulated in FEM/DEM by explicitly modelling crack initiation and propagation according to the principles of non-linear elastic fracture mechanics (Dugdale, 1960; Barenblatt, 1962). As depicted in Fig. 3.1, dedicated four-noded cohesive elements simulate the development of the Fracture Process Zone (FPZ), a zone of non-linear material behaviour that forms ahead of the crack tip due to interlocking and micro-cracking (Labuz et al., 1985). The four-noded cohesive elements (referred hereinafter to as crack elements) are embedded between the edges of all adjacent triangular element pairs from the very beginning of the simulation (i.e., remeshing is not performed as the simulation progresses). Therefore the potential crack paths do not need to be assumed \textit{a priori} and arbitrary fracture trajectories can be captured within the constraints imposed by the initial mesh topology.

In the present study, a modified version of the crack element constitutive response proposed by Munjiza et al. (1999) was adopted. The bonding stresses, $\sigma$ and $\tau$, transferred by the material are decreasing functions of the displacement discontinuity across the crack elements:

$$ \begin{bmatrix} \sigma \\ \tau \end{bmatrix} = f(D) \cdot \begin{bmatrix} f_t \\ f_s \end{bmatrix}, \quad (3.3) $$

where $f_t$ and $f_s$ are the cohesive strengths in tension and shear, respectively, and $f(D)$ is a heuristic scaling function representing an approximation of the experimental cohesive laws proposed by Evans and Marathe (1968):

$$ f(D) = \left[ 1 - \frac{A + B - 1}{A + B} \exp \left( D \frac{A + C \cdot B}{(A + B)(1 - A - B)} \right) \right] \cdot \left[ A(1 - D) + B(1 - D)^C \right], \quad (3.4) $$

\footnote{The modifications include (i) the incorporation of a normal stress dependent term (i.e., $\sigma_n \cdot \tan \phi$) in the calculation of the cohesive shear strength, $f_s$ (eq. (3.6)), and (ii) the distinction between mode I and mode II fracture energy release rates.}
Intrinsic tensile strength, $f_x$, stress-free inelastic (FPZ) elastic normal bonding stress, $\sigma(o)$, opening, $o(x)$, equivalent crack nodal forces, $f_c$,

\begin{align*}
\text{(a) Conceptual model of a tensile crack in a heterogeneous rock material (modified after Labuz et al. (1985)).} \\
\text{(b) Theoretical FPZ model of Hillerborg et al. (1976).} \\
\text{(c) FEM/DEM implementation of the FPZ using triangular elastic elements and four-noded crack elements to represent the bulk material and the fracture, respectively.} \\
\text{(d) FEM/DEM representation of a fracturable body with continuum triangular elements and embedded crack elements indicated in grey and pink, respectively. Triangular elements are shrunk for illustration purposes. Interpenetration of triangular elements is discouraged by the strong stiffening response of the contact penalty formulation.}
\end{align*}

Fig. 3.1. Material failure modelling in FEM/DEM. (a) Conceptual model of a tensile crack in a heterogeneous rock material (modified after Labuz et al. (1985)). (b) Theoretical FPZ model of Hillerborg et al. (1976). (c) FEM/DEM implementation of the FPZ using triangular elastic elements and four-noded crack elements to represent the bulk material and the fracture, respectively. (d) FEM/DEM representation of a fracturable body with continuum triangular elements and embedded crack elements indicated in grey and pink, respectively. Triangular elements are shrunk for illustration purposes. Interpenetration of triangular elements is discouraged by the strong stiffening response of the contact penalty formulation.

where $A$, $B$, $C$ are empirical constants equal to 0.63, 1.8 and 6.0, respectively, and $D$ is a damage factor ranging between 0 and 1. As discussed below, the dimensionless damage factor $D$ describes the displacement jump across the cohesive surface in terms of opening, $o$, and sliding, $s$, between the edges of two adjacent triangular elements\(^2\). Also, $f(D)$ is such that $f(0) = 1$ (i.e., intact crack element) and $f(1) = 0$ (i.e., broken crack element).

Depending on the local stress and deformation field, fractures can nucleate and grow in mode I (i.e., opening mode), mode II (i.e., sliding mode), or in mixed mode I-II. Similar to the cohesive model originally proposed for concrete by Hillerborg et al. (1976), a mode I crack initiates when the crack tip opening, $o$, reaches a critical value, $o_p$, which is related to the cohesive tensile strength of the rock, $f_t$ (Fig. 3.2a). As the fracture propagates and the crack tip opening increases, the normal bonding stress, $\sigma$, is assumed to decrease until a residual opening value, $o_r$, is reached and a traction-free surface is

\(^2\)Opening and sliding between the edges of adjacent triangles are calculated as normal and tangential displacement, respectively, using three integration points located at two end-points and at the mid-point of the four-noded crack element.
created. In this case, the damage factor is therefore defined as

\[ D = \frac{o - o_p}{o_p - o}, \]  

(3.5)

Mode II fracturing is simulated by a slip-weakening model conceptually similar to that of Ida (1972). A tangential bonding stress, \( \tau \), exists between the two fracture walls, which is a function of the amount of slip, \( s \), and the normal stress on the fracture, \( \sigma_n \) (Fig. 3.2b) The critical slip, \( s_p \), corresponds to the cohesive shear strength of the rock, \( f_s \), defined as

\[ f_s = c + \sigma_n \cdot \tan \phi_i, \]  

(3.6)

where \( c \) is the internal cohesion, \( \phi_i \) is the material internal friction angle, and \( \sigma_n \) is the normal stress acting across the crack element. Upon undergoing the critical slip, \( s_p \), the tangential bonding stress is gradually reduced to a residual value, \( f_r \), which corresponds to a purely frictional resistance:

\[ f_r = \sigma_n \cdot \tan \phi_f, \]  

(3.7)

where \( \phi_f \) is the fracture friction angle and \( \sigma_n \) is the normal stress acting across the fracture surfaces. The residual shear strength, \( f_r \), is computed according to eq. (3.7) by the element pair interaction algorithm (Mahabadi et al., 2012a) even after the breakage of the embedded crack element. In this case, the damage parameter is therefore defined as

\[ D = \frac{s - s_p}{s_r - s_p}. \]  

(3.8)

For mixed mode I-II fracturing, the coupling between crack opening and slip is defined by (Fig. 3.2c)

\[ D = \sqrt{\left(\frac{o - o_p}{o_p - o}\right)^2 + \left(\frac{s - s_p}{s_r - s_p}\right)^2}. \]  

(3.9)

As illustrated in Fig. 3.1c, the effect of the crack bonding stress is implemented in FEM/DEM using equivalent crack nodal forces, \( f_c \).

Since the elastic deformation before the onset of fracturing takes place in the bulk material, no deformation should in theory occur in the crack elements before the cohesive strength is exceeded. However, a finite stiffness is required for the crack elements by the time-explicit formulation of FEM/DEM. Such an artificial stiffness is represented by the normal, tangential and fracture penalty values, \( p_n \), \( p_t \) and \( p_f \), for compressive, shear and tensile loading conditions, respectively. For practical purposes, the cohesive contribution to the overall model compliance can be largely limited by adopting very high (i.e., dummy) penalty values (Munjiza, 2004; Mahabadi, 2012).

From an energetic point of view, as there is stress to be overcome in propagating a crack, energy is dissipated during the fracturing process. The material total strain energy release rate, \( G_c \), corresponds to the amount of energy absorbed per unit crack length along the crack edge in displacing a crack
Fig. 3.2. Constitutive behaviour of the crack elements. (a) FPZ model for mode I. (b) Slip-weakening model for mode II. The specific fracture energy values, $G_{Ic}$ and $G_{IIc}$, correspond to the area under the bonding stress-softening curves. The shape of the descending branch of the curves is based upon experimental complete stress-strain curves obtained for concrete in direct tension (eq. (3.4)) (Evans and Marathe, 1968; Munjiza et al., 1999), while the ascending linear branch is incorporated using a penalty method (Munjiza et al., 1999; Munjiza and Andrews, 2000). Note that the residual shear strength, $f_r$, is computed according to eq. (3.7) by the element pair interaction algorithm (Mahabadi et al., 2012a) even after the breakage of the embedded crack element (dashed line in (b)). (c) Graphical representation of the coupling relationship between crack opening, $o$, and crack slip, $s$, for mixed-mode fracturing (eq. (3.9)).

from the critical to the residual value. In general, $G_c$ is obtained by integration of the stress-softening curve (represented by eq. (3.4)) during the debonding process of the crack element and includes the contribution of (i) the surface energy $2\gamma$ of the two newly created discontinuity surfaces, (ii) the energy $G_d$ consumed in the damage process around the crack tip, and (iii) the frictional fracture energy $G_f$. $G_c$ is defined in terms of the material properties, $G_{Ic}$ and $G_{IIc}$, which correspond to the strain energy release rates for mode I and mode II fracturing, respectively. Therefore, the crack residual displacement values, $o_r$ and $s_r$, are such that

$$G_{Ic} = \int_{o_p}^{o_r} \sigma(o)\,do,$$

$$G_{IIc} = \int_{s_p}^{s_r} \left[\tau(s) - f_r\right]\,ds.$$

Upon breakage of the cohesive surface, the crack element is removed from the simulation and replaced by the interaction forces, $f_i$, described in the previous section. At this stage, the transition from continuum to discontinuum is complete, finite displacements and rotations of discrete bodies are allowed and new contacts are automatically recognized as the simulation progresses, as typical of the DEM modelling approach (see Cundall and Hart, 1992).
3.4 FEM/DEM simulation of AE

3.4.1 Static versus dynamic modelling of crack propagation

During a FEM/DEM simulation, the rock is subjected to certain loading conditions and strain energy is stored due to the elastic deformation of the triangular elements. Once the intrinsic strength of the material is locally overcome, a new fracture is initiated and the release of stored strain energy begins. As described in Section 3.3.2, part of this energy is absorbed by the fracturing process itself and its value, $G_c$, is related to the material input parameters $G_{Ic}$ and $G_{IIc}$. If the crack surfaces slide against each other in a compressive stress field, part of the released energy is dissipated as frictional work. Frictional stress develops according to eq. (3.7), while the specific frictional energy dissipated, $E_f$, depends on the total slip, $s$:

$$E_f = f_r \cdot s. \quad (3.12)$$

Under static (or quasi-static) conditions, crack extension is therefore governed by

$$G_{stat} = G_c + E_f, \quad (3.13)$$

where $G_{stat}$ is the static strain energy release rate or crack extension force. Note that ‘rate’ means per unit of newly created fracture surface area. As verified in Section 3.4.3, failure events in FEM/DEM are characterized by an excess of strain energy released with respect to $G_c$ and $E_f$ (i.e., $G > G_{stat} = G_c + E_f$), thus the simulated rupture phenomena are often accompanied by the radiation of kinetic energy, $E_k$, in the form of acoustic emission.

In the framework of continuum fracture mechanics, the mathematical description of the rapid crack propagation process includes the inertial resistance provided by material particles displaced on opposite crack walls (Freund, 1990). Under dynamic conditions, the total energy available for work, $G_{dyn}$, is indeed partitioned into fracture energy, $G_c$, frictional dissipation, $E_f$, and radiated energy, $E_k$. That is, an additional kinetic term is added to the energy equation for crack extension as a mean to dissipate the excess energy resulting from the imbalance in the two driving force terms (Kanamori and Brodsky, 2004):

$$G_{dyn} = G_{stat} - \frac{1}{2} \frac{\partial E_k}{\partial a}, \quad (3.14)$$

where $a$ represents the crack area. Calculating the radiated energy of a propagating crack is in general a challenging task, which involves computing the displacements as a function of the crack length from the equations of motion for the crack tip in a deformable solid (Lawn, 1993). Given the complexities associated with the dynamic stress field and the strain energy flux into the crack tip, simplifying assumptions are generally made. In this context, the rupture speed, $V_r$, assumes a fundamental importance in determining the ratio of the dynamic to static energy release rate, $G_{dyn}/G_{stat}$, for a propagating crack. For instance, for a mode I fracture this ratio can be expressed as (Freund, 1972)

$$\frac{G_{dyn}}{G_{stat}} = 1 - \frac{V_r}{c_R}, \quad (3.15)$$
where \( c_R \) is the Rayleigh wave speed of the material. Under quasi-static conditions (i.e., \( V_r \sim 0 \)), no energy is radiated and all released strain energy is dissipated in the fracture process zone. Conversely, for rupture speed values approaching \( c_R \), all energy is radiated as seismic energy. Furthermore, the rupture speed, \( V_r \), directly affects the characteristics of the emitted stress wave field.

The numerical representation of material damage in FEM/DEM is based on a mesoscopic description of the fracturing process using a cohesive crack approach in combination with discrete elements. The elasto-dynamic problem briefly introduced above is not considered in its entirety and thus the numerical technique does not aim at fully capturing the phenomena occurring during dynamic crack propagation. Nevertheless, quasi-dynamic seismic information associated with the brittle failure process can be extracted from a FEM/DEM simulation despite the simplified representation of the fracturing process. The focus of the FEM/DEM technique is on capturing the brittle fracture process, and the validation of the AE modelling methodology relies mainly on the analysis of the emergent AE statistics for a compression test simulation on rock (Section 3.5).

Two approaches were considered to obtain quantitative information on the acoustic activity of a FEM/DEM simulation. The first approach takes advantage of the discrete representation of the material and of the explicit dynamic solver of the method. This technique, which is described in Section 3.4.2, is based on the internal monitoring of the node motions during crack propagation. An alternative approach employs the standard seismic source inversion techniques based on travel-times picked from recordings at selected locations on the edges of the model, as shown in Section 3.4.3. In general, the latter approach suffers from two major limitations. Firstly, as the simulation progresses, new fractures are generated, more energy is emitted and consequently the level of noise increases. Therefore, in order to be able to record clearly separated events in time, the model needs to be loaded very slowly resulting in running times that are not acceptable at the moment. Secondly, damage accumulation inside the model results in an extensive loss of continuity which makes waveform analysis impractical after the eventual failure. Nevertheless, if particular fracturing conditions such as those of Section 3.4.3 are reproduced, the AE information independently obtained by these two methods can be related.

3.4.2 Internal monitoring of AE sources

The newly-developed AE algorithm directly monitors the relative displacement of crack surfaces and records the kinetic energy of nodes in proximity to propagating fractures. As in seismology, for each acoustic event the following parameters can be numerically assessed: (i) source location, (ii) fracture mode, (iii) initiation time, and (iv) event seismic energy and magnitude. Note that in the context of this paper the term seismic energy refers to a mesoscopic numerical representation of the actual seismic energy radiated from acoustic events in the fracture process zone.

The breakage of each crack element is assumed to be an acoustic event with location coincident with the centroid of the element itself. The fracture mode is derived from the relative displacement of the fracture edges according to the constitutive behavior illustrated in Fig. 3.2. Since crack element failure occurs over a finite time interval, due to its softening behaviour, the assessment of the initiation time is based on the analysis of the kinetic energy of the crack element. It was verified that softening and
rupture of a crack element are typically accompanied by the evolution of the kinetic energy of the four crack nodes reported in Fig. 3.3. The initiation time, $T_i$, is assumed to be the time at which the kinetic energy of the crack element reaches a maximum. The associated event seismic energy, $E_e$, is calculated from the kinetic energy at the initiation time by the following algorithm, similar to the one developed by Hazzard and Young (2000) for a particle-based DEM model:

1. When the peak strength of a crack element is reached (i.e., the element is yielded), the kinetic energy of the four nodes of the crack element is stored in memory as $E_{k,y}$:

   $$E_{k,y} = \frac{1}{2} \sum_{i=1}^{4} m_i v_{i,y}^2,$$

   where $m_i$ and $v_{i,y}$ are the nodal mass and nodal velocity at the time of yielding $T = T_y$, respectively.

2. The kinetic energy, $E_k(t)$, of the four nodes is monitored until the crack residual displacement is reached (i.e., the element fails); the change in kinetic energy is calculated at each time step as

   $$\Delta E_k(t) = E_k(t) - E_{k,y}.$$

3. The seismic energy released by each crack breakage is assumed to be equal to the maximum value of $\Delta E_k$ attained from the time of yielding, $T_y$, to the time of failure, $T_f$, thus corresponding to the initiation time $T_i$:

   $$E_e = \max_{[T_y,T_f]} \Delta E_k(t).$$

4. Finally, the event magnitude, $M_e$, can be calculated from the event seismic energy, $E_e$, using, for
instance, the relationship proposed by Gutenberg (1956):

$$M_e = \frac{2}{3} \left( \log E_e - 4.8 \right).$$ (3.19)

It is noteworthy that, at this stage, the technique considers only the seismic energy radiated from the nucleation of new fractures within intact rock material. Thus, the acoustic emissions derived from crack re-activation, such as stress waves generated by slippage along pre-existing discontinuities, are ignored.

### 3.4.3 Seismic analysis of AE

The simulation of tensile crack initiation and propagation from a pre-existing flaw was used to investigate the correspondence between the AE information extracted using the technique described in Section 3.4.2 and that derived from the analysis of recorded synthetic seismograms. The stress concentration induced in a homogeneous medium by the pre-existing crack was exploited to produce strongly localized acoustic events and hence to facilitate the seismic analysis. However, unlike classic fracture mechanics approaches, FEM/DEM does not require in general the presence of crack-like notches or flaws to simulate fracture nucleation and propagation, as illustrated in Section 3.5.

### Model description

The model consisted of a 50 mm $\times$ 100 mm homogeneous sample containing a 5 mm long linear flaw inclined at 45° and positioned at the center of the model (Fig. 3.4). The sample was discretized by a Delaunay triangulation with an average edge size $h = 0.70$ mm and a total of 21,600 triangular elements.

A constant strain rate was imposed to the model by means of two rigid platens moving in opposite directions at a constant velocity of 0.05 m/s. This loading rate represented the lowest value that could be used for the given element size while keeping the running time within acceptable limits. A constant integration time step of $5 \times 10^{-9}$ s was used to solve eq. (3.1). The material properties reported in Table 3.1 were assumed for this simulation. The results reported in the following subsections were obtained for a damping coefficient value $\mu = 7.4 \times 10^3$ kg/m$\cdot$s, which approximates twice the theoretical critical damping, $\mu_c$, assuming that each element of size $h$ (0.70 mm) behaves as a one-degree-of-freedom mass-spring-dashpot system$^3$:

$$\mu_c = 2h\sqrt{\rho E}.$$ (3.21)

This value represented an acceptable compromise between noise reduction and AE wave amplitude attenuation, as further discussed below.

$^3$In a mass-spring-dashpot system with mass $m$ (in kg), spring constant $k$ (in N/m) and viscous dashpot of damping coefficient $c$ (in kg/s), critical damping is obtained for (Munjiza, 2004)

$$c = c_c = 2\sqrt{mk}.$$ (3.20)

Therefore, eq. (3.21) (with $\mu$ expressed in kg/(m$\cdot$s)) can be directly recovered from eq. (3.20) by replacing $m$ with $\rho h^3$ and $k$ with $E \cdot h$. 
Table 3.1. Sample properties for the wing crack simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, $\rho$ (kg/m$^3$)</td>
<td>2300</td>
</tr>
<tr>
<td>Young’s modulus, $E$ (GPa)</td>
<td>3</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$ (-)</td>
<td>0.29</td>
</tr>
<tr>
<td>Internal friction angle, $\phi_i$ (°)</td>
<td>35</td>
</tr>
<tr>
<td>Internal cohesion, $c$ (MPa)</td>
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</tr>
<tr>
<td>Fracture friction angle, $\phi_f$ (°)</td>
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</tr>
<tr>
<td>Tensile strength, $f_t$ (MPa)</td>
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</tr>
<tr>
<td>Mode I fracture energy, $G_{Ic}$ (J/m$^2$)</td>
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</tr>
<tr>
<td>Mode II fracture energy, $G_{IIc}$ (J/m$^2$)</td>
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</tr>
<tr>
<td>Damping coefficient, $\mu$ (kg/m·s)</td>
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</tr>
<tr>
<td>Normal contact penalty, $p_n$ (GPa·m)</td>
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</tr>
<tr>
<td>Tangential contact penalty, $p_t$ (GPa/m)</td>
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</tr>
<tr>
<td>Fracture penalty, $p_f$ (GPa)</td>
<td>15</td>
</tr>
<tr>
<td>Sample-platen friction coefficient, $k$ (-)</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Analysis of onset of crack growth in the framework of linear elastic fracture mechanics

The nucleation of tension cracks from pre-existing flaws subjected to a compressive stress field and their growth in the direction of maximum compression have been experimentally studied by several authors (e.g., Brace and Bombolakis, 1963; Hoek and Bieniawski, 1965; Nemat-Nasser and Horii, 1982). As discussed by Horii and Nemat-Nasser (1986), this basic micromechanism can be used to explain several features of the failure of brittle rocks, including the transition from axial splitting mode of failure to faulting, if confinement is applied, and the transition from brittle to ductile behaviour, when the confining pressure is suitably large. In the framework of linear elastic fracture mechanics (LEFM), this phenomenon is typically analyzed with reference to the 2D configuration illustrated in Fig. 3.4a. The model consists of a pre-existing straight crack of length $2c$ immersed in a homogenous, isotropic and linear elastic medium, and subjected to the the far-field stresses, $\sigma_1$ and $\sigma_2$. The flaw is inclined at angle $\gamma$ to the direction of $\sigma_1$ and the extended tension cracks are assumed to be straight lines of length $l$. A number of approximate, closed-form solutions of this boundary-value problem have been proposed in terms of stress intensity factors, $K_1$ and $K_{II}$, at the site of wing crack nucleation, and wing crack orientation, $\theta$ (see Lehner and Kachanov (1996) for a review). As shown in Fig. 3.4b, the FEM/DEM model correctly captures the formation of two tensile fractures nucleating from the flaw tips. These cracks, which are induced by the sliding of the flaw surfaces under unconfined compression ($\sigma_2 = 0$), initiate along two crack elements inclined at angle $\theta = 64^\circ$ to the pre-existing discontinuity. The results of the FEM/DEM simulation were compared to a number of LEFM solutions by computing the applied far-field stress, $\sigma_{1c}$, at the onset of wing crack growth with both approaches. In the FEM/DEM simulation, a value of $\sigma_{1c}$ equal to 7.0 MPa was derived from the nodal reaction forces recorded at the loading platens. This value represented about 21% of the ultimate stress at failure of the specimen, $\sigma_{1u} = 33$
Fig. 3.4. (a) Configuration of a pre-existing straight flaw and tension wing cracks growing in a compressive stress field. (b) Zoomed-in view of the center of the FEM/DEM model. Top and bottom wing cracks (shown in red), corresponding to acoustic event 1 and 2 nucleate at \( \sigma_{1c} = 7.0 \) MPa. (c) FEM/DEM fracture pattern corresponding to the specimen ultimate stress at failure, \( \sigma_{1u} = 32 \) MPa.

For the LEFM solutions, \( \sigma_{1c} \) was obtained by imposing the condition

\[
K_1(2c, \gamma, \mu, \theta, l, \sigma_1, \sigma_2) = K_{1c},
\]

where \( K_1 \) was calculated for each analytical model using the parameters reported in Table 3.2 corresponding to the FEM/DEM configuration of Fig. 3.4, and the mode I fracture toughness value, \( K_{1c} = 0.077 \) MPa\( \sqrt{m} \), was estimated by the following relationship (Irwin, 1957):

\[
G_{1c} = \frac{K_{1c}^2}{E},
\]

where \( E \) and \( G_{1c} \) are the Young’s modulus and mode I fracture energy release rate, respectively (Table 3.1). The comparison of \( \sigma_{1c} \) values reported in Table 3.3 indicate that the FEM/DEM result falls within the range predicted by the different LEFM models. Discrepancies between solutions are due to varying modelling assumptions within the LEFM models (Lehner and Kachanov, 1996) and between the LEFM and FEM/DEM approaches. In particular, the LEFM theory is underpinned by the lack of a plastic zone at the tip of a crack which implies a fully elastic behaviour with stress singularities. Conversely, in FEM/DEM, a FPZ develops ahead of the crack tip once the cohesive strength is reached (Section 3.3.2). Also, the angle of crack propagation in the FEM/DEM cohesive fracture model is constrained along the edges of triangular elements and the details of the crack tip stress and strain fields are not resolved by the relatively coarse numerical discretization with constant-strain elastic elements (Fig. 3.4b).

As the simulation progresses, the two fractures tend to align themselves in the direction parallel to
Table 3.2. Parameters used for the wing crack growth analysis using LEFM models.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flaw length, $2c$ (mm)</td>
<td>5</td>
</tr>
<tr>
<td>Flaw inclination, $\gamma$ ($^\circ$)</td>
<td>45</td>
</tr>
<tr>
<td>Flaw friction coefficient, $\mu$ (-)</td>
<td>0.7</td>
</tr>
<tr>
<td>Wing crack inclination, $\theta$ ($^\circ$)</td>
<td>64</td>
</tr>
<tr>
<td>Wing crack length, $l$ (mm)</td>
<td>0.7</td>
</tr>
<tr>
<td>Lateral confining pressure, $\sigma_2$ (MPa)</td>
<td>0</td>
</tr>
</tbody>
</table>

the maximum principal stress. The eventual failure of the sample involves the development of secondary shear fractures and macroscopic axial splitting (Fig. 3.4c).

Simulated AE

The above described wing cracking process was accompanied by the radiation of kinetic energy from the two tensile fractures, as preliminarily indicated by the simulated evolution of particle velocity field in the sample (Fig. 3.5). Hence, the synthetic acoustic activity was simultaneously monitored using the technique illustrated in Section 3.4.2 and two sets of receivers positioned on the left and right side of the sample (Fig. 3.6a). Particle velocities were recorded at these receivers to mimick the effect of piezo-electric transducers used in actual AE experiments.

Travel-time inversions of acoustic emission

The main arrivals of various AE events cluster in time, as highlighted by the $x$-component record section (Fig. 3.6c) for the top half of receivers at the right-side edge (Fig. 3.6a). In particular, four distinct event groups may be identified from the record section before the catastrophic failure of the sample at $T = 9$ ms, corresponding to a sharp increase of fracture nucleation within the model (Fig. 3.4c). Based on the internally recorded energy by FEM/DEM, each group consists of major (i.e., $E_e > 1$ nJ) and minor (i.e., $E_e \leq 1$ nJ) events as listed in Table 3.4. Since events within each group may arrive close in time (Fig. 3.6c), a distinction of individual events can be difficult.

Table 3.3. Comparison of compressive stresses at the onset of crack growth, $\sigma_{1c}$, obtained using different LEFM models with the FEM/DEM simulation result.

<table>
<thead>
<tr>
<th>Analysis type</th>
<th>Critical compressive stress, $\sigma_{1c}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LEFM model</td>
<td></td>
</tr>
<tr>
<td>Cotterell and Rice (1980)</td>
<td>5.1</td>
</tr>
<tr>
<td>Zaitsev (1985)</td>
<td>6.9</td>
</tr>
<tr>
<td>Horii and Nemat-Nasser (1986)</td>
<td>14.6</td>
</tr>
<tr>
<td>Lehner and Kachanov (1996)</td>
<td>8.5</td>
</tr>
<tr>
<td>FEM/DEM simulation</td>
<td>7.0</td>
</tr>
</tbody>
</table>
Fig. 3.5. Contour plot of $x$- and $y$-component of particle velocity in the sample for $T = [1.800, 1.950]$ ms of the wing crack propagation simulation. Background velocity field prior to fracturing ($T = 1.800$ ms) is induced by the loading platens moving in opposite direction with a constant vertical velocity of 0.05 m/s. The lateral expansion of the sample is due to the Poisson’s effect. Notice also the constraint placed on the lateral deformation at the top and bottom sample boundaries by the frictional resistance of the platen-sample interface. Two fracture-induced energy releases occur at $T = [1.860, 1.870]$ ms and $T = [1.890, 1.900]$ ms. These events are associated with two new fractures nucleating from the top and bottom tip of the pre-existing crack and correspond to event 1 and 2 of Fig. 3.6b, respectively.

On the other hand, Fourier analysis of the record section showed dominant frequencies of $8 - 10$ kHz (also see more discussions in the next sections). With a $V_p$ value of 1300 m/s (calculated from the elastic properties of Table 3.1), the dominant wavelengths of seismic waves at the receivers were $130 - 165$ mm, far exceeding the dimensions of the sample. Therefore, mapping fracturing details based on back-projection or adjoint-type of source imaging techniques (e.g., Ishii et al., 2005; Hjörleifsdóttir, 2007) was precluded, as their imaging resolution is generally similar to the dominant wavelength of seismic waves. Seismic event relocation had to rely mainly on the picking of phase onset corresponding to first arrivals of events. However, the close temporal proximity of events within each group and the long-period nature of the recordings limited the picking exclusively to first arrivals for each event group, and in turn provided hints to the location and origin time of only the first event of significant energy in each group.

First-arrival times for event groups 2 and 3 were hand-picked, as shown by the red vertical lines in Fig. 3.6c. The error bar assigned to the arrival times at each receiver was estimated from the difference between the $x$- and $y$-component time picks with a minimum of 0.001 ms for group 2 and 0.002 ms for group 3 (Fig. 3.7). A higher minimum error bar was necessary for group 3 due to the preceding ringings from the coda waves of group 2. Larger error bars are generally observed for stations that are further
Fig. 3.6. (a) Model and receiver geometry for the wing crack propagation simulation together with simulated fracture (i.e., source) pattern. The broken crack elements (shown in red) cluster in two macroscopic fractures originating from the tips of the diagonal flaw. Two sets of receivers placed on the left- and right-side edges are indicated by blue dots. The location of the receiver [25, 0.0] mm is indicated by an orange square. (b) A zoomed-in view of the center of the sample showing the associated acoustic events in circles; minor events with $E_e \leq 1$ nJ are denoted by grey circles and major events are in black (for group 1, 4), blue (for group 2) and green (for group 3) circles. Inverted event locations based on manual travel-time picks for group 2 and 3 and their associated error bars are indicated by blue and green crosses. Note the proximity between the FEM/DEM major event locations and inverted locations. The virtual receiver at [2.5, 2.7] mm is indicated by a red square. (c) $x$-component record section of velocity seismograms between 2 and 9 ms for the top half of the receivers on the right-side edge. Seismograms have been shifted along $y$-axis to allow proper display. Time ranges for the four event groups recorded by the FEM/DEM modelling (listed in Table 3.4) are identified below the recorded section with peak times of individual events indicated by vertical lines. The manually picked first arrivals for group 2 and 3 are indicated by red vertical lines. All seismograms are of the same scale and the maximum amplitude of the bottom velocity seismogram between 4 and 5 ms is 0.04 mm/ms.

away from the wing crack as the diminishing amplitudes of the first arrivals reduce the accuracy of the phase onset picking (Fig. 3.6c and Fig. 3.7).

With first-arrival times picked for 42 receivers on the left and right edges, both event origin times and locations were inverted based on a homogeneous and isotropic background model with a $P$-wave velocity of 1300 m/s. Arrival data were weighted by the associated error bars, and errors on inverted origin times and locations were computed based on data variance estimation from the goodness of fit. The inverted event origin time (circles in Fig. 3.8) falls between the yielding time $T_y$ and peak time $T_i$ of the first major event in each group reported by FEM/DEM modelling. The inverted locations with their associated error bars (crosses in Fig. 3.6b) clearly overlap with the earlier minor events within each group (i.e., events 3 and 4 in groups 2 and 3, respectively), and are only slightly off from the locations of the first major events (i.e., events 6 and 10 in groups 2 and 3, respectively). Given the systematic errors associated with the assumption of homogeneous isotropic background model and the uncertainties in the phase-picking itself, error bars of the inverted locations may be underestimated. Overall, the seismically
Table 3.4. Event groups for the analysis of the record sections for the wing crack simulation. Major events are identified as events with significant internally recorded energy (i.e., $E_e > 1$ nJ), while rest of the events within the defined time ranges are listed under minor events.

<table>
<thead>
<tr>
<th>Group number</th>
<th>Time range (ms)</th>
<th>Major events</th>
<th>Minor events</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[1.8, 2.02]</td>
<td>event 1, 2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>[4.1, 5.0]</td>
<td>event 6, 8, 9</td>
<td>event 3, 5</td>
</tr>
<tr>
<td>3</td>
<td>[5.8, 6.7]</td>
<td>event 10, 11, 12, 13</td>
<td>event 4, 7</td>
</tr>
<tr>
<td>4</td>
<td>[7.7, 8.5]</td>
<td>event 14, 15</td>
<td></td>
</tr>
</tbody>
</table>

Inverted event origin times and locations seem to coincide with the first major event (or earlier minor events) in each event group, thus validating the recordings of acoustic emission.

**Energy scaling**

It will also be interesting to estimate the radiated seismic energy of AE events based on recorded velocity seismograms at receivers, and compare it to the seismic energy $E_e$ computed from eq. (3.18) based on the source kinetic energy (see Section 3.4.2). An event that is of larger magnitude and records higher kinetic energy in general also releases more radiated seismic energy. However, again owing to the large damping value and long-period nature of the arrivals on model edges, it is difficult to estimate the absolute radiated seismic energy, and only relative scaling of seismic energy among different events can be compared in the attempt to validate the FEM/DEM calculations.

On the other hand, due to the spatial and temporal proximity of events in an event group (see Table 3.4), only the total or average seismic energy for an event group could be examined. The instanta-
Fig. 3.8. (a) Temporal distribution of AE events reported by FEM/DEM modelling and divided into four event groups. The origin times for event group 2 and 3 are inverted, each given by two circles indicating the error bar associated with the estimate. However, time errors are generally very small, and the two circles practically overlap. The time extent $[T_y, T_f]$ of major events are indicated by horizontal lines with internally recorded seismic energy, $E_e$ (eq. (3.18)), plotted as vertical lines at their peak times, $T_i$. (b)-(d) Close-up views of (a) for event group 1, 2 and 3.

Neous seismic energy density at a receiver $x_r$ as a function of time is given by

$$E_{is}(x_r, t) \sim \rho [V_x^2(x_r, t) + V_y^2(x_r, t)],$$

where $V_x$ and $V_y$ are the $x$- and $y$-component velocity series recorded at $x_r$, and $\rho$ is the density of the sample reported in Table 3.1. $E_{is}(t)$ for the middle receiver on the right-side edge (orange square in Fig. 3.6a) is plotted in Fig. 3.9a together with the total $E_e$ reported by FEM/DEM for each group. A qualitative scaling relation is visible between the instantaneous seismic energy density, $E_{is}(t)$, for the middle receiver on the right-side edge (orange square in Fig. 3.6a), and the total seismic energy (i.e., sum of $E_e$ for all events within the group) reported by FEM/DEM (Fig. 3.9a). A less crude estimate of
Fig. 3.9. (a) A qualitative linear scaling relation between instantaneous seismic energy density, $E_{is}$, estimated for the center receiver on the right side of the sample (i.e., orange square in Fig. 3.6a) and the total seismic energy, $E_{e}$, calculated by internal kinetic energy monitoring, for all four event groups (see Table 3.4). The total seismic energy values are plotted at the peak times of each event group. Squares of energy values are taken to better present four event groups on the same graph. (b) Linear scaling relation between the squares of seismic energy, $E_{s}$, estimated from receiver recordings and seismic energy, $E_{e}$, calculated by internal kinetic energy monitoring, shown by the red symbols $\times$ for four event groups and a best fitting line.

The radiated seismic energy density requires temporal averaging and spatial integration of the instantaneous energy density for all receivers by

$$E_{s} \sim \frac{\rho}{2\pi T_g} \int_{t}^{t+\Delta T} \left[ V_{x}^2(x_{r}, t) + V_{y}^2(x_{r}, t) \right] \Delta\theta_r \, dt. \tag{3.25}$$

The time integration is done over a length of $T_g$ covering the few oscillations after first arrivals, and $\Delta\theta_r$ is the azimuthal angle spanned by neighboring receivers. As we only seek relative comparisons of radiated energy among different event groups, common factors such as attenuation and geometric spreading are ignored. A linear scaling is observed between the total seismic energy estimated for each event group using eq. (3.25) and eq. (3.18) (Fig. 3.9b), thus helping validate the calculation of the event seismic energy based on the source kinetic energy monitoring performed in the FEM/DEM modelling.

**Effect of numerical damping**

A uniform visco-elastic damping was applied to all triangular elements of the model to dissipate the transient oscillations induced by the moving loading platens and the actual AE sources that would have otherwise been trapped indefinitely within the modelling domain. This numerical damping, together with the geometric spreading effect, reduces the amplitudes of arrivals as seismic waves travel further from the source region, as indicated for instance by the decrease of first arrival amplitudes for receivers towards the top of the right edge for both event group 2 and 3 (Fig. 3.6c).

Higher damping values result in more reduction of AE amplitude and attenuation of high-frequency
content, as highlighted by the $x$-component particle velocities during event 1 and 2 (Fig. 3.10a) and by the corresponding amplitude spectra (Fig. 3.10b), respectively. For comparison, the recordings of a receiver (black line in Fig. 3.10a) close to the AE source of event 1 ([2.5, 2.7] mm) are less affected by the selection of damping value and geometrical spreading, and hence more accurately represent the source time functions of individual events in the fracture process. Its spectrum indicates that the dominant frequencies of the source processes are about 10 to 20 kHz and not much energy is present above 60 kHz (black line in Fig. 3.10b).

The critical damping value as expressed by eq. (3.21) is based on the assumption that each triangular element behaves as a mass-spring-dashpot system. Therefore, theoretically, for waves excited at the sources, damping is most significant at frequencies

$$f \gtrsim \frac{E}{2\pi \mu c}.$$  

It then follows that for a simulation with parameter values listed in Table 3.1 and twice the critical damping $\mu c$, AE events will mostly generate oscillations below 60 kHz (Fig. 3.10b). Even at this frequency limit, it is still difficult to image individual events based on back-projection or adjoint techniques, as locating individual events accurately at sub-mm scale would require frequency content above $\sim 1.3$ MHz. On the other hand, a further reduction in applied damping will result in unwanted persistent oscillations induced by the moving platens and will therefore hamper the seismic analysis.

Finally, although damping affected the recorded waveforms, it was verified that, under the given loading rate, the failure load of the sample was relatively insensitive to this parameter. In other words, breakages of crack elements triggered by acoustic energy (i.e., dynamically) could be neglected.

Rupture speed and AE frequency content

A qualitative explanation of the aforementioned low frequency content of the AE source processes may be provided by considering the propagation speed, $V_r$, of the simulated fractures. For example, events 6, 8, and 9 (i.e., group 2) can be interpreted as a single crack of length $l = 3 \times h = 2.1$ mm. By approximating the duration of crack propagation as $T_{r,9} - T_{r,6} = 0.55$ ms, a rupture speed of about 4 m/s is estimated. A similar analysis for the other sequences of events reveals rupture speed values comprised between 2.5 and 55 m/s. The low values of rupture speed in the FEM/DEM simulation (i.e., $V_r \sim (0.004-0.1)c_R$) imply that most of the released energy is dissipated in the process zone as fracture energy (eqs (3.14) and (3.15)) and that high frequencies are not generated at the source (Fig. 3.10b) as a result of low accelerations of relative displacements along crack elements.

This quasi-dynamic behaviour is a direct consequence of the mechanical assumptions inherent in the cohesive crack approach (Section 3.3.2). More specifically, the bonding stress-softening relationships depicted in Fig. 3.2 lump into a discrete line the effect of inelastic mechanisms, including acoustic events, that, in reality, characterize a finite volume of material ahead of the crack tip (i.e., the FPZ) (Fig. 3.1a). As a consequence, the simulated AE signals are directly influenced by this mesoscopic representation of the process zone, for which the advancement rate is relatively slow. Conversely, acoustic
signals measured in the laboratory are due to the multitude of dynamic micro-failures within the FPZ itself. As experimentally shown by Zietlow and Labuz (1998), these events may be related to the presence of micro-scale inhomogeneities in the material such as mineral grains and pre-existing defects or voids. Owing to the truly dynamic nature of these micro-crack propagation phenomena and their sub-millimeter size, much higher frequencies (e.g., 100 kHz − 2 MHz (Lockner, 1993)) are typically measured in the laboratory.

3.5 Numerical example: AE of a granite sample under unconfined compression

A model of uniaxial compression test was adopted to investigate the acoustic activity associated with the failure process of a heterogeneous crystalline rock, namely Stanstead Granite, and to provide further validation of the FEM/DEM-AE modelling technique.

The mechanical properties of the FEM/DEM model were first calibrated to reproduce the macroscopic stress-strain response observed during standard laboratory tests. The acoustic activity associated with fracturing was then analyzed with particular emphasis on (i) the relation between AE and sample stress-strain response, (ii) the frequency-magnitude statistics and (iii) the spatial clustering of AE sources. Since experimental measurements of AE were not available, the results reported in the following are discussed with reference to the typical behaviour reported in the literature for granitic rocks.
3.5.1 Model description

The modelled rock sample cross section consisted of a 54 mm × 108 mm rectangle, meshed with a uniform, unstructured grid having 0.8 mm average element size and totalling approximately 16000 triangles. Uniaxial loading conditions were obtained by means of two rigid platens moving in opposite directions with a constant velocity equal to 0.125 m/s, which corresponds to a strain rate of 2.3 s\(^{-1}\). Although in actual experiments the sample is loaded at a significantly slower rate, a preliminary analysis revealed that the possible error in the simulated peak strength due to the different loading rate was bound to 0.5% (Mahabadi, 2012). That is, the simulated strengths approached constant values for loading rates smaller than approximately 0.125 m/s, which thus defined the upper boundary of quasi-static loading conditions of the simulation. Conversely, hardening effects were captured for higher strain rate values (i.e., dynamic range). More details on the FEM/DEM simulation of strain rate effects under true dynamic conditions can be found in Mahabadi et al. (2010a). Equations of motion for the discretized system were integrated with a time step of \(5 \times 10^{-6}\) ms; this value was the largest time step size that ensured numerical stability for the explicit time integration scheme of the code. The FEM/DEM Graphical User Interface Y-GUI (Mahabadi et al., 2010b) was used to assign boundary conditions and material properties to the model.

The heterogeneous spatial distribution of mineral phases was stochastically generated based on a discrete Poisson distribution of the rock mineral composition with 71% feldspar, 21% quartz, and 8% biotite (Fig. 3.12a). Material properties adopted for each mineral are summarized in Table 3.5. To simulate the presence of defects within the rock microstructure, the mode I fracture energy values, \(G_{1c}\), for the interfaces between biotite and feldspar, biotite and quartz, and quartz and felspar were reduced to 0.05, 0.05, and 0.6 J/m\(^2\), respectively (Mahabadi, 2012). Note that an equivalent homogeneous distribution of material properties would have resulted in the inability of reproducing any localized crack element failure (i.e., acoustic event) before the macroscopic rupture of the sample. As typical of the DEM modelling methodology, following an iterative trial-and-error calibration procedure, friction, cohesion, and tensile strength of the rock mineral interfaces were varied until the emergent Uniaxial Compressive Strength (UCS) of the model closely matched the value obtained from laboratory testing. Normal contact penalty, tangential contact penalty and fracture penalty values were assumed equal to 10×, 1×, and 5× the Young’s modulus value, respectively (Mahabadi, 2012). A critical viscous damping was applied to the model. Further details on the model calibration procedure and experimental results can be found in Mahabadi (2012).

Since the quality of AE seismograms was heavily influenced by the high loading rate and the relatively diffuse damage pattern, temporally separated events could not be recorded, and thus a seismic analysis, as explained earlier in Section 3.4.3, was not realized. Therefore, AE analysis had to rely only on the internal monitoring of AE sources (Section 3.4.2).
### Table 3.5. Mineral properties of the Stanstead Granite sample for the uniaxial compression test simulation.

<table>
<thead>
<tr>
<th>Property</th>
<th>Feldspar</th>
<th>Quartz</th>
<th>Biotite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume fraction (%)</td>
<td>71%&lt;sup&gt;a&lt;/sup&gt;</td>
<td>21%&lt;sup&gt;a&lt;/sup&gt;</td>
<td>8%&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Density, $\rho$ (kg/m&lt;sup&gt;3&lt;/sup&gt;)</td>
<td>2600&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2600&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2800&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Young’s modulus, $E$ (GPa)</td>
<td>56.4&lt;sup&gt;c&lt;/sup&gt;</td>
<td>83.1&lt;sup&gt;c&lt;/sup&gt;</td>
<td>17.2&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$ (-)</td>
<td>0.32&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.07&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.36&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Internal friction angle, $\phi_i$ (°)</td>
<td>51.8&lt;sup&gt;d&lt;/sup&gt;</td>
<td>51.8&lt;sup&gt;d&lt;/sup&gt;</td>
<td>51.8&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td>Internal cohesion, $c$ (MPa)</td>
<td>24.2&lt;sup&gt;d&lt;/sup&gt;</td>
<td>24.2&lt;sup&gt;d&lt;/sup&gt;</td>
<td>24.2&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td>Tensile strength, $f_t$ (MPa)</td>
<td>5.5&lt;sup&gt;e&lt;/sup&gt;</td>
<td>11.4&lt;sup&gt;e&lt;/sup&gt;</td>
<td>4.2&lt;sup&gt;e&lt;/sup&gt;</td>
</tr>
<tr>
<td>Mode I fracture energy, $G_{Ic}$ (J/m&lt;sup&gt;2&lt;/sup&gt;)</td>
<td>310&lt;sup&gt;f&lt;/sup&gt;</td>
<td>907&lt;sup&gt;f&lt;/sup&gt;</td>
<td>599&lt;sup&gt;f&lt;/sup&gt;</td>
</tr>
<tr>
<td>Mode II fracture energy, $G_{IIc}$ (J/m&lt;sup&gt;2&lt;/sup&gt;)</td>
<td>620&lt;sup&gt;g&lt;/sup&gt;</td>
<td>1814&lt;sup&gt;g&lt;/sup&gt;</td>
<td>1198&lt;sup&gt;g&lt;/sup&gt;</td>
</tr>
<tr>
<td>Platen-mineral friction coefficient, $k$ (-)</td>
<td>0.1&lt;sup&gt;h&lt;/sup&gt;</td>
<td>0.1&lt;sup&gt;h&lt;/sup&gt;</td>
<td>0.1&lt;sup&gt;h&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup> From thin section and µCT analysis (Mahabadi, 2012).
<sup>b</sup> From Mavko et al. (2009).
<sup>c</sup> Measured by micro-indentation testing (Mahabadi, 2012; Mahabadi et al., 2012b).
<sup>d</sup> Average (bulk) rock value from uniaxial and biaxial compression testing (Mahabadi, 2012).
<sup>e</sup> Estimated by scaling the bulk tensile strength of the rock using the fracture toughness values: $f_{t,\text{min}} = f_{t,\text{rock}} \cdot \frac{K_{Ic,\text{min}}}{K_{Ic,\text{rock}}}$. 
<sup>f</sup> Estimated from values of mode I fracture toughness, $K_{Ic}$, measured by micro-indentation testing (Mahabadi, 2012) ($G_{Ic} = K_{Ic}^2/E$).
<sup>g</sup> Assumed equal to $2 \times G_{Ic}$.
<sup>h</sup> Assumed equal to 0.1.

#### 3.5.2 Stress-strain behaviour and acoustic activity

Emergent UCS value, Young’s modulus and Poisson’s ratio of the sample are equal to 142.9 MPa, 49.7 GPa, and 0.25, respectively. These values are in good agreement with the respective experimental values of 147.3 MPa, 52.5 GPa, and 0.23, used as calibration targets. The onset of AE coincides with the initiation of non-linearity in the lateral strain curve while, in the axial direction, the response of the model is linear until a displacement of about 0.250 mm is reached (stage b-c) (Fig. 3.11). With increasing applied strain, more crack elements start to break, more damage is accumulated and acoustic energy emitted, resulting in the load-displacement curve beginning to deviate from linearity. Further increase of displacement leads to an increase in the acoustic event count (stage c to f). Cracking in the pre-peak non-linear stage is diffuse over the sample surface and dominated by extensional failure type (Fig. 3.12b-f). Furthermore, the friction at the interface between rock sample and platens effectively constrains the lateral deformation of the rock sample and, therefore, fracturing tends to be inhibited in the lower and upper part of the sample. Analysis of failure type distribution in stage a to e (Fig. 3.13) indicates that the microfracturing process within the crystalline structure of the numerical sample correlates exclusively with the breakage of weaker interfaces at the biotite-feldspar and biotite-quartz contacts.

As the sample approaches its peak strength, a sensible increase in the acoustic event count is
Fig. 3.11. Axial stress, $\sigma$, versus platen displacement, $\delta_a$, and lateral displacement, $\delta_l$, for the UCS test simulation, also showing counts of acoustic events as columns. Letters a to i indicate the displacement intervals adopted to analyze the evolution of the seismic $b$ value and the fractal dimension $D$ in Section 3.5.3 and 3.5.4, respectively. The platen displacement, $\delta_a$, was used in lieu of the axial strain, $\varepsilon_a$, because of the potential error that can be introduced into the AE count by duplicate values from the post-peak region, where the axial strain decreases.

The AE amplitude distribution during fracturing experiments has been shown to obey the Gutenberg-Richter relationship (Richter, 1958) observed for crustal earthquakes (Mogi, 1962; Scholz, 1968a). Based on this relationship, the distribution of AE size can be expressed by a power law:

$$N(> A) = a A^{-b},$$  \hspace{1cm} (3.27)
Fig. 3.12. (a) Spatial distribution of minerals in the UCS sample. Feldspar, quartz and biotite are indicated in grey, blue and green, respectively. (b)-(f) Cumulative spatial distribution of broken crack elements at increasing platen displacement values, $\delta_a$, during the UCS test simulation: (b) $\delta_a = 0.25$ mm (stage $a$ and $b$), (c) $\delta_a = 0.30$ mm (stage $a$ to $d$), (d) $\delta_a = 0.35$ mm (stage $a$ to $f$), (e) $\delta_a = 0.375$ mm (stage $a$ to $h$), (f) $\delta_a = 0.425$ mm (stage $a$ to $i$). Mode I (i.e., tensile) and mode II (i.e., shear) failures are indicated in orange and blue, respectively. A transition from diffuse-like tensile-dominated cracking to macroscopic spalling is captured as the sample is compressed.

where $A$ is the maximum amplitude of AE, $N$ is the number of events with amplitude greater than $A$, and $a$ and $b$ are constants. In logarithmic coordinates, this relationship becomes linear:

$$\log N(>M) = a - bM,$$

where $M = \log A$ is the AE magnitude and the exponent $b$ represents the scaling of AE magnitude distribution. The evolution of $b$ value has been studied to diagnose the fracture development stage

Fig. 3.13. Relative frequency of failure types during the UCS test simulation. Intergranular failures correspond to the breakage of crack elements bonding together triangular elements representing different mineral phases, whereas intragranular failures correspond to the breakage of crack elements within the same mineral.
during laboratory testing of rock samples (e.g., Lockner et al., 1991) and in non-destructive testing of structures (e.g., Carpinteri and Bocca, 1991). In earthquake seismology, the $b$ value analysis has been used as a earthquake forecasting tool (e.g., Mogi, 1967). In this study, the evolution of $b$ value during the UCS test simulation was analyzed with reference to the nine axial consecutive displacement windows (stage $a$ to $i$) shown in Fig. 3.11. Event magnitudes were calculated from the kinetic energy of the AE sources using eqs. (3.18) and (3.19). Since in actual AE monitoring the size of AE recorded is limited by the resolution, synthetic AE events with magnitude smaller than -9.0 were excluded from the calculation.

The frequency-magnitude distributions (Fig. 3.14) show a good linear behaviour from stage $a$ to $f$, corresponding to the linear and non-linear pre-peak portions of the stress-displacement curve. In the peak and post-peak intervals (stage $g$ to $i$), a marked increase in the mean event magnitude and number of events is accompanied by a loss of linearity in the distributions, which tend to exhibit a large magnitude cut-off indicative of the presence of a finite-size effect. In other words, when the applied stress, $\sigma$, is < 97% of the failure stress (up to stage $g$), the AE population is relatively small and the distribution is fully linear over the entire range of magnitude. For higher applied stresses and in the post-peak region, a polynomial fit would provide a better correlation between event magnitude and frequency. Qualitatively, a similar loss of linearity for increasing applied stress was observed by Rao and Lakshmi (2005) during laboratory uniaxial compression tests on Godhra Granite.

The seismic $b$ values during the UCS simulation, ranging between 0.76 and 1.80 (Fig. 3.15), are in good agreement with published experimental values for granitic rocks ranging between 1.1 and 2.4 (e.g., Lockner et al., 1991; Lockner, 1993). The numerical results indicate two sharp drops in $b$ value during the fracture process of the rock sample. The first drop occurs in the pre-peak region at about 75% of the failure stress (stage $b$) and is characterized by a decrease from 1.80 to 0.99. As further discussed in Section 3.5.4, this unexpected variation is caused by few larger magnitude events clustering close to the bottom left corner of the sample which produce an increase in the share of large events for stage $b$. This localization of failure, which can be attributed to the particular spatial distribution of material properties, contributes to the non-linear behaviour of the sample’s lateral displacement while does not have any sensible effect on its axial deformation response. The second decrease in the $b$ value begins at 97% of the failure stress (stage $g$), with $b$ dropping from 1.59 to 1.08, and continues in the immediate post-peak. This variation of $b$, clearly associated with the macroscopic rupture of the sample, is in agreement with several experimental findings (Scholz, 1968a; Cai et al., 1988; Main and Meredith, 1989; Meredith et al., 1990; Lockner et al., 1991; Amitrano, 2003), which indicate a systematic decrease in $b$ with increasing stress during deformation of intact rock samples. As depicted in Fig. 3.12, the $b$ value decrease in correspondence to the maximum stress marks the transition from diffuse crack nucleation to crack coalescence in a major fracture plane.

### 3.5.4 Spatial clustering of AE

The location of AE sources has been widely used to study the crack redistribution during the rock failure process and, consequently, to obtain information on the fracture mechanisms. In this work, the process
Fig. 3.14. Frequency-magnitude plots for each displacement interval (stage a to i). Only events with magnitude $M_e \geq -9.0$ were considered. The exponent $b$ was calculated for the linear part of each distribution together with the coefficient of determination, $R^2$, of the linear regression. Frequency-magnitude plots display a power law distribution for axial displacement values less than the value at peak (stage a to f). In the peak and post-peak stages, the distributions lose linearity and a finite-size effect can be noticed. The $b$ value for stage i was not calculated. For stage b, an additional analysis was carried by excluding from the distribution the event cluster triggered by the bottom left corner of the sample (see Section 3.5.6).

of spatial clustering of AE source locations, depicted in Fig. 3.16, was quantitatively analyzed using the correlation integral (Hirata et al., 1987):

$$C(R) = \frac{2N_R(r < R)}{N(N - 1)}, \quad (3.29)$$

where $N_R(r < R)$ is the number of AE source pairs separated by a distance $r$ shorter than $R$, and $N$ is the total number of sources analyzed. If the source distribution has a fractal structure, the correlation integral $C(R)$ is proportional to $R^D$, where $D$ is the fractal dimension of the distribution:

$$C(R) \sim R^D. \quad (3.30)$$
Fig. 3.15. Variation of $b$ value during the UCS test simulation. Drops in $b$ value are associated with clustering of higher magnitude events due to either a localized effect (stage $b$) or to crack coalescence in a macroscopic rupture plane (stage $g$ to $i$). For stage $b$, $b^* = 2.1$ was calculated by excluding from the distribution the cluster of events by the bottom left corner of the sample (see Section 3.5.6).

In two dimensions, $D = 2$ indicates complete randomness in the source location distribution, while lower values suggest the presence of clustering. However, note that $D$ does not carry any information about the shape of the spatial distribution: for example, $D = 1.0$ can refer to either a distribution of aligned sources or to a strongly clustered distribution around a point. Hence, to obtain information on the characteristics of the localization, the aforementioned fractal analysis must be accompanied with a visual inspection of the actual source pattern.

For distance $R$ less than 50 mm, which corresponds to the width of the sample, the plots of $C(R)$ against $R$ (Fig. 3.17) follow a good linear trend, indicating the fractal structure of AE source location distribution. Event spatial clustering that can be observed in Fig. 3.16 for stage $b$, $g$, $h$, and $i$, manifests itself in the form of a decrease of fractal dimension to values $1.1 \leq D \leq 1.4$ (Fig. 3.17). The diffuse character of the damage pattern characterizing the other stages ($a$, $c$ to $f$) is reflected in $1.4 \leq D \leq 1.8$. Due to the bi-dimensionality of the FEM/DEM model, the absolute values of fractal dimension could not be directly compared to experimental values, which vary in three dimensions between 0 and 3. Nevertheless, the simulated reduction of $D$ before and after localization is in agreement with the laboratory results reported by Lockner (1993) and Shah and Labuz (1995) for compression tests on Westerly Granite and Charcoal Granite, respectively, and with other numerical simulations (e.g., Amitrano et al., 1999).

Finally, a comparison between the evolution of $b$ value (Fig. 3.15) and fractal dimension $D$ (Fig. 3.18) clearly shows a decrease of $b$ value contemporary to the spatial localization of AE events, represented by a decrease of $D$, as observed by Lockner (1993). Higher $b$ values result from low energy emission due to new crack formation and slow crack growth (i.e., diffuse damage), while lower $b$ values are due to crack coalescence resulting in faster fracture growth accompanied by high energy emission.
Fig. 3.16. AE source locations and associated magnitude for stage a to i of the simulated UCS failure process. The color bar indicates the event seismic magnitude, $M_e$, calculated from the kinetic energy of the sources using the technique illustrated in Section 3.4.2. Several events, with magnitude comprised between -8.5 and -7.5, cluster by the sample bottom left corner during stage b (indicated by an arrow), causing a drop in the correspondent $b$ value and fractal dimension $D$ (see Section 3.5.6). The macro-rupture of the sample (stage g to i) is accompanied by the localization of high-energy events close to the sample lateral free surfaces in the form of spalls, as highlighted also by the fracture pattern depicted in Fig. 3.12f.
Fig. 3.17. Correlation integral, $C(R)$, versus source distance, $R$, for stage $b$, $e$, and $h$ of the simulated UCS stress-displacement curve (Fig. 3.11). A linear regression is applied to the linear descending branch of each distribution ($R < 50$ mm) with slope equal to the fractal dimension $D$. The coefficient of determination, $R^2$, is also indicated.

### 3.5.5 Time evolution of AE rate

The stochastic self-similarity of the simulated microfracturing process was verified for the frequency-magnitude distribution (Section 3.5.3) and spatial distribution of AE sources (Section 3.5.4). As described above, this self-similarity manifests itself as the power laws expressed by eqs (3.27) and (3.30).
in the magnitude and spatial domain, respectively. Similarly, it has been shown that also the rate of AE during rock fracture experiments follows a power law evolution in the time domain (e.g., Scholz, 1968b; Hirata, 1987). This phenomenon is typically described by the Omori’s law, an experimental relationship first introduced to characterize the rate of occurrence of earthquake aftershocks (Omori, 1894). In its generalized form, the Omori’s law is expressed as (Utsu, 1962)

$$\frac{dN}{dt} = \frac{K}{(c + t)^p},$$

(3.31)

where \(dN/dt\) is the aftershock rate, \(t\) is the time after the mainshock, and \(K\), \(c\), and \(p\) are empirical fitting parameters. In the case of foreshocks preceding the main rupture, \(t\) represents the reverse time from the mainshock with the Omori exponent \(p\) directly controlling the event growth rate. In this numerical study, the temporal evolution of the simulated AE triggering was therefore studied with reference to the empirical description provided by eq. (3.31). As described in the following, both aftershocks and foreshocks were initially considered.

During laboratory experiments, a hyperbolic decay of the microfracturing activity with time is commonly recorded after the brittle fracture of rock sample with Omori’s exponent \(p\) values typically ranging between 0.8 and 2.3 (Hirata, 1987). This creep process produced by time-dependent fracturing mechanisms can be followed by AE monitoring provided that the rock sample remains intact (Scholz, 1968b). For example, manual unloading at the onset of dynamic fracture can be performed to save the sample from excessive damage (Lei et al., 2004). In the FEM/DEM simulation, the analysis of aftershock sequences was heavily compromised by the model boundary conditions as well as the brittle behaviour exhibited by the sample under unconfined compression. Since the sample was loaded by means of platens moving at steady speed, a constant strain rate was applied for the entire duration of the simulation. Following the unstable rupture of the sample, this monotonic loading condition greatly enhanced the fragmentation of the rock, thus causing a dramatic increase of breakages in the post-peak stages of the simulation (Fig. 3.11). That is, the simulation was stopped before any decay in the event rate could be observed.

Conversely, acoustic events triggered before the macroscopic failure of the sample could be successfully analyzed. The evolution of AE rate as function of the time prior to the main rupture is reported in the logarithmic scale plot of Fig. 3.19. For time values \(t\) greater than 0.9 ms (i.e., stage \(a\) in Fig. 3.11), very low activity is recorded and the evolution is non-linear. However, as more stress is applied, more events are triggered and a slow growth of microfracturing is followed by a rapid acceleration of AE rate, for which Omori’s law provides a good fit. Due to the above mentioned difficulties, a clear identification of the time, \(t_M\), corresponding to the mainshock was not possible. Therefore, the regression analysis using Omori’s law was repeated for three increasing \(t_M\) values: \(p\) values equal to 0.38, 0.70, and 1.12 were obtained for \(t_M\) equal to 1.45, 1.50, and 1.60 ms, respectively. Given a platen velocity of \(v = 0.125\) m/s, these \(t_M\) values correspond to axial displacements, \(\delta_a\), of 0.3625, 0.375, and 0.400 mm, which in turn correspond to the endpoints of stage \(g\), \(h\) and \(i\), respectively. For comparison, \(p\) values ranging between 0.8 and 2.1 have been reported for foreshocks during actual laboratory tests on rock
Fig. 3.19. Logarithmic scale plot of the rate of acoustic events in the UCS test simulation as function of the time before the main rupture. Omori’s exponent values, \( p \) (eq. (3.31)), equal to 0.38, 0.70, and 1.12 were calculated by assuming the main rupture to occurred at axial displacement values, \( \delta_a \), of 0.3625, 0.375, and 0.400 mm, respectively. These threshold displacement values to the endpoints of stages g, h and i, respectively (Fig. 3.11).

(e.g., Ojala et al., 2004; Schubnel et al., 2007).

### 3.5.6 Analysis of b value anomaly

As described in Section 3.5.3, an anomaly of \( b \) value was recorded during stage \( b \) (0.225 mm ≤ \( \delta_a \) ≤ 0.250 mm) of the UCS test simulation. The \( b \) value, calculated from the frequency-magnitude distribution of all events in the given displacement window, was equal to 0.99, which represented a 40% reduction with respect to the average value in the pre-peak stages of the simulation (\( b = 1.67 \)) (Fig. 3.15). Moreover, the drop in \( b \) value was also accompanied by a reduction in the associated fractal dimension, \( D \), of the hypocenter distribution (Fig. 3.18).

For tectonic earthquakes, correlations between low \( b \) values and regions of increased fault strength have been observed (e.g., Wiemer and Wyss, 1997). In the laboratory, temporal fluctuations of AE statistics have been related to the heterogeneous distribution of grain size and strength within the rock microstructure (Lei et al., 2004). For example, Goebel et al. (2012) showed a clear connection between the spatio-temporal distribution of microseismicity and structural heterogeneities of fracture surfaces during stick-slip laboratory experiments on notched samples of Westerly Granite. More specifically, geometric asperities identified through CT scan images corresponded well with regions of low local \( b \) value.

In the FEM/DEM simulation, a region of high event density was located during stage \( b \) in proximity to the bottom left corner of the sample (Fig. 3.16b). The effect of this cluster of events on the simulated
AE statistics, namely $b$ value and fractal dimension $D$, was assessed by excluding these events from the regression analysis based on eqs (3.28) and (3.30). The modified distributions of event magnitude (Fig. 3.14b) and spatial correlation integral were characterized by $b^* = 2.1$ and $D^* = 1.45$, respectively. As can be observed from Figs 3.15 and 3.18, these values tend to better follow the trend simulated for the other pre-peak stages, thus confirming the influence of the event sequence in causing the simulated anomaly. The local distribution of mineral phases was then investigated in an attempt to provide a mechanical interpretation for the simulated phenomenon (Fig. 3.20a). The acoustic events correspond to the failure of a series of crack elements approximately aligned at about $67^\circ$ from the horizontal. In agreement with the analysis reported in Section 3.5.2, breakages are mainly restricted to the weaker interfaces between biotite and feldspar in the form of mode I fracturing. The visual inspection of the property distribution indicates the presence of two quartz-feldspar clumps located on the top left and bottom right side of the rupture plane. These two mineral clumps, characterized by higher stiffness and strength values (Table 3.5), experience a concentration of maximum principal stress, $\sigma_1$ (Fig. 3.20b). As discussed in detail by Mahabadi (2012), breakage of weaker mineral interfaces is due to higher localized tensile stresses arising from elastic mismatch of the three rock minerals. Based on these observations, it is likely that the simulated higher activity is a direct consequence of the build-up of elastic strain energy in the two clumps which is released as acoustic energy upon failure of the weaker interfaces. Therefore, these numerical results tend to agree with the experimental evidence mentioned above which highlights decreasing $b$ values due to fracture growth around the boundaries of asperities. Nevertheless, further numerical investigation is required to confirm the validity of the postulated mechanism. In this context, a more realistic numerical representation of the rock microstructure, for instance directly derived from \( \mu \)CT images (Mahabadi et al., 2012b), should be adopted.

### 3.6 Summary

Monitoring of acoustic activity has been used to characterize the rock failure process by providing unique information regarding the amount of internal damage, the spatial distribution of microfractures and the magnitude distribution of fracturing events. Therefore, the ability to simulate acoustic activity presents an important tool in the validation of numerical models that aim at quantitatively capturing the deformation and failure process of brittle rocks. Furthermore, the relationship between the simulated seismicity and model parameters (e.g., material properties, loading conditions, degree of heterogeneity) can be numerically investigated. While several models have been developed to date for this purpose, only a limited number explicitly consider acoustic waves, the majority adopting a static approach, whereby the elastic strain energy, dissipated by an elasto-plastic constitutive law, is considered as an equivalent for the radiated seismic energy.

In this work, a new approach to simulate the acoustic activity of brittle failing rocks was presented based on the combined finite-discrete element method (FEM/DEM). Two methods were considered to obtain quantitative information on the acoustic activity: (i) the seismic analysis of waveforms recorded at a distance from the sources and (ii) monitoring of internal variables (e.g., relative displacements and
Fig. 3.20. A zoomed-in view of the squared region of Fig. 3.16b showing (a) the distribution of mineral phases and failed crack elements during stage $b$ of the UCS test simulation and (b) the local distribution of maximum principal stress, $\sigma_1$, before the rupture sequence at $t = 0.68$ ms (i.e., $\delta_a = 0.17$ mm). The approximate alignment direction of the sequence of events is indicated by a dashed line. These events tend to be located at the interface of two clumps of stiffer, stronger material (i.e., feldspar and quartz) contoured by a red line. Note the heterogeneous stress distribution with two major compressive stress concentrations.

Fourier analysis of synthetic seismograms highlighted frequency contents ranging between 8 and 20 kHz. As expected, the amount of applied numerical damping significantly reduced the amplitudes of AE signals recorded at a distance from the source. Low rupture speed values, direct consequence of the adopted mesoscopic model of the fracturing process, resulted in a quasi-dynamic AE behaviour characterized by low frequency content source processes in the FEM/DEM simulations. Although seismic energy is emitted upon failure, the observed low rupture speeds imply that most released energy is dissipated as fracture energy within the FPZ. Furthermore, the seismic analysis of synthetic seismograms suffered from the inability to record temporally distinct events as the event count rate increases, which constrained its application to special fracturing conditions (e.g., wing crack propagation). Nevertheless, event relocation based on travel-time inversion showed good agreement with the internally recorded AE locations. Also, the seismic energy estimated at the receivers via integration of wave amplitude scaled linearly with the kinetic energy of cracks monitored at the source.

Taking advantage of the discrete material representation of FEM/DEM, an alternative algorithm was implemented to obtain seismic information, including source location, mode of fracture, initiation time, and event energy, based on internal monitoring of node motions. As mentioned above, the event energy, estimated based on the crack kinetic energy, was related to the energy carried by the radiated stress waves and recorded at selected locations by the model boundaries. The main limitation of this
technique is represented, at the moment, by its inability to record the energy radiated by slips along pre-existing crack surfaces that do not involve intact material breakage. Lastly, the validity of the aforementioned approach was demonstrated by simulating the AE of an unconfined compression test on Stanstead Granite. The model reproduced the macroscopic mechanical response of the sample (e.g., elastic behaviour, overall strength, post-peak brittle failure), as observed in the laboratory. Simulated event magnitudes tended to display a power law distribution, with $b$ values in agreement with those reported in the literature for granitic rocks. Also, the model showed a correlation between the decrease of $b$ value and the transition of source location distribution from diffuse-like to strongly clustered, as the applied stress increases and macroscopic fractures develop through the sample. A $b$ value anomaly was related to the failure of weaker mineral bonds at the interface of stronger, stiffer clumps within the numerical microstructure of the rock sample. Furthermore, Omori’s law provided a good fit for the evolution of AE rate as function of time before the macroscopic rupture of the sample.

In future studies, the validated FEM/DEM-AE modelling technique will be used to obtain further insights into the micro-mechanics of rock failure with potential applications ranging from laboratory-scale microcracking to engineering-scale processes (e.g., underground excavations, petroleum and geothermal reservoirs) to tectonic earthquakes. Moreover, the approach will be extended to a 3D version of the FEM/DEM code currently under development.
Chapter 4

Numerical modelling of the anisotropic mechanical behaviour of Opalinus Clay at the laboratory-scale using FEM/DEM

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Abstract

The Opalinus Clay (OPA) is an argillaceous rock formation selected to host a deep geologic repository for high-level nuclear waste in Switzerland. It has been shown that the excavation damaged zone (EDZ) in this formation is heavily affected by the anisotropic mechanical response of the material related to the presence of bedding planes. In this context, the purpose of this study is twofold: (i) to illustrate the new developments that have been introduced into the combined finite-discrete element method (FEM/DEM) to model layered materials and (ii) to demonstrate the effectiveness of this new modelling approach in simulating the short-term mechanical response of OPA at the laboratory-scale. A transversely isotropic elastic constitutive law is implemented to account for the anisotropic elastic modulus, while a procedure to incorporate a distribution of preferentially oriented defects is devised to capture the anisotropic strength. Laboratory results of indirect tensile tests and uniaxial compression tests are used to calibrate the numerical model. Emergent strength and deformation properties, together with the simulated damage mechanisms, are shown to be in strong agreement with experimental observations. Subsequently, the calibrated model is validated by investigating the effect of confinement and
the influence of the loading angle with respect to the specimen anisotropy. Simulated fracture patterns are discussed in the context of the theory of brittle rock failure and analyzed with reference to the EDZ formation mechanisms observed at the Mont Terri Underground Research Laboratory.

4.1 Introduction

Opalinus Clay (OPA) is indurated over-consolidated clay shale that has been chosen as a host rock formation for a high-level nuclear waste underground repository in Switzerland. The key characteristics that make this argillaceous rock suitable for radioactive waste storage include: low permeability, low diffusion coefficients and good retention capacity for radionuclides, self-sealing properties, and lack of economic value. Nevertheless, one of the main concerns is that these favourable long-term isolation properties could be negatively affected by the disturbance and damage associated with the underground excavations comprising the repository. The micro-cracked zone surrounding such openings, characterized by damage and permeability increased by several orders of magnitude is termed the excavation damaged zone (EDZ) (Tsang et al., 2005). To determine the shape and extent of the EDZ, a correct understanding and prediction of the mechanical behaviour of OPA is of paramount importance.

Opalinus Clay is characterized by a preferably oriented micro-structure which results in a distinct anisotropy of its hydro-mechanical properties. This material anisotropy has been largely documented by several laboratory testing campaigns on specimens from the Mont Terri Underground Research Laboratory (URL) (e.g., Naumann et al., 2007; Popp and Salzer, 2007a; Bock, 2009; Jahns, 2010). Other recent laboratory results clearly show that the failure process in OPA, including the stress-strain response, fracture mechanisms and acoustic activity, is typical of that for brittle materials (Amann et al., 2011, 2012).

Laboratory evidence regarding the key role played by the material anisotropy in controlling the brittle failure of OPA is confirmed by in situ observations at the Mont Terri URL. Macroscopic excavation-parallel extensional fractures have been reported in the near-field of numerous test tunnels and a distinctive variation of failure mechanism has been observed as a function of the orientation of the tunnel with respect to the bedding plane orientation (Bossart et al., 2002; Blümling et al., 2007). Furthermore, the influence of strength anisotropy on borehole damaged zones has recently been demonstrated by the fracture patterns observed in over-cored resin-injected boreholes (Vietor et al., 2012) and in-hole camera recording (Seeska and Lux, 2012).

The current work is motivated by the need to develop and validate numerical tools that could assist in the design of deep geological repositories. In particular, numerical tools that are capable of reproducing the observed rock mass failure mechanisms, including the shape and extent of the EDZ, are required. Considering the failure process of OPA, the employed numerical model must be able to simulate the intrinsic anisotropy of the material and the localization of failure.

In this paper, new developments that allow geomaterials, with anisotropic deformation and strength characteristics, to be modelled using the combined finite-discrete element method (FEM/DEM) are presented (Section 4.3). The effectiveness of the numerical approach is then demonstrated by quantitatively...
reproducing the short-term response of OPA observed during standard rock mechanics tests. In particular, calibration of the model, based upon unconfined compression and indirect tension test results, is discussed (Section 4.4). In Section 4.5, the model is validated by simulating the effect of confinement and the orientation of specimen anisotropy on the mechanical behaviour of OPA. Modelling results are compared to published laboratory findings for OPA and other anisotropic rocks and are discussed in the context of the EDZ formation mechanisms observed at the Mont Terri URL. Finally, the mesh sensitivity of the proposed FEM/DEM model and its applicability to large-scale problems are discussed (Section 4.6).

4.2 Modelling progressive failure processes of anisotropic rocks

The approaches available in computational geomechanics to model the damage process of anisotropic rock materials are generally classified as: (i) the equivalent continuum approach, (ii) the discrete element method (DEM) and (iii) the hybrid approach.

With the continuum method, the presence of layers is smeared to produce a fictitious continuous material that exhibits mechanical characteristics that are similar to the original discontinuous medium. That is, the effect of layering is implicit in the choice of the material stress-strain constitutive laws. Traditional formulations of the equivalent continuum approach for anisotropic rocks are the Ubiquitous Joint Model, implemented for example in the commercial code FLAC (Itasca Consulting Group Inc., 2012a) and models based on the Cosserat theory (e.g., Adhikary and Dyskin, 1998; Riahi and Curran, 2009). Localization of failure in classic continuum elasto-plastic formulations is captured by either enriching the continuum with micro-structural effects such as the second gradient damage models (e.g., Besuelle et al., 2006; Collin et al., 2006) or using statistical damage models (e.g., Jia and Tang, 2008).

With the DEM approach, layers or joints are explicitly represented in the numerical model. The medium is modelled as an assembly of rigid or deformable particles or blocks with interaction laws governing the emergent behaviour of the material. Examples of anisotropic rock modelling using particle-based DEM codes are given by Potyondy and Cundall (2000), Konietzky et al. (2003), Potyondy and Cundall (2004), and You et al. (2011). Although the large computational demand tends to limit its applicability to problems at the scale of small rock samples in the laboratory, the DEM approach offers unique advantages when the extended loss of continuity inside the material, for example due to the progressive breakdown, makes continuum constitutive models inappropriate.

The third category, hybrid continuum/discontinuum approaches (e.g., Dedecker et al., 2007), combines DEM techniques to represent zones affected by strong non-linear behaviour due to material failure with a continuum approach for the remaining small-strain elastic regions. The hybrid method known as the combined finite-discrete element method (FEM/DEM) (Munjiza, 2004), represents a particular type of hybrid approach whereby the elastic deformation of the material is described using continuum mechanics theory while DEM algorithms and non-linear fracture mechanics principles are employed to capture fracture mechanisms that are typical of brittle and quasi-brittle materials such as concrete and rocks.
4.3 Fundamental principles of the FEM/DEM approach

The combined finite/discrete element method (FEM/DEM) is a numerical method pioneered by Munjiza et al. (1995) for the dynamic simulation of multiple interacting deformable bodies. A unique feature of such a numerical tool is the ability to model the transition from continuum to discontinuum by explicitly simulating fracture and fragmentation processes. In the following sub-sections, the key processes of the method are described with particular emphasis on the approach that was developed to capture the behaviour of anisotropic rocks, including OPA. The anisotropy modelling capability was implemented into the two-dimensional Y-Geo FEM/DEM code (Mahabadi et al., 2012a), which represents an extension of the original Y2D code of Munjiza (2004) undergoing development at the University of Toronto for geomechanical applications.

4.3.1 Interaction of discrete bodies

A FEM/DEM simulation can comprise a very large number of potentially interacting distinct elements. To correctly capture this behaviour, contacting couples (i.e., pairs of contacting discrete elements) must first be detected. Subsequently, the interaction forces resulting from such contacts can be defined. Contact interaction forces are calculated between all pairs of elements that overlap in space. Two types of forces are applied to the elements of each contacting pair: repulsive forces and frictional forces. The repulsive forces between the elements of each contacting pair (i.e., couples) are calculated using a penalty function method (Munjiza and Andrews, 2000). Contacting couples tend to penetrate into each other, generating distributed contact forces, which depend on the shape and size of the overlap between the two bodies and the value of the penalty term. As penalty values tend to infinity, a body impenetrability condition is approached. The frictional forces between contacting couples are calculated using a Coulomb-type friction law. These frictional forces are used to simulate the shear strength of intact material and of pre-existing and newly created fractures.

4.3.2 Material failure

Damage and failure of rock material is simulated in FEM/DEM by explicitly modelling crack initiation and propagation using principles of non-linear elastic fracture mechanics (NLEFM). According to this theory, originally developed for metals by Dugdale (1960) and Barenblatt (1962), when the ultimate strength of the material is reached, a zone characterized by non-linear behaviour starts to form ahead of the crack tip. This zone is known as the fracture process zone (FPZ). In rocks, the FPZ is characterized by interlocking and micro-cracking (Labuz et al., 1985) (Fig. 4.1a). The material in the FPZ, albeit damaged, is still able to transfer load across the crack walls (Fig. 4.1b) while the material outside the FPZ behaves elastically.

In the present study, a modified version of the discrete fracture model originally developed by Munjiza et al. (1999) was employed. With this model, crack walls are assumed to coincide with the edges of the triangular finite elements and the relative crack wall displacements are evaluated using dedicated 4-noded crack elements, as illustrated in Fig. 4.1c. Depending on the local stress and deformation
field, fractures can nucleate and propagate via mode I (i.e., opening mode), mode II (i.e., sliding mode) or mixed mode I-II.

Mode I fracture initiation and propagation is simulated through a cohesive crack model based on the theoretical model originally proposed for concrete by Hillerborg et al. (1976). As shown in Fig. 4.2a, the crack initiates when the crack tip opening, \( o \), reaches a critical value, \( o_p \), which corresponds to the intrinsic tensile strength of the rock, \( f_t \). As the fracture propagates and the crack tip opening increases, the normal stress, \( \sigma_n \), is assumed to decrease until a residual opening value, \( o_r \), is reached and a stress-free surface is created.

Mode II fracture initiation and propagation is simulated by a slip-weakening model. As depicted in Fig. 4.2b, a tangential stress, \( \tau \), exists between the two fracture walls, which is a function of the amount of slip, \( s \), and the normal stress on the fracture. The critical slip, \( s_p \), corresponds to the intrinsic shear strength of the rock, \( f_s \), defined as

\[
f_s = c + \sigma_n \cdot \tan \phi_i, \tag{4.1}
\]

where \( c \) is the internal cohesion, \( \phi_i \) is the intact material friction angle, and \( \sigma_n \) is the normal stress acting across the crack element. Upon undergoing the critical slip \( s_p \), the tangential stress is gradually reduced.
to a residual value, $f_r$, which corresponds to a purely frictional resistance:

$$f_r = \sigma_n \cdot \tan \phi_f,$$

(4.2)

where $\phi_f$ is the fracture friction angle. In the current implementation of the crack element response (Fig. 4.2), the unloading path in the softening branch coincides with the loading path. Therefore, the model is strictly only valid for monotonic loading conditions.

For mixed mode fracturing, the rupture of a crack element is defined by the following coupling criterion between crack opening and slip:

$$\left(\frac{o - o_p}{o_r - o_p}\right)^2 + \left(\frac{s - s_p}{s_r - s_p}\right)^2 \geq 1.$$

(4.3)

The values of residual opening and slip depend on the tensile and shear strength and the mode I and mode II fracture energy release rates, $G_I$ and $G_{II}$, for the material. The values of $G_I$ and $G_{II}$ are defined as:

$$G_I = \int_{o_p}^{o_r} \sigma(o) \, do$$

(4.4)

$$G_{II} = \int_{s_p}^{s_r} \left[\tau(s) - f_r\right] \, ds$$

(4.5)

### 4.3.3 Material anisotropy

As part of this research project, the capabilities of the two-dimensional Y-Geo code were extended such that the mechanical response of anisotropic materials could be simulated. Details of the adopted approach are illustrated in the following subsections.
Anisotropy of stiffness

Like most argillaceous rocks, OPA is a distinctively bedded material with mechanical behaviour that is best described as transversely isotropic (Popp and Salzer, 2007b). That is, the deformability of the rock can be considered isotropic within any plane normal to an axis of rotational symmetry coincident with the normal to the bedding plane orientation (Fig. 4.3a). Therefore, to describe the elastic response of OPA, a stress-strain constitutive law for transversely isotropic elastic solids was implemented in FEM/DEM. For such materials, there are five independent elastic constants (Ting, 1996): $E_1$ and $E_2$ ($= E_3$) are the Young’s moduli in the direction perpendicular, $s_1$, and parallel, $s_2$, to the bedding, respectively; $\nu_{12}$ ($= \nu_{13}$) and $\nu_{23}$ are the Poisson’s ratios that define the lengthening deformation in the directions $s_2$ and $s_3$ due to normal stresses in the directions $s_1$ and $s_2$, respectively; and $G_{12}$ is the shear modulus in the $(s_1, s_2)$ plane. The naming convention of Fig. 4.3b is used in the present work to identify the test specimens according to the direction of anisotropy.

Anisotropy of strength

A large body of experimental evidence (e.g. Popp and Salzer, 2007a; Bock, 2009) clearly indicates that the mechanical strength of OPA during laboratory tests is strongly direction-dependent. The maximum unconfined compressive strength value is generally obtained when samples are loaded in the direction perpendicular to the bedding (S-sample). A local maximum value, lower than the previous one, occurs when samples are loaded in the direction parallel to the layering (P-sample), while a substantial strength reduction is observed for loading angles between these two limiting cases. Similar strength response has been observed for other kinds of anisotropic rocks (Donath, 1972).

To capture this characteristic behaviour in FEM/DEM, a discrete representation of material anisotropy was implemented. This approach follows that which was introduced by Potyondy and Cundall (2000) in a 2D bonded-particle code to simulate the mechanical response of gneissic tonalite and extended to 3D by Wanne (2002). With this approach, the anisotropy of strength is captured as an emergent property of a medium containing a distribution of pre-existing cracks aligned with the bedding planes without introducing any directional dependence in the crack element strength parameters. Since this procedure
can be extended to the general case of multiple arbitrarily-oriented discontinuities, often referred to as a discrete fracture network (DFN), the resulting micro-mechanical model of OPA is referred to herein as the FEM/DEM-DFN model. The newly-developed procedure involves populating a homogenous FEM/DEM model, representing the rock matrix, with a distribution of finite-length discontinuities to represent the bedding planes. This pattern of pre-existing cracks (i.e., DFN) is characterized by two groups of properties:

- **DFN geometry.** The DFN geometry is described by the following parameters Fig. 4.4: fracture length, \( l \), fracture spacing, \( s \), fracture bridge length, \( b \), and crack orientation, \( \gamma \). Initial aperture and tangential slip are set to zero for all cracks.

- **DFN mechanical properties.** After all the cracks have been created, the following mechanical properties are specified for each discontinuity: friction angle, \( \phi_f \), and normal and tangential penalty coefficient, \( p_n \) and \( p_t \), which represent normal and tangential stiffness, respectively (Munjiza, 2004). All the DFN cracks are assumed to have zero cohesion and tensile strength.

The DFN property values are determined during the first step of the model calibration procedure as illustrated in Section 4.4.2.

### 4.4 Model calibration

The FEM/DEM-DFN models were calibrated to averaged laboratory results; namely, uniaxial compression tests and indirect tension (Brazilian) tests reported by Bock (2009) for the shaly facies of the Mont Terri OPA. The model boundary conditions, calibration procedure, and results are discussed in the following subsections.
4.4.1 Geometry and boundary conditions

The two-dimensional laboratory-scale models included 35.8 × 17.4 mm rectangular specimens for the compression test and 29.7 mm diameter disc specimens for the Brazilian test. All the specimen cross-sections were assumed to be oriented perpendicular to the strike of the bedding planes. The direction of anisotropy was then varied by changing the DFN inclination such that loading conditions reported in Fig. 4.3b could be reproduced.

The specimens were discretized with triangular elements having an average edge size of 0.30 mm. Load was applied by means of two rigid triangular platens moving at a constant velocity of $v = 0.1$ m/s. Although this loading rate is much greater than that used in the laboratory tests, a sensitivity analysis of the modelling results to the loading rate revealed that simulated strengths approached constant values for loading rates smaller than approximately 0.25 m/s. An integration time step of $3 \times 10^{-6}$ ms was used to solve the equations of motion for both specimen geometries. Input files for the FEM/DEM simulations were created using the Y-GUI software Mahabadi et al. (2010b).

4.4.2 Calibration procedure and input parameters

Discrete element models synthesize the macroscopic behaviour of the material from the interaction of micro-mechanical constituents. As a result, the measurements from standard laboratory tests cannot, in general, be directly used as input parameters. Instead, input parameters are determined through a calibration process, in which the emergent properties of the model are compared to the relevant measured response of the material (Potyondy and Cundall, 2004). Although Mahabadi et al. (2012b) demonstrated that a micro-mechanical characterization of the investigated medium may reduce the number of input parameters requiring numerical calibration, such a procedure was not attempted for this study.

The following laboratory-scale properties were chosen to characterize the short-term response of OPA and were used as calibration targets for the FEM/DEM-DFN models: elastic modulus, $E$, Poisson’s ratio, $\nu$, uniaxial compressive strength, $UCS$, and indirect tensile strength, $T$. Since each of these properties exhibits a dependence upon the orientation of the material anisotropy, values corresponding to loading parallel (P-sample) and perpendicular (S-sample) to layering were considered. The input parameters required to reproduce these target values were obtained through an iterative process utilizing models of uniaxial compressive strength (UCS) tests and Brazilian disc (BD) tests. The main steps of this process proceeded as follows:

(i) Using the BD models, the average crack length in the DFN was adjusted to match the laboratory-measured anisotropy ratio of the indirect tensile strength, $T_P/T_S$. Given the ubiquitous nature of layering in OPA and the adopted element size (0.3 mm), an average crack spacing and bridge length of 1.0 mm were arbitrarily assumed.

(ii) Using the BD models, the material tensile strength, $T$, and mode I fracture energy, $G_I$, were varied until a good approximation of the indirect strength values, $T_P$ and $T_S$, were obtained.
Table 4.1. Geometrical parameters and mechanical properties of the discrete fracture network of the calibrated FEM/DEM-DFN model

<table>
<thead>
<tr>
<th>Geometrical parameter</th>
<th>Mean value</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crack inclination(^a) (\alpha, \gamma) ((^\circ))</td>
<td>Varying</td>
<td>± 5</td>
</tr>
<tr>
<td>Crack spacing(^b) (s) (mm)</td>
<td>1.0</td>
<td>± 0.1</td>
</tr>
<tr>
<td>Crack length(^c) (l) (mm)</td>
<td>2.0</td>
<td>± 0.2</td>
</tr>
<tr>
<td>Bridge length(^b) (b) (mm)</td>
<td>1.0</td>
<td>± 0.1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mechanical property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal contact penalty(^d) (p_n) (GPa·m)</td>
<td>38</td>
</tr>
<tr>
<td>Tangential contact penalty(^e) (p_t) (GPa/m)</td>
<td>3.8</td>
</tr>
<tr>
<td>Internal cohesion, (c) (MPa)</td>
<td>0</td>
</tr>
<tr>
<td>Tensile strength, (f_t) (MPa)</td>
<td>0</td>
</tr>
<tr>
<td>Friction angle, (\phi_f) ((^\circ))</td>
<td>22</td>
</tr>
</tbody>
</table>

\(^a\) Parallel to the orientation of bedding planes.
\(^b\) Values assumed based on an element size \(h = 0.3\) mm.
\(^c\) Calibrated.
\(^d\) Assumed equal to \(10 \times E_2\) (Mahabadi, 2012).
\(^e\) Assumed equal to \(E_2\) (Mahabadi, 2012).
\(^f\) Assumed equal to zero to decrease the number of variables to calibrate.
\(^g\) From Popp and Salzer (2007b).

(iii) Using the UCS models, the material cohesion, \(c\), and the mode II fracture energy, \(G_{II}\), were adjusted to satisfactorily match the UCS values, \(UCS_P\) and \(UCS_S\).

(iv) Returning to the BD models, the simulations were re-run using the parameters updated during step (iii).

The finalized geometric and mechanical parameters of the DFN are reported in Table 4.1. A uniform distribution was assumed for each geometric parameter. The specified mean crack orientation, with a range of ±5\(^\circ\), was selected to mimic the orientation of layering in the test specimens (Fig. 4.3b). For the remaining three parameters, a range equal to 10\% of the mean value was assumed. An average crack length of 2.0 mm was obtained through step (i) of the calibration process. This value yielded a ratio of crack length to bridge length of 2, which is approximately equal to the anisotropy ratio of the indirect tensile strength, \(T_P/T_S\). Since the anisotropy of stiffness was accounted for through the transversely isotropic elastic law applied to the deformable triangular elements, the discrete fractures were assigned normal and tangential penalty values equal to those of the rock matrix. Zero tensile strength and cohesion were assumed for all fractures. A friction angle of 22\(^\circ\) was selected based on the results of direct shear testing of bedding planes by Popp and Salzer (2007b).

The finalized mechanical and numerical parameters of the rock matrix are reported in Table 4.2. The values of the strength parameters for the rock matrix were obtained as the final result of step (ii), (iii) and (iv) of the calibration process, while the experimental values of the elastic constants measured by Bock
(2009) were used directly as input for the transversely isotropic elastic model. Although the presence of 4-noded crack elements across the interfaces of triangular elements effectively reduces the stiffness of the model, this effect was minimized by selecting appropriate values for the penalty coefficients. Following the recommendations of Mahabadi (2012), normal contact penalty, $p_n$, tangential penalty, $p_t$, and fracture penalty, $p_f$, values were set equal to $10 \times$, $1 \times$ and $5 \times$ the maximum Young’s modulus, respectively. The viscous damping coefficient, $\mu$, was assigned a value according to Munjiza (2004), as:

$$\mu_c = 2h\sqrt{E\rho},$$

which approximates the theoretical critical damping assuming a single element of size $h$ behaves as a one-degree-of-freedom mass-spring-dashpot system. Nevertheless, preliminary analyses revealed a relatively low sensitivity of the model to the applied damping under the given loading rate. That is, dynamic effects due to the propagation of stress waves throughout the model had only minor effects on the overall strength and deformation response of the samples.

**4.4.3 Calibration results**

Table 4.3 compares the emergent macroscopic properties of the calibrated FEM/DEM-DFN models with the experimental values of OPA reported by Bock (2009) which were used as calibration targets.

The indirect tensile stress, $\sigma_t$, in the BD specimens as function of the platen vertical displacement, $\delta_v$, was calculated from the platen reaction forces, according to the ISRM suggested method (Bieniawski and Hawkes, 1978). As shown in Fig. 4.5a, the response of both samples was elastic-brittle with complete loss of strength immediately after reaching the peak strength values. Peak values of 1.20 and 0.71 MPa were obtained for the P- and S-sample, respectively. These values are considered a good match to the respective average experimental values of 1.3 and 0.67 MPa.

Fig. 4.6 depicts the simulated and experimentally observed fracture patterns of the BD tests. As expected, the simulated failure mode was mainly given by brittle tensile splitting along the vertical loading path. For the P-sample, shear fractures were observed in proximity to the loading platens due to the induced compressive stress field. Although this additional failure mechanism was responsible for the oscillations of the indirect tensile stress that can be observed in Fig. 4.5a, a simulation whereby the cohesion was artificially increased to induce tensile failure of the specimen revealed that its influence on the indirect tensile strength value, $T_p$, was minimal.

Fig. 4.5b shows the plot of axial stress, $\sigma_1$, versus axial strain, $\varepsilon_1$, and lateral strain, $\varepsilon_3$, for the UCS simulations. The response of both samples is approximately linearly-elastic until the failure stress is reached and a sudden and complete loss of strength is simulated. Simulated unconfined compressive strength values were equal to 11.9 and 14.0 MPa for the P- and S-sample, respectively. These values were in good agreement with the respective experimental values of 11.6 and 14.9 MPa. As reported in Table 4.3, the numerical response of the UCS models satisfactorily matched the elastic experimental behaviour in terms of axial and lateral deformation. As discussed above, the slight discrepancy between numerical and experimental values was due to the artificial compliance introduced by the 4-noded crack
Table 4.2. Mechanical and numerical parameters for the rock matrix of the calibrated FEM/DEM-DFN model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Triangular elements</strong></td>
<td></td>
</tr>
<tr>
<td>Bulk density$^a$, $\rho$ (kg/m$^3$)</td>
<td>2330</td>
</tr>
<tr>
<td>Young’s modulus perpendicular to bedding$^a$, $E_1$ (GPa)</td>
<td>1.3</td>
</tr>
<tr>
<td>Young’s modulus parallel to bedding$^a$, $E_2$ (GPa)</td>
<td>3.8</td>
</tr>
<tr>
<td>Poisson’s ratio parallel to bedding$^a$, $\nu_{12}$</td>
<td>0.35</td>
</tr>
<tr>
<td>Poisson’s ratio perpendicular to bedding$^a$, $\nu_{23}$</td>
<td>0.25</td>
</tr>
<tr>
<td>Shear modulus$^c$, $G$ (GPa)</td>
<td>0.9</td>
</tr>
<tr>
<td>Viscous damping coefficient$^b$, $\mu$ (kg/m·s)</td>
<td>1.79e3</td>
</tr>
<tr>
<td>Edge length$^d$, $h$ (mm)</td>
<td>0.3</td>
</tr>
<tr>
<td>Time step size$^d$, $t$ (ms)</td>
<td>$3 \times 10^{-6}$</td>
</tr>
<tr>
<td><strong>Crack elements</strong></td>
<td></td>
</tr>
<tr>
<td>Tensile strength$^f$, $f_t$ (MPa)</td>
<td>0.65</td>
</tr>
<tr>
<td>Internal cohesion$^c$, $c$ (MPa)</td>
<td>4.5</td>
</tr>
<tr>
<td>Friction angle of intact material$^f$, $\phi_i$ (°)</td>
<td>22</td>
</tr>
<tr>
<td>Friction angle of fractures$^f$, $\phi_f$ (°)</td>
<td>22</td>
</tr>
<tr>
<td>Mode I fracture energy release rate$^f$, $G_1$ (J/m$^2$)</td>
<td>7.0</td>
</tr>
<tr>
<td>Mode II fracture energy release rate$^f$, $G_{II}$ (J/m$^2$)</td>
<td>35</td>
</tr>
<tr>
<td>Platen-sample friction coefficient$^f$, $k$ (-)</td>
<td>0.1</td>
</tr>
<tr>
<td>Normal contact penalty$^h$, $p_n$ (GPa·m)</td>
<td>38</td>
</tr>
<tr>
<td>Tangential contact penalty$^i$, $p_t$ (GPa/m)</td>
<td>3.8</td>
</tr>
<tr>
<td>Fracture penalty$^i$, $p_f$ (GPa)</td>
<td>19</td>
</tr>
<tr>
<td>Critical crack opening$^k$, $o_p$ (µm)</td>
<td>0.021</td>
</tr>
<tr>
<td>Residual crack opening$^k$, $o_r$ (µm)</td>
<td>32</td>
</tr>
<tr>
<td>Critical crack slip$^k$, $s_p$ (µm)</td>
<td>0.142</td>
</tr>
<tr>
<td>Residual crack slip$^k$, $s_r$ (µm)</td>
<td>23</td>
</tr>
</tbody>
</table>

$^a$ From Bock (2009).
$^b$ Computed according to eq. (4.6).
$^c$ Assumed.
$^d$ Largest value assuring numerical stability.
$^e$ Calibrated.
$^f$ From Popp and Salzer (2007b).
$^g$ Assumed equal to 0.1 (i.e., 5.7°).
$^h$ Assumed equal to $10 \times E_2$ (Mahabadi, 2012).
$^i$ Assumed equal to $E_2$ (Mahabadi, 2012).
$^j$ Assumed equal to $5 \times E_2$ (Mahabadi, 2012).
$^k$ Computed from the cohesive strength parameters, fracture energy values and penalty parameters.
Table 4.3. Comparison between the mechanical laboratory properties of the Mont Terri Opalinus Clay from Bock (2009) and the emergent macroscopic properties of the FEM/DEM-DFN model

<table>
<thead>
<tr>
<th>Macroscopic mechanical property</th>
<th>Experimental value</th>
<th>FEM/DEM-DFN result</th>
<th>Experimental value</th>
<th>FEM/DEM-DFN result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus, ( E ) (GPa)</td>
<td>3.8 ± 1.5</td>
<td>3.6</td>
<td>1.3 ± 0.7</td>
<td>1.3</td>
</tr>
<tr>
<td>Poisson’s ratio, ( \nu ) (GPa)</td>
<td>0.35</td>
<td>0.39</td>
<td>0.25</td>
<td>0.27</td>
</tr>
<tr>
<td>Uniaxial compressive strength, ( UCS ) (MPa)</td>
<td>11.6 ± 3.9</td>
<td>11.9</td>
<td>14.9 ± 5.1</td>
<td>14.0</td>
</tr>
<tr>
<td>Indirect tensile strength, ( T ) (MPa)</td>
<td>1.30</td>
<td>1.13</td>
<td>0.67</td>
<td>0.71</td>
</tr>
</tbody>
</table>

As illustrated in Fig. 4.7a, the numerical response of OPA under unconfined compressive load is characterized by substantially different failure mechanisms when loaded in the direction parallel (P) or perpendicular (S) to the bedding planes. The macroscopic failure mode of the P-sample is given by axial splitting due to fractures initiating from the tips of the DFN cracks, while the failure mode of the S-sample consists of shear fractures, propagating through the rock matrix and inclined at approximately 60°, combined with some tensile fracturing. As can be observed in Fig. 4.7b, the simulated fracture patterns are in excellent agreement with those typically observed in the laboratory.

4.4.4 Analysis of failure process

DFN orientation and anisotropy of strength

For indirect tensile loading conditions (BD model) (Fig. 4.6a), the DFN orientation effectively varies the area in which tensile strength can be mobilized. Hence, the tensile strength anisotropy ratio was

Fig. 4.5. (a) Tensile stress, \( \sigma_t \), versus platen vertical displacement for the BD P- and S-samples, (b) axial stress, \( \sigma_1 \), versus axial strain, \( \varepsilon_1 \), and lateral strain, \( \varepsilon_3 \), for the UCS P- and S-sample.
controlled by the ratio of crack length to rock bridge length in the DFN. Furthermore, numerical results show that the bedding planes tend to arrest crack propagation and off-set the fracture trajectory in the P-sample, but represent the preferred path of new tensile cracks in the S-sample.

For unconfined compressive loading conditions (UCS model) (Fig. 4.7a), the orientation of the DFN directly influences the failure mode of the specimen. In the P-sample, the tensile stress induced by the Poisson’s effect in the direction perpendicular to the maximum compressive stress, $\sigma_1$, causes the nucleation and propagation of extensile fractures from the tips of the pre-existing cracks. This observation is confirmed by the analysis of the fracture mode distribution reported in Fig. 4.8, which reveals that 51% of the UCS P-sample fractures are indeed mode I. Upon propagation of sub-vertical fractures, kinking and buckling of compressed layers can be observed with subsequent lateral ejection of rock slabs. It is noteworthy that a similar buckling failure mechanism has been observed in the laboratory during hollow cylinder experiments on OPA (Labiose, 2012) and in situ around boreholes at the Mont Terri URL (Vietor et al., 2012). In the S-sample, the macroscopic failure mechanism is given by shearing. Although mode II fracturing is predominant, a non-negligible percentage of mode I fractures (33%) is simulated. These numerical results tend to confirm the importance of extensional fracturing in the brittle failure process of samples of OPA under unconfined compression as described and experimentally verified by Amann et al. (2011).
Brittle failure process in unconfined compression

The simulated failure process of OPA in uniaxial compression can be described with reference to the critical stress levels and behaviour stages that are typical of brittle rocks (Bieniawski, 1967). According to Martin (1997), five stages can be identified: (1) closure of micro-cracks and crushing of asperities, (2) linear elastic behaviour, (3) onset of dilation and stable crack propagation, (4) unstable crack growth, and (5) brittle post-peak. The onset of linear elastic behaviour is marked by the crack closure stress threshold, $\sigma_{CC}$. The lower and upper limits of stage 3 are defined by the crack initiation and crack damage stress thresholds, $\sigma_{CI}$ and $\sigma_{CD}$, respectively, while stage 4 falls between $\sigma_{CD}$ and the UCS value. Analysis of the brittle failure process is performed on the stress-strain response of the UCS P-sample reported in Fig. 4.9 and is discussed below with reference to the five stages listed above. Note that an analogous behaviour was simulated for the S-sample.
Fig. 4.8. Relative frequency of fracture mode for the P- and S-sample at increasing confining pressures, $\sigma_3$.

Fig. 4.9. Axial stress, $\sigma_1$, versus axial strain, $\varepsilon_1$, and lateral strain, $\varepsilon_3$, for the UCS P-sample and associated count rate of yielded and failed crack elements as a function of axial strain, $\varepsilon_1$.

The presence of the low-stiffness non-linearity at low strain levels (i.e., stage 1) was first observed in OPA by Bock (2001) and is associated with the breakage of diagenetic bonds following the sample recovery process Corkum and Martin (2007b). The proposed FEM/DEM-DFN model has no means to account for this non-linear effect neither at the matrix level (i.e., continuum) nor at the bedding plane level (i.e., DFN). Since the triangular elements are assumed to follow a linear elastic behaviour and the DFN discontinuities are assumed to have zero aperture and the stiffness of the matrix, no “closure effect” can be reproduced.

The linear-elastic stage (i.e., stage 2), typically observed in samples of OPA under unconfined compression, is captured in the simulation by the elastic deformation of the rock matrix (from point O to A-A’ in Fig. 4.9).

A thorough analysis of stage 3 and 4 for UCS S-samples of OPA can be found in Amann et al.
(2011). Based on acoustic emission measurements and analysis of the stress-strain behaviour, crack initiation and crack damage thresholds were identified at 30% and approximately 70% of the rupture stress, respectively. In the simulated stress-strain response reported in Fig. 4.9, axial and lateral strains start to deviate from linearity at 70% (point A) and 55% (point A') of the UCS value, respectively. As revealed by the count rate of yielded crack elements, this loss of linearity is related to the onset of softening at the crack element level. The linearity in the lateral strain is lost first because crack elements tend to first yield in tension in the direction parallel to the maximum principal stress (i.e., mode I). Although no actual fracturing is reproduced at this stage, in the framework of the fracture model implemented in FEM/DEM, the simulated crack element softening is representative of the micro-cracking that occurs in the FPZ (Fig. 4.1). As the load is increased, the count rate of yielded crack elements increases and damage starts to accumulate in the sample resulting in a non-linear pre-peak response. Therefore, the stress level associated with point A can be interpreted as the equivalent of the crack damage stress threshold, $\sigma_{CD}$.

It is evident that the model cannot capture the stage of stable crack propagation (stage 3), between the crack initiation and crack damage thresholds, that typically causes the lateral strain and volumetric strain response to deviate from linearity at about 30-50% of the uniaxial rupture stress (Brace et al., 1966). This stage has been related to the nucleation of mode I cracks due to local tensile stress fields induced by grain-scale heterogeneities (Tapponnier and Brace, 1976). Although numerous sources of micro-scale heterogeneities have been observed in the OPA, including carbonate bioclasts, pyrite, sandy nodules and calcite veins (Klinkenberg et al., 2009), the rock matrix was assumed to be homogenous in the present study. As other micro-mechanical models of rocks have clearly demonstrated (e.g., Tang and Kaiser, 1998; Diederichs, 2000; Lan et al., 2010; Mahabadi, 2012) it is likely that the explicit incorporation of material heterogeneity into the FEM/DEM-DFN model will overcome this limitation and provide a more accurate simulation of the pre-peak brittle failure process.

Finally, as the load is further increased, the accumulated damage in the sample leads to the failure of crack elements and the sudden drop in stress (point B). This brittle post-peak response is typical of stage 5 and is characterized by the macroscopic fracture pattern depicted in Fig. 4.7a.

### 4.5 Model validation

The calibrated FEM/DEM-DFN model was validated by simulating the effect of confinement and anisotropy direction on the failure process of OPA under compressive loading. The material properties and numerical parameters obtained as a result of the calibration process were left unchanged for this validation. Biaxial loading conditions were obtained by applying a lateral pressure to the specimen boundaries. Numerical results are compared to published experimental findings on OPA and other anisotropic rocks.
Fig. 4.10. Deviatoric stress, $\sigma_1 - \sigma_3$, vs. axial strain, $\varepsilon_1$, at increasing confining pressure values, $\sigma_3$, for the (a) P-sample and (b) S-sample. Fracture patterns associated with point A to E in (a) are illustrated in Fig. 4.12.

### 4.5.1 Effect of confining pressure

**Results**

Fig. 4.10 shows the deviatoric stress, $\sigma_1 - \sigma_3$, as a function of the axial strain, $\varepsilon_1$, at increasing confining pressures, $\sigma_3$, for the P- and S-sample, respectively. For both specimens, the mobilization of friction increases the deviatoric stress at failure as the confining pressure increases. A transition from brittle to ductile post-peak behaviour can be observed at a confining pressure of approximately 7.5 MPa for both samples. This change of response corresponds well with the results of biaxial compression tests on OPA reported by Salager et al. (2010), in which a ductile post-peak was observed in S-samples for $\sigma_3 \geq 10$ MPa.

The failure modes of the P- and S-sample are depicted in Fig. 4.11a,b respectively. Under unconfined conditions ($\sigma_3 = 0$ MPa), the P-sample exhibits axial splitting and buckling of layers. As the confinement is increased ($0.5 \leq \sigma_3 \leq 1$ MPa), longitudinal fractures tend to be suppressed in favour of a well-defined shear plane inclined at about $57^\circ$ from the horizontal. For $\sigma_3 = 5$ MPa, two conjugated shear fractures can be clearly identified. For higher confinements ($\sigma_3 \geq 10$ MPa), the damage pattern consists mainly of a network of short cracks. The S-sample exhibits fracture behaviour similar to the P-sample for confinement values $\sigma_3 \geq 1$ MPa. However, for very low confinements a combination of shear and tensile fracturing is simulated without the characteristic axial splitting and buckling of layers of the P-sample. This overall variation of macroscopic fracture response as a function of the applied confinement is in agreement with the mechanisms described by Jaeger and Cook (1976) and Paterson and Wong (2004).

An example of progressive material breakdown and horizontal displacement field evolution is shown in Fig. 4.12 for the P-sample with $\sigma_3 = 15$ MPa. The appearance of the first macroscopic crack at $\varepsilon_3 = 1.5\%$ is followed by the nucleation throughout the sample of short shear cracks inclined at about
Fig. 4.11. Simulated fracture patterns of the (a) P-sample and (b) S-sample for increasing confining pressure values, $\sigma_3$. 

$\pm 50^\circ$ from the horizontal ($\varepsilon_3 = 2.5$-$3.5\%$). Further increase of applied strain ($\varepsilon_3 = 4.5$-$5.5\%$) leads to the formation of two major through-going fracture planes. The associated horizontal displacement field evolves from lateral contraction at low axial strain levels ($\varepsilon_3 < 2.5\%$) due to the applied confining pressure to lateral expansion and dilation for higher applied deformation. Also, sample barrelling becomes more evident as damage accumulates into the model.

Simulated failure envelopes of the P- and S-samples are plotted in Fig. 4.13. It is noted that for confinement values $\sigma_3 < 2$ MPa the strength of the P-sample is lower than that of the S-sample, while for $\sigma_3 \geq 2$ MPa the opposite response is simulated.

This characteristic variation of strength response is highlighted by the plot of the anisotropy parameter $K_1$, defining the ratio between the deviatoric stress at failure in the direction parallel and perpendicular to the bedding,

$$K_1 = \frac{(\sigma_1 - \sigma_3)_{//}}{(\sigma_1 - \sigma_3)_{\bot}}$$

as a function of the confinement, $\sigma_3$. As depicted in Fig. 4.14, $K_1$ increases from 0.85 to 1.15 as $\sigma_3$ increases from 0 MPa (i.e., unconfined conditions) to 20 MPa and is equal to 1 for a $\sigma_3$ value of about 2.0 MPa. This simulated behaviour is confirmed by the experimental evidence on OPA reported by Popp et al. (2008) and Bock (2009).
Lastly, the quantitative comparison between numerical failure envelopes and experimental values compiled from Popp et al. (2008) and Jahns (2010) (Fig. 4.15) indicates that the FEM/DEM-DFN models correctly reproduce the average mechanical response of P- and S- samples of OPA.

**Non-linear behaviour and brittle-ductile transition**

Overall, the results of the biaxial test models demonstrate a good agreement with published experimental findings in terms of the stress-strain response, fracture pattern, and failure envelope.

Correctly capturing the response of the material under unconfined or moderately confined conditions is crucial when assessing the near-field stability of underground excavations (Diederichs, 2003). Experimental data recently published by Amann et al. (2012), relative to biaxial tests on S-samples of OPA.

![Fig. 4.12. Fracture pattern and horizontal displacement evolution of the P-sample ($\sigma_3 = 15$ MPa) at axial strain levels corresponding to point A to E on the associated stress-strain curve of Fig. 4.10.](image)

![Fig. 4.13. Simulated failure envelopes of the (a) P-sample and (b) S-sample.](image)
OPA, show that a bi-linear or S-shaped Kaiser and Kim (2008) failure criterion should be used to correctly capture the effect of the change in fracture mechanism, from tensile to shear dominated, as the confinement increases.

Although the numerical results relative to the S-sample do not show any non-linearity over the entire range of $\sigma_3$ (Fig. 4.13), the failure envelope of the P-sample clearly exhibits a concave downwards shape

\[ \frac{\Delta \sigma_1}{\Delta \sigma_3} = \frac{1 + \sin \phi}{1 - \sin \phi} \]

This value roughly corresponds to the input value $\phi_i = 22^\circ$. 

\[ \text{Lab values (Popp et al. 2008, Jahns 2010)} \]

\[ \text{FEM/DEM-DFN model} \]
in the stress range $0 \text{ MPa} \leq \sigma_3 \leq 2.5 \text{ MPa}$. This non-linear behaviour can be explained by considering the fracture mode distribution as a function of the applied confinement (Fig. 4.8). In the P-sample, mode I fracturing, induced at low confinement by the preferably oriented DFN, contributes to the rupture of the sample. This fracturing occurs before the shear strength of the material is fully mobilized. As the confinement is increased, tensile fracturing is suppressed in favour of shearing, resulting in a linear Coulomb-type failure envelope. As illustrated in Fig. 4.16, this behaviour manifests itself as a variation of the orientation of the failed crack elements, which from sub-vertical tend to align along two inclined planes of failure. In contrast, the lower percentage of mode I fractures in the S-sample does not seem to have any notable effect on the response of the material. As a result, a Mohr-Coulomb type of behaviour is observed.

As previously discussed in Section 4.4.4, it is possible that the introduction of micro-scale heterogeneities (either in strength or in stiffness) would allow the grain-scale extensional fractures that have been associated with the brittle failure process in OPA to be captured Amann et al. (2011). Consequently, the experimentally observed non-linear strength behaviour of S-samples may also be captured.

The simulated transition of material behaviour from brittle to ductile assumes an increasing importance as the excavation depth increases. The impact of a brittle-ductile transition on the EDZ formation is two-fold. Firstly, as can be observed in Fig. 4.10, the material can sustain increasingly higher strain with increasing load bearing capacity (i.e., strain hardening). Secondly, a variation of fracture pattern, which directly affects the hydraulic properties in the EDZ, may be expected. In particular, the response of the material ceases to involve marked strain localization (i.e., brittle fracturing) in favour of a more pervasive and uniformly distributed deformation field, as shown in Fig. 4.11.
4.5.2 Effect of specimen anisotropy orientation

Results

The simulated values of uniaxial compressive strength, $UCS$, and elastic modulus, $E$, for different loading angles, $\gamma$, are plotted in Fig. 4.17a. As the loading angle increases, the $UCS$ first decreases from the P-sample value of 11.9 MPa ($UCS_P$) to a minimum value of 3.5 MPa for $\gamma = 45^\circ$, and then increases again to reach 14.0 MPa ($UCS_S$). That is, the simulated strength response exhibits the characteristic concave upwards, and parabolic in form, curve that has been typically observed in OPA (Naumann et al., 2007), other shales (McLamore and Gray, 1967; Niandou et al., 1997), and anisotropic metamorphic rocks (Donath, 1972).

The numerical results corresponding to $\gamma = 30^\circ$ show a 65% reduction in strength with respect to $UCS_P$. This reduction is in agreement with the 50 and 80% reduction observed in unconfined or moderately confined compression tests (Naumann et al., 2007; Jahns, 2010). The deformation response as a function of the anisotropy direction is characterized by a decreasing elastic modulus with the loading angle varying from the P-sample value ($E_P = 3.6$ GPa) to the S-sample value ($E_S = 1.3$ GPa). Again, this behaviour is consistent with what observed in OPA (Salager et al., 2010) and other transversely isotropic rocks (Niandou et al., 1997).

To analyze the influence of confinement on the strength anisotropy of OPA, the ratio $K_2$ of the maximum to minimum deviatoric stress at failure was calculated:

$$K_2 = \frac{(\sigma_1 - \sigma_3)_{\text{max}}}{(\sigma_1 - \sigma_3)_{\text{min}}}$$

(4.8)
As can be observed in Fig. 4.14, a decay of $K_2$ from the unconfined compression value of 4.0 is simulated for increasing confining pressures. Qualitatively, this response is consistent with experimental results of Naumann et al. (2007) for OPA and of Niandou et al. (1997) for the Tournemire Shale.

Fracture coalescence and material anisotropy

The results illustrated above further validate the numerical model beyond the cases where specimens are compressed in the direction parallel or perpendicular to the bedding planes (Section 4.4.3, 4.5.1). As expected, the modulus anisotropy follows directly from the assumed constitutive law for the triangular elements and therefore is not discussed any further. However, the strength anisotropy emerges from a complex mechanical behaviour involving the interaction of newly generated fractures and pre-existing DFN cracks (Fig. 4.18) and thereby deserves a more thorough discussion. Conventionally, the variation of strength with respect to the loading angle has been accounted for using discontinuous plane of weakness models (e.g., Jaeger and Cook, 1976; Hoek and Brown, 1980a; Duveau et al., 1998). These conventional models use separate failure criteria to independently characterize the strength of the rock matrix and of the bedding planes. In contrast, with the FEM/DEM-DFN approach, the anisotropy of strength is captured by the variation of rupture mechanism induced by the interaction of the DFN with the rock matrix. Since no clear distinction between failure of the matrix and of bedding planes is made, a smooth transition in the strength response with loading angle is reproduced (Fig. 4.17a).
For loading orientations $0^\circ \leq \theta \leq 15^\circ$, failure of the sample is induced by the extension of the bedding planes according to the process described for the UCS P-sample (Section 4.4.4). For loading orientations $75^\circ \leq \theta \leq 90^\circ$, failure occurs as a combination of shearing and extensional fracturing of the rock matrix as discussed for the UCS S-sample. For intermediate loading angles $15^\circ < \theta < 75^\circ$, a macroscopic shear failure can be observed resulting from the coalescence of the DFN cracks, which undergo mode I propagation from their tips.

This variation in behaviour can be explained using the basis of the theory of brittle failure of hard rock. According to the sliding crack model (Brace and Bombolakis, 1963; Kemeny and Cook, 1986), in a compressive stress field the surfaces of a pre-existing linear flaw tend to slide past each other inducing tensile failure of the rock at the crack tips. This initial tensile failure is followed by the propagation of two fractures, commonly referred to as wing cracks. The wing cracks initiate at an angle to the pre-existing crack and tend to align themselves in a direction parallel to the maximum principal stress. If a multitude of preferably oriented cracks are considered, such as in the FEM/DEM-DFN model, coalescence of the pre-existing cracks results in a characteristic step-path failure surface. The validity of this basic mechanism of fracture coalescence has been confirmed by several experimental and numerical studies (e.g., Bobet and Einstein, 1998; Tang and Kaiser, 1998; Tang et al., 2001; Vesga et al., 2008; Yan, 2008).

The analytical solution of the sliding crack model using linear elastic fracture mechanics principles can provide a qualitative explanation for the simulated variation of strength as a function of the DFN orientation. If failure of the specimen is assumed to be controlled by mode I crack initiation from the tips of pre-existing flaws, the strength of the specimen is ultimately dependent upon the mode I stress intensity factor, $K_I$, and the fracture toughness of the material, $K_{IC}$. Fig. 4.17b shows the variation of $K_I$ as a function of the pre-existing flaw angle, $\gamma$, calculated according to the solution of Horii and Nemat-Nasser (1986) for the case of a ratio of wing crack length to flaw length, $l/c$, equal to 0.01 and zero friction. It can be noticed that the variation of $K_I$ with $\gamma$ follows a curve that is approximately symmetric (with respect to the horizontal axis) of the UCS curve illustrated in Fig. 4.17a. Hence, being that the fracture toughness of the rock matrix is constant, flaw orientations (i.e., DFN) associated with higher $K_I$ values are characterized by tensile crack propagation at lower compressive stress levels therefore resulting in lower UCS values of the specimen.

As shown in Fig. 4.18b, the introduction of confinement strongly affects the failure mode of the inclined samples and consequently the mechanism by which the strength anisotropy is captured by the FEM/DEM-DFN model. As described above, under unconfined compressive loading conditions, the strength anisotropy is dictated by the formation of wing cracks followed by tension-type fracture coalescence. However, under biaxial loading, tensile fracturing is suppressed and the coalescence of the DFN cracks is due to internal shearing. Therefore, as the confinement is increased, the simulated strength anisotropy is governed by the reduced shear strength that can be mobilized in the direction parallel to layering along the cohesion-less DFN discontinuities.
4.6 Mesh sensitivity of the FEM/DEM model

The sensitivity of a FEM/DEM model to the mesh element size and edge orientation arises from the assumptions inherent in the adopted cohesive crack model (Section 4.3.2). To accurately represent the bonding stress close to the crack tip, the element size must be much smaller than the length of the FPZ (Fig. 4.1), defined as the distance from the crack tip to the point where the maximum cohesive strength (i.e., $f_t$ or $f_s$) is attained (Munjiza and John, 2002). The length of the FPZ, $l_{FPZ}$, can be analytically estimated using the following relationship valid for mode I fracturing (Hillerborg et al., 1976):

$$l_{FPZ} = \frac{E}{f_t}$$

Using the parameters reported in Table 4.2 for OPA, $l_{FPZ}$ values of 22 and 64 mm are calculated for $E = E_1$ and $E = E_2$, respectively. Although the exact minimum number of cohesive elements required in the FPZ is not well established, 3-10 elements have generally provided accurate results (Turon et al., 2007). Therefore, the adopted average element size of 0.3 mm, which results in at least 73 elements distributed in the FPZ, should provide an accurate representation of the stress and strain field in the vicinity of crack tips.

However, the simulated failure process of OPA samples in compression is due to a combination of mode I and mode II fracturing together with multiple interactions between newly-created and pre-existing discontinuities. That is, the simulated failure conditions are more complex than the pure opening mode upon which the above discussion is based. Therefore, the element size sensitivity of the FEM/DEM model was further investigated by simulating the response of the UCS P-sample for mesh refinements ranging between 0.2 and 0.4 mm. As shown in Fig. 4.19, the peak strength appears to converge with decreasing element size, which is in agreement with the previous theoretical analysis. Due to excessively long run times, it was not possible to simulate mesh resolutions finer than 0.20 mm. The adoption of smaller element size not only results in a rapid growth of the total number of elements (Fig. 4.19) but also requires smaller time step sizes to satisfy the stability condition of the explicit time integration scheme of FEM/DEM. Conversely, element sizes greater than 0.40 mm could not be used due to the adopted average spacing value of the DFN cracks (1.0 mm).
The mesh topology sensitivity of the cohesive element approach results from the restriction of crack nucleation and growth to the edges of the triangular elements. Although this approach aims at simulating fracturing without any a priori assumption regarding the fracture trajectory, a certain mesh bias is induced by the fact that the direction of crack propagation is not entirely free but restricted to a limited number of predefined angles. To minimize the constraint imposed by the mesh topology on the model behaviour, randomly discretized meshes should be used in place of regularly discretized ones (Tijssens et al., 2000; Mahabadi, 2012). Following this recommendation, an unstructured Delaunay triangulation scheme (Fig. 4.20) was used for all models in the current study.

Fig. 4.21 shows the relative frequency of crack element orientation for the UCS P, S, and Z \((h = 45^\circ)\) models. A spike in the orientation distribution is associated with the bedding plane orientation, \(\gamma\), due to crack elements preferably aligned along the DFN cracks. Also, two symmetric peaks can be observed at approximately \(\gamma \pm 60^\circ\) due to the adoption throughout the model of a uniform crack element size with triangles tending to an equilateral shape.

The spatial discretization sensitivity of FEM/DEM and, in general, of all DEM models represents a major obstacle in their application to engineering-scale models (e.g., simulation of EDZ). For the case

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**Fig. 4.20.** Zoomed-in views of the center the UCS simulation for the (a) P-sample, (b) Z-sample \((h = 45^\circ)\), and (c) S-sample, showing the triangular mesh topology, the distribution of pre-existing cracks (DFN) aligned with the bedding plane orientation and several broken crack elements.

**Fig. 4.21.** Relative frequency of crack element orientation for the UCS (a) P-sample, (b) Z-sample \((45^\circ)\), and (c) S-sample.
of the FEM/DEM-DFN model proposed in this study, the issue is two-fold: (i) element size and (ii) DFN geometry.

As discussed above, a millimetre (or sub-millimetre) element size should be used to correctly capture the mechanical response of the rock material. If such a fine spatial discretization were applied to a model with the size of tens of meters, the total number of triangular and crack elements and associated variables would result in an excessive computational demand. Although increases in computing power have been recently achieved and DEM simulations of entire boundary-values problems attempted (Potyondy and Cundall, 2004), the use of this spatial resolution in a large-scale FEM/DEM model is not feasible at the present time. Therefore, further research is needed to reduce the computational requirements of field-scale FEM/DEM simulations by adopting, for example, a continuum-discontinuum approach, whereby only a small-sized region of interest is treated as a FEM/DEM medium whereas the remainder of the domain is modelled as an elastic, non-fracturing medium.

The simulation of strength anisotropy relies upon a closely spaced distribution of short cracks (Table 4.1). If coarser meshes were to be adopted in the attempt of minimizing the degrees of freedom of the simulation, larger crack spacing and length values will necessarily have to be used. Therefore, the variation of rock representative volume for which the mechanical anisotropy is correctly preserved as the model is up-scaled requires further investigation.

4.7 Summary and conclusions

A new modelling approach for anisotropic rocks was developed based on the combined finite-discrete element method (FEM/DEM) (Munjiza, 2004). In particular, a transversely isotropic elastic constitutive law was implemented in the Y-Geo FEM/DEM code (Mahabadi, 2012) and a procedure to populate the model with a distribution of preferably oriented fractures was developed. It was shown that the proposed approach is able to capture both the stiffness and strength anisotropy that are typical of layered materials.

The said approach was then applied to the laboratory-scale study of the mechanical behavior of Opalinus Clay, an over-consolidated clay shale formation selected to host an underground nuclear waste repository in Switzerland. The model was quantitatively calibrated and validated using experimental values of standard rock mechanics tests.

Following the calibration procedure, a strong agreement between experimentally derived and modeled uniaxial compression test and indirect tension test results was obtained for specimens loaded parallel and perpendicular to layering. Furthermore, a distinctively different crack pattern and failure mechanism was observed for each loading configuration. The simulated stress-strain response exhibited some of the characteristics typically observed in brittle materials, including loss of linearity due to sample damage and post-peak softening.

The effect of confinement on the mechanical behaviour of Opalinus Clay was studied using biaxial compression test models. The simulated failure envelopes corresponded well with the average experimental response of the rock. A characteristic non-linear behaviour was captured for samples loaded in the direction parallel to the bedding at very low confinements due to the transition of the failure mech-
anism from tensile to shear dominated. A transition from brittle to ductile post-peak behaviour was simulated at a confining pressure of about 7.5 MPa.

A distinctive variation of specimen compressive strength, crack pattern and damage mechanism, was captured as a function of the orientation of specimen anisotropy. These emergent properties of the model were shown to be in good agreement with published experimental findings and were discussed in the context of the theory of brittle failure of rock.

The results presented in this paper represent the first necessary step of a broader-scope project that involves using the FEM/DEM numerical tool to aid in the design of a deep geological repository for nuclear waste in Switzerland. Simulated fracture patterns indicate that the model has the potential to reproduce the EDZ formation mechanisms observed at the Mont Terri URL.
Chapter 5

Numerical analysis of failure mechanisms around unsupported circular excavations in clay shales

This chapter has been submitted to the International Journal of Rock Mechanics and Mining Sciences: Lisjak, A., Grasselli, G., and Vietor, T. Continuum-discontinuum analysis of failure mechanisms around unsupported circular excavations in anisotropic clay shales.

Abstract

The stability of circular excavations in clay shales is a key issue in the drilling and tunnelling industries as well as in the field of deep geological waste storage. A large body of experimental evidence indicates that the damaged zone around these cavities is influenced by strong mechanical anisotropy induced by the layered material structure. The vast majority of numerical models adopted to date to analyze the stability of openings in layered rocks have been based on continuum mechanics principles using classic shear failure theory for elasto-plastic materials. However, a number of experimental observations demonstrate that clay shales may fail in a brittle manner under low-confinement conditions such as those characterizing the near-field of the excavation. Therefore, an alternative numerical approach based on non-linear fracture mechanics principles and the discrete element method is adopted to gain new insight into the failure process of this class of geomaterials. In order to account for the influence of clay shale microstructure on its mechanical behaviour a newly-developed approach to capture the anisotropy of strength is proposed. With this numerical approach, the cohesive strength parameters of the fracture model are assumed to be a function of the relative orientation between the element bonds and the layering orientation. The effectiveness of the numerical technique is quantitatively demonstrated by simulating standard rock mechanics tests on an indurated claystone, namely Opalinus Clay. Emergent strength and deformation properties, together with the simulated fracture mechanisms, are shown to be in good agreement with experimental observations. The modelling technique is then applied to
the simulation of the Excavation Damaged Zone (EDZ) around a circular tunnel in horizontally bedded Opalinus Clay. The simulated fracturing process is mainly discussed in the context of the damage mechanisms observed at the Mont Terri URL. Furthermore, the influence of in situ stress on resulting EDZ geometry is analyzed together with possible implications for ground support and tunnel constructability. Modelling results highlight the importance of shear strength mobilization along bedding planes in controlling the EDZ formation process. In particular, slippage of bedding planes is shown to cause rock mass deconfinement which in turn promotes brittle failure processes in the form of spalling. The numerical technique is currently limited to two-dimensional analyses without any thermo-hydro-mechanical coupling.

5.1 Introduction

The stability of underground openings in clay shales is an issue of particular interest for a number of geo-engineering applications, including the geological disposal of nuclear waste, the drilling industry, and the construction of tunnels at depth. Shale formations are currently being assessed as host rocks for the underground storage of solid radioactive waste as they present favourable long-term isolation properties (IAEA, 2003). These properties include: low permeability, good radionuclide retention properties, geological stability over long time periods, and self-sealing capacity. However, one main concern is that these isolation properties may be negatively affected by the rock mass damage associated with the excavations comprising the underground repository, namely the Excavation Damaged Zone (EDZ). In the oil and gas industry, the stability of boreholes is a long-standing problem which results in substantial yearly expenditure (Bradley, 1979). In the presence of instabilities, drilling and production are impacted by several additional costs in the form of time and equipment losses, washouts, problematic logging, and sidetracking (Gazaniol et al., 1995). Depending on the depth and well trajectory, these problems are generally further aggravated when drilling through shales due to their particular geomechanical properties. Finally, construction and ground support difficulties have been reported when excavating road or hydroelectric tunnels in shale formations (Perras and Diederichs, 2009).

The mechanical behaviour of shales is heavily influenced by strong stiffness and strength anisotropy which arises at different spatial scales within the rock. At the mineral scale, textural anisotropy is due to the laminated material microstructure, which consists of preferably-oriented platy clay minerals resulting from the rock formation process (Wenk et al., 2008). At a slightly larger scale, the presence of schistosity, foliation or bedding planes marking the limits of strata further contribute to induce directionality in the rock mechanical response. At the rock mass level, anisotropy can be related to the presence of physical discontinuities such as joints, fractures and tectonic structures.

The mechanical anisotropy of shale specimens has been widely documented by several laboratory studies (McLamore and Gray, 1967; Naumann et al., 2007; Niandou et al., 1997), which typically report a distinctive variation of elastic response, strength characteristics and failure mechanisms with sample layering orientation. At a larger scale, this particular behaviour directly affects the stability of underground structures and the observed failure behaviour. Field observations from the Mont Terri URL
situated in an indurated, overconsolidated clay shale, namely Opalinus Clay, indicate that the shape and extent of the EDZ around tunnels as well as stand-up times are dependent upon the relative orientation between bedding planes and the excavation axis (Bossart et al., 2002). The most unfavourable conditions are encountered when excavating in the direction parallel to the bedding plane strike due to development of delamination mechanisms (e.g., shearing, bending and buckling of layers) in response to the excavation-induced stress redistribution (Blümling et al. (2007); Marschall et al. (2006) (Fig. 5.1). Similarly, several examples of premature borehole collapse have been reported in extended reach and horizontal wells in shale formations with pronounced bedding (Gazaniol et al., 1995; Økland and Cook, 1998; Ong and Roegiers, 1993). Due to the low strength properties of the bedding planes, enhanced instabilities have been observed with failure patterns far more extensive than those predictable under isotropic material conditions (Willson et al., 1999).

Furthermore, several experimental observations clearly indicate that shales may fail in a brittle manner under low-confinement conditions such as those characterizing the near-field of underground openings. For example, a recent laboratory study indicated that the mechanical behaviour of Opalinus Clay under unconfined compression exhibits several features of the failure process of brittle rocks such as staged stress-strain response, strong strain localization and acoustic activity (Amann et al., 2011). These laboratory findings are corroborated by numerous field observations relative to macroscopic extensional fractures (i.e., spalling) in the EDZ of tunnels in argillaceous rocks (Fig. 5.2) (Blümling et al., 2007; Bossart et al., 2002; Millard et al., 2009; Yong et al., 2010). Therefore, an alternative numerical approach based on non-linear fracture mechanics principles, namely the combined finite-discrete element method (FEM/DEM) (Mahabadi, 2012; Munjiza, 2004), was adopted in this study to gain new insight into the failure process around excavations in shales. The technique is, at present, limited to purely mechanical two-dimensional analyses.

The paper is organized as follows. In Section 5.2, a brief overview of the main modelling techniques for anisotropic rocks is provided. In particular, differences between material representation types (i.e., continuum versus discontinuum) are highlighted. In Section 5.3, the fundamental principles of FEM/
5.2 Overview of modelling techniques for layered rocks

The numerical approaches for modelling the mechanical behaviour of layered rocks can be classified according to the type of material representation, as (i) equivalent continuum methods and (ii) discrete element methods (DEM).

With the continuum method, the presence of layers is smeared to produce a fictitious continuous material that exhibits mechanical characteristics that are similar to the original discontinuous medium. While the layering-induced directionality of deformation properties is commonly captured using the theory of elasticity for transversely isotropic materials (Jaeger and Cook, 1976), the treatment of strength anisotropy is sensibly more complex. To evaluate the slip zones around excavations in layered rock masses, a technique often adopted in practice involves calculating a strength factor using an elastic stress-strain analysis together with an ubiquitous distribution of joints characterized by reduced frictional properties (Daemen, 1983; Kumar, 1997). Although this simplified approach can give a good indication of failure development, slippage along bedding planes leads in reality to a stress redistribution which is not accounted for by the elastic model (Tonon and Amadei, 2003). This limitation can be overcome by introducing a failure criterion for anisotropic rocks within elasto-plastic models. Among
these failure criteria, the most common is arguably the discontinuous plane of weakness model (Duveau et al., 1998; Hoek and Brown, 1980a; Jaeger, 1960; Tien and Kuo, 2001), which assumes that shearing along bedding planes and failure of the intact rock matrix are independently characterized. To fully capture the main features of the progressive breakdown of anisotropic rocks, including mechanical degradation, dilatancy, stiffness non-linearity and post-peak softening or hardening, more advanced models have been developed by directly assuming a continuous variation of strength within the continuum mathematical formulation of plasticity for anisotropic solids (Corkum and Martin, 2007b; François et al., 2011; Pietruszczak et al., 2002; Salager et al., 2013). Finally, to overcome some of the limitations of standard continuum formulations when simulating strain localization of brittle materials (e.g., mesh-dependency, ill-posed problems), enriched continuum formulations with microstructural effects (Adhikary and Guo, 2002; Collin et al., 2006; Riahi and Curran, 2009) or statistical damage models (Jia and Tang, 2008) have been proposed.

With the DEM approach, layers or joints are explicitly represented in the numerical model. The medium is modelled as an assembly of rigid or deformable blocks or particles with interaction laws governing the emergent behaviour of the rock. Numerical investigations of the effect of layering in preferably jointed sedimentary rock masses have been carried using both implicit and explicit DEM codes such as the Discontinuous Deformation Analysis (DDA) method and the Universal Distinct Element Code (UDEC) (Bakun-Mazor et al., 2009; Perras and Diederichs, 2010). The main advantage of these techniques is the ability to readily account for the presence of rock mass discontinuities and to capture large displacements and rigid block rotations that typically characterize the failure of jointed rock masses. Furthermore, bonded-particle models have been employed to analyze the progressive failure of brittle foliated and bedded rocks (Konietzky et al., 2003; Wanne, 2002) and to simulate the EDZ around emplacement tunnels for nuclear waste storage (Potyondy and Cundall, 2000). Although the large computational demand tends to limit their applicability to problems at the scale of rock samples, micromechanics-based DEM approaches may offer unique advantages when the extended loss of continuity inside the material, for instance due to the progressive breakdown, makes continuum constitutive models inappropriate.

The combined finite-discrete element method (Mahabadi, 2012; Munjiza, 2004) adopted for this study is a particular type of hybrid approach whereby the elastic deformation of the material is described by continuum mechanics theory while DEM algorithms and non-linear fracture mechanics principles are employed to capture damage mechanisms that are typical of quasi-brittle geomaterials. Original applications of FEM/DEM to the simulation of layered materials can be found in Stefanizzi (2007) and Lisjak et al. (2013c) (see Chapter 4).

5.3 Fundamental principles of FEM/DEM

The combined finite/discrete element method (FEM/DEM) is a numerical method which combines continuum mechanics principles with DEM algorithms to simulate multiple interacting deformable solids (Munjiza et al., 1995). More specifically, the elastic deformation of discrete bodies and the nucleation
of new fractures is described using techniques traditionally employed in continuum finite element (FE) analysis, while the interaction of discrete bodies is captured by discrete element (DE) analysis. For this study, a two-dimensional FEM/DEM code, known as Y-Geo (Mahabadi et al., 2012a), was used. This code represents an extension of the original Y2D code of Munjiza (2004) and is undergoing development at the University of Toronto for rock mechanics applications.

5.3.1 Governing equations

In FEM/DEM, each solid is discretized as a mesh consisting of nodes and triangular elements. An explicit second-order finite-difference integration scheme is applied to solve the equations of motion for the discretized system and to update the nodal coordinates at each simulation time step. In general, the governing equations can be expressed as (Munjiza et al., 1995):

$$\mathbf{M} \frac{\partial^2 \mathbf{x}}{\partial t^2} + \mathbf{C} \frac{\partial \mathbf{x}}{\partial t} + \mathbf{F}_{int}(\mathbf{x}) - \mathbf{F}_{ext}(\mathbf{x}) - \mathbf{F}_c(\mathbf{x}) = 0$$

(5.1)

where $\mathbf{M}$ and $\mathbf{C}$ are the system mass and damping diagonal matrices, respectively; $\mathbf{x}$ is the vector of nodal displacements; $\mathbf{F}_{int}$, $\mathbf{F}_{ext}$ and $\mathbf{F}_c$ are the vectors of internal resisting forces, of applied external loads and of contact forces, respectively.

Numerical damping is introduced in the governing equation to account for energy dissipation due to non-linear material behaviour or to model quasi-static phenomena by dynamic relaxation (Munjiza, 2004). The matrix $\mathbf{C}$ is equal to:

$$\mathbf{C} = \mu \mathbf{I}$$

(5.2)

where $\mu$ is a constant damping coefficient and $\mathbf{I}$ is the identity matrix.

Contact forces, $\mathbf{F}_c$, are calculated either between contacting discrete bodies or along internal discontinuities (i.e., pre-existing or newly created fractures). In the normal direction, body impenetrability is enforced using a penalty method (Munjiza and Andrews, 2000), while in the tangential direction, discontinuity frictional behaviour is captured by a Coulomb-type friction law (Mahabadi et al., 2012a). Internal resisting forces, $\mathbf{F}_{int}$, include the contribution from the elastic forces, $\mathbf{F}_e$, and the crack element bonding forces, $\mathbf{F}_b$, which are used to simulate material elastic deformation and progressive failure, respectively, as further explained in the next section.

5.3.2 Material deformation and failure

The progressive failure of rock material is modelled using a cohesive-zone approach, a technique first introduced in the context of the elasto-plastic fracturing of ductile metals (Barenblatt, 1962; Dugdale, 1960). This approach aims at capturing the non-linear interdependence between stresses and strain that characterizes the zone ahead of a macro-crack tip known as the Fracture Process Zone (FPZ). As depicted in Fig. 5.3, the FPZ in brittle rocks manifests itself in the form of micro-cracking and interlocking related to the presence of micro-scale inhomogeneities (e.g., mineral grains and pre-existing defects or voids) (Labuz et al., 1987). When using cohesive-zone models, the failure of the material
proceeds based solely on the strength degradation of dedicated interface elements (referred herein to as crack elements) and therefore emerges as a natural outcome of the deformation process without employing any additional macroscopic failure criterion. Since the material strain is expected to be localized in the cohesive zone, the bulk material (i.e., the continuum, or unfractured, portion of the model) is treated as linear-elastic using constant-strain triangular elements.

In the Y-Geo FEM/DEM code, the bonding stresses transferred by the material are decreasing functions of the displacement discontinuity across the crack elements according to the cohesive laws illustrated in Fig. 5.4. These constitutive relationships represent a modified version of the crack model response proposed by Munjiza et al. (1999). Mode I (i.e., opening) fracturing is simulated by a cohesive model based on the FPZ model originally developed for concrete by Hillerborg under the name of fictitious crack model (Hillerborg et al., 1976) (Fig. 5.4a). A fracture is assumed to initiate when the crack tip opening, $o$, reaches a critical value, $o_p$, related to the intrinsic tensile strength of the material, $f_t$. When the crack opens, the normal bonding stress, $\sigma$, is not assumed to fall to zero at once, but to

---

**Fig. 5.3.** Cohesive-zone approach for material failure modelling in FEM/DEM. (a) Conceptual model of a tensile crack in a heterogeneous rock material (after Labuz et al. (1987), modified). (b) Theoretical FPZ model of Hillerborg (Hillerborg et al., 1976). (c) FEM/DEM implementation of the FPZ using triangular elastic elements and four-noded crack elements to represent the bulk material and the fracture, respectively. Triangular elements are shrunk for illustration purposes.
Constitutive behaviour of the crack elements. (a) FPZ model for mode I. (b) Slip-weakening model for mode II. In theory no separation/slip occurs until the tensile/shear strength is reached; however, in the actual implementation a penalty function method is used to enforce material continuity. The shape of the cohesive strain-softening curves is based upon experimental curves obtained for concrete in direct tension (Evans and Marathe, 1968; Munjiza et al., 1999). (c) Graphical representation of the coupling relationship between crack opening, $o$, and crack slip, $s$, for mixed-mode fracturing (Eq. 5.5).

decrease with increasing crack opening until a residual opening value, $o_r$, is reached and a stress-free surface is created (i.e., $\sigma = 0$). Mode II (i.e., shear) fracturing is simulated by a slip-weakening model conceptually similar to that of Ida (1972) (Fig. 5.4b). Similarly to what is depicted in Fig. 5.3b for tensile loading conditions, a tangential bonding stress, $\tau$, exists between the two fracture walls, which is a function of the amount of slip, $s$, and the normal stress on the fracture, $\sigma_n$. The critical slip, $s_p$, corresponds to the intrinsic shear strength of the rock, $f_s$, defined as

$$f_s = c + \sigma_n \cdot \tan \phi_i,$$

where $c$ is the internal cohesion, $\phi_i$ is the material internal friction angle, and $\sigma_n$ is the normal stress acting across the crack element. Upon undergoing the critical slip, $s_p$, the tangential bonding stress is gradually reduced to a residual value, $f_r$, which corresponds to a purely frictional resistance

$$f_r = \sigma_n \cdot \tan \phi_f,$$

where $\phi_f$ is the fracture friction angle and $\sigma_n$ is the normal stress acting across the fracture surfaces. In the current crack element implementation, the unloading path in the softening branch coincides with the loading path. Therefore, the model is strictly only valid for monotonic loading conditions.

For mixed mode fracturing, the rupture of a crack element is defined by the following coupling criterion between crack opening and slip (Fig. 5.4c):

$$\left( \frac{o - o_p}{o_r - o_p} \right)^2 + \left( \frac{s - s_p}{s_r - s_p} \right)^2 \geq 1.$$
The mode of fracture, \( m \), associated to a broken crack element can be approximated as:

\[
 m = 1 + \frac{s - s_p}{s_r - s_p}
\]

The external energy required to fully break a unit surface area of cohesive crack corresponds to the input specific fracture energy, \( G_c \). \( G_c \) is defined in terms of the material properties \( G_{Ic} \) and \( G_{IIc} \) which correspond to the strain energy release rates for mode I and mode II fracturing, respectively. The crack residual displacement values, \( o_r \) and \( s_r \), are such that:

\[
 G_{Ic} = \int_{o_p}^{o_o} \sigma(o)do
\]

\[
 G_{IIc} = \int_{s_p}^{s_r} [\tau(s) - f_r]ds
\]

Following an approach similar to that pioneered by Xu and Needleman (1994), the crack elements in FEM/DEM are interspersed throughout the material (i.e., across the edges of all triangular element pairs) from the very beginning of the simulation. Thus, cracks are allowed to nucleate and grow without any additional assumption or criterion other than the crack element constitutive response. Upon breakage of the cohesive surface, the crack element is removed from the simulation and therefore the model locally transitions from a continuum to a discontinuum. The newly created discontinuity is treated by the contact algorithm through the contact forces, \( F_c \), briefly described in the previous section. As the simulation progresses, finite displacements and rotations of discrete bodies are allowed and new contacts are automatically recognized.

### 5.4 Modelling material anisotropy in FEM/DEM

As part of this research project, the capabilities of the two-dimensional Y-Geo code were extended such that the mechanical response of shales could be simulated. In particular, the cohesive fracture model illustrated in Section 5.3.2 was modified to account for directionality of the strength properties. Details of the adopted approach are described in the following subsections. The validation, mesh sensitivity, and application of the approach to a field-scale problem are presented in Sections 5.5, 5.6, and 5.7, respectively.

#### 5.4.1 Elastic behaviour

Several anisotropic rocks (e.g., schists, sandstones, shales, basalts, etc.) are typically described as transverse isotropic bodies (Amadei, 1996). That is, the deformability of these materials show isotropic properties within a plane, called the plane of transverse isotropy, that is normal to an axis of rotational symmetry (Fig. 5.5a). For shales, the plane of transverse isotropy is assumed to be parallel to the bedding planes. Therefore, a stress-strain constitutive law for a linearly elastic, transversely isotropic medium was adopted in this study. With this model, the elastic deformation is fully characterized by
five independent elastic constants (Jaeger and Cook, 1976):

- $E$ and $E'$ are the Young’s moduli in the direction parallel and perpendicular to the plane of transverse isotropy, respectively;
- $\nu$ and $\nu'$ are the Poisson’s ratios that characterize the transverse strain in the plane of isotropy due to a stress applied in the direction parallel and perpendicular to it, respectively;
- $G'$ is the shear modulus for planes normal to the plane of transverse isotropy.

The naming convention of Fig. 5.5b is used in the present work to identify standard laboratory samples according to the relative orientation between the isotropic plane and the loading direction. The loading angle, $\theta$, is related to the bedding dip, $\psi$, by:

$$\psi = 90^\circ - \theta.$$  \hspace{1cm} (5.9)

For the vast majority of anisotropic rocks, higher stiffness values are associated with the direction parallel to the plane of isotropy (i.e., P-sample), with the degree of elastic anisotropy,

$$k = \frac{E}{E'},$$  \hspace{1cm} (5.10)

commonly ranging between 1 and 4 (Amadei et al., 1987).

In general, the elastic response of a FEM/DEM model depends not only on the constitutive relationship of the triangular elements but also on the properties of the crack elements. Since the elastic deformation before the onset of fracturing takes place in the bulk material, no deformation should in
theory occur in the crack elements before the intrinsic strength is exceeded. However, a finite stiffness is required for the crack elements by the time-explicit formulation of FEM/DEM. Such an artificial compliance is represented by the normal, tangential and fracture penalty values, $p_n$, $p_t$ and $p_f$, for compressive, shear and tensile loading conditions, respectively. For practical purposes, the contribution of crack elements to the overall model compliance can be largely limited by adopting very high (i.e., dummy) penalty values (Mahabadi et al., 2012a; Munjiza, 2004). Consequently, no anisotropy in deformation is introduced in the penalty formulation at the crack element level and the elastic response is effectively controlled by the choice of the stress-strain relationship of the continuum triangular elements.

5.4.2 Anisotropy of strength

A number of experimental studies indicate a strong influence of textural anisotropy not only on the deformation response but also on the tensile (Bock, 2009; Liao et al., 1997; Nova and Zaninetti, 1990) as well as compressive (Donath, 1972; Hoek and Brown, 1980a; McLamore and Gray, 1967; Niandou et al., 1997; Popp and Salzer, 2007a) strength of layered materials. The compressive strength generally exhibits a maximum value for configurations in which the loading direction is either perpendicular (i.e., S-sample) or, in certain cases, parallel (i.e., P-sample) to the plane of transverse isotropy. The minimum compressive strength is typically obtained for sample orientations, $\theta$, ranging between 30 and 60°. This directional dependence is associated with the different deformation mechanisms and failure modes that occur depending on the relative orientation between load and plane of isotropy.

Two techniques, referred herein to as the discrete and smeared approach, can be used to capture strength anisotropy in a FEM/DEM model. The discrete approach was originally introduced by Lisjak et al. (2013c) (see Chapter 4) to reproduce the short-term response of the Opalinus Clay observed during standard rock mechanics tests. Motivated by the inability of this approach to correctly capture the delamination observed around large-scale excavations, a new smeared approach was developed for this study, as further described in the following subsections.

Discrete approach

With the discrete approach, the anisotropy of strength emerges as a natural property of an isotropic, homogeneous medium containing a distribution of finite-sized, cohesion-less fractures aligned with the plane of isotropy. As depicted in Fig. 5.6a, macroscopic shear failure along the layering direction, responsible for the reduced strength of Z-samples, is captured as a step-path surface resulting from the coalescence of the pre-existing cracks, which undergo tensile propagation from their tips. The strength of the sample is ultimately controlled by the tensile strength of the intact material, $f_t$, and the fracture set topology (i.e., spacing, length, bridge length) (Lisjak et al., 2013c, see Chapter 4). For this model, the variation of strength as a function of the layering orientation can be analytically explained by the so-called sliding crack models (Fig. 5.6b), proposed in linear elastic fracture mechanics to analyze the onset of extensile fracturing induced by the presence of a linear flaw in a compressive stress regime (Horii and Nemat-Nasser, 1986).
Fig. 5.6. Discrete approach for modelling strength anisotropy in FEM/DEM. (a) Simulated fracture pattern of a UCS Z-sample ($\theta = 45^\circ$). (b) Schematics of a sliding crack model showing wing cracks nucleating from a pre-existing linear defect and associated geometric parameters. (c) Rosette plot of the relative distribution of failed crack elements orientation showing also the inclination of the bedding planes and of the macroscopic failure plane.

The simulated coalescence of pre-existing cracks can be interpreted as a micro-mechanical analogue of the damage process typically observed in foliated rocks (e.g., gneiss). For these rocks, microstructural observations indicate that the strength anisotropy is induced by crack growth around biotite grains favorably oriented for frictional slip (Rawling et al., 2002). Shear deformation on cleavage surfaces in biotite grains causes a stress concentration at the end of the grain, which is relieved by tensile fracturing. Eventually, the mutual interaction of the stress fields of multiple wing cracks leads to macroscopic shear localization (Baud et al., 2005). In shales, a similar effect may be attributed to the presence of preferentially oriented microcracks, high aspect ratio voids or carbonate grains (Renner et al., 2000; Klinkenberg et al., 2009).

Since macroscopic shearing is due to linkage of a number of individual fractures whose individual growth direction does not coincide with the final fault orientation (Fig. 5.6c), with the discrete approach the simulated failure plane is generally steeper than the bedding plane orientation and delamination of bedding planes cannot be captured. This behaviour is further aggravated in field-scale models, where layer spacing values on the order of tens of centimetres must be used due to computational constraints on the mesh resolution. The results of preliminary application of the discrete approach to the simulation of the EDZ around a tunnel in a horizontally bedded shale are summarized in the conceptual model of Fig. 5.7. At this scale, the crack coalescence mechanism cannot capture the slip zones parallel to weaker, critically oriented, bedding planes. As further discussed in Section 5.7, a correct simulation of bedding plane delamination is fundamental to reproduce the fracture patterns typically observed in the field (Fig. 5.1).
CHAPTER 5. ANALYSIS OF FAILURE MECHANISMS AROUND EXCAVATIONS IN SHALES

Smeared approach

In the smeared approach, it is assumed that the macroscopically observed strength anisotropy is induced by a similar anisotropy at the crack element level. Hence, directionality is directly introduced in the fracture model by imposing that the cohesive strength of each crack element is a function of the relative orientation, $\gamma$, between the crack element itself and the bedding orientation (Fig. 5.8a). In particular, the cohesive strength parameters, $f_t$, $c$, $G_{Ic}$, and $G_{IIc}$, assume maximum and minimum values, for $\gamma = 0^\circ$ and $\gamma = 90^\circ$, respectively. A simple linear variation with $\gamma$ between the minimum and maximum value is assumed for each of the above parameters, while the friction angle, $\phi$, is kept constant. Furthermore, to fully capture the bedding plane delamination process described above, the mesh topology must combine a random triangulation for the intra-layer material (i.e., matrix) together with crack elements preferably aligned along the bedding planes (Fig. 5.8b). Further discussion on the mesh sensitivity of the approach is provided in Section 5.6.

5.5 Laboratory-scale simulations

The FEM/DEM models were calibrated to match averaged values obtained through highly controlled unconfined compression tests and indirect tension (Brazilian) tests on the shaly facies of the Mont Terri Opalinus Clay (Bock, 2009). These laboratory results are the same as those employed by Lisjak et al. (2013c) (see Chapter 4) for the calibration of a FEM/DEM model based on the discrete representation of strength anisotropy. The model boundary conditions, input parameters, and results are discussed in the following subsections.

5.5.1 Model description

The two-dimensional laboratory-scale models included a $35 \times 17.5$ mm rectangular specimens for the compression test and $30$ mm diameter circular specimens for the Brazilian test. All the specimen cross-sections were assumed parallel to the $xy$ plane (Fig. 5.5) and, therefore, oriented perpendicular to the strike of the bedding planes. Layering orientation within a particular FEM/DEM model was then set by
specifying the bedding dip, $\psi$.

The specimens were meshed with a uniform, unstructured grid having $h = 0.3$ mm average element edge length and embedded layers with thickness $t = 1.0$ mm (Fig. 5.8b). The equation of motion for the discretized system (Eq. (5.1)) was integrated with a time step of $3 \times 10^{-6}$ ms; this value was the largest time step size that ensured numerical stability for the explicit time integration scheme of the code. Uniaxial loading conditions were obtained by means of two rigid platens moving in opposite directions with a constant velocity $v = 0.05$ m/s. Although this loading rate is significantly greater than that typically used in actual experiments, a preliminary loading rate sensitivity analysis (Fig. 5.9) indicated that the simulated strengths approached constant values for loading rates smaller than approximately 0.25 m/s. The FEM/DEM Graphical User Interface Y-GUI (Mahabadi et al., 2010b) was used to assign boundary conditions and material properties to the model.

**5.5.2 Model calibration and input parameters**

Similarly to other modelling approaches based on DEM (Potyondy and Cundall, 2004), the micromechanical input parameters of the FEM/DEM simulations were calibrated by comparing the emergent properties of the model to the relevant response of the tested rock.

To this end, an iterative, trial-and-error calibration procedure was adopted. The indirect tensile strength, $T$, and the uniaxial compressive strength, $UCS$, were chosen to characterize the short-term, undrained mechanical response of Opalinus Clay and used as calibration targets. Since both macroscopic properties exhibit a strong dependence upon the orientation of bedding, P- and S- values of $UCS$ and $T$ were considered. The $UCS$ value for bedding inclined at $45^\circ$ (Z-sample) was also considered.
Fig. 5.9. Loading rate sensitivity of the FEM/DEM simulations. (a) Indirect tensile strength, $T$, and (b) uniaxial compressive strength, $UCS$, as function of the loading platen velocity, $v$. For $v < 0.125$ m/s the material tends to exhibit rapidly decreasing sensitivity to loading rate and to display a distinct and consistent strength anisotropy.

The finalized model parameters are reported in Table 5.1. The values of the strength parameters were obtained as final result of the calibration process, while the experimental values of the elastic constants reported by Bock (2009) were directly used as input for the transversely isotropic elastic model. A friction coefficient, $k$, equal to 0.1 was assumed at the platen-sample interfaces.

The effect of the crack element compliance on the overall model stiffness (Section 5.4.1) was minimized by selecting appropriate values for the penalty coefficients. Based on the recommendations of Mahabadi (2012), normal penalty, $p_n$, tangential penalty, $p_t$, and fracture penalty, $p_f$, were set equal to $10 \times$, $1 \times$ and $5 \times$ the largest Young’s modulus, $E$, respectively.

A sensitivity analysis was performed in order to assess the effect of the applied viscous damping (Eq. (5.2)) on the stress-strain behaviour of the UCS and Brazilian test models. The results are expressed using the critical damping coefficient, $\mu_c$, as a reference value. This value approximates the theoretical critical damping assuming that each triangular element of size $h$ behaves as a one-degree-of-freedom mass-spring-dashpot system (Munjiza, 2004):

$$\mu_c = 2h\sqrt{E\rho}$$  \hspace{1cm} (5.11)

where $E$ and $\rho$ are the Young’s modulus and the density of the material. As can be observed in Fig. 5.10a for the UCS P-sample, higher $\mu$ values suppress the high-frequency oscillations of the strain-stress curve that are caused by the moving platens. As depicted in Fig. 5.10b, for values larger than $0.01\mu_c$, the failure load of each sample was relatively insensitive to this parameter and variations in the emergent $UCS$ and $T$ could be neglected. Table 5.2 compares the emergent properties of the model with the experimental values for Opalinus Clay used as calibration targets (Bock, 2009).
Table 5.1. FEM/DEM input parameters of the Opalinus Clay model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Continuum triangular elements</strong></td>
<td></td>
</tr>
<tr>
<td>Bulk density, ( \rho ) (kg/m(^3))</td>
<td>2330</td>
</tr>
<tr>
<td>Young’s modulus parallel to bedding, ( E ) (GPa)</td>
<td>3.8</td>
</tr>
<tr>
<td>Young’s modulus perpendicular to bedding, ( E' ) (GPa)</td>
<td>1.3</td>
</tr>
<tr>
<td>Poisson’s ratio parallel to bedding, ( \nu )</td>
<td>0.35</td>
</tr>
<tr>
<td>Poisson’s ratio perpendicular to bedding, ( \nu' )</td>
<td>0.25</td>
</tr>
<tr>
<td>Shear modulus, ( G' ) (GPa)</td>
<td>0.9</td>
</tr>
<tr>
<td>Viscous damping coefficient, ( \mu ) (kg/m( \cdot )s)</td>
<td>1.79e3</td>
</tr>
<tr>
<td>Average edge length, ( h ) (mm)</td>
<td>0.30</td>
</tr>
<tr>
<td><strong>Crack elements</strong></td>
<td></td>
</tr>
<tr>
<td>Tensile strength parallel to bedding, ( f_{t,\text{max}} ) (MPa)</td>
<td>0.65</td>
</tr>
<tr>
<td>Tensile strength perpendicular to bedding, ( f_{t,\text{min}} ) (MPa)</td>
<td>0.16</td>
</tr>
<tr>
<td>Cohesion parallel to bedding, ( c_{\text{min}} ) (MPa)</td>
<td>1</td>
</tr>
<tr>
<td>Cohesion perpendicular to bedding, ( c_{\text{max}} ) (MPa)</td>
<td>9</td>
</tr>
<tr>
<td>Mode I fracture energy parallel to bedding, ( G_{Ic,\text{max}} ) (J/m(^2))</td>
<td>7.0</td>
</tr>
<tr>
<td>Mode I fracture energy perpendicular to bedding, ( G_{Ic,\text{min}} ) (J/m(^2))</td>
<td>0.4</td>
</tr>
<tr>
<td>Mode II fracture energy parallel to bedding, ( G_{IIc,\text{min}} ) (J/m(^2))</td>
<td>10</td>
</tr>
<tr>
<td>Mode II fracture energy perpendicular to bedding, ( G_{IIc,\text{max}} ) (J/m(^2))</td>
<td>35</td>
</tr>
<tr>
<td>Friction angle of intact material, ( \phi_i ) (°)</td>
<td>22</td>
</tr>
<tr>
<td>Friction angle of fractures, ( \phi_f ) (°)</td>
<td>22</td>
</tr>
<tr>
<td>Normal contact penalty, ( p_n ) (GPa( \cdot )m)</td>
<td>38</td>
</tr>
<tr>
<td>Tangential contact penalty, ( p_t ) (GPa/m)</td>
<td>3.8</td>
</tr>
<tr>
<td>Fracture penalty, ( p_f ) (GPa)</td>
<td>19</td>
</tr>
<tr>
<td>Platen-sample friction coefficient, ( k )</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Fig. 5.10. Damping sensitivity of the FEM/DEM simulations. (a) Axial stress, \( \sigma_1 \), vs. axial strain, \( \varepsilon_1 \), of the UCS-P simulation for the several damping coefficient values, \( \mu \). (b) Emergent \( UCS \) and \( T \) values for different applied damping. Results are expressed using the critical damping coefficient, \( \mu_c \) (Eq. (5.2)), as reference value.
Table 5.2. Comparison between the mechanical properties of the Mont Terri Opalinus Clay (Bock, 2009) and the emergent macroscopic properties of the calibrated FEM/DEM model.

<table>
<thead>
<tr>
<th>Macroscopic mechanical property</th>
<th>Experimental value</th>
<th>FEM/DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus parallel to bedding, $E_P$ (GPa)</td>
<td>$3.8 \pm 1.5$</td>
<td>3.6</td>
</tr>
<tr>
<td>Elastic modulus perpendicular to bedding, $E_S$ (GPa)</td>
<td>$1.3 \pm 0.7$</td>
<td>1.3</td>
</tr>
<tr>
<td>Poisson’s ratio parallel to bedding, $\nu_P$</td>
<td>0.35</td>
<td>0.38</td>
</tr>
<tr>
<td>Poisson’s ratio perpendicular to bedding, $\nu_S$</td>
<td>0.25</td>
<td>0.26</td>
</tr>
<tr>
<td>Uniaxial compressive strength parallel to bedding, $UCS_P$ (MPa)</td>
<td>$11.6 \pm 3.9$</td>
<td>11.5</td>
</tr>
<tr>
<td>Uniaxial compressive strength perpendicular to bedding, $UCS_S$ (MPa)</td>
<td>$14.9 \pm 5.1$</td>
<td>15.6</td>
</tr>
<tr>
<td>Uniaxial compressive strength at 45° to bedding, $UCS_Z$ (MPa)</td>
<td>$4.1 \pm 1.7$</td>
<td>3.8</td>
</tr>
<tr>
<td>Indirect tensile strength parallel to bedding, $T_P$ (MPa)</td>
<td>1.30</td>
<td>1.17</td>
</tr>
<tr>
<td>Indirect tensile strength perpendicular to bedding, $T_S$ (MPa)</td>
<td>0.67</td>
<td>0.60</td>
</tr>
</tbody>
</table>

5.5.3 Simulated tensile behaviour

Fig. 5.11 shows the tensile stress, $\sigma_t$, as function of the platen vertical displacement, $\delta_v$, calculated according to the following formula (Bieniawski and Hawkes, 1978):

$$\sigma_t = \frac{2P(\delta_v)}{\piDt},$$  \hspace{1cm} (5.12)

where $P(\delta_v)$ is the applied load, computed as sum of the nodal reaction forces of the top platen; $D$ is the diameter of the sample (30.0 mm); and $t$ is the sample thickness (a unit thickness is assumed in 2D). Although Eq. (5.12) is only strictly valid for isotropic solids, it was used to maintain consistency with the formulation adopted in the laboratory testing (Bock, 2009). In transversely isotropic materials, a more accurate analysis should, however, account for the effect of the loading angle, $\theta$, and the parameter $k$ (Eq. (5.10)) (Barla and Innaurato, 1973).

The response of both samples was elastic-brittle with loss of strength after reaching the peak strength values. Peak values of 1.17 MPa and 0.60 MPa were obtained for the P- and S-sample, respectively. These values are considered a good match to the respective experimental values of 1.30 and 0.67 MPa. A comparison between experimental and simulated fracture patterns is illustrated in Fig. 5.12. For the numerical simulations, the mode of fracture, $m$, calculated according to Eq. (5.6), is also reported. The simulated failure mode was given by brittle tensile splitting along the vertical loading path for both samples. For the P-sample, secondary tensile fractures parallel to the bedding orientation developed at the disc boundary.

5.5.4 Simulated stress-strain behaviour under uniaxial compression

FEM/DEM simulations capture the progressive mechanical failure that is typically observed in rocks under compression (Lisjak et al., 2013c, see Chapter 4). Hence, the stress-strain behaviour of both UCS samples (Fig. 5.14) can be analyzed with reference to the characteristic stress levels and behaviour stages proposed for brittle rocks (Bieniawski, 1967; Eberhardt et al., 1997; Martin et al., 1997) and
Fig. 5.11. Tensile stress, $\sigma_t$, vs. platen vertical displacement, $\delta_v$, for the Brazilian test simulation. Note that the post-peak response is affected by the artificially high platen velocity, which causes the two halves of the sample to remain in contact with the platen for some time after the axial splitting, thus resulting in non-zero reaction forces.

graphically summarized in Fig. 5.13. Experimental investigation of the brittle behaviour of Opalinus Clay can be found in Corkum and Martin (2007b) and Amann et al. (2011).

The simulated curves of applied axial stress, $\sigma_1$, versus sample axial and lateral strain, $\varepsilon_1$ and $\varepsilon_3$, together with the count of yielded/broken crack elements, are displayed in Fig. 5.14 for the UCS P- and S-sample. The corresponding post mortem fracture patterns are depicted in Fig. 5.12d.

From point O to point A-A’ in Fig. 5.14, the response of the model is linear due to the elastic deformation of the continuum triangular elements. Modulus anisotropy is a direct consequence of the adopted transversely isotropic constitutive relationship. In the pre-peak stage (point A-A’ to B), the model exhibits non-linear behaviour due to material softening at the crack element level. The onset of non-linearity manifests itself first in the lateral strain curves ($A’= 55\%$ versus A=70\% of axial strain at peak), as crack elements start to yield in tension in the direction parallel to $\sigma_1$. With respect to Fig. 5.13, point A can be considered representative of the crack damage threshold, $\sigma_{cd}$. Simulated unconfined compressive strength values (point B) were equal to 11.5 MPa and 15.6 MPa for the P- and S-sample, respectively. These values satisfactorily matched the respective experimental values of 11.6 MPa and 14.9 MPa, used as calibration targets. The brittle post-peak behaviour (beyond point B) is characterized by the actual failure of crack elements with consequent macroscopic fractures propagating throughout the model (Fig. 5.12d).

With respect to the stages proposed by Martin et al. (1997), the model cannot capture the low-stiffness non-linearity at low strain levels. In Opalinus Clay, this closure effect has been related to the breakage of diagenetic bonds following the sample recovery process (Corkum and Martin, 2007b). Furthermore, the simulation is unable to reproduce the stable crack propagation stage corresponding the nucleation of extensile cracks induced in a compressive stress field by the presence of micro-scale heterogeneities (Tapponnier and Brace, 1976). It is possible that the latter limitation could be overcome by
Fig. 5.12. Comparison of simulated versus experimentally observed fracture patterns during rock mechanics tests on Opalinus Clay. (a, c) Typical fracture patterns observed during Brazilian tests (disc diameter $\approx 30$ mm, after Jahns (2010), image courtesy of NAGRA) and UCS tests (sample height $\approx 120$ mm, sample diameter $\approx 60$ mm, after Popp et al. (2008), © Elsevier, reproduced with permission) on Opalinus Clay. (b, d) Simulated fracture patterns with associated mode of fracture, $m$, for the Brazilian test and UCS test simulations. The mode of fracture, $m$, of each broken crack element was computed according to Eq. (5.6), where 1 and 2 refer to tensile and shear failure, respectively.

Fig. 5.13. Characteristic stress levels and behaviour stages observed in brittle rocks under unconfined compression (after Martin et al. (1997), redrawn).
5.5.5 Variation of fracture response with loading angle

As further discussed in Section 5.7, the variation of rock deformation and fracture response with loading angle deeply affects the development of damage around circular excavations in bedded rocks. The influence of loading direction with respect to the specimen anisotropy was investigated in the UCS model by rotating the layering orientation at 15° increments, from \( \theta = 0^\circ \) (i.e., P-sample) to \( \theta = 90^\circ \) (i.e., S-sample). Material properties and numerical parameters obtained as a result of the calibration process were left unchanged (Table 5.1). The simulated values of emergent uniaxial compressive strength, \( UCS \), and elastic modulus, \( E \), for the different loading angles, \( \theta \), are plotted in Fig. 5.15.

The deformation response as a function of the anisotropy direction is characterized by a monotonically decreasing elastic modulus with the loading angle varying from the P-sample value \( (E_P = 3.6 \text{ GPa}) \) to the S-sample value \( (E_S = 1.3 \text{ GPa}) \). This behaviour is again consistent with that observed in Opalinus Clay (Salager et al., 2010) and other clay shales (Niandou et al., 1997), and follows directly

**Fig. 5.14.** Simulated stress-strain behaviour under uniaxial compression. Axial stress, \( \sigma_1 \), versus axial strain, \( \varepsilon_1 \), and lateral strain, \( \varepsilon_3 \), for (a) the P-sample and (b) S-sample, also showing counts of yielded/broken crack elements (Fig. 5.4) as columns.

explicitly adopting a heterogeneous material property distribution in the FEM/DEM model (Mahabadi, 2012).

In laboratory experiments, the staged character of the brittle damage process can also be correlated to the variation of acoustic emission (AE) properties (Eberhardt et al., 1997). In FEM/DEM, the simulation of AE associated with the brittle failure of rocks was investigated by Lisjak et al. (2013b) (see Chapter 3). If a homogeneous model is employed to capture the macroscopic stress-strain response of the rock, the seismic response of the Opalinus Clay cannot be reproduced. Capturing localized failures of crack elements and the associated kinetic energy release (i.e., acoustic events) before the macro-rupture of the sample, would require the introduction of element-scale inhomogeneities with a wide spectrum of strength and deformability values. Therefore, in the current study yielding and breakage of the cohesive crack elements can only provide a quasi-static, macroscopic representation of the fracturing process without fully capturing its micro-scale dynamics.
Fig. 5.15. Simulated uniaxial compressive strength value, \( UCS \), and elastic modulus, \( E \), plotted as a function of the loading angle, \( \theta \). Dashed error bars indicate the ranges of experimental \( UCS \) values from Table 5.2.

from the assumed constitutive law for the triangular elements.

With respect to the strength response, as the loading angle increases, the \( UCS \) first decreases from \( UCS_P = 11.5 \) MPa to a minimum value of \( 3.8 \) MPa for \( \theta = 45^\circ \), and then increases again to reach \( UCS_S = 15.6 \) MPa. That is, the simulated strength response exhibits the characteristic concave upwards, and parabolic in form, curve that has been typically observed in Opalinus Clay (Naumann et al., 2007), other shales (McLamore and Gray, 1967; Niandou et al., 1997), and anisotropic metamorphic rocks (Donath, 1972). The simulated \( UCS \) value for \( \theta = 45^\circ \) (\( 3.8 \) MPa) corresponds to a 65% reduction from \( UCS_P \) and therefore agrees well with a 50 to 80% reduction experimentally observed in unconfined or moderately confined compression tests (Naumann et al., 2007; Jahns, 2010).

As mentioned in Section 5.1, when discontinuous plane of weakness models (Jaeger and Cook, 1976; Hoek and Brown, 1980a; Duveau et al., 1998) are employed to capture the variation of strength with respect to the loading angle, two distinct strength criteria are adopted to independently characterize failure due to sliding along the bedding planes and failure in the intact matrix. Conversely, with the FEM/DEM smeared approach, the strength anisotropy is captured by the variation of specimen rupture mechanisms induced by the directionality introduced in the cohesive response of crack elements preferably aligned along the bedding plane direction. Unlike plane of weakness models, since no clear distinction between failure of the matrix and of bedding planes is made, a smooth transition in the strength response with loading angle is reproduced.

The simulated fracture patterns together with the orientation distribution of broken crack elements (Fig. 5.16a,b) highlight a distinct variation of bedding influence on the macroscopic failure response of the sample as a function of the anisotropy direction. For steeply dipping layering (\( \psi = 90^\circ, \theta = 0^\circ \)), the failure of the sample is induced by the extension of the bedding planes. Major cracks develop subparallel to the loading direction consisting of a combination of tensile split along layers and steeply inclined shear fractures. For mid-dip values (\( 30^\circ \leq \psi \leq 75^\circ, 15^\circ \leq \theta \leq 60^\circ \)), the sample fails due to bedding plane delamination. Analysis of the simulated fracture mode indicates almost exclusively
shear fracturing parallel to the preferably oriented layers, in agreement with typical experimental observations (Fig. 5.17). In this case, the strength of the sample is ultimately controlled by the shear strength parameters of crack elements oriented in the direction parallel to the bedding (i.e., $c_{\text{min}}$ and $G_{\text{II, min}}$). As revealed by the strength distribution of Fig. 5.15, the most favourable orientation for shearing is obtained for bedding planes dipping at $30 - 45^\circ$. For loading orientations $75^\circ \leq \theta \leq 90^\circ$ (0° $\leq \psi \leq 15^\circ$), the sample rupture occurs as shearing through the rock matrix. Under these conditions, the inclination of the macroscopic fracture is independent from the bedding plane orientation and equal to about $54^\circ$.

The three main simulated failure modes of the Opalinus Clay sample are summarized in Fig. 5.18 as function of the relative orientation between bedding and macroscopic plane of failure.

### 5.6 Mesh sensitivity

The sensitivity of the failure response of a FEM/DEM model to the size of the spatial discretization and to the mesh orientation naturally arises from the assumptions inherent to the adopted cohesive crack model (Section 5.3.2). On the contrary, the emergent elastic properties are independent of the adopted...
element size and mesh topology, as model deformability is governed by the continuum formulation of triangular elements (Section 5.4.1). The sensitivity of the laboratory-scale simulations to the element size and mesh orientation are therefore discussed in the following sections.

5.6.1 Element size

To accurately represent the bonding stress close to the crack tip, the element size must be much smaller than the length of the FPZ, $l_{FPZ}$, defined as the distance from the crack tip to the point where the maximum cohesive strength (i.e., $f_t$ or $f_s$) is attained (Munjiza and John, 2002). In general, if the FPZ does not spread across a sufficient number of elements the critical load is overestimated. Although analytical relationships are available to estimate the value of $l_{FPZ}$ (Hillerborg et al., 1976), these are strictly only valid for mode I facturing. Instead, the simulated failure process of the rock samples in compression is due to a combination of mode I and mode II fracturing together with multiple interactions between newly-created fractures. Thus, the simulated failure conditions are more complex than the pure opening mode upon which the available analytical estimates are based. Furthermore, the constitutive behaviour of the crack elements was modified by introducing a directional dependence in the strength parameters, which is not accounted for by theoretical models. Therefore, the element size sensitivity of the FEM/DEM model was investigated by simulating the response of the UCS P- and S-samples for mesh refinements ranging between 0.15 and 0.4 mm. As shown in Fig. 5.19, the peak strength appears to tend to a constant value for decreasing values of $h$ and, in general, to exhibit low element size sensitivity. Due to excessively long run times, it was not possible to simulate mesh resolutions finer than 0.15 mm. For example, using an Intel Core i7 920 2.67 GHz CPU with 8 GB of RAM, the total computational time of the UCS-P model ($h = 0.15$ mm, $\approx 42,000$ triangles, 2.5M timesteps, $v = 0.05$ m/s) was equal to approximately 7 days. The adoption of smaller element size not only results in a rapid growth of the total number of elements but also requires smaller time step sizes to satisfy the stability condition of the explicit time-integration scheme of FEM/DEM. On the other hand, element sizes greater than 0.40 mm could not be used due to the adopted layer thickness value of bedding planes ($t = 1.0$ mm). In general, the element size controls the model spatial resolution, but also the strength of the model and, for the case of bedded materials, the minimum layer thickness, $t$, that can be employed.

Fig. 5.17. Typical shear failure observed during compression tests on Z-samples of Opalinus Clay. Bedding plane orientation is indicated by a white line (after Naumann et al. (2007), © Elsevier, reproduced with permission).
Fig. 5.18. Inclination of macroscopic failure plane, $\beta$, versus dip of specimen bedding, $\psi$. Indicated is also the relationship between mesh topology, orientation of bedding planes and fractures.

Fig. 5.19. Variation of $UCS_P$ and of the total number of triangular elements, $N$, as function of the adopted element size, $h$.

5.6.2 Mesh orientation

The sensitivity of the cohesive element approach to the mesh orientation results from restricting crack growth along the edges of the triangular elements (Fig. 5.3). Although this approach aims at simulating fracturing without any a priori assumption regarding the fracture trajectory, a certain mesh bias is induced by the fact that the direction of crack propagation is not entirely free but restricted to a limited number of predefined angles. To minimize the constraint imposed by the mesh topology on the model behaviour, randomly discretized meshes should be used in place of regularly discretized ones (Tijssens et al., 2000; Mahabadi, 2012). Following this recommendation, an unstructured Delaunay triangulation scheme was used for all models in the current study. Moreover, to correctly capture the delamination process along bedding planes, preferably oriented planes are introduced. The resultant
Fig. 5.20. Variation of $UCS$ values and anisotropy ratios as function of the adopted layer thickness, $t$. Input parameters of Table 5.1 were used.

mesh is a combination of a random triangulation for the intra-layer material (i.e., matrix) together with edges preferably aligned along the layering direction for the bedding planes (Fig. 5.8a). The influence of the layer thickness, $t$, on the strength response of Opalinus Clay samples under compression is illustrated in Fig. 5.20. For these simulations, the element size was kept constant ($h = 0.30$ mm). The results indicate that the degree of strength anisotropy is dependent upon the introduction of preferably oriented planes in the mesh topology. As expected the most sensitive model to the element topology is the $Z$-sample. Since failure occurs as sliding along bedding planes, the adoption of a complete random mesh (i.e., no layers, $t > 17.5$ mm) effectively increases the shear strength of the bedding planes by introducing an artificial mesh-induced surface roughness along the potential least-energy failure path. Nevertheless, values of $UCS$ and associated anisotropy ratios appear to tend to constant values as the number of layers increases.

5.7 Simulation of damage process around a circular excavation

5.7.1 Model description

The damage process around a circular excavation in Opalinus Clay was simulated using the FEM/DEM cohesive fracture model approach illustrated in the previous sections. The circular shape and size of the excavation (Fig. 5.21) correspond to those of emplacement tunnels for spent nuclear fuel and vitrified high-level radioactive waste according to the preliminary design of the Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA, 2002, 2010). The axis of the tunnel was horizontal and parallel to the strike of the bedding planes ($z$-axis in Fig. 5.5a). The layering dip, $\psi$, was assumed equal
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Fig. 5.21. Geometry and boundary conditions of the excavation models. Tunnel radius, depth of mesh refinement zone, and model size were assumed equal to $r = 1.4$ m, $d = 4$ m, and $l = 30$ m, respectively.

Given the artificial variation of material strength potentially induced by the increased element size, the input parameters of the FEM/DEM model should be recalibrated based on the newly-adopted spatial discretization. To this end, quantitative field-scale experimental observations (e.g., shape and extent of
EDZ) should be used. Since in this study the input parameters were left unchanged from the values used in the laboratory-scale calibration process (Table 5.1), the simulation results could only be qualitatively analyzed with reference to observed damage mechanisms and fracture patterns available in the literature.

### Boundary conditions

To correctly simulate the prior-to-excavation stress state, each model required two separate runs. In the first run, the vertical and horizontal *in situ* stress conditions, as reported in Table 5.3, were applied to the model. Gravity-induced stress gradients were neglected. To prevent the development of damage in response to this dynamic loading, all the elements were considered perfectly elastic and therefore were not allowed to fracture. The first run was continued until the total kinetic energy of the system decayed to a negligible value (i.e., resulting stress waves were attenuated). The revised nodal coordinates corresponding to the system at rest (i.e., static equilibrium) were then obtained. These revised nodal coordinates were used as the current nodal coordinates (i.e., deformed mesh) of the second run in which the actual material strengths were assigned. By changing the far-field boundaries to be fixed in the horizontal and vertical directions (Fig. 5.21), the first order *in situ* stress conditions were maintained while allowing the excavation to be initiated. Model relaxation induced by the artificial compliance of the crack elements was minimized by the choice of sufficiently large contact and fracture penalty values (Section 5.4.1).

With the correct *in situ* stress conditions achieved, the circular tunnel was excavated using a core replacement technique (Kavvadas, 2005). The progressive deconfinement of the rock mass due to the advancing face was accounted for by reducing the deformation modulus of the tunnel core over time in a step-wise fashion. The total kinetic energy of the model was again monitored to ensure that steady state conditions were reached at every excavation stage. The final stage of the excavation involved the actual removal of material from the tunnel with consequent creation of a traction-free surface at the excavation perimeter. Although the modulus reduction approach is commonly used to correlate the evolution of damage to the excavation advancement rate (Hoek et al., 2008), in the present study it was mainly adopted to avoid damage potentially induced by inertial effects due to a sudden removal of material.

#### 5.7.2 Simulated failure process under isotropic *in situ* stress conditions

For the case of $K_0 = 1.0$, the failure process leading to the formation of the EDZ and the associated stress field evolution are illustrated in the sequence of Fig. 5.22.
Fig. 5.22. FEM/DEM simulation results of the failure sequence around the excavation for the case $K_0 = 1.0$ after (a) 70,000, (b) 120,000 and (c) 210,000 timesteps. Colour contours on the left and right hand side represent maximum and minimum principal stresses, $\sigma_1$ and $\sigma_3$, respectively. Principal stress trajectories are indicated as cross icons with the long and short axis oriented as $\sigma_1$ and $\sigma_3$, respectively. Mode of fracture of crack elements is calculated according to Eq. (5.6), where 1 and 2 refer to tensile and shear failure, respectively.
Failure around the excavation boundary initiates in the haunch area at angles $\alpha$ approximately equal to $\pm 45$ and $\pm 135$ in the form of shear-dominated fractures along the bedding planes (Fig. 5.22a). This distinctive location of failure and fracturing behaviour can be explained by considering the polar distribution of elastic circumferential stress, $\sigma_\alpha$, together with the compressive strength value, $UCS$, and macroscopic failure mode of a hypothetical rock core oriented along the tunnel perimeter (Fig. 5.23). The distribution of $\sigma_\alpha$ exhibits a slight anisotropy deriving from the assumed transversely isotropic elastic behaviour and elastic parameters (Table 5.1). Compared to the isotropic case, whereby $\sigma_\alpha$ is equal to $2 \cdot \sigma_v = 4$ MPa regardless of the choice of the elastic parameters (Kirsch, 1898), a reduction of about 12.5% and 25% is estimated in the sidewalls and back, respectively. However, when considering the orientation of the $\sigma_\alpha$ with respect to the layering, a great variation in material strength is observed along the perimeter of the excavation. As described in Section 5.5.5, the presence of bedding planes inclined at an angle of about $30 - 60^\circ$ to $\sigma_1$ drastically reduces the strength of the rock resulting in premature bedding slip.

The slippage of bedding planes in the haunch area causes a local perturbation in the stress field which results in the nucleation of extensional (i.e., mode I) fractures in the direction perpendicular to the layering (Fig. 5.22b). As the delaminated layers tend to bend and slide past each other, brittle spalling is promoted in the tunnel sidewalls. The failure of rock in the sidewalls causes in turn the deflection and inwards sliding of other unsupported layers of rock in the back and invert. The final
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Fig. 5.24. Total displacement field, $\delta$, around the circular excavation corresponding to the stress field distribution and fracture pattern of Fig. 5.22c. Note that, owing to the lack of support, static equilibrium conditions could not be reached within the heavily fragmented zone around the tunnel and the relative displacement contour should be therefore be treated as transient.

The excavation disturbed zone (EdZ) is characterized by reversible processes which, in this context, are represented by the excavation-induced elastic stress redistribution. The excavation damaged zone (EDZ) is dominated by irreversible processes in the form of damage and failure. Within the EDZ, an inner and
an outer shell can be identified according to the characteristics of the simulated damage process (Kaiser and Kim, 2008). The inner shell is characterized by brittle failure triggered by bedding plane slips in the haunch area that lead to loss of material continuity, open fractures and consequent rock mass bulking. In this area, the confining stress, $\sigma_3$, is low to moderately negative (i.e., tensile stress). In the outer shell, mode II fractures can still nucleate but the relative sliding along the fracture surfaces is limited by higher values of confining stress, $\sigma_3$. Consequently, the growth of extensional fractures is effectively inhibited.

A quantitative comparison of the simulated damage pattern with specific in situ observations is beyond the scope of this work. Nevertheless, the failure mechanisms here simulated are, at least from a qualitative point of view, supported by a number of field or laboratory observations in excavations in laminated shale formations. In particular, the characteristic shear failure of bedding planes has been observed in Opalinus Clay during hollow cylinder experiments (Labiouse and Vietor, 2013), and around boreholes, microtunnels and drifts at the Mont Terri URL (Blümling et al., 2007; Marschall et al., 2006). Also, the importance of weakness planes in controlling the rock mass behaviour and the stability of underground openings is confirmed by observations from the construction of a hydroelectric tunnel in laminated sedimentary formations (Perras and Diederichs, 2009). Characteristic square-shaped fractured zones have also been reported in the hydrocarbon exploration industry when drilling horizontal boreholes in laminated shales (Gazaniol et al., 1995; Økland and Cook, 1998; Edwards et al., 2004; Willson et al., 1999). Furthermore, brittle failure in the form of extensional fractures parallel to the tunnel walls have been typically observed around excavations at the Mont Terri URL (Bossart et al., 2002; Stefanizzi, 2007; Yong et al., 2010).

**Fig. 5.25.** Schematic illustrating the shape and extent of the simulated EdZ and EDZ for the case $K_0 = 1.0$. 
Fig. 5.26. Effect of *in situ* stress anisotropy. Final stress distribution and fracture pattern for the cases of (a) $K_0 = 0.60$ and (b) $K_0 = 1.67$. Colour contours on the left and right hand side represent maximum and minimum principal stresses, $\sigma_1$ and $\sigma_3$, respectively. Principal stress trajectories are indicated as cross icons with the long and short axis oriented as $\sigma_1$ and $\sigma_3$, respectively. Mode of fracture of crack elements is calculated according to Eq. (5.6), where 1 and 2 refer to tensile and shear failure, respectively.

5.7.3 Effect of *in situ* stress anisotropy

The influence of *in situ* stress anisotropy on the EDZ development in Opalinus Clay was simulated for the cases $b$ and $c$ reported in Table 5.3. The final fracture patterns with associated principal stress contours and principal stress directions are depicted in Fig. 5.26. Based on the distribution of circum-
ferential stress around the tunnel (Fig. 5.23), the rock mass failure initiates for both cases in the haunch area due to the presence of planes of weakness favourably oriented for slippage, according to the process described above for $K_0 = 1.0$. Although extensional brittle fracturing can be observed in the sidewalls for both cases, the interaction between newly-created shear fractures and *in situ* stress field results in sensibly different stress redistributions, which in turn deeply affect the final shape and extent of the EDZ. For $K_0 = 0.60$, the lateral growth of bedding plane delamination is suppressed by the increase in shear strength due to the maximum principal stress, $\sigma_1$, locally oriented in the direction perpendicular to the layering. Consequently, the flow of maximum principal stress around the hole tends to promote further failure in the roof and invert resulting in a vertically elongated damaged zone, with maximum depth equal to $1.5r$. Conversely, for $K_0 = 1.67$ the lateral development of bedding slippage from the haunch is greatly enhanced by the orientation of the far field stresses with $\sigma_3$ oriented perpendicular to the direction of fracture propagation. The fracture-induced stress redistribution limits the flow of $\sigma_1$ around the back and invert. Therefore, the vertical development of EDZ is reduced in favour of further bedding slippage in the horizontal direction up to a depth of $2r$ from the haunch area.

Based on the above results, both fracture patterns differ from damaged zones typically observed in massive isotropic rocks whereby spalling is generally observed at the intersection of the minimum principal stress axis and the hole boundary (Hoek et al., 1995). Given the strong influence of material anisotropy on the rock mass response, classic stress stability analyses (Diederichs et al., 2004; Martin et al., 1999) may not be applicable as premature failure and distinctive failure kinematics induced by the bedding planes are not correctly accounted for.

### 5.7.4 Implications for constructability, ground support and nuclear waste storage

The above illustrated modelling results clearly indicate that for support design purposes the rock mass should not be treated as an isotropic medium. As observed by others (Bewick and Kaiser, 2009; Perras and Diederichs, 2009), the mobilization of shear strength along bedding planes in the haunch area plays a key-role in the EDZ formation process in laminated rocks. That is, the slippage of bedding planes causes a substantial reduction of confining stress, $\sigma_3$, in the sidewalls and therefore promotes brittle failure processes in the form of spalling. Subsequently, fracturing propagates in the crown and invert resulting in loss of cohesion due to the formation of small rock blocks, typically of tabular shape, and consequent rock mass bulking. If the excavation is left unsupported, this damage growth process may have severe effects on the tunnel constructability due to a drastic reduction of stand-up time. Delaying the installation of the support system may result in gravitational fall-outs of loose blocks in the crown together with floor heave. Also, if a Tunnel Boring Machine (TBM) were used for the excavation, failure of rock in the sidewalls may negatively impact the stability of the gripper system (Kaiser, 2006).

Therefore, to minimize the short-term development of the EDZ and associated overbreaks, pre-convergence of excavation boundary should be controlled by installing a lining system (e.g., shotcrete, steel arches) as close as possible to the tunnel face. If the liner were to be coupled with rock bolting, the anchoring elements in the crown and invert should be long enough to reach the stronger, confined rock in the outer shell or beyond (Kaiser and Kim, 2008).
In the context of the long-term underground storage of nuclear waste, the hydraulic and transport behaviour of the rock mass within the EDZ should also be considered. In Opalinus Clay, the permeability in the EDZ may increase by several orders of magnitude with respect to the highly impermeable intact rock (Bossart et al., 2002). In this regard, the assessment of performance and long term safety of a repository system, including the simulation of radionuclide transport towards the biosphere, may benefit from the geometric information (e.g., fracture aperture and network interconnectivity) that could be extracted from FEM/DEM simulations for a range of different geomechanical scenarios. In this context, the evolution of hydraulic properties with time (e.g., self-sealing effects) due to the waste-generated thermal transient and hydro-mechanical processes (Blümling et al., 2007) should, however, be taken into account.

### 5.7.5 Model limitations

#### Three-dimensional effects

In this study, a two-dimensional FEM/DEM analysis was adopted to simulate the fracturing behaviour of unsupported circular openings excavated in anisotropic clay shales. Although the simulations did not attempt to match any experimental in situ deformation field, the excavation modelling procedure via core modulus reduction can, in general, be used to indirectly account for the supporting action of the excavation face occurring during the tunnel advancement, thus allowing to calibrate the FEM/DEM model using, for instance, measurements of tunnel wall convergences. However, only a three-dimensional stress analysis would be able, in general, to capture the evolution of the primary stress field and associated ground deformation as the tunnel approaches and passes through a volume of rock. That is, two-dimensional models neglect several factors that are inherently three-dimensional, including the influence of stress path and loading history, and the effect of the axial (i.e., intermediate) principal stress (Pan and Hudson, 1988). In this regard, Eberhardt (2001) showed that the progressive advancement of a tunnel face is associated with a spatio-temporal evolution of the three-dimensional stress field which undergoes a series of deviatoric stress increases and/or decreases as well as several rotations of the principal stress axes. Consequently, since rock mass damage and strength degradation is largely dependent upon the deviatoric stress magnitude and the orientation of the principal stresses, the tunnel behaviour in the near-field will be necessarily influenced by three dimensional effects occurring ahead of the face. In clay shales, the situation is further complicated because damage may arise from a complex interaction between the aforementioned three-dimensional stress field and geological structures such as bedding planes and tectonic faults. At the Mont Terri URL, experimental evidence suggests that the excavation yielded/fractured zone does not develop exclusively along the tunnel periphery behind the excavation face but surrounds the excavation face itself of which it may affect the stability (Nussbaump et al., 2011; Yong et al., 2013). In conclusion, a more accurate analysis of the fracturing behaviour of underground openings would require adopting a three-dimensional FEM/DEM model. However, such type of analysis is at present hindered by the excessively high computational demand of hybrid finite-discrete element simulations.
Hydro-mechanical coupling and time-dependent behaviour

The FEM/DEM models presented in this work consisted of purely mechanical analyses without any consideration for pore pressure variation such as instantaneous hydro-mechanical coupling or fluid flow effects. Conversely, the rock-water interaction may, in reality, lead to several phenomena that will alter the EDZ as function, for instance, of the water content and the degree of saturation (Blümling et al., 2007). In the short-term, instantaneous poromechanical effects may occur when the mechanical loading rate is higher than the fluid pressure dissipation rate (i.e., undrained conditions). Firstly, if the spikes of pore pressure are such that the intact tensile strength of the rock is overcome, pore-pressure-induced yielding (i.e., hydraulic fracturing) may occur. However, in rocks, the material contraction in the direction of the maximum principal stress is typically associated with the onset of dilatancy which causes a pore pressure decrease (Brace and Martin, 1968). Therefore, material dilation may be associated with a decrease or even negative fluid pressure owing to dilatancy occurring at a faster rate than the pore fluid diffusion into the dilated zones. This phenomenon may result in significant suction pressures which, in turn, can increase the effective stress of the rock and, consequently, its strength (i.e., dilatant hardening). Due to the low hydraulic conductivity of clay shales and the relatively fast advancement rate, the excavation-induced response is typically treated as an undrained response (Martin and Lanyon, 2003). However, modelling fluid flow and associated phenomena (e.g., de-saturation, swelling, re-consolidation) is an essential component of simulations aimed at studying the long-term evolution of the EDZ, which characterizes the open drift, exploitation, and post-closure stages of an underground repository for nuclear waste (Tsang et al., 2012). Also, visco-plastic effects (e.g., sub-critical crack growth, creep), neglected in this study, may contribute to the long-term evolution of deformations in argillaceous rocks (Egger, 2000).

5.8 Concluding remarks

A new modelling approach based on the combined finite-discrete element method (FEM/DEM) was used to investigate the damage process and failure mechanisms around underground openings in clay shales. Unlike continuum-based methods, FEM/DEM explicitly simulates the growth of fractures in rocks, thus allowing to reproduce typical brittle failure processes involving loss of material continuity, large displacements and rigid block rotations.

The anisotropic strength response characteristic of clay shales was captured with a simple directional dependence in the cohesive strength parameters of the crack elements. When modelling large-scale problems, this approach was shown to overcome some of the limitations of a previously-developed discrete approach based on an explicit incorporation of pre-existing cracks oriented along the direction of bedding (Lisjak et al., 2013c, see Chapter 4). The numerical model was validated by simulating indirect tensile and unconfined compression tests on Opalinus Clay, a shale formation in Switzerland chosen to host a deep geological repository for high-level nuclear waste. A distinct variation of strength and fracture response as function of the layering angle was captured as an emergent property of the model. In agreement with experimental observations, three main macroscopic modes of failures were
reproduced: (i) shearing through intact matrix, (ii) bedding plane delamination, and (iii) axial splitting.

A mesh sensitivity study indicated that element size and grid topology are not entirely free parameters of the model. The element size influences not only the model spatial resolution, but also the strength of the material and, for the case of bedded materials, the minimum layer thickness that can be incorporated into the model. However, it has been demonstrated that the simulated strength response tends to a constant value for decreasing values of the element size and layer thickness. Nonetheless, when the method is applied to field-scale problems, computational demands require an increase of element size. Therefore, the cohesive strength parameters of the model should be checked and eventually recalibrated to match the evolution and extent of damage at the scale of interest.

The simulation of a circular tunnel excavation in horizontally bedded Opalinus Clay under isotropic pre-excavation stress conditions showed an EDZ formation process consisting of a combination of shearing along bedding planes and extensional brittle fracturing. Failure around the hole initiated in the haunch area due to the presence of bedding planes favourably oriented for shearing. With the rock mass left unsupported, inwards movement of layers tended to promote spalling in the tunnel sidewalls and buckling of other layers in the back and invert. The resulting EDZ could be divided into an inner shell and an outer shell. The vertically elongated inner shell was characterized by rock mass fragmentation, bulking and large deformations. The outer shell extended out in the horizontal direction with brittle fracturing effectively limited by the increase of confining stress. Under anisotropic in situ stress states, the combination of rock inherent anisotropy and anisotropy induced by newly-developed preferably-oriented fractures resulted in fracture patterns substantially different than those typically observed in massive isotropic rocks in similar stress conditions.

In future work, further model validation will take advantage of EDZ measurements relative to a full-scale emplacement test tunnel recently excavated at the Mont Terri Underground Research Laboratory (St-Ursanne, Switzerland). Also, the influence of joints and tectonic faults on the rock mass response will be simulated as well as the effect of tunnel support on the excavation stability.
Chapter 6

The excavation of a circular tunnel in a bedded argillaceous rock (Opalinus Clay): short-term rock mass response and numerical analysis using FEM/DEM

This chapter will be submitted to the journal Tunnelling and Underground Space Technology as:

Abstract

The Opalinus Clay formation is currently being investigated as a potential host rock for the deep geological storage of radioactive waste in Switzerland. Recently, a full-scale emplacement (FE) test tunnel was excavated at the Mont Terri underground research laboratory (URL) as part of a long-term research project aimed at studying the hydro-thermo-mechanical effects induced by the presence of an underground repository. The objective of this paper is two-fold. Firstly, the results of the rock mass monitoring program carried out during the construction of the 3 m diameter, 50 m long FE tunnel are presented, with particular focus on the short-term deformation response. Secondly, the deformational behaviour observed in the field is analyzed using a hybrid finite-discrete element (FEM/DEM) analysis to obtain further insights into the formation of the excavation damaged zone (EDZ). The deformation measurements, including geodetic monitoring of tunnel wall displacements, radial extensometers and longitudinal inclinometers, indicate a strong directionality in the excavation response induced by the presence of bedding planes striking parallel to the tunnel axis. In particular, radial convergences ranging between 0.6 and 2.5% are observed, with the most severe deformation occurring in the direction approximately perpendicular to the material layering. Likewise, strong displacement gradients are mea-
sured in proximity to the excavation boundary in the direction perpendicular to the bedding likely due to rock mass fracturing. Three-dimensional effects associated with the tunnel advance are highlighted by vertical deflections in the crown starting to develop on average 1.0–1.2 tunnel diameters ahead of the excavation face. The FEM/DEM simulation using the Y-Geo code (Mahabadi et al., 2012a) is calibrated based on the average short-term response observed in the field. Deformation and strength anisotropy are accounted for in the model by a transversely isotropic, linear elastic constitutive law and cohesive elements with orientation-dependent strength parameters. An overall good agreement is obtained between convergences measured in the field and numerical results. The simulated EDZ formation process highlights the importance of bedding planes in controlling the failure mechanisms around the underground opening. In particular, failure is initiated due to shearing of bedding planes critically oriented with respect to the compressive circumferential stress induced around the tunnel. Slippage-induced rock mass deconfinement promotes extensional fracturing in the direction perpendicular to the bedding orientation. The simulated EDZ comprises an inner shell, dominated by severe rock fragmentation and bulking and characterized by large deformations, and an outer shell, whereby an increase of confining stress suppresses extensional fracturing and thus causes a sensible decrease of deformations. The numerical fracture pattern is consistent with previous experimental evidence from the Mont Terri URL.

6.1 Introduction

The deep geological disposal of nuclear waste in an indurated clay formation, namely Opalinus Clay, is currently being assessed in Switzerland. Owing to its very low hydraulic conductivity, high radionuclide retention capacity, and potential for self-sealing of fractures, Opalinus Clay is indeed well suited for the long-term storage of radioactive waste (Blümling et al., 2007). However, the formation of an excavation damaged zone (EDZ) around the underground structures, including emplacement tunnels and shafts, needs to be considered when assessing both short and long term safety of the repository. Apart from directly affecting the stability of the excavation during construction, the EDZ is typically associated with a permeability increase of several orders of magnitude due to the formation of newly connected porosity in response to fracturing of intact rock and shearing along structural features such as tectonic faults and bedding planes. Therefore, the formation of the EDZ and its evolution with time need to be evaluated as part of the safety assessment of any potential storage site.

Over the past 15 years, an extensive experimental research program has been conducted at the Mont Terri underground rock laboratory (URL) aimed at characterizing the EDZ in Opalinus Clay. As further described in Section 6.3.1, a distinctive feature of damage development in this type of argillaceous rock is the fundamental role played by the material anisotropic behaviour. In particular, the shape and extent of the EDZ around tunnels and boreholes are strongly dependent upon the relative orientation between excavation axis and bedding planes.

At the same time, field and laboratory investigations of the Opalinus Clay failure behaviour have been supported by the development of several numerical models with the goal of providing an interpretation for the response observed in the field (see Section 6.3.2 for a review). However, modelling the
creation and evolution of the EDZ remains an open research topic as to date no single set of consistent modelling approaches has been able to reproduce all the observations from the URL (Tsang et al., 2012). Due to the complexity of the observed phenomena, a complete description of the processes in the EDZ would require, in general, to consider hydro-mechanical, thermal, as well as chemical effects.

For this study, the short-term rock mass response of a newly-excavated, full-scale emplacement (FE) test tunnel at the Mont Terri URL was characterized based on monitoring data collected during the tunnel construction. Despite several important differences between the Mont Terri URL and the actual repository site candidates (e.g., depth, stress state and tectonic imprint), the FE experiment offered the opportunity to analyze for the first time the behaviour of Opalinus Clay under geometric (i.e., same tunnel shape and dimensions) and structural-geological (i.e., tunnel oriented parallel to the bedding strike) conditions similar to those of the planned repository tunnels. Subsequently, a mechanical total stress analysis of the tunnel response was carried out using a hybrid finite-discrete element (FEM/DEM) code (Munjiza, 2004; Mahabadi et al., 2012a; Lisjak et al., 2013a). Unlike traditional continuum-based models, the adopted FEM/DEM Y-Geo code presented the characteristic feature of explicitly simulating the spontaneous nucleation and propagation of cracks within the rock mass and could therefore be used to gain original insight into the brittle fracturing process around the underground excavation.

The paper is organized as follows. In Section 6.2, a brief description of the Mont Terri URL is provided, including geological setting, rock material and rock mass characterization, and in situ stress field. In Section 6.3, an overview of the published experimental observations regarding the EDZ in Opalinus Clay is given together with a summary of the major related simulation studies. In Section 6.4, the recent excavation of the FE tunnel is described together with the results of the monitoring campaign using geodetic measurements of tunnel wall displacements, radial extensometers, and longitudinal inclinometers. In Section 6.5, an experimental model of the average tunnel wall deformation is created and preliminary linear elastic, finite element modelling accounting for modulus anisotropy carried out. This is followed in Section 6.6 by the calibration of the aforementioned FEM/DEM model. The calibrated FEM/DEM model is then used as a tool to provide a mechanical interpretation of the observed anisotropic rock mass deformation response in terms of fracturing evolution around the opening. Furthermore, the influence of support stiffness and in situ stress anisotropy on the development of damage is analyzed.

6.2 Site description: Mont Terri URL

6.2.1 Geological setting

The Mont Terri URL is located northwest of the town of St-Ursanne in the Canton Jura, Switzerland. Access to the underground facilities is provided through the security gallery of the Mont Terri tunnel along the A16 motorway connecting Biel and Porrentruy. As shown in Fig. 6.1, the URL lies in the southeastern limb of the Mont Terri anticline at an average overburden depth of 300 m. The stratigraphy of Mont Terri consists of limestones, marls, and shales, with the URL entirely located in the Opalinus Clay formation, a sequence of dark grey, silty, micaceous clays, sandy, and locally marly (to limy) shales
Fig. 6.1. Vertical geological section of the Mont Terri anticline along the motorway tunnel (after Freivo- gel and Huggenberger (2003), © Springer, reproduced with permission).

having thickness of 90 m (Nussbaum et al., 2011). The lithostratigraphic sub-units of Opalinus clay can be grouped into three main facies (Thury and Bossart, 1999): (i) a sandy facies in the middle and upper part of the formation, (ii) a carbonate-rich, sandy facies in the middle of the formation, and (iii) a shaly facies in the lower part. A site map of the URL is shown in Fig. 6.2. The FE tunnel starts from the FE niche at an azimuth of 242° from North and it is entirely located within the shaly facies of the Opalinus Clay formation.

6.2.2 Rock material and rock mass characterization

The most prominent geological feature of the Opalinus Clay at Mont Terri is a bedding structure moderately dipping towards the SSE. At the location of the FE tunnel, the average bedding orientation of 139/33 (Jaeggi et al., 2013) results in the excavation axis approximately parallel to the strike of bedding planes. This bedded structure has been shown to affect the mechanical behaviour of the rock material by inducing strong directionality in its deformation and strength characteristics (Popp and Salzer, 2007a; Bock, 2009; Jahns, 2010). Overall, Opalinus Clay can therefore be classified as a soft, brittle rock with mechanical behaviour best described as transversely isotropic (Table 6.1). In addition to the presence of layering, the rock mass at the Mont Terri URL is typically characterized by numerous tectonic structures, which can be grouped into three different fault systems (Nussbaum and Bossart, 2008): (i) moderately SSE-dipping reverse faults, (2) low angle SW-dipping fault planes and sub-horizontal faults, and (iii) moderately to steeply inclined N to NNE-striking sinistral strike-slip faults. A thorough description of the structural geological investigations carried out during the construction of the FE tunnel can be found in Jaeggi et al. (2013). In brief, a variety of different tectonic structures were mapped along the tunnel. Based on a combination of manual measurements and digital photogrammetric surveying of the rock mass surfaces, three fault orientation subsets could be identified:

- a gently to moderately SE-dipping fault subset (mean: 139/33) and thus roughly parallel to the Opalinus Clay mean bedding plane orientation;
Fig. 6.2. Geological map of the Mont Terri underground rock laboratory showing the location of underground facilities, including the newly-excavated FE tunnel (image courtesy of Dr. Christophe Nussbaum (swisstopo)).

- a fault system (dip < 20°) consisting of gently SW- (mean: 221/19) and NE-dipping (mean: 042/12) faults;
- a gently NW-dipping fault subset (mean: 306/12).

Furthermore, excavation-induced fractures were observed as further described in Section 6.3.1.

6.2.3 In situ stress field

Since 1996, several measuring campaigns have been carried out at the Mont Terri URL to characterize the in situ stress field in Opalinus Clay. To this end, a number of different techniques have been employed, including borehole slotter (Cottour et al., 1999), undercoring (Bigarré and Lizeur, 1997), and hydraulic fracturing (Evans et al., 1999). Moreover, direct measurements have been complemented by extensive geological mapping of fractured zones in niches (Bossart and Adler, 1999) and borehole
breakouts (Bossart and Wermeille, 2003), and by numerical back-analyses of deformations around instrumented excavations (Martin and Lanyon, 2003). In general, the determination of the in situ stress in clay shales such as Opalinus Clay has been a challenging task mainly owing to the strong deformation and strength anisotropic behaviour of the rock mass as well as the non-elastic response of underground openings. These difficulties are also further aggravated by the variation of rock properties with moisture uptake (i.e., swelling), which have made in situ tests hard to conduct (Martin and Lanyon, 2003).

The most likely in situ stress field available to date is based on original undercoring measurements, subsequently constrained by 3D elastic simulations and hydrogeological arguments (Martin and Lanyon, 2003; Corkum, 2006) (Table 6.2). The maximum principal stress, $\sigma_1$, is sub-vertical and its magnitude, varying between 6 and 7 MPa, agrees well with the lithostatic pressure value at a depth of 250 m. The minimum and intermediate principal stresses, $\sigma_1$ and $\sigma_2$, are sub-horizontal with magnitude equal to 2-3 and 4-5 MPa. Undisturbed pore pressure values are approximately equal to 2 MPa. As discussed by Bossart and Wermeille (2003), the magnitude of principal stresses are better constrained than the respective directions. In particular, the minor and intermediate principal stress directions are those with the highest degree of uncertainty.

The in situ stress field adopted for the numerical analyses of the FE tunnel excavation (Table 6.3) was based on the average values from Table 6.2 and the relative orientation between principal stresses and tunnel axis shown in Fig. 6.3.

### Table 6.1. Mechanical properties of the shaly facies of Mont Terri Opalinus Clay reported by Bock (2009).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus parallel to bedding, $E_P$ (GPa)</td>
<td>$3.8 \pm 1.5$</td>
</tr>
<tr>
<td>Elastic modulus perpendicular to bedding, $E_S$ (GPa)</td>
<td>$1.3 \pm 0.7$</td>
</tr>
<tr>
<td>Poisson’s ratio parallel to bedding, $\nu_P$ (-)</td>
<td>0.35</td>
</tr>
<tr>
<td>Poisson’s ratio perpendicular to bedding, $\nu_S$ (-)</td>
<td>0.25</td>
</tr>
<tr>
<td>Shear modulus perpendicular to bedding, $G_S$ (GPa)</td>
<td>3.7</td>
</tr>
<tr>
<td>Uniaxial compressive strength parallel to bedding, $UCS_P$ (MPa)</td>
<td>$11.6 \pm 3.9$</td>
</tr>
<tr>
<td>Uniaxial compressive strength perpendicular to bedding, $UCS_S$ (MPa)</td>
<td>$14.9 \pm 5.1$</td>
</tr>
<tr>
<td>Uniaxial compressive strength at 45$^\circ$ to bedding, $UCS_Z$ (MPa)</td>
<td>$4.1 \pm 1.7$</td>
</tr>
<tr>
<td>Indirect tensile strength parallel to bedding, $T_P$ (MPa)</td>
<td>1.30</td>
</tr>
<tr>
<td>Indirect tensile strength perpendicular to bedding, $T_S$ (MPa)</td>
<td>0.67</td>
</tr>
</tbody>
</table>

### Table 6.2. In situ stress tensor at the Mont Terri rock laboratory (Corkum and Martin, 2007b).

<table>
<thead>
<tr>
<th>Principal stress</th>
<th>Orientation</th>
<th>Trend ($^\circ$)</th>
<th>Plunge ($^\circ$)</th>
<th>Range (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_1$</td>
<td>Sub-vertical</td>
<td>210</td>
<td>70</td>
<td>6-7</td>
</tr>
<tr>
<td>$\sigma_2$</td>
<td>NW–SE</td>
<td>320</td>
<td>7</td>
<td>4-5</td>
</tr>
<tr>
<td>$\sigma_3$</td>
<td>NE–SW</td>
<td>052</td>
<td>18</td>
<td>2-3</td>
</tr>
</tbody>
</table>
6.3 The EDZ in the Mont Terri Opalinus Clay

6.3.1 Experimental evidence of failure patterns around openings in Opalinus Clay

The experimental characterization of the EDZ in Opalinus Clay has been the objective of several research projects at the Mont Terri URL. A summary of the main results focusing on \textit{in situ} observations relative to the short-term response of excavations in Opalinus Clay is provided in the following. Although time-dependent phenomena, including hydro-mechanical processes (e.g., de-saturation, swelling, consolidation) and visco-plastic effects (e.g., sub-critical crack growth, creep), have been shown to play an important role in the long-term evolution of the EDZ in argillaceous rocks (Blümling et al., 2007), the review of these processes was beyond the scope of this work, as the numerical mod-
elling focused only on purely mechanical simulations without any time-dependency. Similarly to other anisotropic rocks, a distinct variation of rock mass response has been typically observed in Opalinus Clay as function of the relative orientation between the excavation axis and the bedding plane direction. Based on the geometrical layout of the Mont Terri URL (Fig. 6.2), the cases of excavations parallel and perpendicular to the bedding strike were therefore distinguished and the failure patterns classified accordingly. Excavations perpendicular to the bedding strike (e.g., Security Gallery, Gallery 98, Gallery 04, and Gallery 08) generally exhibited stable conditions without the need for heavy support measures. Conversely, excavation driven parallel to the bedding strike (e.g., HG-A microtunnel, MB niche, FE tunnel) were characterized by deformation response strongly affected by the reduced strength properties of the bedding planes which often resulted in construction and ground control difficulties.

Openings perpendicular to the strike of bedding planes

The first conceptual model of EDZ in Opalinus Clay was proposed by Bossart et al. (2002) based on the geological mapping of over-cored, resin-injected boreholes and hydraulic testing around the Security Gallery (Fig. 6.4a). The model, developed on the basis of a 4 m diameter, NNW-SSE oriented tunnel, consists of a inner and an outer shell, extending approximately 1 and 2 m from the tunnel wall, respectively. The inner zone is characterized by an interconnected fracture network of extensional fractures sub-parallel to the tunnel walls and small-scale shear fractures. The outer zone consists of non-interconnected, extensional fractures. The validity of the EDZ model proposed by Bossart et al. (2002) was confirmed by field observations relative to Gallery 98 (Bossart et al., 2004), whereby the presence of unloading fractures parallel the excavation boundary was again reported together with excavation-induced bedding plane reactivation. Also, the tunnel performance of the ED-B section of Gallery 98 and associated EDZ characteristics was discussed by Martin et al. (2002). The absence of ground support problems was confirmed by low values of tunnel strain and pressure in the shotcrete lining, ranging between 0.2 and 1%, and 0.025 to 1 MPa, respectively. The EDZ characterization was carried out using a number of techniques, including hydraulic testing from radial boreholes, ultrasonic velocity profiles, core logging and resin injection, and geoelectric tomography. The results indicated a pattern of slip-related deformation in the roof and floor, and extensile brittle fractures in the sidewalls, with an overall extension of damaged zone less than one tunnel radius from the excavation boundary (Fig. 6.4b).

A detailed analysis of the fracture network around Gallery 04 from the EZ-B niche was carried out by Yong et al. (2010). Three sets of EDZ fractures were reported: (i) extensional fractures parallel to the sidewall of Gallery 04, (ii) oblique striking, tensile fractures with respect to the axis of Gallery 04, and (iii) reactivated bedding planes in proximity to the tunnel wall. A quantitative analysis of this EDZ geometry, including fracture density, trace orientation, and trace lengths, was subsequently performed in an attempt to generate a statistical fracture network model of the EDZ around Gallery 04 (Thovert et al., 2011). More recently, new insights into the EDZ formation process in Opalinus Clay have been provided by Nussbaum et al. (2011) based on the geological mapping of Gallery 08. In particular, shear fractures striking parallel to the excavation face and systematically more inclined than the bedding by 20° – 40° have been clearly identified. These fractures were interpreted as originating from the reactivation of
bedding planes and/or pre-existing SSE-dipping faults as normal faults in response to the excavation-induced stress redistribution ahead of the tunnel face (Fig. 6.4c).

**Openings parallel to the strike of bedding planes**

Original experimental investigations regarding the effect of the mechanical anisotropy on the development of damage around openings in Opalinus Clay were carried out by Bossart and Werneille (2003). Using in-hole camera recording, breakout directions were analyzed in boreholes drilled in three orthogonal directions from the Security Gallery. For the case of horizontal boreholes drilled parallel to the strike of bedding, three breakout directions were observed. Among these, the most prominent (i.e., 75% of the cases) could be directly related to the strength anisotropy of the rock and, in particular, to the reduced shear strength of the bedding planes. As depicted in Fig. 6.5a, these breakouts occurred at a polar angle, $\theta$, of about $135^\circ$ and $315^\circ$, roughly corresponding to the bedding planes oriented tangentially to the hole boundary. Less frequently, other two breakout directions were observed at $0^\circ$ ($180^\circ$) and $90^\circ$. While the former orientation agreed well with the expected zone of high deviatoric stress concentration induced by a vertically oriented, maximum principal far-field stress, the latter was only observed in proximity to the borehole mouth and therefore directly related to the steeply-inclined unloading fractures of the EDZ of the Security Gallery. Similar failure mechanisms were observed around the 1 m long HG-A micro-tunnel drilled sub-parallel to the bedding strike (Marschall et al., 2006) and reported in Fig. 6.5b and 6.6a. More specifically, the mechanical anisotropy of Opalinus Clay manifested itself in the form of slab-like breakouts at $\theta = 120 - 150^\circ$ due to bending and buckling of layers oriented parallel to tunnel boundary, and wedge-shaped breakouts at $\theta = 330 - 360^\circ$. The visual inspection of breakout locations was confirmed by the recordings of extensometers located around the excavation which consistently
showed significant ground deformation associated with the above angular positions. Furthermore, the formation of extensional fractures at 0° and 90°, roughly corresponding to the direction of the minimum principal *in situ* stress, was also observed. Subsequently, a conceptual model of EDZ was developed by Blümling et al. (2007) based on several cases of borehole failures induced by bedding plane delamination (Fig. 6.6b), such as the SELFRAC experiment boreholes (Bernier et al., 2007), and a larger scale example of progressive failure in the direction perpendicular to bedding around a horseshoe-type tunnel (Fig. 6.6c). As shown in Fig. 6.5c, the failure pattern schematic consisted of a combination of extensional failure in the sidewalls together with bedding plane failure in the floor and roof. The influence of rock mass anisotropy and heterogeneity in the form of small scale faults on the development of the EDZ around Gallery 04 via mapping of the EZ-B niche was investigated by Yong et al. (2010). In particular, the kinematic freedom of faults was shown to control the development and orientation of extensional fractures in the tunnel sidewalls. Convergences higher than expected and ground control difficulties were experienced during the construction of the 4.5 m diameter MB niche oriented parallel to the bedding strike (Vietor et al., 2010). The subsequent analysis of excavation-induced fractures using a resin impregnation technique (Jaeggi et al., 2012b) identified a number of different sets, including N-S striking sub-vertical fractures intersecting the tunnel-sidewalls at high angles and fractures associated to bedding plane slippage or bedding parallel fault reactivation. Some of the failure mechanisms illustrated above have found experimental confirmation from hollow-cylinder tests on Opalinus Clay (Labiouse and Vietor, 2013). The laboratory results indicated a distinctive variation in behaviour between samples cored in the directions parallel and perpendicular to the bedding plane orientation. While in specimens cored perpendicular to bedding failure was not observed, a characteristic buckling of layers with bedding plane delamination resulting in strong hole ovalization in the direction parallel to bedding was reported for holes drilled parallel to the orientation of layering (Fig. 6.6d). From a qualitative point of view, a similar response was also observed *in situ* using in-hole video recording of the evolution of deformation of small boreholes (Seeska and Lux, 2012). An experimental investigation of the EDZ fracture pattern around the FE tunnel based on resin-impregnated drillcore logging is currently on-going. Nevertheless, a preliminary EDZ model based on excavation-induced fractures mapped during tunnel construction (Jaeggi et al., 2013) can be formulated. In particular, the presence of a pattern of shortly spaced, vertically oriented, extensional fractures on the excavation face and tunnel sidewalls tends to confirm a three-dimensional fracture pattern surrounding the advancing tunnel, as originally described by Jaeggi et al. (2012a) for the FE niche.

### 6.3.2 Related modelling studies

The large body of research for the experimental characterization of the EDZ in Opalinus Clay (Section 6.3.1) has been accompanied by a number of modelling studies aimed at capturing the response of the rock mass observed *in situ*. A brief review of selected simulation methodologies and modelling assumptions adopted to date is provided in the following with reference to several case studies from the Mont Terri URL (Table 6.4). In this context, only modelling studies targeting the short-term (i.e., undrained) rock mass behaviour and EDZ formation process were considered. With reference to the
Fig. 6.5. Conceptual models of failure patterns around openings oriented in the direction parallel to the strike of bedding planes. (a) Typical breakout orientations observed around horizontal boreholes normal to the Security Gallery (after Bossart and Wermeille (2003), redrawn), (b) schematic representation of the damaged zone around the HG-A microtunnel (after Marschall et al. (2006), © Society of Petroleum Engineers, reproduced with permission), and (c) conceptual EDZ model for openings parallel to the bedding plane strike (after Blümling et al. (2007), redrawn).

Fig. 6.6. Examples of fracture patterns observed around openings parallel to the strike of bedding planes. The trace of bedding planes is indicated by a dashed line. (a) HG-A microtunnel (after Marschall et al. (2006), © Society of Petroleum Engineers, reproduced with permission), (b) small borehole (after Blümling et al. (2007), © Elsevier, reproduced with permission), (c) horseshoe-shaped access drift (after Blümling et al. (2007), © Elsevier, reproduced with permission), and (d) hollow-cylinder experiment (after Labiouse and Vetric (2013), © Springer, reproduced with permission).

life-cycle of an underground repository for nuclear waste described by Tsang et al. (2012), the short-term rock mass response is limited to the construction stage, defined as the period of time which extends from the tunnel excavation to a few days after the lining installation. Simulation studies aimed at investigating the temporal evolution of the EDZ during the open drift, exploitation, and post-closure stages (e.g., Boidy et al., 2002; Billaux et al., 2004; Shao et al., 2008; Levasseur et al., 2010) were excluded from this review.

Martin and Lanyon (2003) carried out three-dimensional, linear-elastic, boundary element simulations of multiple boreholes drilled from the ED-B section of Gallery 98. By comparing the stress con-
centrations around the borehole walls with the observed breakout orientations, the in situ stress tensor measured with undercoring techniques was numerically constrained. Although material anisotropy was not taken into account, the model was able to reproduce the extensometer data recorded around the ED-B niche. Two-dimensional, finite element numerical simulations of the ED-B mine-by test were performed by Corkum and Martin (2004) using a number of different material constitutive relationships, including linear-elastic, elasto-plastic and elastic-brittle-plastic. Although the latter model provided an overall good fit to the inclinometers data, none of the approaches was able to correctly capture the development of extensional fractures observed along the tunnel sidewalls. These modelling results were further refined by three-dimensional, finite-difference simulations adopting a variety of constitutive models, including linear elastic, elasto-plastic, ubiquitous joint anisotropic elasto-plastic, and non-linear elastic with stress dependent modulus (SDM) (Corkum and Martin, 2007a). Again, none of the approaches was able to correctly capture the effect of dilation associated with extensional fracturing. Nevertheless, the SDM phenomenological model provided the best fit for the zones of high deformation, non-plastic rock mass response. The fracturing behaviour around the Security Gallery was investigated by Stefanizzi (2007) using a hybrid finite-discrete element code, namely ELFEN (Rockfield Software Ltd., 2004). In particular, the study focused on the conceptual modelling of the transition from stress-driven to strain-driven fracturing behaviour around a tunnel containing either two parallel discontinuities or layers with elastic mismatch to mimick the effect of bedding planes. Discrete element simulations using UDEC (Itasca Consulting Group Inc., 2004) were carried out by Popp et al. (2008) in an attempt to capture the failure mechanisms observed around the Security Gallery, such as extensional fracturing in the sidewalls and shear failure in the roof and floor (Fig. 6.4b). Yielding of sidewalls was captured using an elasto-plastic model, while the introduction of pre-existing, horizontal joints allowed to reproduce the slippage of bedding planes in the roof and floor of the tunnel. The influence of small-scale faults on the development of the EDZ in the entrance walls of the EZ-B niche was investigated by Yong et al. (2010) by two-dimensional, finite element analysis. The rock matrix was assumed to behave as a Mohr-Coulomb, elasto-plastic medium with elastic deformability governed by a transversely isotropic law, while the tectonic faults were captured by continuous joint elements. A three-dimensional, discrete element simulation using 3DEC (Itasca Consulting Group Inc., 2003) under isotropic, elastic conditions was then carried out to account for the complex geometry of the problem due to the proximity of HG-A niche, the non-orthogonal intersection of the EZ-B niche with Gallery 04, and the skewed alignment of the niche axis with the principal stress axes. More recently, Yong et al. (2013) integrated 3D continuum simulations with geophysical measurements to characterize the rock mass response ahead of the EZ-B niche. To the author knowledge, the only two modelling studies of excavations in the direction parallel to the bedding strike, where material anisotropy has been shown to govern the EDZ formation, are those of Konietzky and te Kamp (2004) and Konietzky and te Kamp (2006) which simulate the HG-A niche and EZ-A niche, respectively. In these models, the effect of material layering was captured by a bi-linear, strain-softening ubiquitous joint model implemented in a 2.5D, FLAC3D model (Itasca Consulting Group Inc., 2000).

In this study, a preliminary analysis of the FE tunnel excavation response was carried out using a
linear elastic, finite element model (Section 6.6). The adoption of a transversely isotropic elastic constitutive model allowed to qualitatively reproduce the anisotropic deformation response of the tunnel. However, the lack of plasticity resulted in the inability to capture the large deformations measured in the field (Section 6.4.2). For this reason, a numerical approach that explicitly simulates fracture propagation, namely the hybrid finite-discrete element method (FEM/DEM) (Munjiza, 2004), was adopted. As further described in Section 6.6, the FEM/DEM simulation of the anisotropic behaviour of Opalinus Clay followed the approach developed by Lisjak et al. (2013a) (see Chapter 4) for the FEM/DEM Y-Geo code (Mahabadi et al., 2012a).

### 6.4 Rock mass response during the FE tunnel excavation

The full-scale emplacement (FE) experiment at the Mont Terri URL simulates the construction, waste emplacement and backfilling of an emplacement tunnel for spent fuel (SF) and vitrified high-level waste (HLW) as realistically as possible. Given the site-specific conditions of Mont Terri (e.g., past tectonic activity), extrapolation to real storage site should however be handled carefully. The experiment is considered full-scale as the planned size of an emplacement tunnel is reproduced according to the Swiss reference concept for a geological repository (Fig. 6.7a). The entire implementation as well as the post-closure thermo-hydro-mechanical (THM) evolution are monitored with several hundred sensors. The FE experiment is lead by NAGRA (Switzerland) in collaboration with other five partners, including ANDRA (France), the Department of Energy (USA), NWMO (Canada), GRS and BGR (Germany), in the

<table>
<thead>
<tr>
<th>Study</th>
<th>case</th>
<th>code</th>
<th>dimensions</th>
<th>anisotropy</th>
<th>stiffness</th>
<th>strength</th>
<th>constitutive models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Martin and Lanyon (2003)</td>
<td>ED-B tunnel</td>
<td>Examine3D</td>
<td>3D</td>
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<td>no</td>
<td>linear elastic</td>
<td></td>
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<td>ED-B tunnel</td>
<td>Phase2</td>
<td>2D</td>
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<td>no</td>
<td>linear elastic, elastoplastic, elastoplastic-brittle-plastic</td>
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<tr>
<td>Corkum and Martin (2007a)</td>
<td>ED-B tunnel</td>
<td>FLAC3D</td>
<td>3D</td>
<td>no</td>
<td>no</td>
<td>linear elastic, elastoplastic, non-linear elastoplastic (SDM), elastoplastic with ubiquitous joints</td>
<td></td>
</tr>
<tr>
<td>Stefanizzi (2007)</td>
<td></td>
<td>ELFEN</td>
<td>2D</td>
<td>no</td>
<td>no</td>
<td>elastoplastic with crack insertion</td>
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</tr>
<tr>
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<td>2D</td>
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</tr>
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<td>no</td>
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<td>FLAC3D</td>
<td>3D</td>
<td>yes</td>
<td>no</td>
<td>elastoplastic with ubiquitous joints</td>
<td></td>
</tr>
<tr>
<td>Konietzky and te Kamp (2004)</td>
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<td>FLAC3D</td>
<td>2.5D</td>
<td>yes</td>
<td>yes</td>
<td>elastoplastic with ubiquitous joints</td>
<td></td>
</tr>
<tr>
<td>Konietzky and te Kamp (2006)</td>
<td>EZ-A niche</td>
<td>FLAC3D</td>
<td>2.5D</td>
<td>yes</td>
<td>yes</td>
<td>elastoplastic with ubiquitous joints</td>
<td></td>
</tr>
<tr>
<td>This work</td>
<td>FE tunnel</td>
<td>Phase2</td>
<td>2D</td>
<td>yes</td>
<td>no</td>
<td>linear elastic</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Y-Geo</td>
<td>2D</td>
<td>yes</td>
<td>yes</td>
<td>linear elastic with cohesive elements</td>
<td></td>
</tr>
</tbody>
</table>

* a Rocscience Inc., Toronto, Canada
  b Itasca Consulting Group Inc., Minneapolis, USA
  c Rockfield Software Ltd., Swansea, UK
  d Mahabadi et al. (2012a) and Lisjak et al. (2013a) (see Chapter 4)
framework of the Mont Terri Project. With this experiment, NAGRA also participates in the EURATOM (7th framework programme) project “Large Underground Concept Experiments” (LUCOEX). This work focuses on the analysis of the short-term rock mass response as monitored during the excavation phase of the FE experiment (Fig. 6.7b).
Fig. 6.8. Simplified longitudinal cross section of the FE tunnel showing the installed support measures, the convergence measuring sections (C0-C9), and the location of radial extensometers (E1 and E2). The tunnel nominal diameter, $D$, is equal to 3.0 m.

### 6.4.1 Tunnel construction and monitoring program

The 50 m long FE tunnel was excavated full-face between April 25 and July 10 (2012) from northeast to southwest direction starting from the FE niche (Fig. 6.2). The excavated and final tunnel diameter (including lining) were approximately equal to 3.0 and 2.7 m, respectively. The excavation method consisted of a combination of pneumatic hammer and roadheader, with a typical advance rate varying between 1.0 and 1.5 meter/day, depending on the adopted support measures (Fig. 6.8). From TM 0 to TM 38 (i.e., access, plug and test sections), the support in the tunnel consisted of mesh reinforced, low pH shotcrete with nominal thickness ranging between 160 and 240 mm and applied right behind the excavation face. Steel sets with a spacing of 0.5–1.0 m were installed between TM 0 and 9 and TM 38 and 50 (i.e., access and interjacent sealing sections). Between TM 9 and 38, a combination of 22 mm diameter, 2.5 m long fibreglass solid bolts and 32 mm diameter, 7.5 m long hollow steel anchors were installed in correspondence of areas experiencing high convergence values, typically in the lower part of the right and left sidewalls (see Section 6.4.2).

To quantitatively characterize the rock mass response, an extensive monitoring program was carried out before, during, and after the construction of the FE tunnel. The monitoring campaign included:
• geodetic monitoring of tunnel wall displacements during the tunnel excavation (section C0 to C9 in Fig. 6.8);

• five radial extensometers installed from the tunnel walls during the tunnel excavation (section E1 and E2 in Fig. 6.8);

• inclinometer chains installed two months before the excavation phase in two 45 m long boreholes drilled sub-parallel to tunnel axis from the FE niche (Borehole BFEA-10 and BFEA-11 in Fig. 6.9);

• pore water pressure monitoring from six boreholes drilled from the FE niche two months before the excavation phase and forming an umbrella around the roof of FE tunnel (Borehole BFEA-02 to BFEA-07 in Fig. 6.9);

Furthermore, a detailed geological and structural mapping of the tunnel face was carried out daily immediately after each excavation round (Jaeggi et al., 2013) and complemented by a digital photogrammetric survey of the excavation surfaces using ShapeMetriX3D (3G Software and Measurements GmbH, 2010).

### 6.4.2 Tunnel wall deformation

The displacements of the tunnel walls were measured in three dimensions by geodetic surveying using total stations with integrated distance measurements (Eiholzer, 2012). As depicted in Fig. 6.8, a total of ten convergence sections were installed during the excavation of the FE tunnel at an average spacing of 6 m. While the typical radial measuring configuration consisted of five observation targets (P1-P5), two additional targets (P6 and P7) were installed in the right sidewall from section C5 to C9. In this study, we focused only on sections C1 to C5 which correspond to the tunnel sections where shotcrete and anchors were used as support. Furthermore, those sections were far enough from the entrance and end of the tunnel (i.e., more than 3 diameters) to neglect three-dimensional effects due to the presence of the niche.
As described by Lunardi (2008), the deformation behaviour of an advancing tunnel is characterized by three main deformation typologies (Fig. 6.11): (i) pre-convergence of the advance core, (ii) extrusion of the face, and (iii) convergence of the cavity. The intensity of each deformation behaviour depends in general on the relationship between strength and deformation properties of the rock mass as well as the stress field at which it is subjected. In the case of the FE tunnel, the optical reflectors were put in place at a certain distance, typically $1.0 - 1.5$ m (i.e., $0.3 - 0.5D$), behind the excavation face. Therefore, neither the convergence occurring between the measuring section and excavation face, nor the rock mass pre-convergence were picked-up during monitoring with the optical reflectors. Since a great portion of the total tunnel deformation typically takes place in close proximity to the excavation face (Kavvadas, 2005), the magnitude of the two unmeasured deformation components had to be estimated to allow a direct comparison between field measurements and numerical results, as further discussed in Section 6.6.

The graphs of measured $x$ and $y$ displacement components, $\delta_x$ and $\delta_y$, and displacement magnitude, $\delta$, as function of the normalized distance from the excavation face, $Z/D$, are reported in Fig. 6.12. The observed displacement response was typical of a full-face excavated, advancing tunnel whereby the
excavation-induced, progressive rock mass deconfinement resulted in a closure of the tunnel walls behind the excavation face. Exception to this general trend was represented by the downward displacement recorded at P1 and P5 (at C5), which could be related to the presence of a bedding-parallel fault zone discovered during the excavation. Furthermore, while the deformation response was fairly homogenous for a given radial position along the tunnel axis, substantial differences in displacement magnitudes could be observed around the tunnel boundary at a given cross section. In particular, displacements measured at P5 were consistently higher than others. The typical evolution of displacements observed between TM 10.6 and TM 34.3 is well exemplified by the time and distance history of total wall displacement, $\delta$, measured at section C3 (TM 21.8) (Fig. 6.13). In proximity to the excavation face, the response was characterized by progressively decreasing displacement rates occurring as elasto-plastic deformations directly induced by the excavation of the tunnel. Short-term deformations tended to stabilize at approximately three tunnel diameters (i.e., 9 m) behind the excavation face, corresponding to roughly 11 days for the given advance rate of 1.0 m/day. This observed behaviour was in good agreement with previous measurements at the Mont Terri URL relative to the ED-B tunnel (Martin et al., 2002; Martin and Lanyon, 2003; Corkum and Martin, 2007b). Distant from the excavation face, the rock mass underwent deformation at a much slower rate due to visco-plastic effects and hydro-mechanical consolidation of Opalinus Clay. Such time-dependent deformations, typically observed in argillaceous rocks, have been shown to follow a linear trend on a logarithmic time scale (Egger, 2000).

6.4.3 Radial extensometers

Radial measurements of ground movements around the FE tunnel were carried out by mechanical multi-point extensometers installed from within the tunnel wall at TM 14.6 (section E1) and TM 43.1 (section E2) (Fig. 6.8). Similarly to the geodetic measurements of tunnel convergence, extensometers were installed as soon as possible after the pass of the excavation face. Since the extensometers did not capture the entire strain evolution within the rock mass from pre-mining conditions to the post-excavation stage, a straightforward comparison of experimental measurements with numerical simulations was not possible. Nevertheless, extensometer data could be used to assess the extent of the zone of influence around the tunnel and the influence of anisotropy on the rock deformation response.

The time evolution of relative displacements measured at section E1 by two four-point extensometers, BFEC-01 and BFEC-02, inclined at $30^\circ$ and $120^\circ$ (i.e., parallel and perpendicular to bedding) is reported in Fig. 6.14. As the excavation advances, a short-term rapid increase of deformation is followed by either a long-term stabilization or a secondary increase, likely due to time-dependent processes. Qualitatively, the extensometer response is similar to the time evolution of tunnel wall displacement shown in Fig. 6.13. By assuming negligible the displacement of the anchors located at 6 m from the tunnel wall, the relative displacement measurements were then used to plot the curves of radial displacement as function of the distance from the excavation walls. To this end, the short-term displacement values recorded on June 6 were considered for consistency with the wall convergence analysis (Section 6.4.2). As depicted in Fig. 6.15a, the radial displacement profile in the direction parallel to bedding ($\theta = 30^\circ$) was approximately linear along the entire length of the drillhole. Conversely, the displace-
Fig. 6.12. History plots of tunnel wall displacements, $\delta_x$, $\delta_y$, and $\delta$, as function of the normalized distance between the measuring section and the excavation face, $Z/D$. $Z$ and $D$ correspond to the distance from the face and the nominal diameter of the tunnel, respectively. Graphs (a) to (e) are relative to measuring sections C1 to C5, respectively (Fig. 6.8). Displacements directed towards the tunnel axis are taken as positive. For P3, $x$ component displacements are positive when directed towards right.
Fig. 6.13. Short-term vs. time-dependent displacements. Total displacement, $\delta$, as function of date and normalized distance from the excavation face, $Z/D$, measured at section C3 (TM 21.8).

Fig. 6.14. Time evolution of radial displacements recorded by two four-point extensometers installed at TM 14.6 (section E1). Time of tunnel advance at the measuring section is indicated by a red circle corresponding to May 22. Extensometers were installed on May 25.
Fig. 6.15. Radial (a) displacement and (b) strain profiles at TM 14.6 (Section E1) in the direction parallel and perpendicular to bedding. Displacement profiles were obtained from the short-term differential displacement readings reported in Fig. 6.14 by assuming a zero displacement at the 6 m anchor point. For comparison, equivalent displacement values at the tunnel wall from the geodetic measurements are also plotted. Strain profiles were obtained from the respective radial displacement profiles by dividing the differential displacement between two consecutive points by the length of the interval.

rigid body motion of discrete blocks. The radial displacements derived from the extensometer data were compared to geodetic measurements of tunnel wall displacements at section C2 (Fig. 6.12) in attempt to verify the validity of the nil displacement assumption of the furthest anchor. More specifically, the radial component of the displacement recorded from April 25, corresponding to day of the extensometer installation, and June 6 were derived for the reflectors P2 (θ = 150°), P3 (θ = 90°), and P4 (θ = 30°).

For the case of E1, a value of 5 mm was obtained from the analysis of P4 which was almost double the extensometer value of 2.6 mm. This discrepancy indicated that a differential displacement might have arisen owing to deformation occurring further than 6 m from the excavation wall. A similar conclusion may also be drawn by observing the radial strain profile profile along BFEC-01 (Fig. 6.15b), which, unlike BFEC-02, shows no decrease in deformation with distance. For the case of E2, a good agreement was instead obtained between the extensometer value (4.2 mm) and the average displacement of 4.5 mm calculated by averaging the P2 and P3 values equal to 5 and 4 mm, respectively.

6.4.4 Inclinometers

The ground vertical displacement, \( \delta_v \), above the crown of the FE tunnel was continuously monitored by inclinometer chains permanently installed in two 45 m long boreholes (BFEA-10 and BFEA-11) drilled sub-parallel (dip = 1°) to the tunnel axis (Fig. 6.9 and 6.10). The radial distance of the inclinometer probes from the tunnel wall varied between 1.4 and 2.4 m. Unlike convergence reflectors and radial extensometers, inclinometers were installed from the FE niche prior to the start of the excavation and thus the entire deformation history before and after the pass of the excavation face could be recorded (Fig. 6.16). The deformation trend was characterized by a general increase of maximum displacement...
Fig. 6.16. Ground vertical displacement, $\delta_v$, above the crown of the FE tunnel measured by two inclinometer chains. Displacement evolution is represented for different positions of the excavation face (in TM). The vertical displacement recorded at the excavation face and the corresponding maximum short-term values are indicated by orange and green circles, respectively. The maximum short-term value was obtained by considering the displacement recorded at a given section when the excavation face was approximately 9 m (i.e., $3D$) ahead of it.

with distance. The sharp decrease in the rate of deformation, identified between TM 10 and 15, was likely due to the gradual reduction of support effect of the reinforced FE niche walls in combination with the installation of steel sets in the access section (Fig. 6.18). Maximum vertical displacements equal to 29 and 32 mm were recorded in borehole BFEA-010 and BFEA-011, respectively. The evolution of displacement with excavation advance was consistent with the typical tunnel deformation behaviour described in Section 6.4.2. A sharp increase in $\delta_v$ was usually recorded at about 3 – 4 m ($1.0 – 1.3D$) ahead of the excavation face. The progressive reduction of distance between isolines indicated that the deformation in the crown tended to stabilize as the excavation face moved further away from the sensor. This behaviour was in agreement with the deformation response measured at the tunnel walls. The vertical displacement recorded above the excavation face was on average 43 and 29% of the maximum short-term (i.e., time-dependent deformation excluded) vertical displacement experienced at the given section, for BFEA-010 and BFEA-011, respectively. The latter values, again averaged between TM 9 and 38, were equal to 22 and 21 mm for BFEA-010 and BFEA-011, respectively. Inclinometers data were subsequently used to validate the estimate of the tunnel wall pre-convergence obtained from numerical tunnel longitudinal profiles.

6.5 Preliminary analysis

6.5.1 Average short-term response

The short-term tunnel wall displacements measured between sections C1 and C5 were averaged in order to create an experimental model to be used as reference for the numerical simulations of Section 6.5.3
**Fig. 6.17.** Displacement vector plot of short-term values averaged in longitudinal direction from TM 10.6 to TM 34.3 (sections C1–C5) at different radial positions along the tunnel boundary. Shaded areas indicate the range of variation at each point based on minimum and maximum value of $x$ and $y$ components (Table 6.5). An exaggeratedly deformed excavation profile (amplitude factor = 20) is qualitatively indicated by a black dashed line. The trace of bedding planes is indicated by a green dashed line.

and 6.6. The displacement vector plot of the average experimental cross-section is depicted in Fig. 6.17 based on the values reported in Table 6.5. From these values, the radial strain of the tunnel, defined as

$$\varepsilon_r = \frac{\delta_r}{R},$$

where $R = 1.5$ m is the tunnel radius and $\delta_r$ is the radial component of the displacement vector, was calculated. Depending on the radial position, values ranging between 0.6 and 2.5% were obtained. As revealed by the finite element analysis (Section 6.5.3), the magnitude of the measured displacement field

<table>
<thead>
<tr>
<th>Measuring target</th>
<th>$\delta_{x,\text{min}}$ (mm)</th>
<th>$\delta_{x,max}$ (mm)</th>
<th>$\delta_{x,\text{mean}}$ (mm)</th>
<th>$\delta_{y,\text{min}}$ (mm)</th>
<th>$\delta_{y,max}$ (mm)</th>
<th>$\delta_{y,\text{mean}}$ (mm)</th>
<th>$\delta_{\text{mean}}$ (mm)</th>
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</thead>
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<tr>
<td>P1</td>
<td>9</td>
<td>17</td>
<td>13</td>
<td>-12</td>
<td>7</td>
<td>-5</td>
<td>14</td>
</tr>
<tr>
<td>P2</td>
<td>7</td>
<td>11</td>
<td>9</td>
<td>10</td>
<td>24</td>
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<td>3</td>
<td>8</td>
<td>16</td>
<td>11</td>
<td>12</td>
</tr>
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<td>10</td>
<td>7</td>
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<td>8</td>
<td>40</td>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>20</td>
</tr>
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</table>
at the tunnel boundary was not compatible with a purely linear elastic rock mass behaviour. Instead, the measured material strain softening was likely due to a combination of factors including material yielding, in the form of dilation induced by extensional fracturing or deformation along pre-existing rock mass discontinuities (e.g., faults), and non-linear elastic behaviour in proximity to the excavation surfaces. The heterogeneity in the radial displacement field indicated a probable strong influence of the rock material textural anisotropy, rock mass fabric (e.g., faults, bedding planes), and in situ stress orientation on the tunnel behaviour. Furthermore, the high displacements recorded at P5 ($\delta = 40$ mm) caused a substantial deviation of the strain field from polar symmetric conditions, thus suggesting possible heterogeneities within the rock mass, a non-circular tunnel geometry, or a poorly supporting shotcrete invert. The larger closure registered at the bottom half of the tunnel with respect to the top is also highlighted by the three longitudinal profiles of tunnel wall deformation shown in Fig. 6.18.

### 6.5.2 Anisotropy of tunnel wall deformation

In an attempt to further investigate the anisotropy of the tunnel deformation, convergences values were calculated by projecting the displacement vectors of Table 6.5 along six virtual convergence lines (Fig. 6.19). The absolute convergence values are reported in Table 6.6 together with the associated relative values defined as

$$d_c = \frac{d_{P_i - P_j}^0 - d_{P_i - P_j}^f}{d_{P_i - P_j}^0},$$

(6.2)

where $d_{P_i - P_j}^0$ and $d_{P_i - P_j}^f$ are the distances between points $P_i$ and $P_j$ ($i, j = 1 - 5$) at the time of instrument installation and at the end of the short-term deformation response (Fig. 6.19), respectively.

Minimum and maximum mean convergence values equal to 14 mm and 53 mm were obtained along
line 1-3 and 2-5, respectively, thus yielding a convergence ratio $\delta_{2-5}/\delta_{1-3}$ equal to 3.9. A convergence ratio as high as 2.3 was obtained for $\delta_{2-5}/\delta_{1-4}$, which approximately represented the ratio of deformation in the direction parallel and perpendicular to the bedding orientation. The average relative closure values varied between a minimum of 0.5% and maximum of 2.0% along line 1-3 and 1-5, respectively. Overall, this analysis shows that larger tunnel wall closures tended to occur along lines oriented approximately in the direction perpendicular to the bedding plane orientation (i.e., 5-3, 2-5, 1-5) and were influenced by the larger displacement measured at P5.

### 6.5.3 Elastic modelling

A preliminary elastic analysis of the FE tunnel excavation was carried out aimed at providing a reference model for the interpretation of the deformation response observed in the field (Section 6.4.2) and for the subsequent FEM/DEM simulations (Section 6.6). In this context, highly-simplifying assumptions were made regarding the material constitutive behaviour. More specifically, the deformability of Opalinus

### Table 6.6. Absolute and relative convergence values obtained by projecting the displacement vectors of Table 6.5 along the virtual convergence lines depicted in Fig. 6.19.

<table>
<thead>
<tr>
<th>Line</th>
<th>Convergence (mm)</th>
<th>Relative convergence, $d_c$ (%)</th>
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<tr>
<td></td>
<td>min</td>
<td>max</td>
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<tr>
<td>1-3</td>
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<td>49</td>
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<td>28</td>
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<tr>
<td>1-5</td>
<td>40</td>
<td>67</td>
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</tbody>
</table>
Fig. 6.20. Two-dimensional finite element mesh of the FE tunnel with 8-noded quadrilateral elements.

Clay was captured using a transversely isotropic, linear elastic medium with properties reported in Table 6.1, while material damage was not taken into account. Also, the effect of the tunnel lining was not incorporated into the model. The analysis was carried out using the finite element program Phase2, Version 8.0 (Rocscience Inc., 2011). The model consisted of a two-dimensional, plane-strain cross-section of the tunnel discretized with a graded, radial mesh of 8-node quadrilateral elements (Fig. 6.20). The boundary conditions were uniform pre-mining stress of state throughout the domain (Table 6.3) and zero displacement condition at the external boundary.

Excavation-induced stress and displacement fields

The distribution of elastic stresses is illustrated in Fig. 6.21a using the contour of deviatoric stress, $\sigma_1 - \sigma_3$. Upon tunnel excavation, the normal stress perpendicular to the excavation walls becomes zero and the excavation boundary a principal plane. Owing to the vertical orientation of the in situ maximum principal stress, an extensive stress redistribution is simulated in the sidewalls of the tunnel while a zone of low deviatoric stress developed in the roof and floor. As shown in Fig. 6.22, the circumferential stress around the opening wall, $\sigma_\theta$, is affected by the transversely isotropic elastic behaviour of the material with plane of isotropy oriented at $\psi = 33^\circ$. In particular, minimum and maximum values of 6.2 and 15.7 MPa are obtained at $\theta = 162^\circ$ ($342^\circ$) and $\theta = 108^\circ$ ($288^\circ$), respectively. For comparison, the stress distribution in the case of a linear elastic isotropic medium is characterized by minimum and maximum values of 7.0 and 15.0 MPa, respectively, located at the intersection of the principal field stress axes with the excavation boundary (i.e., $\theta = 90^\circ$ ($270^\circ$) and $\theta = 0^\circ$ ($180^\circ$)).

The analysis of the associated displacement field (Fig. 6.21b) reveals an even stronger influence of the material elastic anisotropy on the tunnel convergence. Due to the relatively low stiffness of Opalinus Clay in the direction perpendicular to the bedding, a maximum inward displacements of 7 mm is
obtained at \( \theta = 108^\circ \) and \( \theta = 288^\circ \), while a minimum value of 3 mm is simulated in the direction sub-parallel to the bedding (\( \theta = 18^\circ \) and \( \theta = 198^\circ \)). Based on the aforementioned displacement vector magnitudes, the elastic model clearly under-predicted the values measured in the field (Table 6.5). Had the numerical model incorporated also the confining effect of the liner and the simulated displacement values been reduced to account for the fact that rock mass convergence occurring prior to support installation was not picked-up by the geodetic monitoring, this discrepancy would have been even higher. In conclusion, although elastic models have met with some success in predicting the deformation response of excavations at the Mont Terri URL (e.g., Martin and Lanyon, 2003; Corkum and Martin, 2007b), this was not the case for the FE tunnel excavation. Consequently, numerical models that can capture deformation sources different than elastic strain, such as plastic yielding or rock dilation induced by brittle fracturing, should be adopted to capture the deformation response of the FE tunnel as measured in the field.

**Analysis of slip zones**

Slip zones are areas in a layered medium where the shear strength is reached point-wise along weakness planes of given dip and strength (Kumar, 1997). Despite the fact that the failure-induced stress redistribution is not taken into account when assessing the slip zones, this type of analysis has been typically adopted to identify regions of potential problem around excavations in layered rock masses (Daemen, 1983; Hoek and Brown, 1980b; Tonon and Amadei, 2003). In the case of the FE tunnel, the analysis of slip zones was carried out using the stresses calculated from the finite element analysis by assuming a set of ubiquitous joints with a friction angle \( \phi_b = 21^\circ \) and cohesion \( c_b = 1 \) MPa (Bock, 2009) accounting for the presence of bedding planes. The contours of strength factor against sliding is shown in Fig. 6.23. Two major slip zones develop in symmetric position with respect to the tunnel axis in the upper and
Chapter 6. Numerical analysis of the FE tunnel excavation

Fig. 6.22. Polar plot of elastic circumferential stress, $\sigma_\theta$, around the FE tunnel wall and hypothetical uniaxial compressive strength, $UCS$, for a transversely isotropic material such as Opalinus Clay. The circumferential stress, $\sigma_\theta$, coincides with the deviatoric stress, $\sigma_1 - \sigma_3$, at the tunnel boundary (Fig. 6.21). The hypothetical distribution of $UCS$ was obtained by amplifying 1.5 times the strength values obtained using calibrated laboratory-scale FEM/DEM models of Opalinus Clay with varying bedding orientation (Lisjak et al., 2013a, see Chapter 4). Indicated are also the typical failure modes of a hypothetical Opalinus Clay specimen oriented parallel to the tunnel wall and loaded in unconfined compression.

Fig. 6.23. Analysis of slip zones. Contours of strength factors against sliding along joints inclined at $\psi = 33^\circ$. The strength factor is calculated as the ratio of the shear strength, defined by a Mohr-Coulomb criterion with $\phi_b = 21^\circ$ and $c_b = 1$ MPa, to the shear stress from the elastic analysis. The strength of intact matrix is not considered.
lower part of the left and right sidewall, respectively (i.e., $126^\circ \leq \theta \leq 189^\circ$ and $306^\circ \leq \theta \leq 9^\circ$). These two zones extend in the rock mass for about 0.9 m from the tunnel walls. Moreover, two slip zones of shorter extension (0.45 m) are simulated in the tunnel back and invert for $63^\circ \leq \theta \leq 117^\circ$ and $243^\circ \leq \theta \leq 297^\circ$.

The polar orientation of the aforementioned slip zones correspond to critical values of relative orientation between compressive stress around the excavation boundary and bedding favourably oriented for slippage. Therefore, the angular position of the slip zones can be analyzed with reference to the polar distribution of circumferential stress, $\sigma_\theta$, and the uniaxial compressive strength, $UCS$, of a hypothetical rock core oriented parallel to the excavation boundary (Fig. 6.22). Slip zones correspond roughly with $UCS$ values smaller than $\sigma_\theta$. The location of slip zones is consistent with zones of high tunnel wall convergences measured in the field.

### 6.6 Combined finite-discrete element analysis

#### 6.6.1 Brief description of FEM/DEM

The combined finite/discrete element method (FEM/DEM) is a numerical method which combines continuum mechanics principles with DEM algorithms to simulate multiple interacting deformable bodies (Munjiza et al., 1995; Munjiza, 2004). In FEM/DEM, each solid is discretized as a mesh consisting of nodes and triangular elements. An explicit time integration scheme is applied to solve the equations of motion for the discretized system and to update the nodal coordinates at each simulation time step.

The progressive failure of rock material is captured by a cohesive-zone approach. With this technique, the failure of the material progresses based solely on the strength degradation of dedicated interface elements (referred hereinafter to as crack elements), which are inserted between each pair of triangular elements at the very beginning of the simulation (Fig. 6.24a). Therefore, material damage emerges as a natural outcome of the deformation process without employing any additional macroscopic failure criterion. The constitutive response of a crack element is defined in terms of variation of the bonding stresses, $\sigma$ and $\tau$, between the edges of the triangular element pair as function of the crack relative displacements, $o$ and $s$, in the normal and tangential direction, respectively (Fig. 6.24b). In tension (i.e., mode I), the response of each crack element depends on the cohesive tensile strength, $f_t$, and the mode I fracture energy release rate, $G_{Ic}$. In shear (i.e., mode II), the behaviour is governed by the peak shear strength, $f_s$, and the mode II fracture energy release rate, $G_{IIc}$. The peak shear strength is defined as

$$f_s = c + \sigma_n \tan \phi_i$$

where $c$ is the cohesion, $\phi_i$ is the internal friction angle, and $\sigma_n$ is the normal stress acting across the crack element. Upon breaking a crack element, a purely frictional resistance, $f_r$, is assumed to act along each newly-created discontinuity:

$$f_r = \sigma_n \tan \phi_f$$

where $\phi_f$ is the fracture friction angle. For mixed mode I-II fracturing, an elliptical coupling relationship
is adopted between crack opening, \( o \), and slip, \( s \) (Fig. 6.24c).

Since the material strain is expected to be localized in the cohesive zone, the bulk material is treated as linear elastic using constant-strain triangular elements. Although no deformation should in theory occur in the crack elements before the cohesive strength is exceeded, a finite stiffness is required by the time-explicit formulation of FEM/DEM. Such an artificial stiffness is represented by the normal, tangential and fracture penalty values, \( p_n \), \( p_t \) and \( p_f \), for compressive, shear and tensile loading conditions, respectively. For practical purposes, the cohesive contribution to the overall model compliance can be largely limited by adopting very high (i.e., dummy) penalty values (Munjiza, 2004; Mahabadi, 2012).

In this study, the simulation of material anisotropy followed the approach first developed by Lisjak et al. (2013a) (see Chapter 4) to model the mechanical response of Opalinus Clay and implemented in the two-dimensional Y-Geo code (Mahabadi et al., 2012a). In particular, the modulus anisotropy is captured by a transversely isotropic, linear elastic constitutive law implemented at the triangular element level. The elastic deformation is therefore fully characterized by five independent elastic parameters: two Young’s moduli, \( E_P \) and \( E_S \), and Poisson’s ratios, \( E_P \) and \( E_S \), for the direction parallel and perpendicular to the plane of isotropy, and the shear modulus, \( G_S \). The anisotropy of strength is instead introduced at the crack element level by imposing that the cohesive strength of each crack element is a function of the relative orientation, \( \gamma \), between the crack element itself and the bedding orientation (Fig. 6.25a). The cohesive strength parameters and the fracture energy release rates are assumed to vary linearly between a minimum value for \( \gamma = 0^\circ \) (i.e., \( f_{t,\text{min}}, c_{\text{min}}, G_{Ic,\text{min}}, G_{IIc,\text{min}} \)) to a maximum value for \( \gamma = 90^\circ \) (i.e., \( f_{t,\text{max}}, c_{\text{max}}, G_{Ic,\text{max}}, G_{IIc,\text{max}} \)). Furthermore, the mesh topology combines a random triangulation for the intra-layer material (i.e., matrix) together with crack elements preferably aligned

\[
\begin{align*}
\sigma & = \text{Normal Bonding Stress}, \\
\tau & = \text{Tangential Bonding Stress}, \\
\phi & = \text{friction angles}, \\
f_p, c & : \text{cohesive strengths}, \\
p_n, p_t, p_f & : \text{penalty parameters}, \\
o, s & : \text{crack opening and sliding}, \\
h & : \text{element size}, \\
n, r & : \text{normal, tangential}, \\
G_{Ic}, G_{IIc} & : \text{fracture energy release rates}, \\
\theta & : \text{crack relative displacement}, \\
\text{Mode I}, \text{Mode II} & : \text{fracture modes}.
\end{align*}
\]
Fig. 6.25. FEM/DEM modelling of strength anisotropy. (a) Linear variation of cohesive strength parameters with the angle, $\gamma$, between crack element and bedding. (b) Example of mesh combining a Delaunay triangulation for the intra-layer material with edges preferentially aligned along the bedding plane direction. (Source: Lisjak et al. (2013a))

along the bedding planes (Fig. 6.25b).

6.6.2 Model description

Geometry, mesh generation and input parameters

The model geometry for the FEM/DEM analysis consisted of the 3.0 m diameter, circular cross-section of the FE tunnel placed at the centre of a 50 m $\times$ 50 m square domain (Fig. 6.26). The cross-section was assumed perpendicular to the strike of bedding planes with layering inclined at $\psi = 33^\circ$ (Section 6.2.2). To maximize the model resolution in the EDZ while keeping the run times within practical limits, a mesh refinement zone, with average element size of 0.03 m, was adopted around the excavation boundary. In this zone, the layering thickness, $t$, was set to 10 cm. The refinement zone extended radially for $d_r = 4.0$ m around the tunnel walls. From the refinement zone the element size was then graded towards the external boundaries, where an element size equal to 0.6 m was used. The total number of triangular elements employed was approximately 180,000. Equations of motion for the discretized system were integrated with a time step of $5 \times 10^{-4}$ ms; this value was the largest time step size that ensured numerical stability for the explicit solver of the code. The FEM/DEM Graphical User Interface Y-GUI (Mahabadi et al., 2010b) was used to assign boundary conditions and material properties to the model.

The choice of cohesive strength parameters was initially based on the laboratory-scale calibration process carried out by Lisjak et al. (2013a) (see Chapter 4) for the shaly facies of the Mont Terri Opalinus Clay (Bock, 2009). Given the coarser spatial discretization of the field-scale models, the input strength parameters were then re-calibrated to match the average field measurements reported in Section 6.4. On
the other hand, the experimental values of the elastic constants reported in Table 6.1 were directly used as input for the transversely isotropic elastic model, as the material deformability is governed by the continuum formulation of the triangular elements and is therefore independent of the adopted element size and topology (Munjiza, 2004). The finalized input parameters of the crack elements are reported in Table 6.7. Both the cohesive strength parameters and the fracture energy values were increased by 2.75 times with respect to the laboratory-calibrated ones. Conversely, the friction angles, \( \phi_i \) and \( \phi_f \), were left unchanged. Based on the recommendations of Mahabadi (2012), the penalty values, \( p_n \), \( p_t \) and \( p_f \), were set equal to \( 10 \times \), \( 1 \times \) and \( 5 \times \) the largest Young’s modulus, \( E_P \), respectively, to minimize the effect of the crack element compliance on the overall model stiffness (Mahabadi, 2012). Also, a critical viscous damping coefficient, \( \mu = 1.79 \times 10^3 \) kg/m·s, was applied to the model to dissipate dynamic oscillations and thus approximate a quasi-static behaviour.

In first approximation, bedding-parallel tectonic faults (Section 6.2.2) were not explicitly included into the model. By doing so, any kinematic constraint potentially imposed on the rock mass response by the presence of these discontinuities could not be captured. However, the associated reduction of strength from the intact material values was implicitly accounted for via calibration of equivalent homogenous material properties.

**In situ stress and boundary conditions**

The in situ stress field reported in Table 6.3 was used for the calibration of the FEM/DEM model. Since the adopted crack elements do not account for the influence of an out-of-plane stress during the simulation of fracture nucleation and growth, only the in-plane stresses were effectively used in the analysis. Also, gravity-induced stress gradients were neglected in all models. The effect of varying the orientation and magnitude of the in-plane in situ stress field was also investigated and the results

---

**Fig. 6.26.** Geometry and boundary conditions of the FEM/DEM model of the FE tunnel excavation.
Table 6.7. Input parameters of the crack elements for the FEM/DEM simulation of the FE tunnel excavation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cohesive strengths</td>
<td></td>
</tr>
<tr>
<td>Tensile strength parallel to bedding, $f_{t,\text{max}}$ (MPa)</td>
<td>1.8</td>
</tr>
<tr>
<td>Tensile strength perpendicular to bedding, $f_{t,\text{min}}$ (MPa)</td>
<td>0.44</td>
</tr>
<tr>
<td>Cohesion parallel to bedding, $c_{\text{min}}$ (MPa)</td>
<td>2.8</td>
</tr>
<tr>
<td>Cohesion perpendicular to bedding, $c_{\text{max}}$ (MPa)</td>
<td>24.8</td>
</tr>
<tr>
<td>Fracture energy release rates</td>
<td></td>
</tr>
<tr>
<td>Mode I fracture energy parallel to bedding, $G_{Ic,\text{max}}$ (J/m$^2$)</td>
<td>19.5</td>
</tr>
<tr>
<td>Mode I fracture energy perpendicular to bedding, $G_{Ic,\text{min}}$ (J/m$^2$)</td>
<td>1.0</td>
</tr>
<tr>
<td>Mode II fracture energy parallel to bedding, $G_{IIc,\text{min}}$ (J/m$^2$)</td>
<td>27.5</td>
</tr>
<tr>
<td>Mode II fracture energy perpendicular to bedding, $G_{IIc,\text{max}}$ (J/m$^2$)</td>
<td>96.5</td>
</tr>
<tr>
<td>Friction angles</td>
<td></td>
</tr>
<tr>
<td>Friction angle of intact material, $\phi_i$ ($^\circ$)</td>
<td>22</td>
</tr>
<tr>
<td>Friction angle of fractures, $\phi_f$ ($^\circ$)</td>
<td>22</td>
</tr>
<tr>
<td>Cohesive stiffnesses</td>
<td></td>
</tr>
<tr>
<td>Normal contact penalty, $p_n$ (GPa·m)</td>
<td>38</td>
</tr>
<tr>
<td>Tangential contact penalty, $p_t$ (GPa/m)</td>
<td>3.8</td>
</tr>
<tr>
<td>Fracture penalty, $p_f$ (GPa)</td>
<td>19</td>
</tr>
</tbody>
</table>

reported in Section 6.6.5.

The initialization of each model with the prescribed *in situ* stress field was accomplished by a preliminary elastic run (i.e., without crack elements) which aimed at obtaining the revised nodal coordinates of the non-excavated model subjected to the prescribed far-field stresses. These revised nodal coordinates were subsequently used as the current nodal coordinates (i.e., deformed mesh) of the actual FEM/DEM simulation run in which crack elements were inserted into the model to capture material failure. By changing the far-field boundaries to be fixed in the horizontal and vertical directions, the first order *in situ* stress conditions were maintained while allowing the excavation sequence to be modelled.

**Modelling procedure for excavation advance**

It is common engineering practice to carry out stress-strain analyses of tunnel cross-sections distant from the face under two-dimensional, plane strain conditions. However, solving the distribution of stresses in the rock mass surrounding an advancing tunnel in proximity to the excavation face is a three-dimensional problem. If a support system is installed behind the excavation face, part of the load re-distributed around the excavation is carried by the face itself. Consequently, the direct application of two-dimensional numerical models to the evaluation of the stress and strain fields in the cross-section of a supported tunnel may result in non-negligible inaccuracies (Curran et al., 2003). As the tunnel advances, the supporting action of the face decreases and, at a certain distance, plane strain conditions are attained (Carranza-Torres and Fairhurst, 2000). A two-dimensional analysis can be realistically
Fig. 6.27. Modelling procedure for excavation advance and support installation using the core replacement technique in FEM/DEM. (a) Replacement of core with reduced elastic modulus material. (b) Installation of tunnel lining. (c) Qualitative example of ground reaction curve simulated via stepwise modulus reduction and support characteristic curve for a linear elastic lining.

employed only if the displacements of the excavation boundary prior to support installation can be estimated. Furthermore, in the case of the FE tunnel, the amount of tunnel deformation occurring before the installation of lining and convergence points needed to be estimated to allow a direct comparison of numerical results with field measurements.

To capture the supporting effect of the tunnel face in the two-dimensional FEM/DEM model, a core replacement technique was implemented for this study based on the approach first developed by Curran et al. (2003). With this technique, the three-dimensional face effect, which causes a gradual reduction of radial resistance around the excavation boundary, is captured by a fictitious, softening elastic material in the tunnel core. That is, the deformation modulus of the excavated material is progressively reduced from the original rock mass values, corresponding to an undeformed section far ahead of the face, to a value that results in the wall displacements at the time of support installation. The general procedure for modelling excavation advance and support installation in FEM/DEM consisted of the following main steps, graphically summarized in Fig. 6.27:

1. The amount of tunnel wall deformation that occurred prior to support installation was estimated from the longitudinal displacement profile (LDP) of the tunnel and compared with the inclinometer measurements. In practice, the determination of the LDP is often based on a finite element analysis using either axisymmetric or three-dimensional models is often carried out, depending on the level of complexity of the tunnel geometry (i.e., circular vs. non-circular shape), in situ stress field (i.e., isotropic vs. anisotropic), and material property distribution (i.e., homogeneous vs. heterogeneous). Alternatively, analytical or numerical parametric solutions have been proposed for the cases of linear elastic (Panet, 1995; Unlu and Gercek, 2003) or elasto-plastic material behaviour (e.g., Panet and Guenot, 1982; Vlachopoulos and Diederichs, 2009).

In the present study, the LDPs proposed by Vlachopoulos and Diederichs (2009) were adopted in an attempt to estimate the percentage of convergence that occurred before the simultaneous
installation of the measuring targets and application of the shotcrete layer. The simulated displacements were then reduced by this percentage for direct comparison with field measurements. Firstly, the normalized closure at tunnel face, \( u_0^* \), was determined as

\[
u_0^* = \frac{u_0}{u_{\text{max}}} = \frac{1}{3} e^{-0.15 R^*},
\]

where \( u_0 \) is the radial displacement at the tunnel face, \( u_{\text{max}} \) is the maximum, short-term radial displacement distant from the face, and \( R^* \) is the ratio of the plastic radius, \( R_P \), to the tunnel radius, \( R \). A value of \( u_0^* \) equal to 27% was obtained by assuming \( R_P = 2 \) m and \( R = 15 \) m. For comparison, the inclinometer recordings reported in Section 6.4.4 indicated that the vertical displacement in the crown measured above the excavation face (i.e., \( z = 0 \) m) was, on average, 36% of the maximum short-term displacement experienced at the given tunnel section (Fig. 6.16). Then, the amount of convergence at a distance \( z = 1.0 \) m behind the tunnel face, which corresponded to the distance of support and measuring targets installation (Section 6.4.2), was estimated to be equal to 55% from

\[
\frac{u}{u_{\text{max}}} = 1 - (1 - u_0^*) \cdot e^{-(3z)/(2 R^*)}.
\]

This value is in agreement with 3D modelling results relative to the ED-B tunnel (Corkum and Martin, 2007b), indicating that approximately 50% of convergence occurred prior to installation of a convergence array.

2. Using the core replacement technique, the modulus reduction necessary to obtain the amount of tunnel wall displacement calculated in Step 1 was determined. To this end, a FEM/DEM simulation was run whereby the elastic parameters of the fictitious core material (i.e., \( E_x, E_y, G \)) were reduced in a stepwise fashion over time by a softening ratio, \( \alpha_s \), and the wall displacements recorded. The result was the plot of the tunnel wall displacements, \( \delta \), as function of the core softening ratio, \( \alpha_s \), depicted in Fig. 6.28.

3. The FEM/DEM simulation was then re-run by allowing the excavation boundary to relax up to the point where the prescribed wall displacements, equal to the convergence measured at the time of support installation, were obtained and by subsequently adding the support. The tunnel deformation was again monitored for comparison with experimental measurements.

**Modelling procedure for support installation**

The application of shotcrete on the walls of the FE tunnel was modelled using the constant-strain, triangular elements implemented in FEM/DEM (Munjiza, 2004). Since the constitutive response of the support is at present limited to isotropic, linear elastic conditions (i.e., fracturing is not allowed), the mechanical behaviour of the shotcrete was fully characterized by Young’s modulus, \( E_c = 8 \) GPa, and Poisson’s ratio, \( \nu_c = 0.20 \). The support installation consisted of specifying the liner thickness,
Fig. 6.28. Simulated ground response curve for the FE tunnel excavation. Total displacement, $\delta$, vs. softening ratio of the core material, $\alpha_s$, at five points along the tunnel boundary.

$t_c = 16$ cm, and the installation time from the appropriate core softening ratio, $\alpha_s$. Since the delayed installation of shotcrete was accomplished by varying the elastic properties of the liner from those of the rock mass to those of the shotcrete (Fig. 6.27b), the deformation in the liner had to be zeroed to avoid an artificial build-up of stress in response to an instantaneous increase of material stiffness in a pre-stressed medium. This was accomplished by a newly-implemented routine, which sets the nodal coordinates of the deformed configuration (i.e., at the installation time) as new initial (i.e., undeformed) coordinates for the triangular mesh of the support. The radial reinforcement of the rock mass using rock bolts was not included in the model.

### 6.6.3 Simulated deformational response

The FEM/DEM model was calibrated to match the averaged short-term tunnel wall displacements measured between TM 10.6 and 34.3 (Section 6.5.1). For this purpose, an iterative, trial-and-error calibration procedure was adopted which involved varying material properties, and support installation time and stiffness. The best overall fit to the in situ observations was obtained for the input parameters reported in Table 6.7 by applying a core softening ratio $\alpha_s = 0.01$ (Fig. 6.28) before activating the 16 cm thick support layer with a Young’s modulus $E_c = 10$ MPa.

### Tunnel wall convergence

The evolution of total displacement, $\delta$, at the five measurement sites corresponding to the position of the convergence targets P1 to P5 is depicted in Fig. 6.29a together with the corresponding averaged experimental values (Table 6.5). To allow a comparison with field values, the displacements recorded since the start of the simulation were discounted by the deformation component occurring before the activation of the support. This component was on average equal to 50% of the overall deformation and thus satisfactorily matched the target value of 55% estimated from the tunnel LDP. As expected, the
numerical model tended to exhibit a polar symmetric deformation behaviour induced by the assumptions of homogeneous, transversely isotropic material and circular excavation shape. That is, the displacement evolution at P1 and P2 followed that of P4 and P5, respectively. As illustrated below, large displacements developing at P2 and P5 were a direct consequence of rock mass dilation induced by brittle fracturing.

With respect to the field measurements, the FEM/DEM model underestimated the wall displacements at P1 and P4 by approximately 9 mm, while captured the lower bound of the response at P3. The displacement at P2 matched the associated experimental value, while the displacement of P5 was again underestimated by about 15 mm with respect to the average field value. Overall, the point-wise comparison of numerical and experimental values was, to a certain degree, skewed by the heterogeneous response of the actual excavation (possibly due to the presence of tectonic faults), which the homogenous model had no means to capture. Therefore, an alternative comparison was carried out by considering the relative displacements between the target points in lieu of absolute displacements. To this end, a comparison between measured and simulated convergences is shown in Fig. 6.29b. As expected, values obtained from the elastic analysis (Section 6.5.3) substantially under-predicted the field measurements, thus suggesting the fact that linear elasticity was not the main source of deformation. Conversely, an overall good fit of the experimental data was provided by the FEM/DEM model, which reproduced well the anisotropic response of the rock mass. The most notable exception was Convergence Line 1-5, along the bottom of the tunnel, which was under-predicted by approximately 30 mm. This discrepancy may be explained by several factors, including the presence of an area of local material weakness around P5 (e.g., fault zone), a high deviatoric stress concentration induced by a sharp corner in the excavation geometry due to the presence of a flat temporary invert, and poor quality and/or reduced thickness of the shotcrete layer. Note that three months after the completion of the tunnel the invert had to be re-excavated and new reinforcement installed. Furthermore, a less fit was obtained along Line 1-4 for which the model predicted a mainly elastic behaviour while again dilation might have resulted in larger than predicted inward deformations.

**Support stiffness**

As described in Section 6.3.1, large tunnel wall displacements were measured in the field in response to the rock mass squeezing conditions. Since these deformations occurred while a layer of mesh-reinforced shotcrete was applied to the tunnel surfaces, the effect of the tunnel support stiffness on the rock mass response was further investigated. Upon activation of the support, increasingly larger displacements were captured for decreasing values of the elastic modulus of the shotcrete, $E_c$ (Fig. 6.30), while higher $E_c$ values resulted in higher support stiffness, $K_s$, and consequently steeper support characteristic curves (Fig. 6.27c) which in turn prevented further tunnel wall displacements. For very low $E_c$ values (1 MPa), equilibrium was not reached and tunnel collapse simulated. In the field, testing on shotcrete cores indicated an average Young’s modulus equal to 8 and 14 GPa at 1 and 7 days, respectively. As demonstrated by Fig. 6.30, if such high values were directly used as input in the model, the deformation observed in situ could not be reproduced. This seemingly inconsistent behaviour may be explained by several factors. Firstly, the model did not account for a time-dependent increase of material stiffness due to cur-
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Fig. 6.29. Comparison of simulated tunnel wall deformation with averaged field measurements. (a) Evolution of total displacement, $\delta$, at five points along the tunnel boundary. Error bars indicate the range of variation of the correspondent field measurements (Table 6.5). (b) Convergences associated with the displacements of the elastic finite element model, the final displacements at equilibrium of the FEM/DEM analysis, and the average field measurements (Section 6.5.2).

Instead, a steady value was adopted immediately after the activation of the support layer. Secondly, the squeezing conditions of the rock mass might have resulted in yielding and failure of the shotcrete layer. Yielding of the shotcrete layer is indeed consistent with stress measurements from the load cells installed at TM 14 which indicated average compressive stress values of about 6 MPa with a maximum value as high as 16 MPa. Conversely, a fully elastic formulation was adopted in the numerical model for the support. Finally, large tunnel convergences might have been due to poor adhesion of the shotcrete coating to the rock surfaces (Reinhold, 2012), or to a non-perfectly-circular cross section of the excavated tunnel.

Radial deformation and vertical deflection in the crown

The simulated radial displacement, $\delta_r$, along two orthogonal lines, EXT-01 and EXT-02, corresponding to the location of extensometers BFEC-01 and BFEC-02 (Section 6.4.3), is shown in Fig. 6.31. A quantitative comparison of the simulated values with the in situ values shown in Fig. 6.15 was not possible due to the relative character of field measurements and the fact that radial extensometers captured only a limited portion of the total deformation field within the rock mass. Nevertheless, the similar variation in response as function of the polar direction increases the confidence in the numerical results and thus can be used to provide further insight into the fracturing process around the tunnel. In the direction parallel to bedding (EXT-01), the FEM/DEM model predicted a relatively smooth decrease in radial deformation with increasing distance from the tunnel wall. This behaviour reflected the general absence of fracturing and consequent deformation behaviour associated mainly with the elastic redistribution of stress around the tunnel. Conversely, a number of displacement jumps were simulated in the direction...
perpendicular to bedding (EXT-2) due to extensive loss of material continuity occurring in close proximity to the excavation boundary (i.e., within about 1.0 m). This behaviour is consistent with rock mass bulking due to open fractures and inward movement of rigid rock blocks.

Following the evolution of vertical displacement, $\delta_v$, of two measuring points, INCL-10 and INCL-11, in the crown of the tunnel corresponding to the sub-horizontal inclinometers BFEA-10 and BFEA-11 (Section 6.4.4) (Fig. 6.31b), displacement values of 8 and 10 mm were recorded at equilibrium in correspondence of EXT-10 and EXT-11, respectively. For comparison, an average displacement equal to 21.5 mm was measured by the inclinometer chains between TM 9 and 38, corresponding to the reference section for the numerical calibration (Fig. 6.16).

### 6.6.4 Simulated fracturing behaviour

The evolution of fracturing around the FE tunnel responsible for the simulated deformation response described in Section 6.6.3 is reported in the sequence of Fig. 6.32. Failure around the excavation boundary initiates at approximately $120^\circ \leq \theta \leq 195^\circ$ and $-60^\circ \leq \theta \leq 15^\circ$ in the form of shear-dominated (i.e., mode II) fractures along the bedding planes (Fig. 6.32a). The azimuthal position and extension of these two damaged zones roughly correspond to the two major slip zones captured by the elastic analysis with ubiquitous joints (Fig. 6.23). As discussed in Section 6.5.3, failure around the tunnel is triggered by the excavation-induced stress redistribution in combination with the reduced strength of bedding planes favourable oriented for slip. As the simulation progresses, the slippage of bedding planes causes a local perturbation in the stress field which results in the nucleation of strain-driven, mode I fractures in the direction perpendicular to the layering (Fig. 6.32b). Also, further bedding-parallel sliding is simulated at about $70^\circ$ and $250^\circ$, thus corresponding to the secondary slip zones in the back and roof of the ubiquitous joint, elastic model (Fig. 6.23). Further rock mass deconfinement triggers further delamination.
**Fig. 6.31.** Simulated rock mass deformation around the FE tunnel. (a) Total radial displacement, $\delta_r$, along two lines, EXT-01 and EXT-02, corresponding to the location of extensometers installed in boreholes BFEC-01 and BFEC-02, and (b) evolution of vertical displacement, $\delta_v$, measured at two points, INCL-10 and INCL-11, corresponding to inclinometers BFEA-10 and BFEA-11.

**Fig. 6.32.** Simulated evolution of fracture growth around the FE tunnel at increasing simulation times corresponding to different stages of the core modulus reduction sequence.
Fig. 6.33. Final stress distribution simulated for the FE tunnel. Colour contours in a) and b) represent maximum and minimum principal stress, $\sigma_1$ and $\sigma_3$, respectively. Associated principal stress directions are indicated by short straight lines.

of bedding planes (Fig. 6.32c) with formation of wing-shaped fractured zones that tend to extend out in the direction parallel to the bedding to a distance of about 3 m from the sidewalls. After installing the support, the propagation of damage away from the opening is suppressed in favour of fragmentation in close proximity to the excavation boundary until new equilibrium conditions are reached (Fig. 6.32d).

The stress and displacement fields corresponding to the final stable configuration of Fig. 6.32d are shown in Fig. 6.33 and 6.34, respectively. The redistribution of compressive stress in response to the tunnel excavation is influenced by the in situ stress anisotropy as well as the characteristic fracture pattern with bedding-parallel discontinuities and a heavily fractured zone around the tunnel. The lateral extension of the EDZ due to bedding delamination is suppressed by the re-orientation of $\sigma_1$ in the direction perpendicular to bedding. In proximity to tunnel boundary, bedding plane slippage promotes a drastic reduction of confining stress, $\sigma_3$, with low to moderately negative values responsible for the observed extensional fracturing.

The total displacement field associated with the tunnel configuration at equilibrium is depicted in Fig. 6.34 together with the location of the virtual extensometers, EXT-01 and EXT-02, and the inclinometers, INCL-10 and INCL-11 (Section 6.4.2). At a distance from the excavation, the rock mass behaves elastically and therefore small strains, induced by the stress redistribution around the damaged zone, are simulated. Due to the highly anisotropic rock mass response, this distance varies between a minimum of 0.5 m to a maximum of 3 m in the direction parallel to bedding and in the sidewalls, respectively. Furthermore, elastic deformations of higher intensity are captured in the direction sub-perpendicular to the bedding orientation due to the high rock compressibility in the said direction (Ta-
ble 6.7). In the excavation near-field, an inner and an outer shell can be identified. The shape of the inner zone is roughly a 4.5 m × 4.5 m square with edges oriented in the direction parallel and perpendicular to the bedding and centre coincident with the tunnel axis. In this zone, the rock mass deformation is governed by a combination of mode I and mode II fracturing and bulking, thus resulting in large displacements (i.e., \( \delta > 3 \) cm). In the outer shell, while mode II fractures can still nucleate, the relative sliding along the fracture surfaces is limited by higher values of confining stress, \( \sigma_3 \). Consequently, the growth of extensional fractures is effectively inhibited.

The radial extension of the fractured zone in the direction parallel (i.e., along EXT-01) and perpendicular (i.e., along EXT-02) to bedding is equal to approximately 0.5 and 1.5 m. These estimations are consistent with the possible experimental limits of the EDZ estimated from pore water pressure measurements and equal to 2.3 and 2.8 m, respectively (Garitte and Vietor, 2012).

A quantitative comparison of the simulated fracture pattern and damage mechanism with in situ observations was at present not possible due to the lack of experimental data. This limitation will likely be overcome thanks to a currently on-going investigation program aimed at characterizing the shape and extent of the EDZ around the FE tunnel. Nevertheless, the simulated fracturing behaviour is in good qualitative agreement with previous experimental observations from the Mont Terri URL described in Section 6.3.1. A remarkable similarity between breakout location and types of fractures (i.e., bedding plane delamination and extensional fractures) can indeed be noticed between Fig.s 6.6 and 6.5 and the simulated fracture pattern reported in Fig. 6.32d.

### 6.6.5 Effect of varying in situ stress conditions

The influence of in situ stress anisotropy and magnitude on the fracture development around the FE tunnel was simulated for the three cases reported in Table 6.3. The final fracture patterns with the associated contours of total displacement, \( \delta \), are depicted in Fig. 6.35. Under highly anisotropic in situ stress conditions \( (K_0 = 0.38, \text{Fig. 6.35a}) \), secondary slip zones in the roof and floor are suppressed in favour of further bedding parallel fracturing in the direction parallel to bedding in the upper left and lower right parts of the tunnel section. A zone of heavy rock mass fragmentation is associated with the high concentration of deviatoric stress in tunnel sidewalls. Under isotropic far-field stresses \( (K_0 = 1.0, \text{Fig. 6.35b}) \) the failure pattern is symmetric with respect to the bedding orientation and consists of a heavily fragmented square zone of size 5 m × 5 m together with bedding-parallel shear fractures extending out from its corner in the direction parallel to bedding. Finally, if the horizontal stress is increased to 8.5 MPa while keeping the overburden depth unaltered \( (K_0 = 1.31, \text{Fig. 6.35c}) \), equilibrium cannot be reached, thus indicating that additional support should be applied to stabilize the rock mass. An intermediate fracture pattern shows again bedding plane slippage in the sidewalls and haunch areas accompanied by spalling in proximity of the tunnel boundary. Additionally, the flow of maximum principal stress around the opening promotes extensive fracturing in the back and invert, resulting in a vertically elongated damaged zone which will eventually lead to the collapse of the hole.
Fig. 6.34. Simulated total displacement field, $\delta$, around the FE tunnel corresponding to the fracture pattern and stress distribution of 6.32d and Fig. 6.33, respectively. The radial displacement, $\delta_r$, along lines EXT-01 and EXT-02 is reported in Fig. 6.31a. The evolution of vertical displacement, $\delta_v$, at points INCL-10 and INCL-11 is shown in Fig. 6.31b. Indicated is also the location of the two boreholes, BFEA-02 and BFEA-05, with the closest piezometers to the tunnel walls.

Fig. 6.35. Effect of *in situ* stress conditions on the fracture pattern and total displacement field around the FE tunnel. Note that for $K_0 = 1.31$ equilibrium could not be reached.


### 6.6.6 Model limitations

#### Three-dimensional effects

In this study, a two-dimensional FEM/DEM analysis was adopted to provide an interpretation of the FE tunnel deformation response observed in the field in terms of possible fracturing behaviour. In particular, the numerical model was calibrated based on measurements of tunnel wall convergence carried out during the excavation advancement. Both excavation sequence and distance to the face were indirectly taken into account by an equivalent two-dimensional model section with variable support pressure obtained through a core replacement technique. By accounting for the effect of stress release before the activation of the lining resistance, the technique allowed to compare the numerical results with the experimental data. However, only a three-dimensional stress analysis is able, in general, to capture the evolution of the primary stress field and associated ground deformation as the tunnel approaches and passes through a volume of rock (Duddeck, 1991). That is, two-dimensional models neglect several factors that are inherently three-dimensional, including the influence of stress path and loading history, and the effect of the axial (i.e., intermediate) principal stress (Pan and Hudson, 1988). In this regard, Eberhardt (2001) showed that the progressive advancement of a tunnel face is associated with a spatio-temporal evolution of the three-dimensional stress field which undergoes a series of deviatoric stress increases and/or decreases as well as several rotations of the principal stress axes. Consequently, since rock mass damage and strength degradation is largely dependent upon the deviatoric stress magnitude and the orientation of the principal stresses, the tunnel behaviour in the near-field will be necessarily influenced by three-dimensional effects occurring ahead of the face. As discussed by Diederichs et al. (2004), the rotation of stresses can induce damage oriented at angles other than the final boundary-parallel crack directions as well as affect the conditions for further crack propagation. If these three-dimensional effects are significant, errors may arise in the two-dimensional FEM/DEM analysis, which by nature allows to capture only fractures striking in the direction parallel to the tunnel axis.

In Opalinus Clay, the situation is further complicated because damage arises from a complex interaction between the aforementioned three-dimensional stress field and geological structures such as bedding planes and bedding-parallel tectonic faults. At the Mont Terri URL, experimental evidence suggests that the excavation yielded/fractured zone does not develop exclusively along the tunnel periphery behind the excavation face but surrounds the excavation face itself of which it may affect the stability. For example, Nussbaum et al. (2011) observed a pattern of bedding-parallel, shear-dominated fractures on the tunnel face of Gallery 08 excavated against the layering dip (Fig. 6.4c). Likewise, by integrating geophysical measurements with 3D numerical simulations, Yong et al. (2013) showed that the characteristics of the perturbation zone ahead of the EZ-B niche was dependent upon the distance beyond face. For the case of excavations parallel to the bedding strike, such as the FE tunnel and the FE niche, the existence of a pattern of spherical fractures developing around the excavation face was postulated based on field mapping of exposed excavation-induced, rock mass discontinuities (Jaeggi et al., 2012a, 2013).

In conclusion, a more accurate analysis of the fracturing behaviour around the FE tunnel would require adopting a three-dimensional FEM/DEM model. However, such type of analysis is at present...
impractical due to the excessively high computational demand of hybrid finite-discrete element simulations (Munjiza et al., 2012).

**Hydro-mechanical coupling**

Changes in pore water pressure were recorded in the rock mass surrounding the FE tunnel as the excavation progressed (Garitte and Vietor, 2012). Qualitatively, this evolution of pore pressure was consistent with the elastic stress redistribution occurring in response to the excavation. Conversely, the FEM/DEM model did not account for any sort of pore pressure variation such as instantaneous hydro-mechanical coupling or fluid flow effects.

Modelling fluid flow and associated phenomena (e.g., rock mass desaturation and pore pressure dissipation with time) is an essential component of simulations aimed at studying the the long-term evolution of the EDZ. However, the short-term response of Opalinus Clay considered in this study is typically analyzed using a total stress analysis. As discussed by Martin and Lanyon (2003), the excavation-induced response can be treated as an undrained response because of the fast advancement rate involved and the low hydraulic conductivity, \( K \), of Opalinus Clay, ranging between \( 2 \times 10^{-14} \) and \( 2 \times 10^{-12} \) m/s (Marschall et al., 2004), which cause stress-induced pore pressure disturbance to dissipate over a relatively large timescale. In clay shales, drained conditions are to be expected when the \( K \) value is higher than \( 10^{-7} \) to \( 10^{-6} \) m/s and the net excavation advance rate is less than \( 0.1 - 1 \) m/h (Anagnostou and Kovári, 1996). Failing to capture the instantaneous poromechanical effects occurring when the mechanical loading rate is higher than the fluid pressure dissipation rate (i.e., undrained conditions) may result in model inaccuracies. Firstly, if the spikes of pore pressure are such that the intact tensile strength of the rock is overcome, pore-pressure-induced yielding (i.e., hydraulic fracturing) may occur. However, in rocks, the material contraction in the direction of the maximum principal stress is typically associated with the onset of dilatancy which causes a pore pressure decrease (Brace and Martin, 1968). Secondly, material dilation may be associated with a decrease or even negative (i.e., suction) fluid pressure owing to dilatancy occurring at a faster rate than the pore fluid diffusion into the dilated zones. This phenomenon is typically observed in low-porosity rocks (Martin, 1980) and can increase the effective stress of the rock and, consequently, its strength (i.e., dilatant hardening).

### 6.7 Summary and concluding remarks

The Opalinus Clay formation is currently assessed as a host rock formation for the deep geological disposal of radioactive waste. Recently, an instrumented 3 m diameter, 50 m long tunnel was excavated at the Mont Terri URL as part of a long-term project aimed at investigating the thermo-hydro-mechanical effects induced by the construction of an underground repository. Given the tunnel geometry and the relative orientation with respect to the bedding planes of Opalinus Clay, the observed deformation response may provide useful indications regarding the behaviour to be expected during the excavation of actual emplacement tunnels under similar geological conditions.

Tunnel wall displacements were monitored by three-dimensional geodetic surveying. Despite the
installation of a mesh-reinforced shotcrete layer and rock bolting, radial convergences comprised between 0.6 and 2.5%, and absolute displacements as high as 40 mm were recorded. A strong anisotropic response of the tunnel cross section was measured with an average convergence in the direction perpendicular to the bedding orientation about 4 times bigger than the convergence in the direction parallel to the layering. Radial displacements were obtained from multi-point extensometers installed from within the tunnel walls. Again, a distinct variation of behaviour as function of the orientation was observed, thus confirming the influence of mechanical anisotropy on the rock mass response. In particular, strong displacement gradients were measured in proximity to the excavation boundary in the direction perpendicular to bedding possibly due to brittle failure processes and rock mass bulking. Inclinometer chains were installed in the crown sub-parallel to the tunnel axis before the start of the excavation, thus allowing to monitor the complete evolution of displacement from undisturbed conditions. On average, deformations initiated about 3–4 m ahead of the excavation face. The vertical deflection as the excavation passed underneath each probe was ranging between 29 and 43% of maximum deflection experienced at the given section.

A preliminary interpretation of the excavation response was attempted by a linear elastic analysis accounting for modulus anisotropy of Opalinus Clay. The model substantially under-predicted the deformation response as the largest displacement value was 10 mm despite the unsupported tunnel conditions. Analysis of slip zones using a ubiquitous joint model captured location and size of potential areas of material failure in agreement with the experimental model.

Subsequently, a combined finite-discrete element method (FEM/DEM) model was developed and calibrated based on the tunnel deformation measurements. To allow a direct comparison of in situ convergence measurements with numerical results, a core replacement technique with modulus reduction was implemented. The point-wise comparison of absolute displacements was hindered by the heterogeneous response observed in the field likely due to a non-homogenous distribution of rock mass properties and/or non-circular geometrical shape, which were not taken into account by the numerical model. Instead, the comparison of relative displacements (i.e., convergences) indicated an overall good agreement between experimental data and numerical model. Also, the vertical displacement in the crown was satisfactorily matched. Qualitatively, the response of the virtual extensometers resembled that observed in the field with prevalently elastic deformation in the direction parallel to the bedding and displacement jumps associated with open fractures in the perpendicular one. The simulated evolution of fracturing was characterized by failure initiating due to shearing of bedding planes oriented at a critical angle to the induced maximum principal stress around the excavation. As bedding planes slid past each other tensile fracturing was induced in the direction parallel to the bedding orientation. The potentially catastrophic development of damage in the direction perpendicular to bedding was prevented by the activation of the support layer. Although the numerical fracture pattern was in agreement with damage patterns typically observed around excavations parallel to the bedding strike in Opalinus Clay, further validation of the numerical model will take advantage of a currently on-going EDZ characterization research program. The simulated displacement field around the tunnel indicated the formation of a square shaped inner shell oriented along the bedding planes and dominated by rock mass fragmentation.
and bulking, and of an outer shell characterized by sensibly smaller deformation magnitude with extensional fracturing inhibited by an increase of confining stress. Finally, the possible effects of varying in situ stress conditions on the final fracture pattern were highlighted.

Currently, the main limitations of the adopted FEM/DEM model consist of the inability of the 2D simulation to capture 3D effects potentially associated with a rotation of the stress field ahead of the excavation face, as well as the lack of hydro-mechanical coupling in the stress-strain formulation.
Chapter 7

Discussion

7.1 Overall conclusions

The main goal of this thesis was to develop and validate a new robust numerical approach to model the effect of mechanical anisotropy on the fracturing behaviour of brittle clay shales. A newly-extended finite-discrete element (FEM/DEM) technique was employed to analyze the deformation and failure mechanisms of Opalinus Clay typically observed in the laboratory during standard rock mechanics tests and in the field around deep underground tunnels. Numerical investigation of the short-term mechanical response of Opalinus Clay was integrated with field measurements from the full-scale emplacement (FE) test tunnel recently excavated at the Mont Terri URL (Switzerland). The following topics were investigated: damage processes and acoustic activity of brittle materials, fundamental failure and deformation mechanisms in anisotropic rocks, anisotropic response of deep underground excavations, and formation of excavation damaged zones (EDZ) around emplacement tunnels for nuclear waste.

Previous research has shown that continuum approaches, based on classic shear failure theory for elasto-plastic materials, are limited in their ability to reproduce the mechanical response of the Opalinus Clay, specifically its brittle failure mechanisms. On the other hand, the hybrid finite-discrete element approach has the inherent ability to capture continuum and discontinuum behaviours as well as the transition from one to the other via fracturing and fragmentation processes. However, validation of the method and of its ability to quantitatively model how energy is dissipated and redistributed during brittle failure processes have never been accomplished before this work.

Acoustic emissions (AE) have been commonly used in the laboratory to characterize the rock failure process by providing unique information regarding the amount of internal damage, the spatial distribution of microfractures and the magnitude distribution of fracturing events. AE are also directly related to the amount of energy released during failure processes in brittle materials. While several models have been developed to simulate AE, the majority adopt a static approach, whereby the elastic strain energy, dissipated by an elasto-plastic constitutive law, is considered as an equivalent for the radiated seismic energy; and thus fail to explicitly consider acoustic waves. Expanding the approach first developed by Hazzard and Young (2000), a new algorithm to model synthetic AE was therefore proposed based on the monitoring of displacements and kinetic energy in proximity to propagating cracks within the FEM/
DEM model (Chapter 3). In agreement with laboratory observations, the numerical results highlighted the stochastic self-similarity of the microfracturing process in terms of frequency-magnitude distribution of acoustic events (i.e., Gutenberg-Richter relationship), spatial distribution of hypocenters (i.e., fractal character), and time evolution of AE rate in the pre-peak stage (i.e., Omori’s law for foreshocks). Furthermore, a qualitative energy-based validation of the simulated fracturing process was obtained by recovering realistic seismic $b$ values. Also, the frequency-magnitude signature of simulated AE showed a correlation between the macroscopic rupture of the sample and the decrease of seismic $b$ value. Furthermore, $b$ value anomalies could be related, as observed during laboratory experiments, to the failure of weaker mineral bonds at the interface of stronger, stiffer clumps (i.e., asperities) within the numerical microstructure of the rock sample. A transition of AE spatial distribution from diffuse, in the pre-peak stage, to strongly localized at the peak and postpeak stages, was also observed. All these results compared well with typical experimental findings, thus increasing the confidence that the adopted modelling technique could capture the fundamental aspects of the failure process in brittle rocks.

Once the FEM/DEM ability to capture brittle failure phenomena was validated, it was necessary to substantially extend the original method to account for the highly anisotropic characteristics of Opalinus Clay as typically exhibited during laboratory testing and around underground excavations (Chapter 5). Specifically, new modelling procedures and associated algorithms were developed to account for both elastic and strength anisotropy by: (i) smearing the transversely isotropic elastic deformation of the material in the continuum formulation of FEM/DEM, (ii) preconditioning the triangular mesh along the bedding plane direction, and (iii) developing a directional cohesive fracture formulation to reproduce the variation of failure mechanisms and strength response as function of the layering orientation. An early modelling attempt included also capturing the strength anisotropy of Opalinus Clay as an emergent property of a homogeneous medium containing a distribution of finite-sized, cohesionless cracks aligned with the plane of isotropy (Chapter 4). The presence of micro-cracks oriented along the bedding direction allowed to reproduce key damage mechanisms such as extensional fracturing and coalescence of pre-existing cracks. However, due to computational constraints associated with the mesh resolution, the technique was found unsuitable for field-scale models. Conversely, the adoption of the aforementioned directional cohesive fracture model allowed the upscaling of the numerical approach to the tunnel scale. Using this approach, the contribution of different failure mechanisms to the EDZ formation process around circular tunnels was studied. In particular, it was possible to observe that, for tunnels excavated parallel to the bedding strike, failure initiates with shearing along bedding planes and later evolves with extensional fracturing in the direction perpendicular to the layering (Chapters 5 and 6). Spalling and buckling failures were also simulated and shown to be promoted by bedding planes delamination. The numerical models also proved that the EDZ development could be controlled by minimizing the rock mass deconfinement induced by bedding slippage. This could be achieved, for example, by installing the support system (e.g., shotcrete) close to the excavation face. Under anisotropic in situ stress states, the combination of material textural anisotropy and fracturing-induced rock mass anisotropy resulted in fracture patterns and damage locations substantially different than those typically observed in massive isotropic rocks in similar stress conditions.
Lastly, the proposed approach was verified against the results of the 2012 full-scale emplacement (FE) experiment at the Mont Terri URL. The numerical models were able to quantitatively reproduce the rock mass deformation response measured during the excavation of the FE tunnel (Chapter 6). In particular, field monitoring of rock mass displacements indicated squeezing conditions and mechanical response strongly controlled by the local orientation of bedding planes. The simulated fracture pattern and displacement fields around the tunnel showed the formation of (i) a square shaped inner shell oriented along the bedding planes and dominated by rock mass fragmentation and bulking and of (ii) an outer shell characterized by sensibly smaller deformation magnitudes with extensional fracturing inhibited by an increase of confining stress.

### 7.2 Contributions

This thesis resulted in several original contributions:

1. Two new numerical algorithms were developed and validated against experimental results:
   - A numerical procedure to extract seismic information from a FEM/DEM model by monitoring internal variables, such as relative displacements and kinetic energy, in proximity to spontaneously nucleating cracks (Chapter 3).
   - A directional cohesive fracture model formulation (Chapter 5).

2. This research is the first study to provide a complete numerical description of the mechanical response of an anisotropic rock, namely Opalinus Clay, in terms of overall stiffness and strength as well as fracturing behaviour. The simulations illuminate the processes governing fracture development in clay shales under tensile and compressive stress fields for varying confining stresses (Chapters 4 and 5).

3. This research represents the first quantitative simulation of the EDZ formation process around openings in Opalinus Clay with direct application to the design of a deep underground repository. The numerical results highlight the importance of bedding plane delamination and subsequent strain-driven extensional fracturing in the formation of the EDZ fracture network (Chapters 5 and 6).

### 7.3 Future work

Based on the results reported in this thesis and the experience gained in the last four years, the following recommendations for future research directions are outlined:

1. Establish a quantitative relationship between laboratory- and field-scale input parameters.

   At present, owing to computational constraints on the element size and the mesh sensitivity of the numerical method, the input parameters of the EDZ models must be calibrated based on experimental observations at the scale of interest. The mesh sensitivity of FEM/DEM represents a
major limitation of the current work as it prevents the straightforward use of laboratory-scale calibrated input parameters for prediction purposes in field-scale models. Such a shortcoming could be minimized by enhancing the computation efficiency of FEM/DEM by developing, for instance, a cluster version of the current code or by adopting a coupled continuum-discontinuum approach, whereby only a small-sized region of interest is treated as a FEM/DEM medium whereas the remainder of the domain is modelled as an elastic, non-fracturing solid. Efforts in this direction may allow the adoption in field-scale models of element sizes of the same order of magnitude as in the calibrated laboratory-scale models, thus reducing substantially the mesh sensitivity of the simulations. Nevertheless, the existence of upscaling relationships for the FEM/DEM input parameters should be the subject of future research.

2. Numerically investigate the effect of geological heterogeneity and presence of faults on the response of underground excavations.

In particular, it would be interesting to refine the FEM/DEM model of the FE tunnel by including specific geological features mapped during the tunnel construction. This study might shed some light on the influence of geological structures, reinforcement quality, and support strategy on tunnel deformations, which in turn could help explain the large convergences observed in the bottom part of the left sidewall and their potential effects on the EDZ development.

3. Compare the 2D modelling results with 3D simulations.

The comparison between 2D and 3D results should at first focus on the fundamental fracture mechanisms observed during laboratory-scale models (e.g., compression and tension tests) and subsequently be extended to the analysis of EDZ development around underground excavations. The 3D extension of the FEM/DEM code will likely allow a more accurate analysis of the rock fracturing behaviour around advancing tunnels. Inherently three-dimensional factors were indeed neglected by the two-dimensional FEM/DEM simulations, including the influence of stress path and loading history (e.g., rotation of principal stress axes ahead of the excavation face), and the effect of the axial (i.e., intermediate) principal stress.

4. Investigate the influence of poromechanical effects on the short-term (i.e., undrained) behaviour of Opalinus Clay.

The current FEM/DEM model should be enriched with the introduction of an instantaneous hydro-mechanical coupling aimed at analyzing phenomena potentially occurring in Opalinus Clay when the mechanical loading rate is higher than the fluid pressure dissipation rate (e.g., hydraulic fracturing, dilatant hardening).

5. Integrate the FEM/DEM modelling methodology within the long-term safety assessment procedure for the planned underground repository.

In Opalinus Clay, the long-term evolution of the EDZ seems to be characterized by several hydro-mechanically coupled processes, including rock mass desaturation, time-dependent pore pressure
dissipation, and swelling. Future studies should aim at taking these important processes into account. Also, a methodology to extract information about the secondary (i.e., excavation induced) porosity and fracture inter-connectivity from a FEM/DEM simulation should be developed. The information could be used to provide further validation of the FEM/DEM model and used as input for long-term simulations of fluid flow and radionuclide transport around emplacement tunnels for nuclear waste.


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## Appendix A

### Source code of the FEM/DEM algorithms

The implementation of the algorithmic procedures described in this thesis is given in the form of code listings in the following sections. These algorithms have been implemented in the open-source FEM/DEM Y-Geo code (Mahabadi, 2012), which represents an extension of the original Y2D-code (Munjiza, 2004). The adopted programming language is C.

```c
/* Global variables */

double *d1ncix; // Array of initial x coordinates of nodes
double *d1nciy; // Array of initial y coordinates of nodes
double *d1ncex; // Array of current x coordinates of nodes
double *d1nccy; // Array of current y coordinates of nodes
double *d1nvcx; // Array of current x velocities of nodes
double *d1nvcy; // Array of current y velocities of nodes
double *d1nfcx; // Array of x components of nodal forces
double *d1nfcy; // Array of y components of nodal forces
int *i1pnfx; // Array of boundary conditions in x-direction
int *i1pnfy; // Array of boundary conditions in y-direction

int **i2elto; // Array of element topology
double nelem; // Total number of elements
double d1peex; // Young’s modulus in x-direction
double d1peey; // Young’s modulus in y-direction
double d1pemx; // Poisson’s ratio in x-direction
double d1pemy; // Poisson’s ratio in y-direction
double d1peg; // Shear modulus
double dpeks; // Viscous damping coefficient
double dpela; // First Lame’ constant
double dpemu; // Second Lame’ constant
double dpero; // Material density

double dcsstx; // In situ stress component sigma_xx
double dcsstxy; // In situ stress component sigma_xy
double dcstyy; // In situ stress component sigma_yy
double dcsyxx; // In situ stress gradient delta(sigma_xx)/(delta y)
double dcsxyy; // In situ stress gradient delta(sigma_xy)/(delta y)
double dcsyy; // In situ stress gradient delta(sigma_yy)/(delta y)
double dcsrfy; // y coordinate of zero stress surface
```

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# Appendix A. Source Code of the FEM/DEM Algorithms

```c
double dpealp;  // Inclination of layering (in degrees)
double dpeftp;  // Maximum tensile strength
double dpefr;   // Minimum tensile strength
double dpegtpt; // Maximum mode I fracture energy
double dpegttr; // Minimum mode I fracture energy
double dpecop;  // Maximum cohesion
double dpecor;  // Minimum cohesion
double dpegsp;  // Maximum mode II fracture energy
double dpegsr;  // Minimum mode II fracture energy
double dpefr;   // Internal friction coefficient
double dpepe;   // Fracture penalty
double dlnmct;  // Nodal mass
double *d1els;  // Array of element friction
int *i1esftf;  // Array of yielded crack element flags
double *dledke; // Seismic energy of broken crack elements
double *dletmke; // Event initiation time
```

## A.1 Transversely isotropic, linear elastic triangular element

```c
/* Local variables */
int ielem;
int i, j, k, in, jn, kn;
double nx, ny;
double voli, volc;
double F0[3][3];  // initial local base
double FX[3][3];  // current local base
double LX[3][3];  // velocity gradient in current local base
double F0inv[3][3]; // global base in initial local base
double FXinv[3][3]; // global base in current local base
double F[3][3];    // deformation gradient in global base
double L[3][3];    // velocity gradient in global base
double B[3][3];    // left Cauchy–Green strain tensor
double D[3][3];    // rate of deformation tensor
double E[3][3];    // strain tensor
double T[3][3];    // Cauchy stress tensor

/* Loop over triangular elements */
for (ielem = 0; ielem < nelem; ielem++)
{
    for (i = 1; i < 3; i++)
    {
        F0[0][i-1]=dlnxcx[(i2elto[i][ielem])-dlnxcx[(i2elto[0][ielem])];
        F0[1][i-1]=dlnncy[(i2elto[i][ielem])-dlnncy[(i2elto[0][ielem])];
        FX[0][i-1]=dlnccx[(i2elto[i][ielem])-dlnccx[(i2elto[0][ielem])];
        FX[1][i-1]=dlnccy[(i2elto[i][ielem])-dlnccy[(i2elto[0][ielem])];
        LX[0][i-1]=dlnvcx[(i2elto[i][ielem])-dlnvcx[(i2elto[0][ielem])];
        LX[1][i-1]=dlnvcy[(i2elto[i][ielem])-dlnvcy[(i2elto[0][ielem])];
    }
    YMATINV2(F0, F0inv, voli);
    YMATINV2(FX, FXinv, volc);
}
```
for (i=0; i<2; i++)
    { for (j=0; j<2; j++)
        { F[i][j] = 0.0;
          L[i][j] = 0.0;
          for (k=0; k<2; k++)
            { F[i][j]=F[i][j]+FX[i][k]*F0inv[k][j];
              L[i][j]=L[i][j]+LX[i][k]*FXinv[k][j];
            }
          }  }
/* Calculation of strain */
for (i=0; i<2; i++)
    { for (j=0; j<2; j++)
        { B[i][j] = 0.0;
          for (k=0; k<2; k++)
            { B[i][j]=B[i][j]+F[i][k]*F[j][k];
            }
          D[i][j] = 0.5*(L[i][j]+L[j][i]);
          E[i][j] = 0.5*B[i][j];
          if (i==j) E[i][j]=E[i][j]−0.5;
        }
    }
/* Apply transversely isotropic, linear elastic constitutive law */
T[0][0]=(d1peex/(1−d1pemx*d1pemy))*(E[0][0]+d1pemy*E[1][1])
         +dpeks*D[0][0];
T[1][1]=(d1peey/(1−d1pemx*d1pemy))*(E[1][1]+d1pemx*E[0][0])
         +dpeks*D[1][1];
T[0][1]=(2*d1peg)*E[0][1]+dpeks*D[0][1];
T[1][0]=(2*d1peg)*E[1][0]+dpeks*D[1][0];
/* Update nodal forces */
for (i=0; i<3; i++)
    { j=i+1; if (j>2) j=0;
      k=j+1; if (k>2) k=0;
      in=i2elto[i][ielem];
      jn=i2elto[j][ielem];
      kn=i2elto[k][ielem];
      nx=d1nccy[kn]−d1nccy[jn];
      ny=d1nccx[jn]−d1nccx[kn];
      /* Nodal forces due to elastic reaction */
      dlnfcx[in]=dlnfcx[in]+(T[0][0]*nx+T[0][1]*ny)/2.0;
      dlnfcy[in]=dlnfcy[in]+(T[1][0]*nx+T[1][1]*ny)/2.0;
    }
A.2 In situ stress initialization routine

/* Local variables */
int ielem;
int i,j,k,in,jn,kn;
double nx,ny;
double voli,volc;
double F0[2][2];      // initial local base
double FX[2][2];      // current local base
double LX[2][2];      // velocity gradient in current local base
double F0inv[2][2];       // global base in initial local base
double FXinv[2][2];       // global base in current local base
double F[2][2];           // deformation gradient in global base
double L[2][2];           // velocity gradient in global base
double B[2][2];           // left Cauchy–Green strain tensor
double D[2][2];           // rate of deformation tensor
double E[2][2];           // strain tensor
double T[2][2];           // Cauchy stress tensor
double Tinsitu[2][2];     // In situ stress tensor

/* Loop over triangular elements */
for (ielem=0; ielem<nelem; ielem++)
{
  for (i=1; i<3; i++)
  {
    F0[0][i-1]=d1nci{[i2elt0[i][ielem]]}−d1nci{[i2elt0[0][ielem]]};
    F0[1][i-1]=d1nciy{[i2elt0[i][ielem]]}−d1nciy{[i2elt0[0][ielem]]};
    FX[0][i-1]=d1ncx{[i2elt0[i][ielem]]}−d1ncx{[i2elt0[0][ielem]]};
    FX[1][i-1]=d1ncy{[i2elt0[i][ielem]]}−d1ncy{[i2elt0[0][ielem]]};
    LX[0][i-1]=d1ncx{[i2elt0[i][ielem]]}−d1ncx{[i2elt0[0][ielem]]};
    LX[1][i-1]=d1ncy{[i2elt0[i][ielem]]}−d1ncy{[i2elt0[0][ielem]]};
  }
  YMATINV2(F0, F0inv, voli);
  YMATINV2(FX, FXinv, volc);

  for (i=0; i<2; i++)
  {
    for (j=0; j<2; j++)
    {
      F[i][j]=0.0;
      L[i][j]=0.0;
      for (k=0; k<2; k++)
      {
        F[i][j]=F[i][j]+FX[i][k]*F0inv[k][j];
        L[i][j]=L[i][j]+LX[i][k]*FXinv[k][j];
      }
    }
  }

/* Calculation of strain */
for (i=0; i<2; i++)
{
  for (j=0; j<2; j++)
  {
    B[i][j]=0.0;
    for (k=0; k<2; k++)
    {
      B[i][j]=B[i][j]+F[i][k]*F[j][k];
    }
    D[i][j]=0.5*(L[i][j]+L[j][i]);
    E[i][j]=0.5*B[i][j];
    if (i==j) E[i][j]=E[i][j]−0.5;
  }
}

/* Apply transversely isotropic, linear elastic constitutive law */
T[0][0]=(d1pex/(1−d1pemx*d1pemy))*(E[0][0]+d1pemy*E[1][1])
+dpeks*D[0][0];
T[1][1]=(d1pex/(1−d1pemx*d1pemy))*(E[1][1]+d1pemx*E[0][0])
+dpeks*D[1][1];
T[0][1]=(2*d1peg)*E[0][1]+dpeks*D[0][1];
T[1][0]=(2*d1peg)*E[1][0]+dpeks*D[1][0];

/* Update nodal forces */
for (i = 0; i < 3; i++)
{
    j = i + 1;
    if (j > 2) j = 0;
    k = j + 1;
    if (k > 2) k = 0;
    in = i2elto[i][ielem];
    jn = i2elto[j][ielem];
    kn = i2elto[k][ielem];
    nx = dlnccy[kn] - dlnccy[jn];
    ny = dlnccx[jn] - dlnccx[kn];

    /* Nodal forces due to elastic reaction */
    dlnfcx[in] = dlnfcx[in] + (T[0][0] * nx + T[0][1] * ny) / 2.0;
    dlnfcy[in] = dlnfcy[in] + (T[1][0] * nx + T[1][1] * ny) / 2.0;

    /* Element in situ stress tensor */
    Tinsitu[0][0] = - dcsstxx - dcsstxy * ((dlnsci[i2elto[0][ielem]]
        + dlnsci[i2elto[1][ielem]]
        + dlnsci[i2elto[2][ielem]]) / 3.0 - dcsrfy);
    Tinsitu[0][1] = - dcsstxy - dcsstyy * ((dlnsci[i2elto[0][ielem]]
        + dlnsci[i2elto[1][ielem]]
        + dlnsci[i2elto[2][ielem]]) / 3.0 - dcsrfy);
    Tinsitu[1][0] = - dcsstxy - dcsstyy * ((dlnsci[i2elto[0][ielem]]
        + dlnsci[i2elto[1][ielem]]
        + dlnsci[i2elto[2][ielem]]) / 3.0 - dcsrfy);
    Tinsitu[1][1] = - dcsstxx - dcsstxy * ((dlnsci[i2elto[0][ielem]]
        + dlnsci[i2elto[1][ielem]]
        + dlnsci[i2elto[2][ielem]]) / 3.0 - dcsrfy);

    /* Nodal forces due to in situ stress */
    dlnfcx[in] = dlnfcx[in] + (Tinsitu[0][0] * nx + Tinsitu[0][1] * ny) / 2.0;
    dlnfcy[in] = dlnfcy[in] + (Tinsitu[1][0] * nx + Tinsitu[1][1] * ny) / 2.0;
} }

A.3 Cohesive element with direction-dependent strength parameters and AE recording

/* Local variables */
int ielem;
int i, j, k;
int i0, i1, i2, i3;
double elx, ely, h, area;
double small = 1.0e-10;
double s1, s2, o1, o2;
double beta, gamma;
double dpeft; /// Tensile strength
double dpegf; /// Mode I fracture energy
double dpefs; /// Shear strength
double dpegs; /// Mode II fracture energy
int nfail; /// Number of broken integration points
int nsoft; /// Number of yielded integration points
int integ;
double op, sp; /// Peak opening and sliding
double ot, st; /// Residual opening and sliding
double o, s, sabs; /// Crack opening and sliding
double z; /// Damage factor
```c
double dpfe = 0.63;
double dpfeb = 1.8;
double dpfec = 6.0;

double sigma;  // ! Normal bonding stress

double tau;  // ! Tangential bonding stress

double joint_ke;  // ! Kinetic energy of crack element (Ek)

double delta_ke;  // ! Differential kinetic energy (=Ek−Ek,y)

/** Loop over crack elements */
for (ielem=0; ielem<nelem; ielem++)
{
    dpefs=d1elsf[ielem];
    i0=i2elto[0][ielem];
    i1=i2elto[1][ielem];
    i2=i2elto[2][ielem];
    i3=i2elto[3][ielem];
    elx=0.5*(d1nccx[i1]+d1nccx[i2]−d1nccx[i0]−d1nccx[i3]);
    ely=0.5*(d1nccy[i1]+d1nccy[i2]−d1nccy[i0]−d1nccy[i3]);
    h=sqrt(elfx*elfx+elfy*elfy);
    elfx=elfx/(h+small);
    elfy=elfy/(h+small);
    sl=(d1nccy[i0]−d1nccy[i3])*elfy+(d1nccx[i0]−d1nccx[i3])*elfx;
    s2=(d1nccy[i1]−d1nccy[i2])*elfy+(d1nccx[i1]−d1nccx[i2])*elfx;
    s1=(d1nccy[i0]−d1nccy[i3])*elfx−(d1nccx[i0]−d1nccx[i3])*elfy;
    s2=(d1nccy[i1]−d1nccy[i2])*elfx−(d1nccx[i1]−d1nccx[i2])*elfy;

    /** Compute cohesive strength parameters based on relative orientation */
    beta=atan((d1nccy[i1]−d1nccy[i0])/(d1nccx[i1]−d1nccx[i0]))*180/3.14159;
    if (beta<0.0)
    { beta=beta+180.0; }
    gamma=abs(dpealp−beta);
    if (gamma>90.0)
    { gamma=180.0−gamma; }
    dpeft=dpeft+ppeft−dpefr*(gamma/90.0);
    dpegf=dpegf+ppegf−dpegf*(gamma/90.0);
    dpegs=dpegs+ppegs−dpegs*(gamma/90.0);

    /** Compute peak and residual crack relative displacements */
    op=2.0*h*dpeft/dpepe;
    sp=2.0*h*dpefs/dpepe;
    ot=fmax(small,(3.0*dpegf/dpeft));
    st=fmax(small,(3.0*dpegs/dpefs));

    nfail=0;
    nssoft=0;

    /** Loop over three integration points */
    for (integ=0; integ<3; integ++)
    {
        if (integ==0)
        { o=o1; s=s1; }
        else if (integ==2)
        { o=o2; s=s2; }
        else
        { o=0.5*(o1+o2); s=0.5*(s1+s2); }
```
sabs = abs(s);

/* Yielding in tension and shear */
if ((o>op) && (sabs>sp))
{ z = sqrt(((o-op)/ot)*((o-op)/ot)+((sabs-sp)/st)*((sabs-sp)/st));
  nsoft = nsoft + 1;
  if ((nsoft>2) && (ilesftf[ielem]==0))
  { /* Kinetic energy of the crack element at yielding (E_k, y) */
    dleike[ielem] = 0.5*(dlnmct[0]*(dlnvc[0]*dlnvc[0])
       +dlnvcy[0]*dlnvcy[0])
       +dlnmct[1]*(dlnvc[1]*dlnvc[1])
       +dlnvcy[1]*dlnvcy[1])
       +dlnmct[2]*(dlnvc[2]*dlnvc[2])
       +dlnvcy[2]*dlnvcy[2])
       +dlnmct[3]*(dlnvc[3]*dlnvc[3])
       +dlnvcy[3]*dlnvcy[3]) ;
    ilesftf[ielem] = 1;
  }
  /* Yielding in tension only */
  else if (o>op)
  { z = (o-op)/ot;
    nsoft = nsoft + 1;
    if ((nsoft>2) && (ilesftf[ielem]==0))
    { /* Kinetic energy of the crack element at yielding (E_k, y) */
      dleike[ielem] = 0.5*(dlnmct[0]*(dlnvc[0]*dlnvc[0])
         +dlnvcy[0]*dlnvcy[0])
         +dlnmct[1]*(dlnvc[1]*dlnvc[1])
         +dlnvcy[1]*dlnvcy[1])
         +dlnmct[2]*(dlnvc[2]*dlnvc[2])
         +dlnvcy[2]*dlnvcy[2])
         +dlnmct[3]*(dlnvc[3]*dlnvc[3])
         +dlnvcy[3]*dlnvcy[3]) ;
      ilesftf[ielem] = 2;
    }
  }
  /* Yielding in shear only */
  else if (sabs>sp)
  { z = (sabs-sp)/st;
    nsoft = nsoft + 1;
    if ((nsoft>2) && (ilesftf[ielem]==0))
    { /* Kinetic energy of the crack element at yielding (E_k, y) */
      dleike[ielem] = 0.5*(dlnmct[0]*(dlnvc[0]*dlnvc[0])
         +dlnvcy[0]*dlnvcy[0])
         +dlnmct[1]*(dlnvc[1]*dlnvc[1])
         +dlnvcy[1]*dlnvcy[1])
         +dlnmct[2]*(dlnvc[2]*dlnvc[2])
         +dlnvcy[2]*dlnvcy[2])
         +dlnmct[3]*(dlnvc[3]*dlnvc[3])
         +dlnvcy[3]*dlnvcy[3]) ;
      ilesftf[ielem] = 3;
    }
  }
  /* No yielding */
  else
{ z = 0.0; }

/* Broken integration point */
if (z>=1.0)
{ nfail=nfail+1;
  if ((nfail>1)&(ielpr[ielem]>=0))
  { /* Compute failure mode */
    if ((o>=(op+ot))&((sabs>=(sp+st)))) // Mode I + mode II
      { d1ebrkf[ielem]=3.0; }
    else if (o>=(op+ot)) // Mode I
      { d1ebrkf[ielem]=1.0; }
    else if (sabs>=(sp+st)) // Mode II
      { d1ebrkf[ielem]=2.0; }
    else
      { d1ebrkf[ielem]=1.0+(sabs-sp)/(st); } // Mixed mode I–II
  }
  z=1.0;
}

/* Compute scaling factor for bonding stresses */
z=(1.0-(dpefa+dpefb-1.0)/(dpefa+dpefb))*
  exp(z*(dpefa+dpefc*dpefb)/((dpefa+dpefb)*(1.0-dpefa-dpefb))))
  *(dpefa*(1.0-z)+dpefb*pow((1.0-z),dpefc));

/* Calculate bonding stresses */

/* Normal stress */
if (o<0.0)
{ sigma=2.0*o*dpeft/op; }
else if (o>op)
{ sigma=dpeft*z;
  nsoft=nsoft+1; }
else
{ sigma=(2.0*o/op–(o/op)*(o/op))*z*dpeft; }

/* Compute shear strength according to Mohr–Coulomb */
if (sigma>0.0)
{ dpefs=dpecor+(dpecop–dpecor)*(gamma/90.0); }
else
{ dpefs=dpecor+(dpecop–dpecor)*(gamma/90.0)–sigma*dpefr; }

/* Shear stress */
if ((sigma>0.0)&(sabs>sp))
{ tau=z*dpefs; }
else if (sigma>0.0)
{ tau=(R2*(sabs/sp)–(sabs/sp)*(sabs/sp))*z*dpefs; }
else if (sabs>sp)
{ tau=z*dpefs–dpefm*sigma; }
else
{ tau=(2.0*(sabs/sp)–(sabs/sp)*(sabs/sp))*(z*dpefs); }

/* Update shear strength of crack element */
d1elefs[ielem]=dpefs;
if (s < 0.0)
    { tau = -tau; }

/* Update nodal forces */
if (integ == 0)
    { area = h / 6.0;
      dlnfcx[i0] = dlnfcx[i0] - area * (tau * ex - sigma * ey);
      dlnfcx[i3] = dlnfcx[i3] + area * (tau * ex - sigma * ey);
      dlnfcy[i0] = dlnfcy[i0] - area * (tau * ey + sigma * ex);
      dlnfcy[i3] = dlnfcy[i3] + area * (tau * ey + sigma * ex);
    }
else if (integ == 1)
    { area = h / 3.0;
      dlnfcx[i0] = dlnfcx[i0] - area * (tau * ex - sigma * ey);
      dlnfcx[i3] = dlnfcx[i3] + area * (tau * ex - sigma * ey);
      dlnfcy[i0] = dlnfcy[i0] - area * (tau * ey + sigma * ex);
      dlnfcy[i3] = dlnfcy[i3] + area * (tau * ey + sigma * ex);
    }
else
    { area = h / 6.0;
      dlnfcx[i1] = dlnfcx[i1] - area * (tau * ex - sigma * ey);
      dlnfcx[i2] = dlnfcx[i2] + area * (tau * ex - sigma * ey);
      dlnfcy[i1] = dlnfcy[i1] - area * (tau * ey + sigma * ex);
      dlnfcy[i2] = dlnfcy[i2] + area * (tau * ey + sigma * ex);
    }

/* If joint is yielded, compute kinetic energy */
if (i1esftf[ielem] > 0)
    { joint_ke = 0.5 * (dlnmct[i0] * (dlnvcx[i0] * dlnvcx[i0] + dlnvcy[i0] * dlnvcy[i0]) +
                      dlnmct[i1] * (dlnvcx[i1] * dlnvcx[i1] + dlnvcy[i1] * dlnvcy[i1]) +
                      dlnmct[i2] * (dlnvcx[i2] * dlnvcx[i2] + dlnvcy[i2] * dlnvcy[i2]) +
      delta_ke = joint_ke - delta_ke[ielem];
      if (delta_ke > delta_k[elem])
          { dledke[ielem] = delta_k;
            dletmk[elem] = dtime;
          }
    }

A.4 Absorbing boundary condition

/* Local variables */
double nx, ny;
int ielem;
int i,j,k, in, jn, kn;
double cp; /* ! P-wave velocity */
double cs; /* ! S-wave velocity */

/* Loop over triangular elements */
for (ielem = 0; ielem < nelem; ielem++)
    { for (i = 0; i < 3; i++)
        { j = i + 1; if (j > 2) j = 0;
\begin{verbatim}
\textbf{APPENDIX A. SOURCE CODE OF THE FEM/DEM ALGORITHMS}

k = j+1; \textbf{if}(k>2) k=0;

in = i2elt[i][ielem];
jn = i2elt[j][ielem];
kn = i2elt[k][ielem];

nx = d1nccy[kn]− d1nccy[jn];
ny = d1nccx[jn]− d1nccx[kn];

\textbf{cp} = \textbf{sqrt}((2*dpemu+dpela)/dpero);
\textbf{cs} = \textbf{sqrt}(dpemu/dpero);

\textbf{/* Nodal forces due to absorbing boundary */}
\textbf{if} ((ilpnfx[jnopr]==4)\&\&(ilpnfx[knopr]==4))
{ 
d1nfex[jn] = d1nfex[jn]− dpero*cp*dlnvex[jn]*abs(nx)/3.0−
dpero*cp*dlnvex[kn]*abs(nx)/6.0−
dpero*cs*dlnvex[jn]*abs(ny)/3.0−
dpero*cs*dlnvex[kn]*abs(ny)/6.0;

d1nfex[kn] = d1nfex[kn]− dpero*cp*dlnvex[jn]*abs(nx)/6.0−
dpero*cp*dlnvex[kn]*abs(nx)/3.0−
dpero*cs*dlnvex[jn]*abs(ny)/6.0−
dpero*cs*dlnvex[kn]*abs(ny)/3.0; }

\textbf{if} ((ilpnfy[jnopr]==4)\&\&(ilpnfy[knopr]==4))
{ 
d1nfey[jn] = d1nfey[jn]− dpero*cp*dlnvey[jn]*abs(ny)/3.0−
dpero*cp*dlnvey[kn]*abs(ny)/6.0−
dpero*cs*dlnvey[jn]*abs(nx)/3.0−
dpero*cs*dlnvey[kn]*abs(nx)/6.0;

d1nfey[kn] = d1nfey[kn]− dpero*cp*dlnvey[jn]*abs(ny)/6.0−
dpero*cp*dlnvey[kn]*abs(ny)/3.0−
dpero*cs*dlnvey[jn]*abs(nx)/6.0−
dpero*cs*dlnvey[kn]*abs(nx)/3.0; }
\}
\end{verbatim}
Appendix B

Computational time of the FEM/DEM simulations

B.1 Run times of selected FEM/DEM models

The simulations presented in this thesis were carried out using the open-source Y-Geo FEM/DEM code (Mahabadi et al., 2012a), which is developed at the University of Toronto based on the original Y-Code of Munjiza (2004). The Y-Geo code and its Graphical User Interface, Y-GUI (Mahabadi et al., 2010b), can be downloaded at http://www.geogroup.utoronto.ca. The run times of selected simulations are reported in Table B.1. All models were run on Ubuntu 11.04 (64 bit) using a Intel Core i7 920 2.67 GHz CPU with 8 GB of RAM.
### Table B.1. Run times of selected FEM/DEM models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
<th>Number of triangles</th>
<th>Number of nodes</th>
<th>Physical time</th>
<th>Number of time steps</th>
<th>Total run time</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Chapter 3</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Section 3.4.3</td>
<td>Wing crack (0.1 m/s)</td>
<td>21k</td>
<td>64k</td>
<td>12.5 ms</td>
<td>2.5M</td>
<td>4 d</td>
</tr>
<tr>
<td>Section 3.5</td>
<td>UCS (0.25 m/s)</td>
<td>16k</td>
<td>48k</td>
<td>2 ms</td>
<td>400k</td>
<td>12 h</td>
</tr>
<tr>
<td><strong>Chapter 4</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Section 4.4.3</td>
<td>BD-S (0.1 m/s)</td>
<td>15k</td>
<td>45k</td>
<td>1.25 ms</td>
<td>750k</td>
<td>15 h</td>
</tr>
<tr>
<td>Section 4.4.3</td>
<td>BD-P (0.1 m/s)</td>
<td>15k</td>
<td>45k</td>
<td>2.5 ms</td>
<td>1.25M</td>
<td>30 h</td>
</tr>
<tr>
<td>Section 4.4.3</td>
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