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**FDEM analysis of shale anisotropy and its
effect on EDZ fracturing in deep buried tunnels**

By

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Abstract

Fractures form and propagate in the excavation damage zone (EDZ) due to underground excavation, degrading the rock's mechanical properties and permeability, and resulting in excavation problems such as collapse, seepage, rock burst and large deformations. In addition to affecting the choice of excavation method and design of supporting structures in underground engineering projects, understanding the formation and evolution of the EDZ, especially its fracturing mechanism, is also an important assessment index for the design of permeability sensitive excavations (such as hydroelectric power generation stations or nuclear waste repositories). However, the study of the fracturing mechanism and fracturing conditions of the EDZ still remains as an open topic, especially under shale formation. As one of the most encountered rocks during underground construction, shale poses many geotechnical problems due to its special properties (e.g., anisotropic behaviours, creeping and self-sealing). Shale is difficult to study because of its complex mechanism response. Shale matrix strength and fracture mechanism are affected significantly by bedding planes with lower stiffness and cohesion. This research adopted the finite discrete element method (FDEM) to create anisotropic shale models in ABAQUS.

Based on FDEM laboratory-scale models, fracturing mechanics, fracturing behaviour, and brittleness of shale have been studied from a microscopic perspective with taking shale anisotropy into account. Three failure modes for shale in uniaxial compressive test have been identified, in terms of tensile splitting (T-S), bedding plane delamination (B-D) and shearing through matrix (S-M). Two novel new brittleness indices, in terms of Bl_f and Bl_{CD} , have been proposed in this study to help researchers to assess shale frac-ability and provides an easy approach to evaluate rock brittleness based on

uniaxial compression test. In addition, an empirical relationship has been proposed in this study to predict the tensile strength, σ_t based on the uniaxial compression tests. The shale layer thickness shows great impact on the mechanical strength, fracturing conditions, and brittleness. However, it varies among shale models with different failure modes.

For new insights into EDZ fracturing behaviours in shale, this research studied the short-term response of the EDZ in anisotropic shale after tunnel excavation under different environment conditions (i.e., in-situ stress, layer thickness, and bedding plane inclinations). Three general fracturing modes of EDZ in shale formation under different conditions have been classified. By analysing the EDZs' locations, depth, and fracturing behaviours in the three fracturing modes, the results can help researchers and engineers in future to predict the depth of the EDZ, optimize the supporting methods and parameters. Bl_f is capable of predicting the fracturing conditions in the EDZ. The greater the Bl_f , the more severe fracturing conditions in the EDZ (e.g., fracture number and depth of EDZ).

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List of abbreviations

Full Form	Abbreviation
Excavation damage zone	EDZ
Finite discrete element method	FDEM
Uniaxial Compressive Strength	UCS
Brazilian disc	BD
Discrete element method	DEM
Finite element method	FEM
Notched deep beam	NDB
Brittleness index	BI
Cohesive element model	CZM
Fracture Process Zone	FPZ
Megapascal	MPa
Gigapascal	GPa
Millimetre	mm
Crack damage stress	CD
Crack initiation stress	CI
Tensile splitting	T-S
Bedding plane delamination	B-D

Shearing through rock matrix	S-M
Central spilt	C-S
Inclined arch fracturing	I-A
Central arch fracturing	C-A
Acoustic emission	AE
X-ray computed tomography	CT
Tensile-splitting spalling	TS-S
Bedding plane delamination notches	BD-N
Shearing through layers notches	SL-N
Cohesive element	COH

List of symbols

Description	Symbol
Young's modulus	E
Shear modulus	G
Poisson's ratio	ν
Principal stress	σ
Shear stress	τ
Strain	ε
Normal stress	N
Shear strength	S
Angle between weakening plane and maximum principal stress	β
Weight	W
Force	F
Length	L
Displacement	δ
Stress-strain Energy	U
Uniaxial compressive strength	σ_u
Tensile strength	σ_t
Diameter of tunnel	D

Cohesion	c
Internal friction coefficient	$\tan f_i$
Stiffness	k
Fracture opening width	δ_f
Traction stress	t
Internal friction angle	ϕ_i
Fracture energy	G_f
Dip angle	θ
Loading rate	v
The length of the fracture process zone	l_{cz}
Sliding friction coefficient	μ
Cohesive element tensile strength	f_t
Element/Loading platen friction coefficient	f_l
Density	ρ
Indirect tensile strength	T
Coefficient of lateral earth pressure	K_0
Reduction factor	λ
Ratio between the post-support displacement and the total displacement at the tunnel crown	δ^*

Angle between the failure plane and the maximum principal stress	α
Total number of the fractures	M
Mean value of a data set	X_{mean}
Critical value of the data set	t_c
Sample size	n
Layer thickness	λ_t

Chapter 1 INTRODUCTION

1.1 Research Background

Throughout the world, using underground space in the form of tunnels and caverns for transportation, mining, hydroelectric power generation station, and nuclear waste disposal repository has become increasingly popular due to the development of the economy and technology (Orellana et al., 2019 and Li et al., 2023). During the excavation, it is inevitable to form massive fractures near the tunnel wall, especially under high in situ stresses. An excavation damage zone (EDZ) is identified in this highly fractured area near the tunnel wall. In the EDZ, fractures form and propagate, which degrades the mechanical properties and permeability of the rock mass, even leading to excavation failures such as collapse, seepage, large deformation, and rock burst as shown in Figure 1.1 (Blümling et al., 2007b, Chen et al., 2019 and Perras 2009).

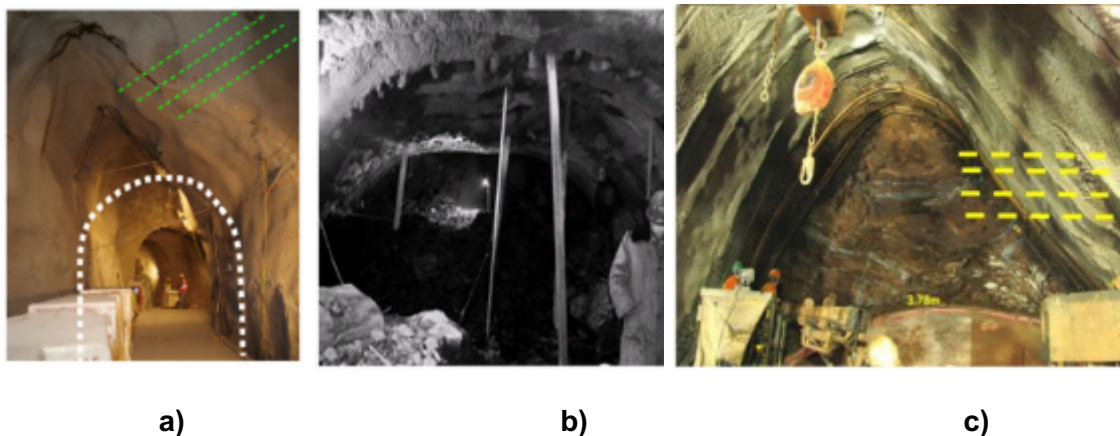


Figure 1.1 Excavation failure observed from different projects; a) Blümling et al., 2007 b) Chen et al., 2019 c) Perras 2009 (the dot line in the pictures indicate the inclination of the shale bedding planes).

As shale exhibits low permeability, geological stability, and self-sealing capabilities, it has attracted particular attention for geo-engineering applications such as nuclear waste disposal repository and hydroelectric power stations. It is generally considered that self-sealing rocks reduce their permeability over time (Williams, 2021). The excavation induced EDZ, however, could negatively impact these properties. Research facilities around the world have investigated the EDZ's properties and its impact on surrounding rocks and structures, including the Mont Terri project (Switzerland), the underground research laboratory (France), HADES (Belgium), KAERI (Korea), and Baihetan hydropower station (China) (Hao et al., 2016, Bossart et al., 2004, Armand et al., 2007, Kwon et al., 2009 and Mertens et al., 2004). The Mont Terri project has selected Opalinus clay at a depth ranging from 500m - 900m as the site for the nuclear waste disposal repository (Bossart et al., 2004). The excavation induced EDZ has been identified as a big threat to the project due to the increased permeability and reduced mechanical strength of the EDZ based on field studies. (Chandler et al., 1996, Bossart et al., 2004 and Fu et al., 2014). The priorities in the shale gas extraction industry lie in increasing fractures and keeping fractures open during hydraulic fracturing to increase productivity (Bing et al., 2014 and Hou et al., 2019). EDZ has, meanwhile, caused several tunnel construction problems and failures, such as tunnel collapses, rock bursts, and pathways for groundwater flow, that have been reported in many projects (Perras et al., 2009, Perras et al., 2014 Khalymendyk et al., 2019). Hence, a better understanding of fracturing conditions and behaviours in the EDZ in shale formation, not only affects the choice of the excavation method and support design of the underground engineering projects, but it is also a significant assessment index for the design of permeability sensitive drilling and excavation projects. For the geotechnical projects already mentioned, studying

fracturing conditions and behaviour in the EDZ in shale formation is both academically and economically valuable.

As one of the most encountered rocks during underground construction, shale poses many geotechnical challenges due to its specific properties (e.g., anisotropic behaviours, creeping). Shale is difficult to model, test in the laboratory or conduct field experiments because of its complex mechanism behaviour and the variability. The existence of bedding planes with lower stiffness and cohesion acts as weakening planes in the shale matrix, significantly affecting the strength, and fracturing mechanism of the shale. The orientation of these bedding planes within the shale leads to the most important property of the shale, anisotropy. Among the largest shale gas extraction sites in China, Longmaxi shale has been extensively studied (Xu et al., 2017, Wang et al., 2020 and Yang et al., 2020). The impact of Longmaxi shale anisotropy on its mechanical strengths and fracturing mechanism have been evaluated in several studies (Ma et al., 2016, Wang et al., 2020 and Zhai et al., 2021). This strong directionality mechanism behaviour of shale will significantly contribute to the fracturing preference in the EDZ. However, most field studies on EDZ have only primarily examined the response of excavations aligned with certain dip direction of bedding planes (Bradley, 2013). The study of the fracturing mechanism of the EDZ under the impact of shale anisotropy still remains an open topic.

With the above-mentioned geotechnical challenges, the understanding of the shale anisotropic properties and its effect on the forming and evolution of EDZ in deep tunnel is clearly important for scholars and engineers to predict the depth of the EDZ and optimize the supporting parameters in future.

1.2 Aim and Objectives

This study aims to improve the knowledge of anisotropic behaviour of shale and its effect on the EDZ fracture mechanisms of deep buried tunnels using numerical simulations based on finite and discrete element method (FDEM). To achieve the goal, the main objectives of this thesis are presented as follows:

- 1) To conduct a critical literature review determining the state-of-the-art and any gaps in the literature in relation to the shale anisotropy, EDZ in tunnel excavation and available numerical approaches to simulate anisotropic shale. This will also identify appropriate numerical approaches to simulating shale.
- 2) To select and develop the most appropriate numerical modelling approach identified from the literature which is capable to create anisotropic shale laboratory scale models which accurately captures the short-term mechanical behaviours using Longmaxi shale mechanical strengths data (Uniaxial Compressive Strength (UCS); Brazilian disc (BD)).
- 3) To create and calibrate a field scale FDEM tunnel excavation model to analyse the fracturing mechanism of Full-scale Emplacement tunnel in Opalinus clay shale. The mechanical behaviour (i.e., displacement fields) of the surrounding rock in FDEM model is compared to the FEM model and field measuring in order to evaluate the short-term deformation fields during shale excavation.
- 4) To analyse the effects of the anisotropy on shale mechanical behaviours from a micro crack level. To evaluate the brittleness of the shale through the calibrated FDEM shale laboratory scale model with different bedding plane inclinations to provide a new perspective of shale anisotropy effects on its

macro-mechanical strengths from micro crack level. This objective would focus on fracturing mechanism, fracturing behaviours and brittleness.

- 5) To investigate the anisotropic properties of shale effect on the fracturing mechanism of EDZ using the calibrated field scale FDEM model exposed to different environmental conditions in terms of lateral stress, dip angle of bedding planes and layer thickness thereby providing an in-depth understanding of the fracturing modes of EDZ in shale formation.
- 6) To analyse the failure modes of the EDZ due to shale anisotropy to provide useful information, such as predicting the location the depth of the EDZ to scholars and engineers in the future to optimise the tunnel design and supporting parameters.

1.3 Thesis layout

There are six chapters in this thesis that contains literature review, methodology, the study of shale anisotropy from micro crack level based on FDEM simulation, FDEM simulation of the fracturing behaviours of EDZ under anisotropy shale formation, and conclusions and recommendations for future research. Each chapter is described briefly below:

Chapter 2: This chapter illustrates the state-of-the-art research of shale anisotropy, EDZ in tunnel excavation and available numerical simulation methods for modelling shale anisotropy. In addition, a summary of the gaps in knowledge is also discussed.

Chapter 3: This chapter provides methodology for the developing of the shale models of laboratory tests and tunnel excavation. Using data collected from previous studies, this chapter also reports the calibration of the models.

Chapter 4: The failure modes of shale with different bedding plane inclinations in the laboratory tests (i.e., UCS test and BD test) are recognized. The layer thickness of shale effects on the mechanical strengths is also investigated. In addition, the relationship between the failure modes and fracturing mechanism, and brittleness are discussed.

Chapter 5: Based on the calibrated model for the tunnel excavation in anisotropic shale formation, different environment conditions influence on the EDZ are discussed. Based on the identified fracturing modes in EDZ under different environmental conditions, the fracture conditions and depth of the EDZ in each fracturing mode are analysed.

Chapter 6: This chapter presents the main conclusions from the research. Meanwhile, it highlights the contributions of the research to the field of knowledge and provides recommendations for future studies.

A flow chart for the structure of the thesis is shown in Figure 1.2.

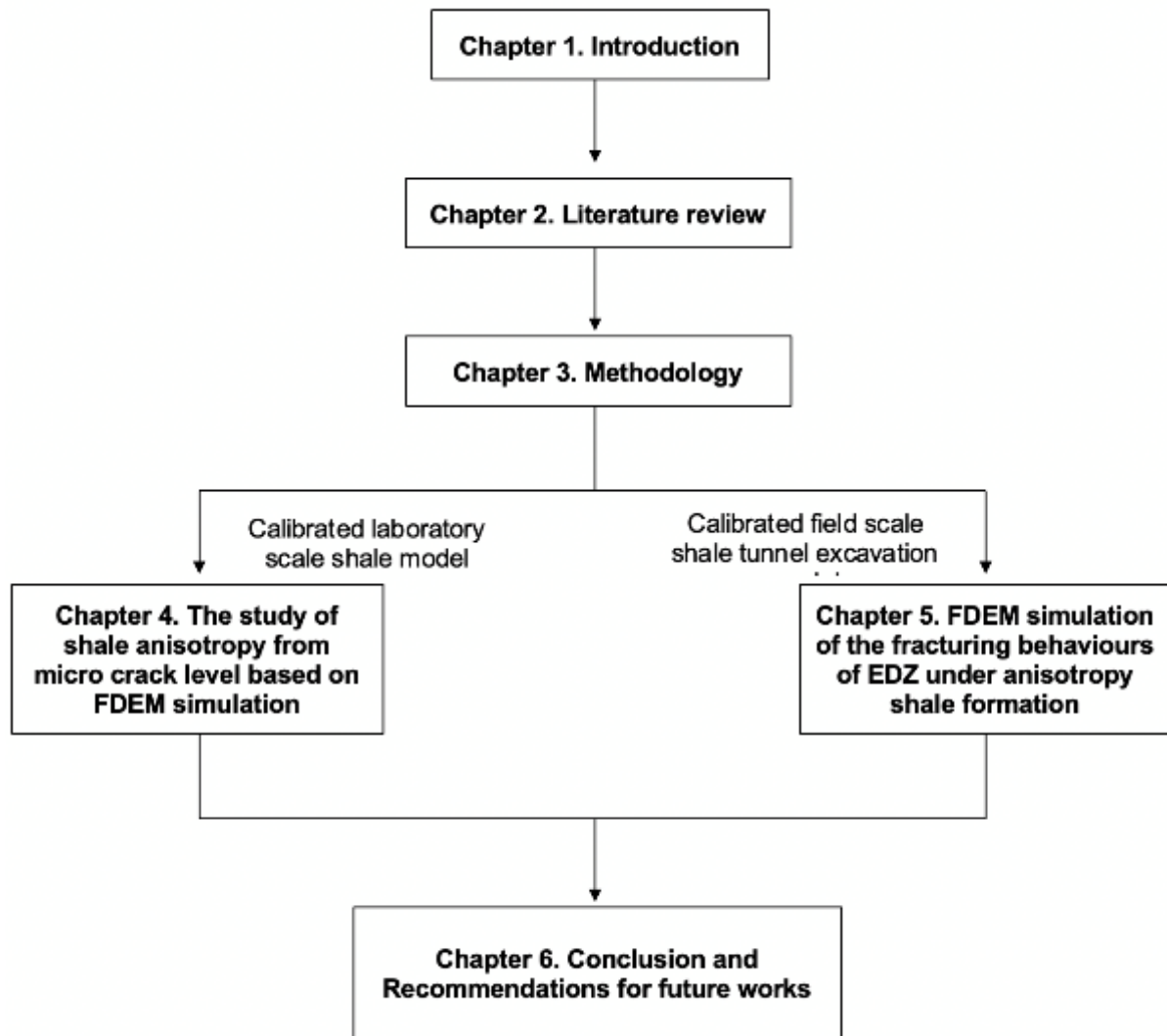


Figure1.2 The structure of the thesis.

Chapter 2 LITERATURE REVIEW

2.1 Introduction

Based on the aforementioned challenges and limitations related to understanding shale anisotropic properties and its effect on the forming and evolution of EDZ in deep tunnels in the Chapter 1, a review of past research studies on shale anisotropy and EDZ properties is presented in this chapter. In addition, due to the difficulties in conducting both laboratory experiments and field studies, this project plans to use numerical simulations to study the EDZ in shale formations. In this case, numerical methods for simulating anisotropic shale are also presented in this chapter. This chapter describes the current state of the art and identifies gaps in previous studies, i.e., areas that haven't been explored.

There are four main sections in this chapter. The former three sections (section 2.2, 2.3 and 2.4) illustrate the previous studies based on shale anisotropy, EDZ properties, and numerical methods for simulating anisotropic shale. In section 2.5, gaps in previous studies are presented and discussed. The arrangement of each section is as follows:

Section 2.2 has been divided into four subsections covering the shale anisotropy, influence of shale anisotropy on the mechanical behaviours, fracturing behaviours and brittleness. The purpose of this is to illustrate what shale anisotropy is and how it affects shale properties.

There are three subsections included in section 2.3, in terms of the characteristics of the EDZ, the forming and evolution of the EDZ and the influence factors of EDZ characteristics. It is the purpose of this section to provide an understanding of what

EDZ is, its properties, its fracturing mechanism, as well as the factors that control EDZ's properties.

Section 2.4 has been divided into three subsections which covers the continuum method, discrete element method (DEM) and also finite discrete element method (FDEM). The purpose of this section is to illustrate the numerical approaches available for simulating layered rocks and assist in selecting the most appropriate numerical modelling approach for creating anisotropic shale laboratory models.

In section 2.5, the gaps spotted in the knowledge regarding previous studies are discussed.

2.2 Shale anisotropy

2.2.1 Shale Anisotropy

Anisotropy characteristics of rock are described as the material exhibiting a variety of mechanical properties depending on the direction in which it is loaded. As a distinctively layered material, shale is widely introduced as transversely isotropic rock (Lisjak et al., 2014a, Yang et al., 2020). As shown in Figure 2.1, the properties of the shale (such as hydraulics, stiffness, permeability, and mechanical strength) in a plane parallel to the bedding planes are considered isotropic, whereas those at other angles to the plane have different values. The plane is called plane of transverse.

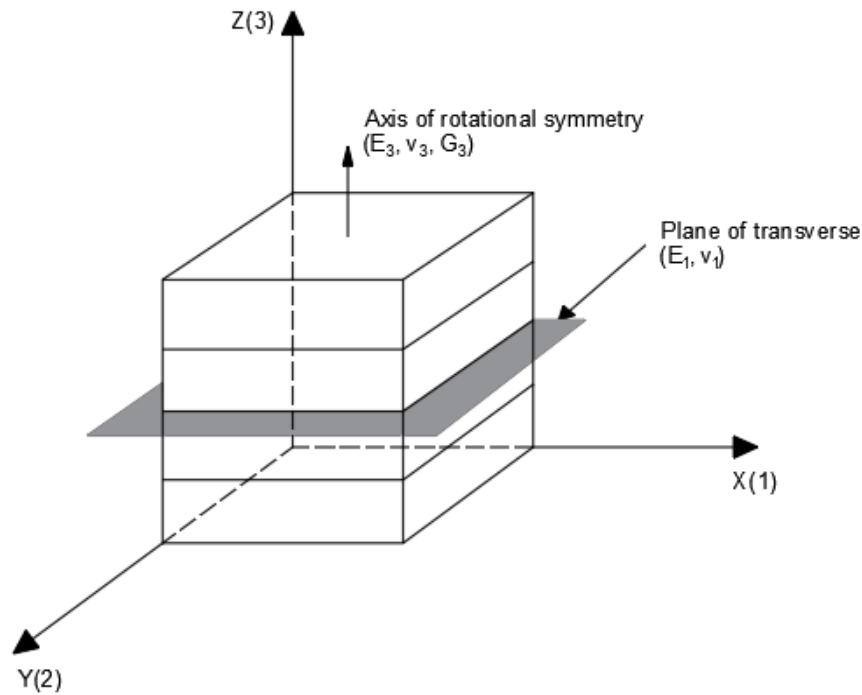


Figure 2.1 Elastic constants of transversely isotropic rock.

Numerous researchers have conducted uniaxial compression strength test (UCS) tests on different shales in order to gain a better understanding of rock mechanical behaviour under compression (Yan et al., 2015, Lu et al., 2021, Duan et al., 2019 and Lisjak et al., 2014a). Figure 2.2 illustrates a typical stress-strain curve for shale rock with identified behaviour stages during compression (Lisjak et al., 2014a and Bieniawski, 1967). According to Figure 2.2, the mechanical response of shale sample under UCS test can be divided into four main phases: crack closure phase (I), linear elastic deformation phase (II), crack propagation phase (III) and post-peak phase (IV). Phase one involves compressing pre-existing flaws or micro-cracks under applied pressure, resulting in a nonlinear stress-strain response. Phase two occurs when the pre-existing flaws in the sample are closed, resulting in a linear elastic phase until point A is reached, where fracture propagates and coalesces. Phase three after point A

results in a non-linear response due to plastic deformation caused by fractures propagating. Point B marks the peak strength of the shale sample at the end of this phase. The evolution of fractures formed within shale samples is significantly related to the mechanical strength of shale, as shown by the stress-strain behaviour of the UCS test sample. Fractures forming inside samples are the primary cause of inelastic strain accumulation.

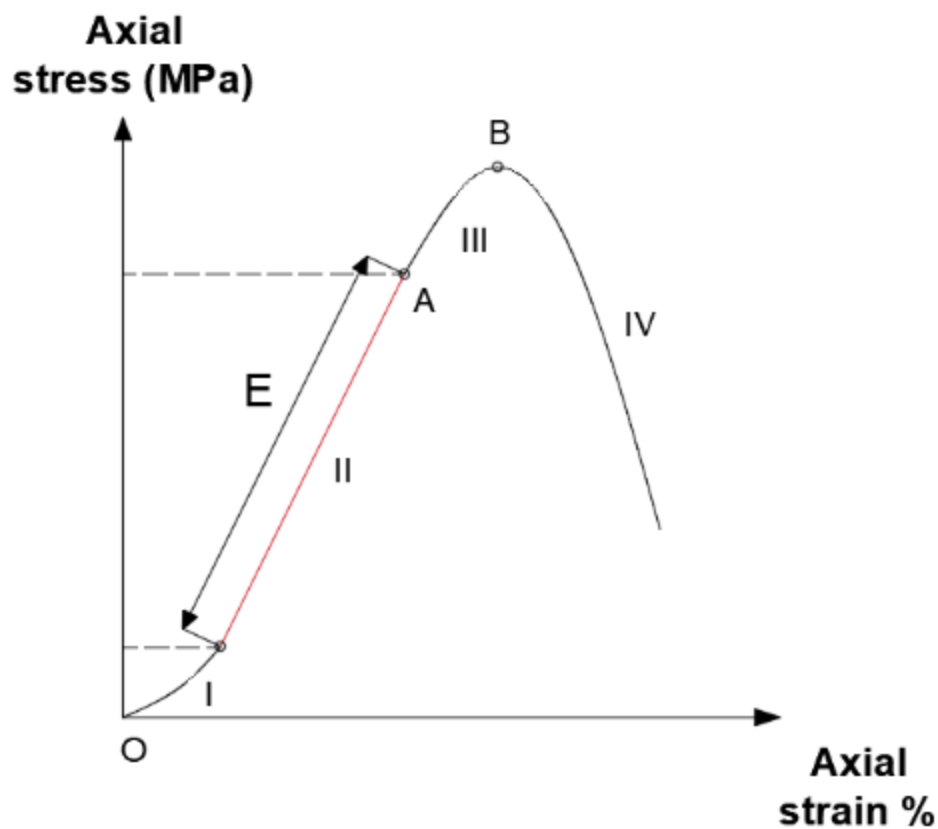


**Figure 2.2 Typical stress-strain curve obtained in shale sample under UCS test
(modified after Lisjak et al., 2014a and Bieniawski, 1967).**

To capture the linearly elastic behaviour of shale, there are numerous works on the mathematical derivation of elastic parameters from its samples (Graham and Houlsby, 1983, Siggins and Dewhurst, 2007 and Jaeger et al., 2007) . The generalized form of Hooke's law for elastic stress-strain relationships is as follows:

$$\{s\} = \{e\}|C| \quad \text{Eq. 2.1}$$

Where $|C|$ is a 6×6 stiffness matrix, $\{s\}$ and $\{e\}$ represents 1×6 stress and strain column vectors, respectively (Voigt, 1928). Equation 2.1 can be written in a matrix form as follows:

$$\begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{xy} \\ \tau_{zy} \\ \tau_{xz} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \varepsilon_{xy} \\ \varepsilon_{zy} \\ \varepsilon_{xz} \end{bmatrix} \quad \text{Eq. 2.2}$$

Where σ_x , σ_y and σ_z are normal stresses in the axis directions, and τ_{xy} , τ_{zy} and τ_{xz} are shear stresses on the XY, ZY and ZX planes. Meanwhile, ε_x , ε_y and ε_z are normal strains in the axis directions, and ε_{xy} , ε_{zy} and ε_{xz} are shear strains on the XY, ZY and ZX planes. Based on Equation 2.2, there are 21 independent stiffness parameters. Due to the rotational symmetry of transverse isotropic materials, the independent stiffness parameters can be reduced to 5, as shown in Equation 2.3. Z (3) is the rotational symmetry axis of the material in Figure 2.1.

$$\begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{xy} \\ \tau_{zy} \\ \tau_{xz} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \varepsilon_{xy} \\ \varepsilon_{zy} \\ \varepsilon_{xz} \end{bmatrix} \quad \text{Eq.2.3}$$

Where $C_{66} = \frac{(C_{11}-C_{12})}{2}$. Thus, the elastic deformation of transversely isotropic rock is characterized by five independent elastic constants (axis z as the rotational symmetry axis: E_1 , ν_1 , E_3 , ν_3 , G_3 (Jaeger et al., 2007). E_1 and ν_1 are the Young's Modulus and Poisson's ratios in the plane of the transverse isotropy, respectively. E_3 , ν_3 and G_3 are

the Young's Modulus, Poisson's ratios and shear modulus in the direction of parallel to the axis of rotational symmetry, as shown in Figure 2.1.

2.2.2 Influence of shale anisotropy on the mechanical behaviours

In the past decades, many researchers have conducted various laboratory tests to study the anisotropic properties of shale effects on the mechanical strength. Researchers around the world have studied the mechanical response of shale under uniaxial compression strength (UCS) tests with samples obtained from various places (Yang et al., 2020; Cao et al., 2021 and Popp et al., 2008). The experimental results suggest that the maximum uniaxial compressive strength is normally found in the sample with bedding planes parallel or perpendicular to the major principal stress, while the minimum value is obtained in the sample with bedding planes 30° to the major principal stress (Heng et al., 2015). Based on results from UCS tests on shale from around the world, the curve of the shale uniaxial compressive strengths with variation of bedding planes dipping angles can be generally classified into three types, i.e., "U-shaped", "shoulder shaped" and "wavy shaped", as shown in Figure 2.3 (Ramamurthy, 1993).

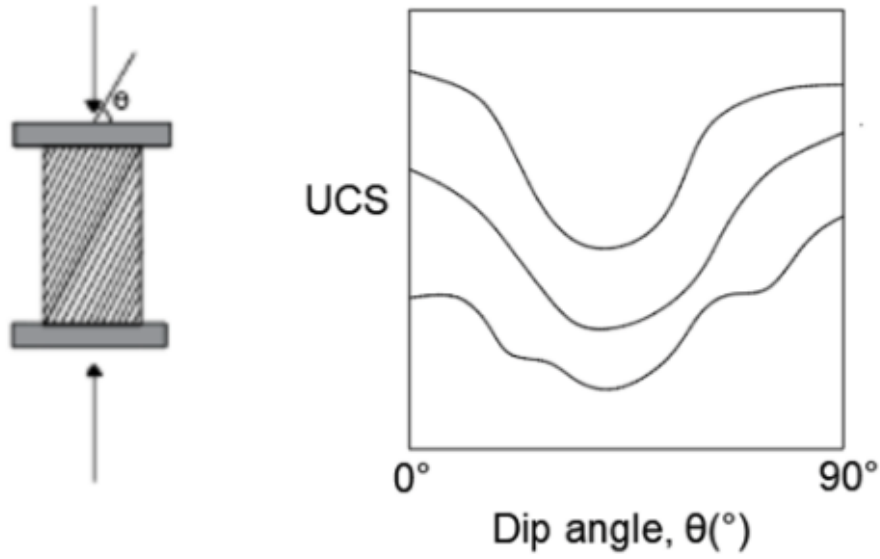


**Figure 2.3 Variation of UCS values with changing of the bedding planes dip angles
(Modified after Ramamurthy (1993))**

In 1960, Jaeger first proposed a failure criterion to describe shale strength anisotropy by introducing a single weakening plane in the shale matrix (Jaeger, 1960), as shown in Figure 2.4. Using the linear Mohr-Coulomb failure criterion, the failure of geomaterials appears to slip along the plane when the shear stress, τ , on the plane reaches a critical value to overcome a "frictional" resistance force, plus an additional material shear strength, S . The criterion for the failure along the plane is as follows:

$$\tau = S + N \tan \phi_i \quad \text{Eq. 2.4}$$

ϕ_i is the internal friction angle, N is the normal stress on the plane. With a plane inclined β to the maximum principal stress, σ_1 ,

$$N = N_m - \tau_m \cos 2\beta \quad \text{Eq. 2.5}$$

$$\tau = \tau_m |\sin 2\beta| \quad \text{Eq. 2.6}$$

Where N_m is the maximum normal stress, and τ_m is the maximum shear stress.

$$\tau_m = (\sigma_1 - \sigma_3)/2 \quad \text{Eq. 2.7}$$

$$N_m = (\sigma_1 + \sigma_3)/2 \quad \text{Eq. 2.8}$$

The σ_1 and σ_3 are the maximum and minimum principal stresses, as shown in Figure 2.4. The Jaeger single weak plane failure criterion, expressed in terms τ_m and N_m (found by inserting Equation 2.5 and Equation 2.6 into Equation 2.4), is

$$\tau_m = (S \cos \phi_i + N_m \sin \phi_i) / [\sin(2\beta + \phi_i)] \quad \text{Eq. 2.9}$$

The minimum values happened when $\beta = 45^\circ - \phi_i/2$. In the UCS test with zero minimum principal stress, σ_3 , Equation 2.9 can be written as:

$$\sigma_1 = \frac{2S}{(1 - \tan \phi_i \cot \beta) \sin 2\beta} \quad \text{Eq. 2.10}$$

Based on Equation 2.10, the maximum principal stress needed to produce slip along the weak plane is changing with β . When β is getting close to 90° , the principal stress required for shearing along the plane tends to infinity, which does not comply with the mechanical behaviours of shale (Yang et al., 2020; Cao et al., 2021 and Popp et al., 2008). Bewick (2008) suggested that this is because the failure mode of the model changes from shearing along the plane to a combination of slipping along the plane and failure through the rock matrix or only failure through the rock matrix.

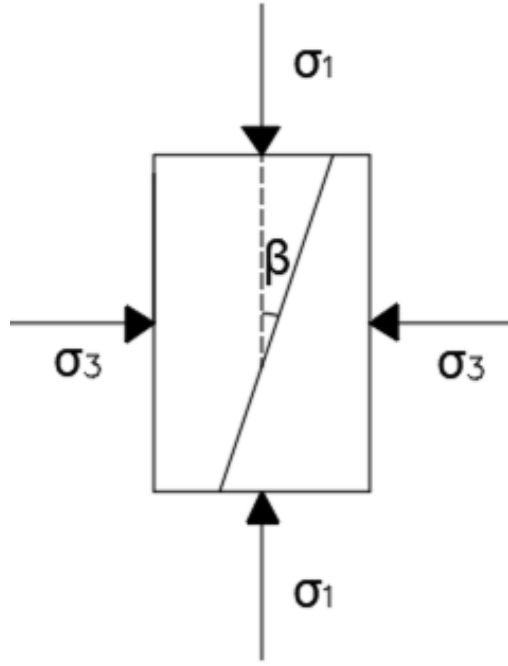


Figure 2.4 Rock with single weak plane under a triaxial compression test (β is the angle between the weak plane and maximum principal stress).

Based on the above failure criterion, many researchers have developed further failure criterions considering the changing of the shear strength of the plane and the friction coefficient $\tan\phi$ with the changing of the angle β (Jaeger, 1960, Mclamore and Gary, 1967).

Li et al. (2020) have evaluated shale samples with seven different bedding layer orientations (0° , 15° , 30° , 45° , 60° , 75° , 90°) in a triaxial compressive laboratory test. In their study crack initiation stress (CI) and crack damage stress (CD) thresholds were collected using the stress-axis strain curve and the lateral strain-axis strain curve, which showed that the crack initiation stress is independent of the bedding layer orientation. In contrast, crack damage stress of shale is significantly affected by the shale anisotropy (Li et al., 2020).

The influence of the anisotropic behaviours of shale on the tensile strength is also studied by a few researchers. The tensile strength of the shale decreases with the increasing dip angles of the bedding planes (Wang et al., 2017 and Feng et al., 2020). Meanwhile, the elastic modulus of the shale increases with increasing dip angles of the bedding planes (Yang et al., 2020; Cao et al., 2021).

Ren et al. (2021) have studied the shale anisotropy effect on the fracture toughness and energy. The chevron-notched deep beam (CNDB) was used to test 12 longmaxi samples of different dip angles (i.e., 0° and 90°). It was found that the fracture toughness of the shale sample with 0° and 90°, is 1.116 MPa $m^{1/2}$ and 0,781 MPa $m^{1/2}$, respectively. Meanwhile, the fracture energy for the 0° and 90°, is 44.44 N/m and 23.12 N/m, respectively. The mechanical response of the fracture inside of the shale sample is significantly affected by the shale anisotropy.

By studying the permeability of Barnett shale in two different bedding layer inclinations (i.e., 0° and 90°), the ratio between the horizontal to the vertical permeability is approximately 40 with a confining stress of 10.3 MPa (Bhandari et al., 2015). Moreover, the horizontal-vertical permeability ratio was observed to remain the same under different confining stresses, which indicates that permeability anisotropy of shale is independent from the effective stress.

Xu et al. (2017) monitored the wave velocity of the Longmaxi shale samples cored horizontally and vertically to the bedding planes under UCS tests. The results showed that the velocity of the P-wave and S-wave for horizontally cored samples is considerably higher than for vertically cored samples. In addition, the P-wave values remained stable with increasing confining stress in the horizontally cored samples compared to the S-wave values.

Using acoustic emission, Guo et al. (2021) examined the changes in P-wave velocity in five shale samples with different bedding plane inclinations (0° , 30° , 45° , 60° and 90°). P-wave velocity increases with increasing bedding plane inclination, as indicated by the obtained values. With increasing thermal temperature, the velocity in each model decreased.

The previous studies have demonstrated that shale anisotropy affects the mechanical behaviour of shale samples. The aforementioned literature review shows, however, that the mechanical response of shale under tests has primarily been studied at the macroscale peak value of strengths. Based on the stress-strain curve of the shale sample under compression, it appears that the mechanical response of shale is under the effects of fracture initiation and propagation. Additionally, the sensitivity of CD threshold to shale anisotropy indicates that the micro crack level underlies the effect of shale anisotropy on macro mechanical strength. The evolution of fractures inside of rocks have a significant impact on its macro mechanical strength apparently. However, the understanding of shale macro mechanical strength from micro-crack level (e.g., fracturing mechanism and fracturing conditions) still remains as an open book. Shale anisotropy effects on its macro mechanical strength can be better understood by studying the mechanisms and conditions of fracturing at the micro crack level.

2.2.3 Influence of shale anisotropy on the fracturing behaviours

EDZ is characterized by fractures that form inside, which makes understanding the behaviour of shale fracturing (e.g., size and shape) crucial to evaluating its properties. Meanwhile, literatures in the last section have shown the macro mechanical strengths of shale are under the effects of shale anisotropy from micro crack level. Hence, understanding shale anisotropy effects on fracturing behaviours is important.

Li et al. (2021) compared the fracturing behaviour of 7 Longmaxi shale models with different bedding plane inclinations (0° , 15° , 30° , 45° , 60° , 75° and 90°) in notched deep beam (NDB) tests. Figure 2.5 shows that when the bedding dip angle is greater than 45° , crack propagation tends to follow the bedding plane rather than proceeding straight along the crack direction. According to Li et al. (2021), this is due to the energy principle, in which fractures propagate along the path that consumes the least amount of energy.

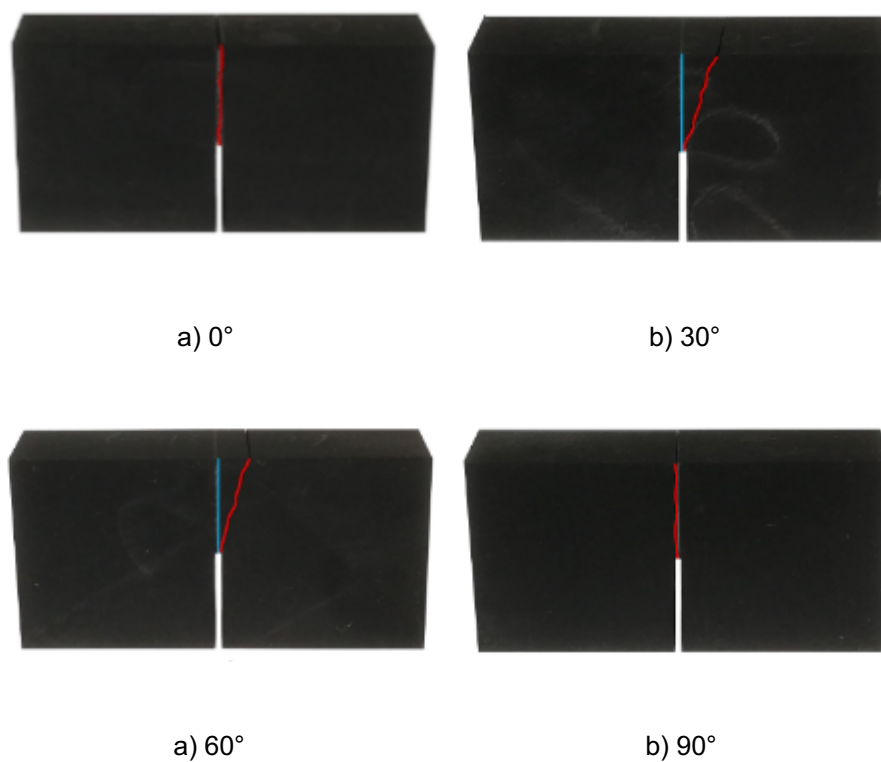


Figure 2.5 Crack propagation of shale with different bedding plane inclinations in NDB test (the white line is the pre-existed crack direction, red line is the crack propagation path, and blue line indicates the extending of the crack along the crack direction) (Li et al., (2021)).

Based on the observation of the failure modes of the Longmaxi shale samples with different dip angles under UCS test, Wang et al. (2020) have noticed that for shale

samples with lower dip angles ($\theta = 0^\circ$ and 15°), the macro-fractures are mainly located inside of the shale matrix. With increasing dip angles, the shale samples fracture more along the bedding planes, as shown in Figure 2.6.

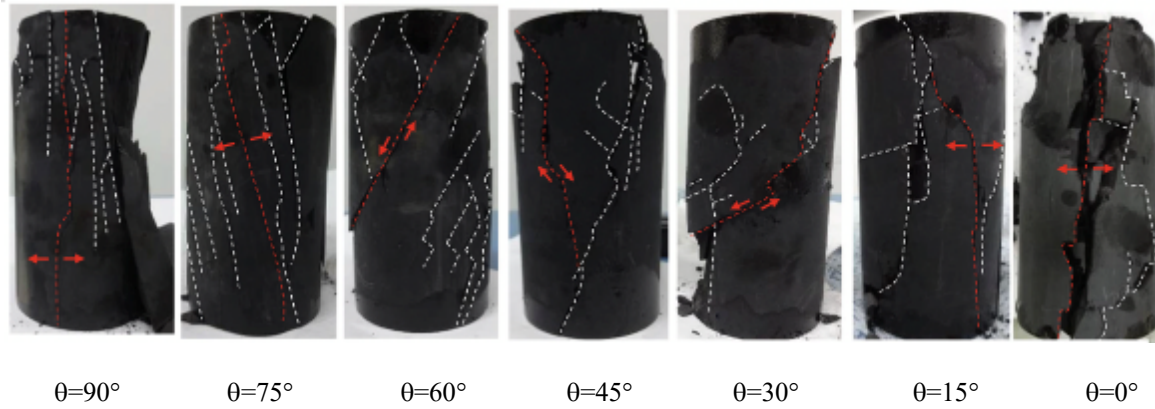


Figure 2.6 Failure modes of shale samples with different inclination angles under UCS test (Wang et al., 2020).

In addition, the shale anisotropy effect on the fracturing behaviour can also be noticed in the Brazilian disc (BD) tests. The failure modes of Chongqing Longmaxi shale samples with 4 different inclination angles under BD test are shown in Figure 2.7 (Wang et al., 2017). The bedding planes have a significant influence on the fracturing of the shale sample, especially when the bedding planes are steep. The fractures tend to propagate along the bedding plane in shale sample with a bedding plane inclination of 90° .

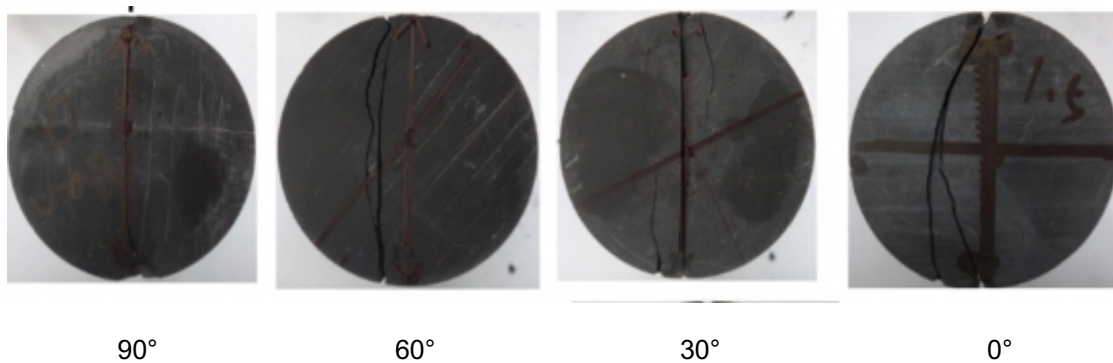


Figure 2.7 Failure modes of shale samples with different inclination angles under BD test (Wang et al., 2017).

Meanwhile, many researchers have conducted experiments to study shale borehole stability. Meier et al (2015) have found that the failure of the shale samples within boreholes is starting with fracturing along the bedding planes by using X-ray CT scan. The borehole stability is strongly affected by the slip along the bedding planes in inclined shale samples (Økland and Cook 1998; Russell et al. 2003). Shale samples with bedding planes perpendicular to the maximum principal stress show V-shaped notch failures (Choens et al., 2019).

In field-based experiments, V-shape notches have been found in the crown and invert of a tunnel constructed in shale with 0° bedding planes (Dammyr, 2016). The regions perpendicular to the bedding planes that point towards the tunnel wall are prone to experience large deformations (Cui et al., 2014 and Xu et al, 2020). Compared to the isotropic rock masses, tunnels in shale formations tend to have asymmetric deformation and slip along bedding planes (Do et al., 2019).

As a result of its anisotropic properties, the fracturing behaviour of shale in both laboratory experiments and field tunnel excavation shows great directionality. However, there are still some limitations. Aforementioned laboratory experiments have simply focused on its final macro fractured failure modes under shale anisotropy, and the reasons behind the fracturing behaviour from micro crack level still remain. Furthermore, few studies have explored the relationship between the fracturing behaviour and mechanical properties of shale (Young's modulus, shale strengths). As discussed in section 2.2.3, the failure of shale rock in experiment tests is caused by the formation and propagation of fractures, and the mechanical strengths (for example,

CD, uniaxial compressive strength, and tensile strength) are significantly influenced by shale anisotropy at the microcrack level. The study of the fracturing behaviour of shale in the field focuses on case studies, which make it difficult to gain general laws and conclusions about fracturing behaviours in shale formations as it only analyses one specific engineering case.

2.2.4 Shale brittleness

Brittleness is a term commonly adopted in geotechnical engineering to describe potential failure characteristics of rocks (Zhang et al. 2016). It has been used in many engineering projects to predict and evaluate the rock fracturing conditions (Holt et al., 2015, Gong and Zhao, 2007, Hucka and Das, 1974 and Yarali and Kahraman, 2011). Scholars and engineers have faced one of the common issues of rockburst during underground construction, and they have used brittleness indices as one of the major criteria methods to predict it (Wang et al., 2020). Based on comparisons of the burst proneness index (ratio of strain energy retained to dissipated strain energy obtained from UCS tests) and the brittleness index (ratio between uniaxial compressive strength and tensile strength) obtained from granite, Singh (1987) found that brittle failure is an important condition for a rockburst to occur. In addition, brittleness is also commonly used in hydraulic fracturing to evaluate shale properties. Fracture work in shale during hydraulic fracturing depends on a variety of factors, including brittleness of the shale. Shale can be classified into two different types, in terms of brittle and ductile, based on its mechanical behaviour (Rybacki et al., 2016 and Jaeger et al., 2007). Compared to ductile shale, brittle shale is more susceptible to fracture, and the induced fractures are more likely to remain open (Zhang et al., 2016). To this date, there still is no general definition for brittleness. Generally, a sudden failure is more likely to occur

with massive fractures in brittle rocks, with a sudden drop in strength (Zhang et al., 2016). The following characteristics are commonly observed in brittle rocks, based on Hucka and Das (1974) and Zhang et al. (2016):

- 1) low value of elongation along the loading direction;
- 2) distinct fracture surface at the failure area;
- 3) higher elastic modulus;
- 4) large strength reduction after failure;
- 5) multiple fractures;
- 6) higher ratio of compressive strength to tensile strength.

A large body of research has studied the shale brittleness influencing factors, such as material internal geological factors, environment factors and geo-stress differences (Wang et al., 2016, Jarvie et al., 2007, Ai et al., 2016 and Hucka and Das, 1974). On that basis, many researchers have proposed different rock brittleness indices (BI) based on, for example, rock strength, stress strain curve, energy balance and components analysis (Jarvie et al., 2007, Bishop et al., 1971 and Munoz et al., 2016).

1) Mineral composition based *BIs*

As the formation and evolution of fractures within the rock is strongly controlled by the mineral composition, the brittle and ductile properties of shale are highly influenced by it (Li, 2022). In comparison to ductile shale, brittle shale is believed to contain more brittle minerals, however brittle mineral still lacks a unified definition (Li, 2022). The study of Barnett shale by Jarvie et al. (2007) found quartz to be one of the main

minerals responsible for simulating the brittleness of shale, and proposed the brittleness index BI_{qz} , as shown in Equation 2.11.

$$BI_{qz} = \frac{W_{qz}}{W_{qz} + W_C + W_{cl}} \quad \text{Eq. 2.11}$$

Where W_{qz} , W_C and W_{cl} are the weight of the quartz, carbonate and clay minerals, respectively.

As shale with high content of dolomite shows high Young's modulus, dolomite also has been classified as brittle minerals (Wang and Gale, 2009). The Young's modulus decreases with the increase of limestone and organic matter, which have been recognized as ductile minerals. Wang and Gale (2009) modified Equation 2.11 to include brittle dolomite, ductile limestone, and organic matter, as shown in Equation 2.12.

$$BI_b = \frac{W_{qz} + W_{dol}}{W_{qz} + W_C + W_{cl} + W_{dol} + W_{lm} + W_{TOC}} \quad \text{Eq. 2.12}$$

Where W_{dol} , W_{lm} and W_{TOC} are the weight of the dolomite, limestone and organic matter respectively.

This approach, however, has its limitations. Firstly, there is insufficient physical basis for this index since it is simply based on field data. Secondly, testing all types of minerals in rocks is time-consuming.

2) Stress-strain curve based BI s

Stress-strain curves can give a full representation of rock failure and can show the mechanical characteristics of rocks before and after failure. Hence, stress-strain curves are used frequently nowadays for determining the mechanical properties of

rocks (Chen et al., 2017). A brittle rock mass can be quantified by its strength and deformation performance under stress, which are indicators of its brittleness. The strain generated by brittle rocks is mostly elastic before failure, while ductile rocks are mostly inelastic (plastic) before failure without losing their bearing capacity (Li, 2022). Therefore, the ratio between the elastic strain and total strain before failure has been adopted as a brittleness index, as shown in Equation 2.13 (Hucka and Das, 1974).

$$BI_s = \varepsilon_e / \varepsilon_u \quad \text{Eq. 2.13}$$

Where ε_e is the elastic strain and ε_u is the total strain before failure, as shown in Figure 2.8.

Brittleness indices obtained from stress-strain curves normally only take strain or strength behaviours into account separately. According to Hajiabdolmajid and Kaiser (2003), two rocks with the same BI_s values have the same strain paths, but their peak strengths are different. Therefore, using strain and stress parameters alone may not always be accurate to predict the brittleness of a rock.

By measuring the mutual effect of stresses and strains within a rock mass, Young's modulus and Poisson's ratio obtained from stress-strain curve provide more accurate measurements of its brittleness than measuring them individually. Compared to ductile material, brittle materials are more likely to experience shear fracturing with small displacement, which means the brittle rock shear modulus, G , has larger values (Jahandideh and Jafarpour, 2016).

$$G = \frac{FL}{A\Delta x} \quad \text{Eq. 2.14}$$

where F is the applied shear force, L is the initial length, A is the area where the force acts and Δx is the transverse displacement. The shear modulus for the isotropic material can be calculated from the Young's modulus, E , and Poisson's ratio, ν , as follow equation:

$$G = \frac{E}{2(1+\nu)} \quad \text{Eq. 2.15}$$

Based on Equation 2.15, rocks with a high Young's modulus and low Poisson's ratio have more potential for brittle failure along the shear planes (Jahandideh and Jafarpour, 2016). Hence, Luan et al. (2014) used the ratio between the Young's modulus and the Poisson's ratio to calculate the brittleness index of rock.

$$BI_L = \frac{E}{\nu} \quad \text{Eq. 2.16}$$

However, the adopting of the elastic modulus only representing the elastic phase of the stress-strain curve. It disregards the plastic phase of the stress-strain curve. Hence, the accuracy of this index is limited.

3) Energy based BI s

Rock failure is essentially a balance between energy absorption and release. With stress-strain curves, the energy evolution of the rock failure process can be clearly depicted, as shown in Figure 2.8 (Li, 2022). Prior to failure, the rock specimen keeps absorbing external energy, resulting in significant amounts of elastic energy (the green area) being stored inside, and also the unrecoverable plastic deformation with internal damage (fracture forming and propagating) caused by the dissipation of some other energies (the grey area) (Ai et al., 2016 and Yang et al., 2020). Before the peak strength, most of the absorbed energy is stored in the form of the strain energy (Ai et

al., 2016). Hukka and Das (1974) first introduced Bl_{et} , in terms of the ratio between the consumed elastic energy (U_{et}) and total energy ($U_P + U_{et}$) during compression, to describe brittleness, as shown in Equation 2.17.

$$Bl_{et} = U_{et} / (U_P + U_{et}) \quad \text{Eq. 2.17}$$

As the rock fails, the stress decreases, and the stored energy is released. The release of the stored elastic energy and post-peak energy leads to macro-fractures, which leads to specimen full damage (Munoz, et al., 2016).

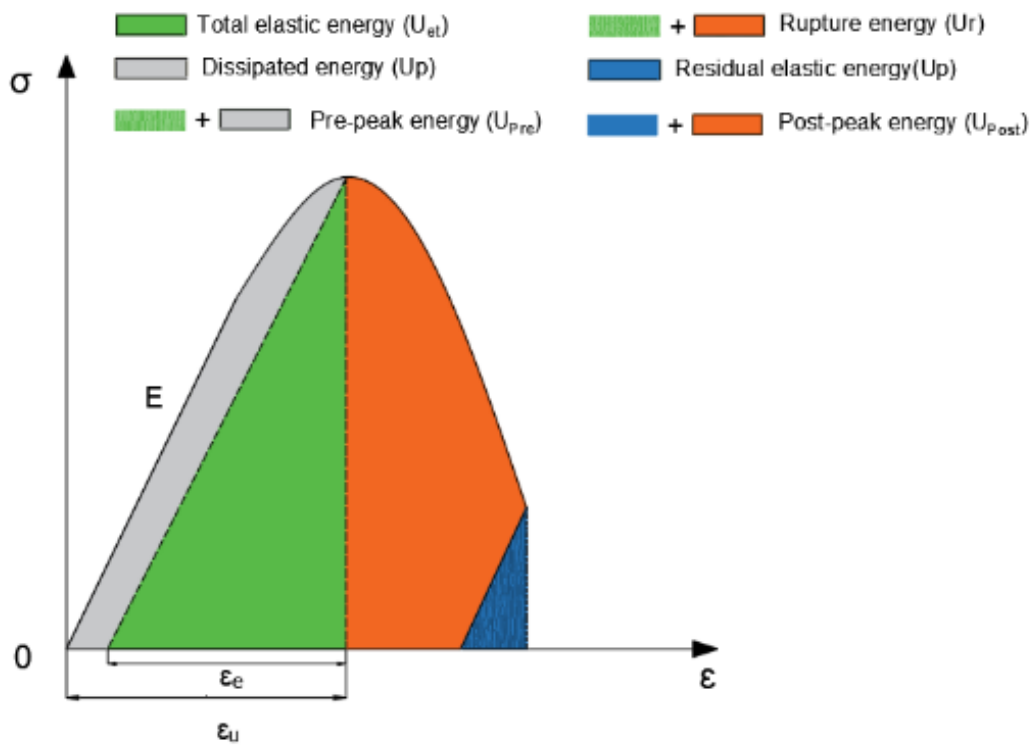


Figure 2.8 Energy evolution of rock failure process on stress-strain curve (Li, 2022).

To fully use the stress-strain curve and understand the post-peak rock failure behaviours, Munoz et al. (2016) used the pre-peak strength energy (U_{pre}) and post-peak energy (U_{post}) to create new brittleness indices, Bl_{M1} and Bl_{M2} as shown in Equation 2.18 and Equation 2.19.

$$BI_{M1} = U_{et}/(U_{Pre} + U_{Post}) \quad \text{Eq. 2.18}$$

$$BI_{M2} = U_{et}/U_{Post} \quad \text{Eq. 2.19}$$

A rise in post-peak energy indicates a rise in stability, Munoz et al. (2016) claim. Brittle rocks tend to have a sudden drop of strength with small strain after peak strength, which shows less post-peak stability with less post-peak energy. Therefore, bigger value of BI_{M1} and BI_{M2} values indicate more brittle rocks.

4) Strength parameters based BIs

The uniaxial compressive strength (σ_u) and tensile strength (σ_t) are two common rock mechanic strength properties, and it has been observed that the ratio between the compressive and the tensile strengths is related to the brittleness (Hucka and Das, 1974). Based on this, Hucka and Das (1974) proposed two brittleness indices as follows:

$$BI_{s1} = \frac{\sigma_u}{\sigma_t} \quad \text{Eq. 2.20}$$

$$BI_{s2} = \frac{\sigma_u - \sigma_t}{\sigma_t + \sigma_u} \quad \text{Eq. 2.21}$$

Because these two BIs are based on easily obtained laboratory parameters, they are widely used by researchers today to evaluate the brittleness of rocks (Tarasov and Potvin, 2013, Altindag, 2002, Gong and Zhao, 2007 and Wang and Park, 2001). However, there are some limitations with using of the BI_{s1} and BI_{s2} . First, BI_{s1} and BI_{s2} build on the ratio between the two values, in terms of uniaxial compressive strength and tensile strength, which means two different rocks with different uniaxial compressive strength and tensile strength could have same values of BI_{s1} and BI_{s2} . Moreover, a study by Meng et al. (2015) found that BI_{s1} falls within the range of value

8-22 across various data sets. This limited variation range of BI_{s1} makes it insufficient for describing the difference in brittleness between various rocks based on the analysis (Meng et al., 2015). Therefore, Altindag (2002) proposed a new brittleness index, BI_{s3} , as shown in Equation 2.22.

$$BI_{s3} = \frac{\sigma_u \sigma_t}{2} \quad \text{Eq. 2.22}$$

Compared to BI_{s1} and BI_{s2} , BI_{s3} is better in relating the brittleness and penetration rate based on data collected by Altindag (2002). Penetration rate describes the drillability of rocks. It equals the ratio between the total depth drilled (m) and total time taken (min).

Table 2.1 summarises the brittleness indices mentioned in this section. As mentioned above, the proposed brittleness indices are usually included in the four methods, in terms of mineral composition based, stress-strain curve based, strength parameter based, and energy based. Excepting mineral composition, other three methods are all related to the stress-strain curve. The compressive strength, strain and energy balance parameters can all be obtained from the stress-strain curve.

Table 2.1 Summary of mentioned brittleness indices, BI

Method	Formulae	References
Mineral composition	$BI_{qz} = \frac{W_{qz}}{W_{qz} + W_C + W_{cl}}$ $BI_b = \frac{W_{qz} + w_{dol}}{W_{qz} + W_C + W_{cl} + W_{dol} + W_{lm} + W_{TOC}}$	Jarvie et al. (2007) Wang and Gale (2009)
Stress-strain curve	$BI_S = \varepsilon_e / \varepsilon_u$ $BI_L = \frac{E}{V}$	Hucka and Das, 1974 Luan et al. (2014)
Energy balance	$BI_{et} = U_{et} / (U_P + U_{et})$ $BI_{M1} = U_{et} / (U_{Pre} + U_{Post})$ $BI_{M2} = U_{et} / U_{Post}$	Hucka and Das (1974) Munoz et al., (2016)
Strength parameters	$BI_{s1} = \frac{\sigma_u}{\sigma_t}$ $BI_{s2} = \frac{\sigma_u - \sigma_t}{\sigma_t + \sigma_u}$	Hucka and Das (1974)

$$BI_{s3} = \frac{\sigma_u \sigma_t}{2}$$

Altindag (2002)

As discussed above, there is no general definition of brittleness of rock. Different brittle indices were proposed based on different characteristics of rock brittleness. Based on its mechanical properties, shale can be classified as either brittle or ductile (Nygard et al., 2006). Comparing to ductile shale, brittle shales are more easily fracture (Sui et al., 2019). Brittleness of rock has been used to evaluate rock cutability, drill-ability, and frac-ability in hydraulic fracturing, mining, and tunnelling (Altindag, 2002, Dursun and Gokey, 2016 and Kahraman and Altindag, 2004). Since this research focuses on fracturing conditions in EDZ, fracturing behaviour in shale is the primary concern. Therefore, investigating the brittleness of shale is important from the aspect of rock fracturing. Although some researchers have conducted studies on the relationship between the rock failure mechanical characteristics (cutability, drill-ability, and frac-ability) and brittleness of rocks, but few studies have studied the shale anisotropy effects on its brittleness. Based on the discussion of last section, shale anisotropy shows a great impact on its fracturing conditions. The changing of the frac-ability of shale under the influence of shale anisotropy will undoubtedly impact on the brittleness. In the presence of shale anisotropy, the frac-ability and brittleness of shale changes. Therefore, studying shale anisotropy effects on brittleness from a micro-crack level can provide an additional perspective to further understand shale anisotropic behaviour.

2.3 Excavation Damage Zone (EDZ) studies

2.3.1 The characteristics of the EDZ

The concept of EDZ was first introduced in the early 1980s in relation to nuclear waste disposal (Kelsall et al., 1984). As a result of excavation methods and redistribution of stresses, the EDZ occurs near the tunnel wall where the mechanical, and hydraulic properties of the rocks have been seriously impacted due to the excavation-induced fractures (Malmgren et al., 2007). In the past decades, many researchers have studied the EDZ in shale formation in various sites (e.g., HADES-Belgium, Mont Terri-Switzerland, Tournemire-France, Lac du Bonnet-Canada) because shale formations are widely considered to be suitable for radioactive waste disposal. Bossart et al. (2004) have found that EDZ in the new gallery of the Mont Terri Rock Laboratory can be classified into two zones – an inner zone and an outer zone, based on the fracturing pattern through borehole observation, as shown in Figure 2.9.

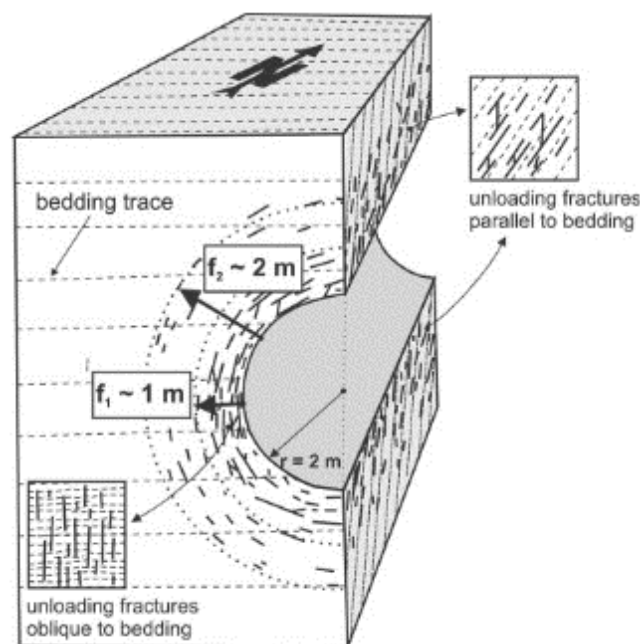


Figure 2.9 Structural model of EDZ with fractures in Mont Terri Laboratory (f_1 is the area with interconnected fractures, and f_2 is the area which is less fractured and not connected to the tunnel wall) (Bossart et al., 2004).

The inner zone is defined as a zone consisting of an interconnected fracture network with connections to the tunnel wall, while the outer one is less fractured and not connected to the tunnel wall (Bossart et al., 2004). The permeability of clay shale samples obtained from the inner zone and outer zone has increased 10 times and 5 times, respectively, as compared to the Opalinus clay shale far outside of the damaged zone (Nagra, 2002). Based on borehole samples in HADES, Belgium, an increase in hydraulic conductivity is measured up to approximately 2-3m into the surrounding rock (Bastiaens et al., 2007). The average permeability of samples obtained outside and inside of the EDZ are 10^{-21} m/s and 4×10^{-14} m/s, respectively. As shown in Table 2.2, the increasing of the gas permeability of the surrounding rock in EDZ at several locations has been found.

Table 2.2 Gas permeability in EDZ after excavation in different locations (m/s)

Locations	Intact rock	EDZ
Callovo-Oxfordian clay, Meuse (France) (Armand et al., 2013)	$10^{-22} \sim 10^{-21}$	4×10^{-16}
Opalinus Clay, Mont Terri (Switzerland) (Zhang and Rothfuchs, 2008)	10^{-21}	10^{-14}

Boom Clay

(Belgium)

$10^{-21} \sim 10^{-20}$

4×10^{-14}

(Delage et al., 2011)

Moreover, the Young's modulus in the EDZ of the Kiirunavaara iron mine were 50%-90% reduced compared to the undamaged rock through P-wave measurements (Malmgren et al., 2007). This has also been found in the EDZ of KAERI shale underground research tunnel (KURT) (Kwon and Cho, 2008). Young's modulus of samples from the EDZ decreased about 37% compared to samples obtained before excavation, based on laboratory tests (Kwon and Cho, 2008).

In addition to the mechanical properties of rocks in the EDZ, capturing the depth is also important to scholars and engineers. The depth of the EDZ refers to the extent of the EDZ from the tunnel wall. Researchers have conducted studies to explore the depth of the EDZ in different projects through different geophysical methods (e.g., borehole observation, seismic measurements) (Schuster and Alheid, 2007; Kwon et al., 2008). However, due to the difficulty of conducting field tests during the tunnel excavation, the studies of the extent of the EDZ are limited. Table 2.3 shows the depth of the EDZ collected from different sites. From Table 2.3, it can be noted that the depth of the EDZ in shale formation is larger than other rocks, ranging from 0.5-1.4D, with the depth of the EDZ normalised to the tunnel diameter.

Table 2.3 The depth of the EDZ in different projects through field measurements

Projects	Rock type	Burial depth (m)	Excavation size (m)	EDZ depth (m)	Methods
Baihetan hydropower station China (Hao et al., 2016)	Columnar Jointed Rock Mass	100	24	6.5~7m	seismic measurements
Mont Terri Project Security gallery, Switzerland (Bossart et al., 2004)	Shale	250	4	1~2.2	Borehole observation
The Underground research laboratory(URL) Meuse/Haute- Marne, France (Armand et al., 2007)	Clay rock	490	2.2	2~2.2	seismic measurements
KAERI, Korea (Kwon et al., 2009)	Granite	255	6	1.5	Borehole observation
HADES, Belgium (Mertens et al., 2004)	Clay shale	223	2	2.9	Borehole observation

Aforementioned literatures have shown the properties of the surrounding rocks in EDZ have changed due to the excavation induced fractures. Increased permeability and decreased mechanical strength may cause serious engineering problems (e.g., rockburst and seepage). On the other hand, studies on the depth of EDZ have been conducted by a few researchers. However, they are all case studies. There is no general laws and conclusions about the fracturing conditions (e.g., location, depth, and fracture frequency) of the EDZ.

2.3.2 The forming and evolution of the EDZ in shale formation

Since the EDZ is characterized by fractures that form inside, understanding its fracturing behaviour is crucial to exploring its characteristics. Yong et al. (2017) have found that over 80% of excavation induced fractures in the EDZ are made by fractures parallel to the bedding planes through borehole mapping in Opalinus clay. Using 400 boreholes, Armand et al. (2007) collected over 4000 excavation-induced fractures from the EDZ at Meuse/Haute-Marne URL and identified two zones (outer and inner). It is same to the two zones spotted by Bossart et al (2004). The inner zone contains both tensile fractures and shear fractures, while the outer zone only has shear fractures.

It is hard to monitor the evolution of the EDZ in shale formations during the excavation through field surveys. In this case, many researchers have adopted numerical simulation approach to investigate the fracturing behaviours in EDZ. Lisjak et al. (2014b) have simulated the EDZ failure evolution during the excavation of a 3m tunnel in shale with horizontal bedding planes through FDEM. As depicted in Figure 2.10, the fractures inside of the EDZ are dominated by the fractures along the bedding planes.

The shear fractures are mainly located at the tunnel crown and invert, and the tensile fractures are mainly formed on the sidewalls.

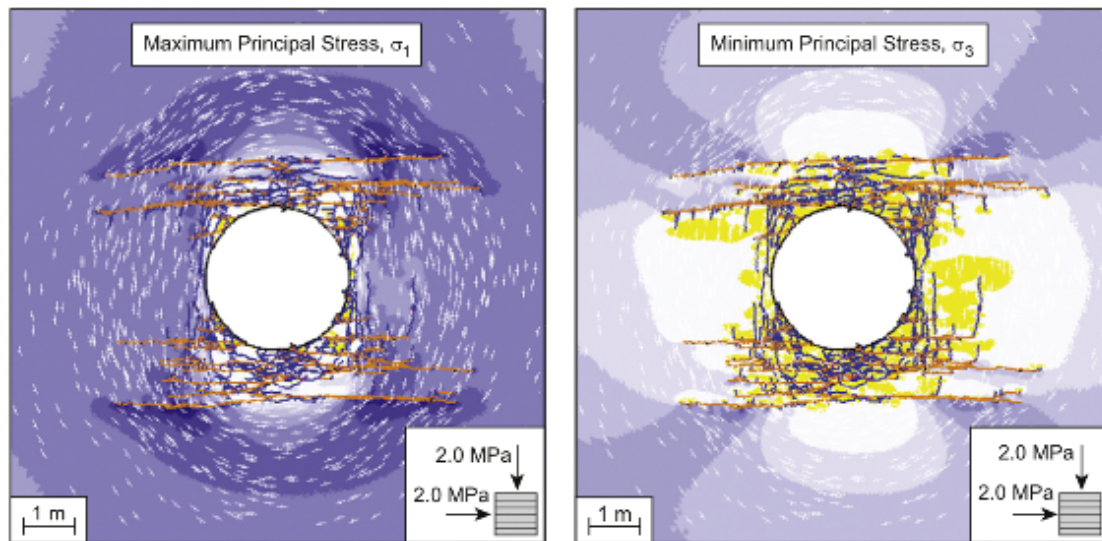


Figure 2.10 The fracturing patterns around the tunnel wall (Lisjak et al., 2014b, orange lines indicate fractures along the bedding planes).

Deng et al. (2022) have further analysed the tunnel shape effect on the EDZ in shale formation. As shown in Figure 2.11, the depth of the EDZ in the square tunnel is bigger than in the circular tunnel. They also have studied the rock strength (i.e., cohesion, tensile strength, and internal friction coefficient) effect on the EDZ evolution, as illustrated in Figures 2.12-14. With increasing shale cohesion, internal friction coefficient and tensile strength, the depth of the EDZ initially decreases before stabilising as the parameters continue to increase.

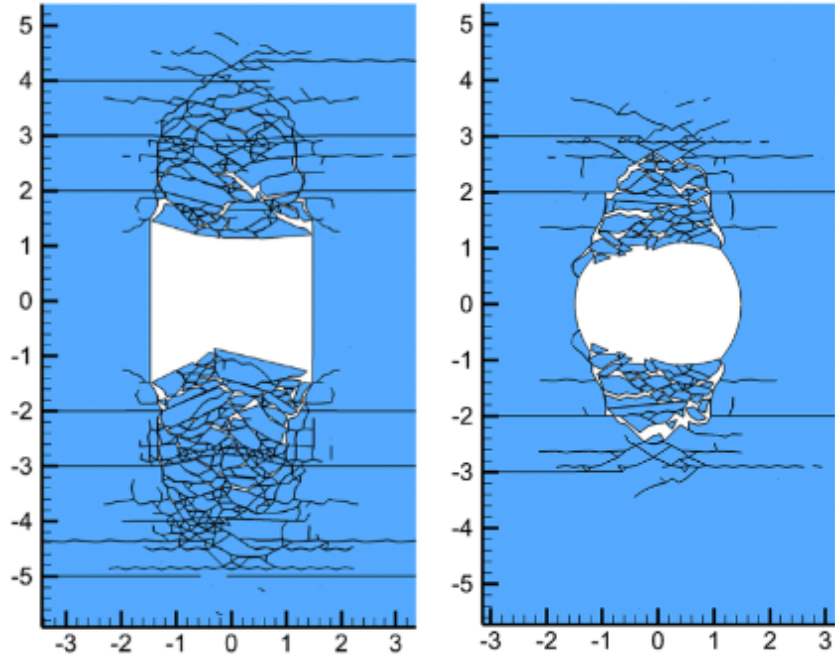


**Figure 2.11 The fracturing pattern of the EDZ between two different tunnel shape
(Deng et al., 2021).**

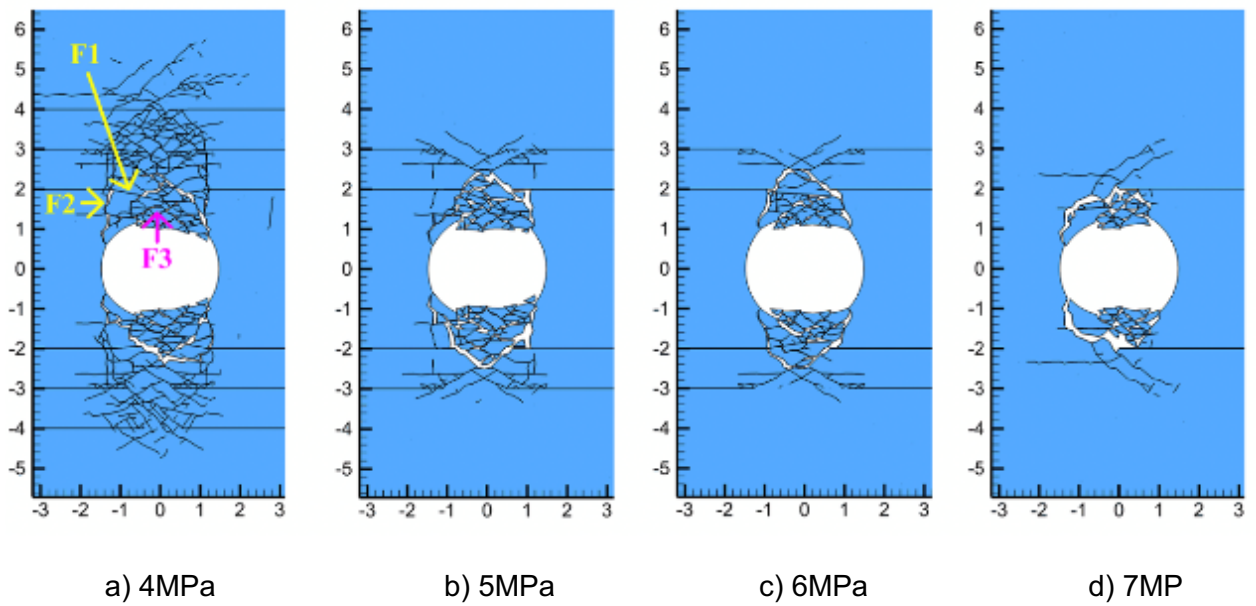


**Figure 2.12 The fracturing pattern of the EDZ with different cohesion, c (F1, F2 and F3
are the shear fractures along the bedding plane, tensile fractures, shear fractures
inside of shale matrix) (Deng et al., 2021).**

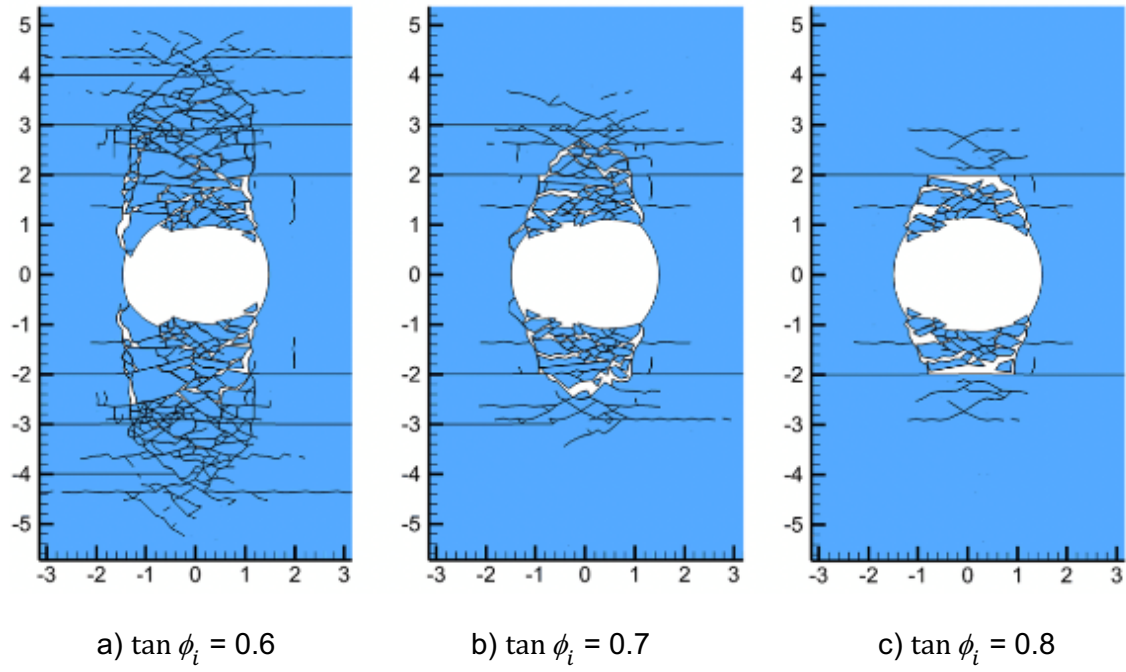


Figure 2.13 The fracturing pattern of the EDZ with different internal friction coefficient, $\tan \phi_i$ (Deng et al., 2021).

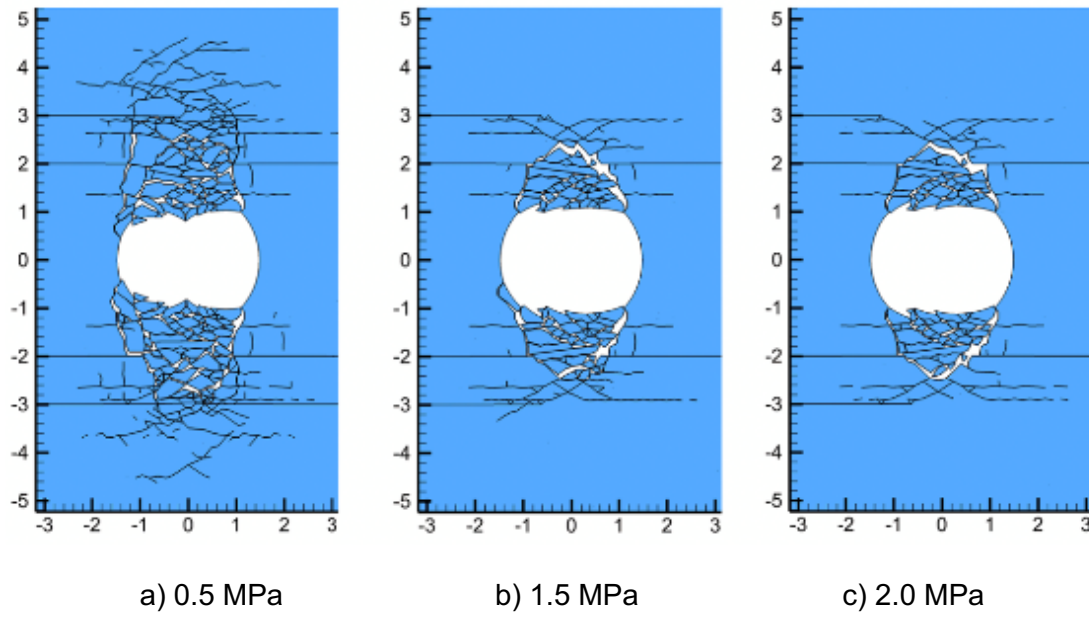


Figure 2.14 The fracturing pattern of the EDZ with different tensile strength, σ_t (Deng et al., 2021).

Although Lisjak et al. (2015) and Deng et al. (2022) both have used the FDEM approach to study the fracturing mechanism of EDZ in shale formation under different environmental conditions (e.g., rock strength, dip angle of rock layers and layer thickness), they did not examine how these conditions affect the properties of the EDZ (i.e., EDZ location, depth, fracturing number, and frequency) during tunnel excavation in anisotropic shale formation. Under different environmental conditions, the properties of the EDZ in shale formation remain unclear.

2.3.3 The influence factors of EDZ characteristics

The forming and evolution of the EDZ inside of the surrounding rock is due to the excavation and stress redistribution (Martino and Chandler, 2004). Additionally, literatures in the previous section have shown that rock strength parameters are highly influential on EDZ fracture behaviour. Therefore, the characteristics of the EDZ are related to the rock mass strength parameters, in-situ stress, excavation and support method. These three factors have been widely accepted by scholars (Backblom and Martin, 1999 and Tsang et al., 2005).

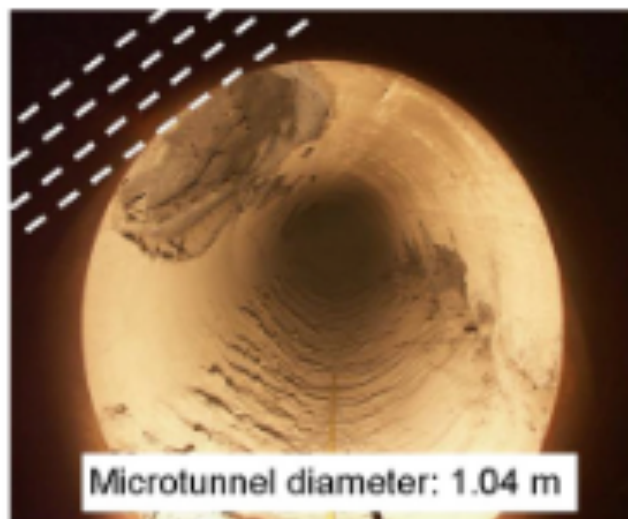
As field studies of the EDZ were mostly based on a single case study, it is difficult to vary any in situ parameters and carry out studies on the parameters influencing the EDZ such as in-situ stress and rock mass strength parameters. Therefore, Deng et al. (2021) have used numerical simulation to study the rock mass strength parameter effect on the EDZ. The hydraulic properties of a vault in Canada excavated by drill and blast and mechanical methods were examined by Chandler et al. (1996). The results show that the permeability in the EDZ excavated by drill and blast and mechanical are bigger than that of the intact rocks with 6-7 and 2-3 orders of magnitude, respectively. Fu et al. (2014) investigated the influence of two different detonators on the EDZ depth;

electronic detonators which allow the delay time to be controlled and hence reducing the blasting impact on the environment and nonel detonators which do not have the same control. They found that the average depth of the EDZ excavated by nonel detonators blast and electronic detonators blast is 1.9m and 1m, respectively. Further, the P-wave of the EDZ of the tunnel excavated using nonel detonators blast and electronic detonators blast methods decreased by 36% and 18%, respectively, in comparison to the intact rock.

The EDZ around tunnels is shaped and extended by the inclination of the bedding planes, as observed from the Mont Terri underground research laboratory (Bossart et al., 2004). Based on borehole mapping, the fractures in the crown and invert were formed along the bedding planes, while those on the side walls were pedicular to the bedding planes, as shown in Figure 2.15a. When excavating or drilling in shale formations, it is easy to observe the surrounding rocks with shear fracturing along the bedding planes and then spalling off into tunnel, as shown in Figure 2.15b.



a) Borehole experiment



b) Micro-tunnel

Figure 2.15 Two experiment tests on Opalinus Clay (Mont Terri) with different bedding plane inclinations (green lines in a) and white lines in b) indicate the inclination of the bedding planes) (Blümling et al., 2007 and Marschall et al., 2006).

According to the literatures cited above, the fractures in the EDZ have changed the properties of the surrounding rock. The increased permeability and decreased mechanical strengths contributed to certain engineering problems (e.g., rockburst and seepage and tunnel failure). The characteristics of the EDZ in shale formation are influenced by the bedding planes. Fractures are more easily formed and propagated inside of bedding planes due to their low stiffness and cohesion. The influence of shale anisotropy on the fracturing behaviour of EDZ is, however, overlooked. According to the literatures from section 2.2, shale anisotropy has a great impact on the fracturing behaviour of shale samples, suggesting that the fracturing behaviour of EDZ in shale formation should also be affected. Furthermore, most studies on the fracturing behaviour of EDZ in shale were based on field cases. It is limited to certain engineering conditions. There is no general laws and conclusions about fracturing behaviours in shale formations in different environment occurrences.

2.4 Numerical simulation of the layered rock

Based on the above literature, field surveys can only study one single specific case with specific engineering conditions. Hence, there is no general conclusions of fracturing behaviours in EDZ in shale formations. To overcome the limitations of field study, numerical modelling has become increasingly popular in recent decades for analysing some complex geotechnical issues (Lisjak et al., 2014b, Deng et al., 2021 and Lisjak et al., 2020). As computer hardware and software have become more prevalent, numerical modelling has become widely used to simulate geotechnical

conditions. Numerical approaches used in computational geomechanics can be classified as (i) continuum methods; (ii) discrete element methods (DEM); and (iii) hybrid finite-discrete element methods (FDEM).

2.4.1 Continuum methods

Continuum methods create models based on treating the computational domain as a continuous entity. Continuous bodies are composed of infinitesimal elements that share the same properties as bulk materials. It captures the evolution of microstructure changes by incorporating mechanisms such as elastics, plastics, and damage mechanics into the small elements.

In the past few decades, Finite element method (FEM) has been a popular continuum method for studying geotechnical problems (Doležalová, 2001 and Hao et al., 2016). In FEM models, discontinuities inside rocks are typically accounted for using two approaches, explicit and implicit. Typically, the implicit techniques are used when there are a large number of discontinuities. The implicit approach, also called the smeared approach, considers the rock with joints as a fictitious homogenised material that exhibits similar mechanical properties compared to the original rocks (Mosler and Meschke, 2004). Huang et al. (2009) adopted this approach to study the deformation of the surrounding rock after the tunnel excavation in shale formations. In this study, vertical displacements around tunnel in left side, right side and crown were analysed both computationally and in the field. The model deformation at the three points does not match the field values well. Wang et al. (2009) created a mathematical model of anisotropic rock with ubiquitous joints. This approach simulates the deformation of the rock mass by incorporating it into existing FEM numerical models.

Unlike the matrix, discontinuities have much lower strength, resulting in progressive failure mechanisms around the discontinuities. Most fractures formed along the bedding planes in the EDZ are shearing fractures, as reported in the literature by Armand et al. (2007) and Bossart et al. (2004). These failures then lead to stresses redistribution and large deformation (Hammah et al., 2008). However, the localised large deformation around discontinuities (e.g., slip, rotations, and separation) cannot be captured by this homogenisation approach (Hammah et al., 2008).

Explicit approaches, on the other hand, consider discontinuities separately from continuum formations. Modelling discontinuities inside rocks explicitly can also be classified in two methods. Goodman et al. (1968) introduced the first approach to modelling discontinuities using specific elastic elements. This zero-thickness elastic element, also called a 'joint element', has a linear stress-strain elastic relationship, as shown in Figure 2.16a. With the development of this theory, more joint elements with different mechanical properties, such as plastic behaviour and elastoplastic behaviour, have been proposed (Zienkiewicz et al., 1970). In addition, Zienkiewicz et al. (1970) proposed a six-node joint element to allow the element to bend, and Desai et al. (1984) proposed a 'thin-layer' solid joint element with a thickness.

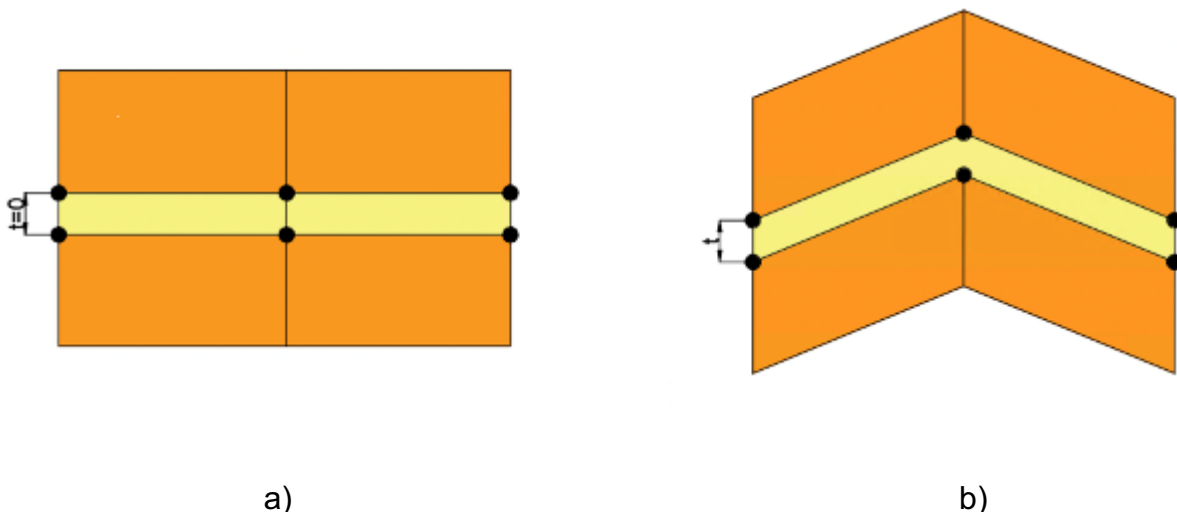


Figure 2.16 Joint elements. a) Goodman et al. (1968) and b) Zienkiewicz et al. (1970).

However, a second approach where zero thickness with reduced friction fractures directly inserted into the continuum formations has also been recently adopted (Panthee et al., 2016). This approach was originally introduced from DEM, however because of the fixed interconnectivity between the fractures and the continuum elastic elements, only small displacements can be captured.

The two explicit approaches both allow reasonably localised deformation happening around the discontinuities; however, this large deformation is limited. Firstly, large, localised deformation of the elements is not allowed in FEM due to the continuum assumption. Rotation and separation between elements cannot be considered. Secondly, slipping can only occur around discontinuities, the large deformations inside intact rock will not be captured. Despite the significant improvements offered by the aforementioned FEM models, standard FEM cannot be used to model discontinuities in rock due to the continuum assumption. Furthermore, since FEM models lack an internal fracture mechanism, fracture formation and propagation cannot be explicitly represented.

2.4.2 Discrete element methods (DEM)

DEM was first introduced by Cundall et al. (1971) as an alternative numerical approach to solve rock mechanical problems (Cundall et al., 1971). With this approach, the macro-scale failure of the rock can be investigated from a microscopic particle scale (Duan et al., 2015 and Ivars et al., 2011). In DEMs, discrete particles can be displaced, rotated, and detached completely. As the simulation progresses, it recognizes new contacts automatically.

The bond particle model (BPM) as one of the widely used models in DEM, extends the ability to trace the propagation of cracks inside rocks from a microscale to a macroscale without involving parameter assumptions or complicated constitutive laws (Potyondy and Cundall, 2004). Two types of bond exist in BPM, in terms of the contact bond and parallel bond. At the contact point, the contact band acts like elastic spring with normal and shear stiffnesses between two particles. As a result of the bonded contact, forces are transmitted, and particles cannot overlap. The discrete particles in the BPM are also bonded parallel together in both the normal and shear directions, and once their applied strength exceeds their corresponding bond strength, they can move relative to one another, as shown in Figure 2.17. The parallel bond provides a general method for presenting cement between grains (Lisjak and Grasselli, 2014).

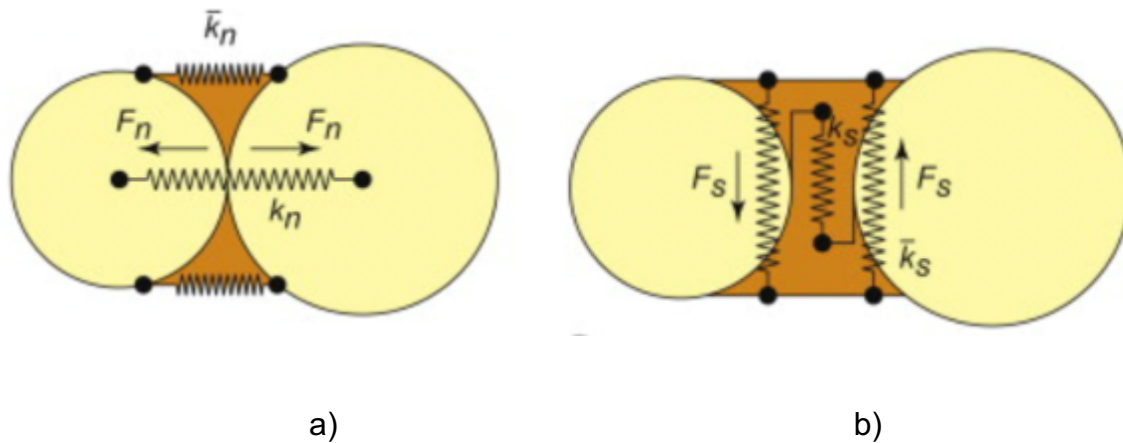


Figure 2.17 The parallel bond between two particles. k_n and k_s represents particles contact stiffnesses, while $\bar{k}_s$ and $\bar{k}_n$ represent bond stiffnesses; a) Normal direction, b) Shear direction (Lisjak and Grasselli, 2014).

Previous research has shown that the crack formation and propagation in shale rock is mainly due to the relative movement of the clay particles (Fabre and Pellet, 2006).

Under a scanning electron microscope (SEM), the face-to-face clay particle adjustment along these micro-cracking planes has been observed (Raynaud et al., 2008). In this case, DEM can capture this feature of the rock perfectly as it treats the material directly as an assembly of bonded blocks or particles.

Liu et al. (2019) have adopted BPMs to investigate the effects of the bedding planes of shale on the forming and evolution of tensile fractures through a semi-circular bend (SCB) test. The micro-properties of the particle and bond values were obtained through trial-and-error process based on the experimental macroscopic strength values. As shown in Figure 2.18, the SCB numerical model contains over 22000 particle elements with sizes ranging between 0.10 and 0.12 mm. Based on the results, the bedding planes have a significant effect on the propagation of the fractures. Shale samples with 30° inclinations tend to fracture along the bedding plane, in contrast to samples with horizontal bedding planes. Meanwhile, it was also found that the strength of the bedding planes has a great effect on the fracturing path. With smaller strength of the bedding planes, the tensile fractures were more likely to fracture along the bedding planes (Liu et al., 2019).

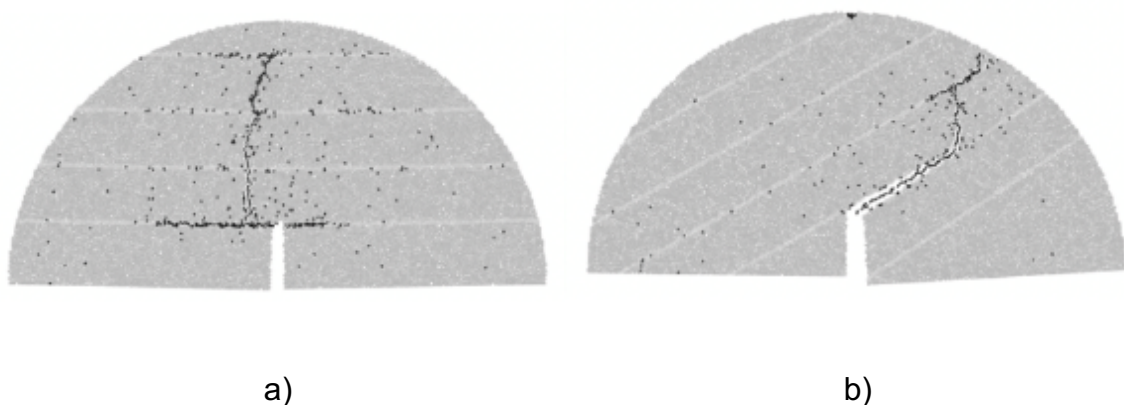


Figure 2.18 The failure of the SCB models for a) horizontal bedding planes, b) bedding planes with 30° inclination (Liu et al., 2019).

Most geotechnical DEM modelling is conducted at a laboratory-scale due to the limitations of computational capacity (Ivars et al., 2011 and Yimsiri et al., 2010). The size of the shale rock particles can be discretised to micrometre clay sized particles. However, there would be millions of particles and in a field-scale model with the size of tens of metres, this would result in a significant workload in building the model and unacceptable computation time. Xiang et al. (2018) have used DEM to study the failure mode of a shallow tunnel during excavation. This model only has a tunnel size of 50mm in order to reduce computation time. Meanwhile, the particle size varies from 2.5 to 5.0mm, which are far bigger than the real soil size with size 0.5mm-1.0mm. As shown in Figure 2.19, a $120 \times 120 \times 120$ mm model with 21495 particles were created. To achieve a reasonable time in creating model and running through DEM, researchers have to compromise on certain things (e.g., model scale and particles size).

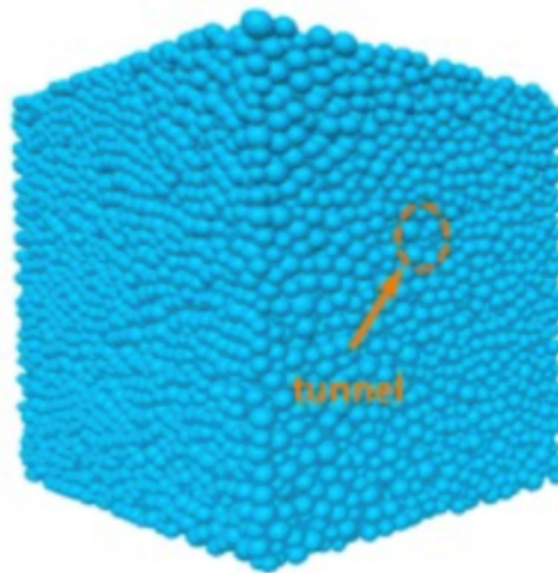


Figure 2.19 The DEM model of the tunnel excavation (Xiang et al., 2018).

2.4.3 Finite-discrete element methods (FDEM)

The finite-discrete element method was first introduced by Munjiza (2004). The FEM can capture the elastic deformability of the domain well, and the DEM can show fractures within the domain explicitly, so the FDEM combines the two advantages of both models. The domain in FDEM is discretised into elastic and cohesive elements, as shown in Figure 2.20. The hybrid FDEM has adopted the principles of continuum mechanics to govern the small strain changes in the elastic and cohesive elements, while the DEM algorithms are used to trace the interaction of the elastic elements once the cohesion crack elements are broken.

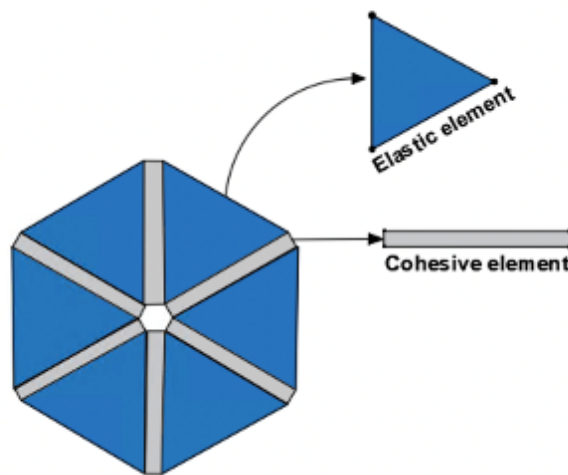


Figure 2.20 The diagram of a domain meshed by FDEM.

As this method can explicitly show the fractures inside the model, the last decade has seen increasing popularity of FDEM to simulate the fracturing in different fields (Chen et al., 2020; Fukuda et al., 2021 and Ma et al., 2019).

The fracture energies of UCS test samples were studied using FDEM by Deng et al. (2021). They found that the peak strength increases as tensile fracturing Mode I energy (G_I) or shear fracturing Mode II energy (G_{II}) increases, while the failure mode

(fracturing) remains stable. This suggests that calibrating G_{II} and G_I values in the simulation is reasonable given the two microparameters have a significant impact on the macro-parameters.

This method has been increasingly used to simulate different geo-mechanical problems in recent years. Lisjak et al. (2014a) first used FDEM to study the anisotropic behaviour of Opalinus clay. Seven different FDEM UCS test models with different bedding plane inclinations have been created to compare with laboratory tests. The simulation results matched well with the laboratory experiments. After the successful modelling of the laboratory results, Lisjak et al. (2014b) then used FDEM to investigate the failure mechanisms around tunnels in anisotropic clay shales with horizontal bedding planes. As shown in Figure 2.21, the excavation induced fractures tend to form shearing along bedding planes. Based on the fracturing in the EDZ, the EDZ can be divided into two fracturing zones. Shearing along bedding planes and extensional tensile fractures present in the inner zone, while fractures in the outer zone manifested as only horizontal shearing fractures. Lisjak et al. (2020) have continued studying the influence of rock bolts on the EDZ of an 8m × 8m tunnel in a highly fractured formation. Based on the simulation of different numbers of rock bolts (6, 11, 21) within the rock mass, it was shown that the rock bolts greatly affected the depth of the EDZ. The overall stability of the excavation improved when a denser pattern of rock bolts consisting of 11 and 21 rock bolts was used instead of six. Fracturing and displacement decreased as the number of rock bolts increased within the rock mass.

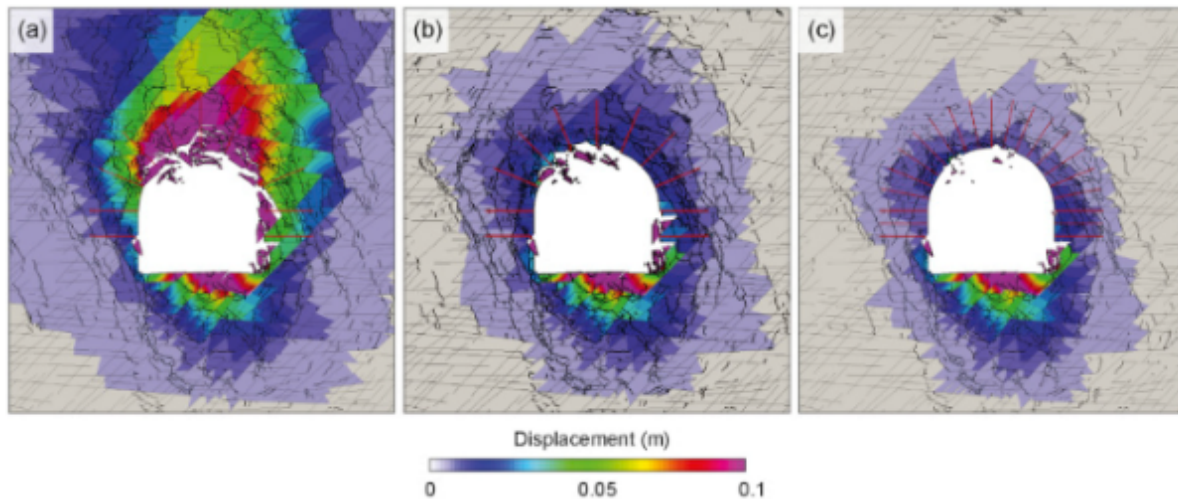


Figure 2.21 The displacement field of rock masses with 6, 11, 21 rock bolts. a) 6 rock bolts, b) 11 rock bolts, c) 21 rock bolts. (Lisjak et al., 2020).

Ha et al. (2021) compared the simulation results of tunnel excavation in shale with horizontal bedding planes in FEM and FDEM. With no fractures formed with a lateral coefficient $k=3$, the displacement fields were similar. A lateral coefficient, K , is determined by the ratio between horizontal and vertical effective stresses. When the lateral coefficient increased to 5, fractures formed around tunnel wall. It is evident that the displacement around the tunnel wall in FDEM is much greater than FEM, with an increase of up to 50%. In contrast to the FEM results, the displacement in the FDEM model is asymmetric due to fracturing. The fracturing in the EDZ caused by the excavation contributes to the large displacements, which cannot be captured by FEM. The rock response in FDEM is more realistic (Ha et al., 2021).

Liu and Deng (2019) studied the effects of the element sizes on the fractures forming around the tunnel due to the excavation by comparing four tunnel excavation models with different element size. According to the study, the fracturing depth and broken cohesive element number tend to converge when the element size is smaller than the fracture process zone. It is a zone where micro-cracks form in front of macro-crack

tips within rocks. When the element size exceeds the fracture process zone, multiple elements may bear the stress at the crack tip based on the distribution of the stress field. Consequently, the distributed stresses in each cohesive element were not sufficient to cause further fracturing, resulting in a small EDZ depth, which was detrimental to crack development.

Ma et al. (2022) used FDEM to study the large deformation of the tunnel face during excavation in a high in-situ stress. Because of the stress redistribution, excavation induced fractures led to the moving of the rock mass and increasing of the rock mass volume, representing severe squeezing. The simulated deformation of the rock mass in FDEM matched well with field monitoring result.

Studies in the literature have demonstrated that FDEM can be used to model rock engineering problems with explicit descriptions of fracture formation. Lisjak et al. (2015) have successfully modelled the excavation of Full-scale Emplacement tunnels in shale formations using FDEM. However, the researchers did not further examine the effects of shale anisotropy on the fracturing characteristics of EDZ and the fracturing characteristics of EDZ under different occurrences (e.g., in situ stress and layer thickness).

2.5 Key gaps in knowledge

As part of this chapter, this research reviewed previous studies on shale anisotropy, EDZ properties, and numerical methods for simulating anisotropic shale to understand the state-of-the-art studies related to shale anisotropy behaviours and EDZ in anisotropic shale formations. It has been identified, however, there are still some gaps in knowledge.

1) Shale anisotropy was previously studied in terms of its effect on macro mechanical properties. There are only a few studies that have examined the relationship between shale anisotropy and failure modes during compression, and none have examined how shale anisotropy affects brittleness. Brittleness indices are widely used by researchers to evaluate rock failure conditions. Although some researchers have conducted studies on the relationship between the rock failure mechanical characteristics (cutability, drill-ability, and frac-ability) and brittleness of rocks, but few studies have studied the shale anisotropy effects on its brittleness. Based on the aforementioned literatures, shale anisotropy shows a great impact on its fracturing conditions. The changing of the frac-ability of shale under the influence of shale anisotropy will naturally impact on the brittleness.

2) Based on previous research, the study of EDZ is typically limited to case studies of specific projects. There is lack of general conclusions and laws to the fracturing mechanism, or even fracturing conditions of EDZ in shale formation under different environment occurrences. Scholars and engineers can predict better the depth of EDZ and optimise supporting parameters in the future with an understanding of the fracture modes of the EDZ in shale.

3) There are several factors that affect the EDZ properties, including rock mass strength parameters, in-situ stress, excavation method, and support method. However, no researcher has studied the shale anisotropy effects on the properties of the EDZ (e.g., depth and shape). As a result of the anisotropy of shale properties, the forming of fractures in the shale occurs directionally due to the existence of the bedding planes. In this case, the EDZ in shale formation should also presents anisotropy.

4) Due to the limitation of field case studies, it is difficult to vary any in situ parameters and carry out studies on the parameters influencing the EDZ such as in-situ stress and rock mass strength parameters. On the other hand, numerical simulation probably can be used as an effective approach for studying the aforementioned problems due to its low cost, high efficiency, repeatability, and practicality. However, the current numerical modelling approaches that have been used to study the EDZ in anisotropic shale have some limitations. Not only can the discontinuous features of the rock (e.g., joint and fractures) not easily be simulated in the FEM because of the continuum assumptions, but also the most significant post-excavation properties of fracture forming, and growth cannot explicitly be represented in the model, as it lacks an internal fracturing mechanism. Additionally, the large computation times limit the use of DEMs in field scale projects. By explicitly simulating brittle fracture processes, FDEM is capable of modelling the transition of domain changing from continuum to discontinuum with requesting reasonable computation time for field scale simulation. It has been only a decade since FDEM was introduced, so it has been limited to problems related to geoengineering. Lisjak et al. (2015) have successfully modelled the excavation of Full-scale Emplacement tunnels in shale formations using FDEM. The effects of different environmental conditions on its fracture mechanisms were further examined by Deng et al. (2022). However, the researchers did not further examine the effects of shale anisotropy on the fracturing characteristics of EDZ and the fracturing characteristics of EDZ under different occurrences (e.g., in situ stress and layer thickness). There is no general conclusions or laws about the fracturing conditions of EDZ in shale formations.

2.6 Summary

A thorough review of previous studies on shale anisotropy, EDZ properties, and numerical methods for simulating anisotropic shale has been conducted in this chapter. Shale anisotropy shows great influence on its fracturing behaviours. It was found that brittleness, as one key parameter to evaluate the failure behaviours of rocks, was affected by several factors. However, shale anisotropy has been overlooked. Meanwhile, previous studies have looked into the rock mass strength parameters, in-situ stress, excavation method, and support method effects on EDZ. However, the shale anisotropy effects on the EDZ were neglected. Meanwhile, research methods typically limit the study of the fracturing mechanism of the EDZ to case studies of specific projects. There are no general conclusions or laws about the fracturing conditions of EDZ in shale formations.

This research's objectives were developed based on the summarization and highlighting of all above-mentioned issues and gaps.

Chapter 3 METHODOLOGY

3.1 Introduction

In the last chapter, several key gaps were identified as follows: 1) Only a few studies have investigated the relationship between shale anisotropy and failure modes during compression from micro crack level, additionally, none have examined the effect of shale anisotropy on brittleness; 2) The study of EDZ is typically limited to case studies of specific projects. There is a lack of general conclusions and laws governing the fracturing mechanism, or even fracture modes of EDZ in shale formation under different environment occurrences; 3) The effects of shale anisotropy on the properties of the EDZ (e.g., depth and shape) have not been studied previously; 4) The current common numerical modelling approaches (i.e., FEM and DEM) that have been used to study the EDZ have some limitations to track the fracture propagation during the tunnel excavation. On the other hand, FDEM is capable of modelling the excavation of tunnels by explicitly simulating fracture propagation at a reasonable computational cost. However, previous research did not further examine the effects of shale anisotropy on the fracturing characteristics of EDZ and the fracturing characteristics of EDZ under different occurrences (e.g., in situ stress and layer thickness). Therefore, the purpose of this chapter is to present and develop a methodology for analysing the anisotropic behaviours of shale at the micro-crack level and how they affect EDZ fracture mechanisms in deep-buried tunnels.

In light of the difficulty of preparing samples for model testing and the limitations of the field survey, this study has chosen to use numerical simulation to study the fracturing mechanism of shale under anisotropy. Numerical simulation is widely adopted by

researchers to study complex geotechnical problems because of its low cost, high efficiency, repeatability and practicality for parametric investigations. As discussed in Chapter 2, the discontinuous features of the rock cannot easily be simulated in FEM because of the continuum assumptions, and post-excavation fracture forming and growth cannot be explicitly represented in FEM models, which lack internal mechanisms for fracturing. Meanwhile, the use of DEM field models is limited due to large computation times. The FDEM has been adopted by few researchers as an appropriate tool for modelling the transition of domains from continuum to discontinuum within a reasonable computation time. Hence, to achieve the aim, this research has mainly designed two types of FDEM models, in terms of small-scale laboratory shale models and large-scale shale field tunnel models. Small-scale laboratory models are designed to validate the effectiveness of the FDEM by quantitatively reproducing the short-term behaviour of Longamxi shale in laboratory tests (i.e., uniaxial compression strength (UCS) tests and Brazilian disc (BD) tests). In addition, the effects of shale anisotropy on the failure mechanism and brittleness from micro-crack level were analysed through the verified FDEM small-scale laboratory shale model with different bedding plane inclinations. After that, a large-scale shale field tunnel model is simulated and qualitatively reproduces the short-term excavation deformation fields observed in the field. FDEM's verified large-scale shale field tunnel model was then used to study EDZ fracturing behaviour in relation to shale anisotropy. Finally, an analysis of the fracturing law of EDZ in shale formation was carried out using the validated large-scale shale field tunnel model applied to a variety of environmental conditions.

This chapter, split into three main sections, presents the methodology for this research. The three sections (section 3.2, 3.3 and 3.4) illustrate the methodology of modelling

shale in FDEM, the development of the laboratory scale and field scale model. The arrangement of each section is as follows:

Section 3.2 has been divided into four subsections covering the methodology of FDEM, the chosen software, FDEM in ABAQUS and modelling shale through FDEM. The purpose of this section is to illustrate how to build a shale FDEM model in ABAQUS.

Section 3.3 has five subsections, in terms of model description, model calibration and input parameters, calibration results, sensitivity study and methods for determining the brittleness of shale. The purpose of this section is to describe how laboratory scale shale models are created and validated.

Section 3.4 has been divided into five subsections which covers the project background, description of FEM and FDEM field scale model, in situ stress and input parameters, modelling excavation procedure and validation. This section explains the process of creating and validating field scale shale models.

3.2 Creating shale FDEM model in ABAQUS

3.2.1 Software selection

As mentioned in section 2.4, this research has adopted an FDEM approach to study the fracturing mechanism in shale. Currently there is only one software, Y-GEO, which specifically supports the FDEM approach to study rock materials. Many scholars have conducted research using this software. However, due to the significant cost of the software (>£7,000) and computing power needed, combined with a limited budget, this software was not considered for this research. Based on the literature review, it was shown that ABAQUS, freely available at the university, can also support the FDEM

approach to conduct research on geotechnical engineering problems (Zhou et al., 2015 and Ye et al., 2021).

3.2.2 FDEM in ABAQUS

According to previous studies, ABAQUS can provide cohesive elements to simulate FDEM (Zhou et al., 2016 and Jiang et al., 2016). However, ABAQUS does not support abundant cohesive elements freely embedded into the adjacent elastic elements. Normally, it only provides limited cohesive elements inserted along fixed directions. Therefore, this thesis introduces a novel additional code using python to realise this process in ABAQUS. The source code is listed in appendix A.

To create an FDEM model, the rock material is first meshed into triangular elastic elements using ABAQUS software based on mesh topology (Zhang et al., 2016 and Lisjak et al., 2014a). To insert cohesive elements into adjacent elastic elements, the nodes' information from the elastic model was extracted and put into the Python code program. The inserting process is shown in Figure 3.1. It should be noted that there is no gap between the adjacent elastic elements in the model. The gap shown in Figure 3.1b and 3.1c is used to better illustrate the relationship of the elastic and cohesive elements. The additional scheme can be described as:

- 1) Following the meshing of an ABAQUS continuous domain, the node information of the elastic elements 1-8 is read out in ABAQUS input files (Figure 3.1a).
- 2) Each node's number in all elements is counted, and then a new set of nodes is defined with new numbers based on these old nodes. As shown in Figure 3.3a, Node 9 appears 8 times in 8 different elements. During the dividing steps, Node 9 has split

into 7 new nodes: 19,29,39,49,59,69,79, as shown in Figure 3.1b. Equation 3.1 was used to prevent the numbering of the new nodes being the same as the old ones.

$$N_{\text{new}} = (n-1) \times (a \times 10) + N_{\text{old}} \quad \text{Eq.3.1}$$

where N_{old} is the dividing node, n is the appearing times of node (N_{old}), N_{new} is the new number of node (N_{new}), and a is the place of the first digit of the maximum number among all old nodes. For example, the maximum number in Figure 3.1a is 9, which means a is 1. As node 9 appears eight times, the new nodes that divide from it are 19,29,39,49,59,69,79.

3) After renumbering the nodes, each element is assigned new numbered nodes. The element 2 was formed by the nodes 2-9-3, as an example. Figure 3.1b shows that element 2 is formed by 12-19-3 after steps 2 and 3.

4) After assigning new nodes for each elastic element, if two elements share the same node numbers from the original node number, it means they share the same side. For example, element 1 (1-2-9) and element 8 (11-8-79) share two nodes, nodes 1 and 9 in element 1 and nodes 11 and 79 in element 8. Nodes 11 came originally from nodes 1, and 79 came from original node 9. Based on this, Nodes 1-9-79-11 forms a new cohesive element, as shown in Figure 3.1c. This system helps inserting cohesive elements into elastic elements.

5) By processing this program for all elastic elements, an FDEM model with zero-thickness cohesive elements can be realized in ABAQUS software as shown in Figure 3.2.

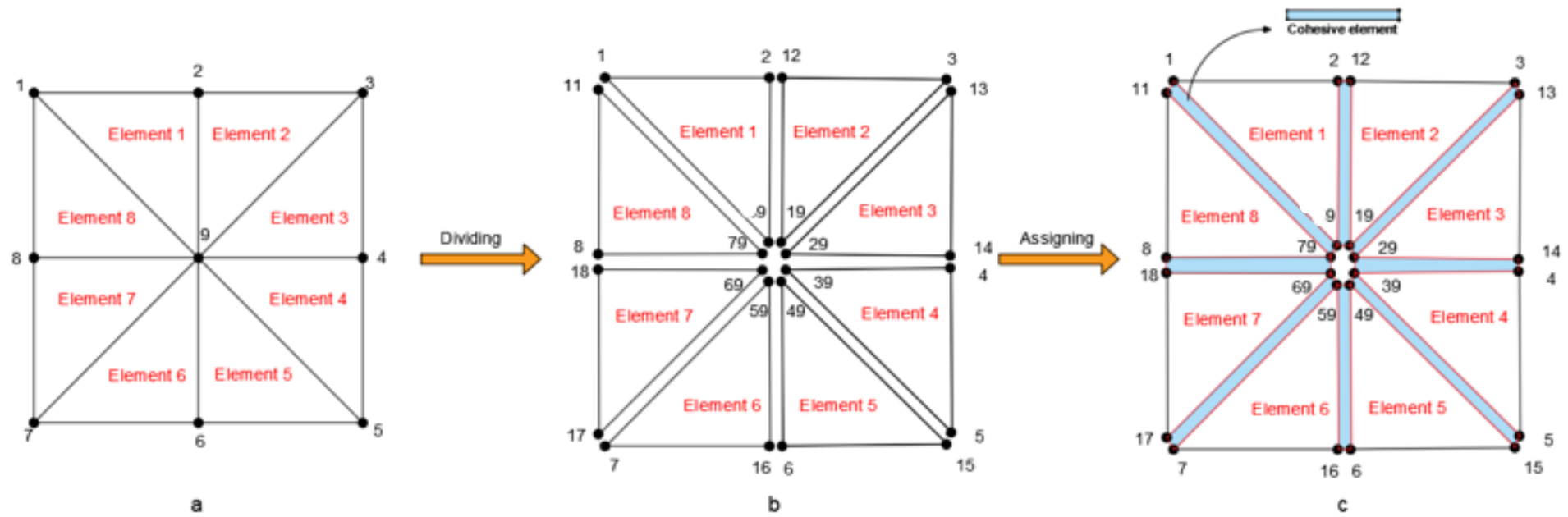


Figure 3.1 Process of inserting zero thickness cohesive elements into adjacent elastic elements in ABAQUS.

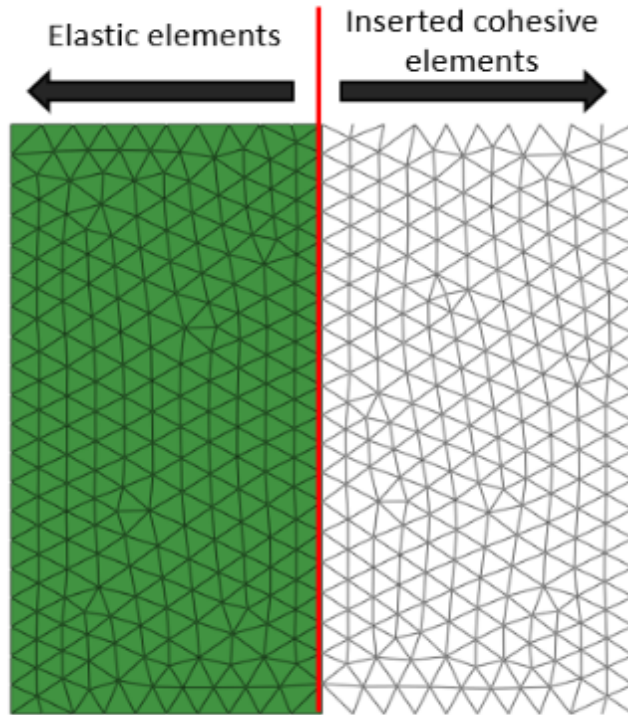


Figure 3.2 Schematic of the FDEM model with cohesive elements in ABAQUS (Zero thickness cohesive elements between elastic elements are displayed on the right of the domain, while elastic elements are displayed on the left).

3.2.3 Modelling shale through FDEM

Modelling domains in FDEM are discretised into four-node triangular cohesive elements interconnected by three-node rectangular elastic elements, as shown in Figure 3.3.

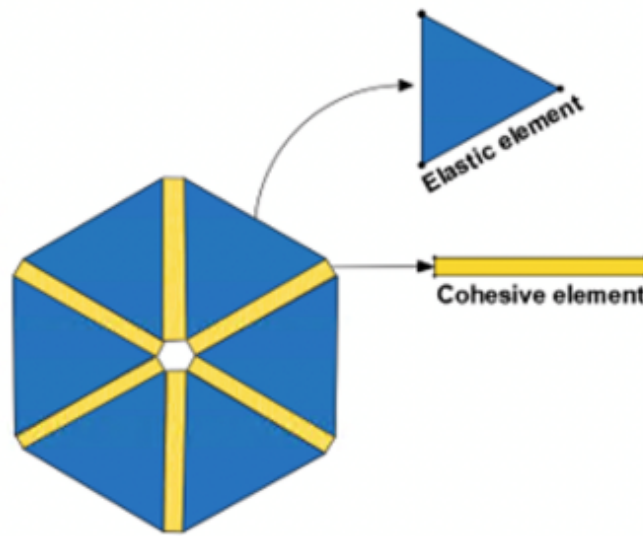


Figure 3.3 Diagram of a domain meshed by FDEM.

The anisotropic characteristics of shale are mainly controlled by the bedding planes distributed within it, which leads to the deformation of the shale showing strong anisotropic properties within the bedding planes (Hakala et al., 2007 and Amadei, 1996). Shale, in this case, has been classified as a transversely isotropic material. Due to their lower stiffness and strength, these bedding planes act as discontinuities or joints within the shale matrix. As with shale, in the hybrid finite and discrete element method (FDEM), cohesive elements serve as interfaces between adjacent elastic elements, which is similar to the composition of the shale. Due to the discretization of the shale matrix by bedding planes, the FDEM approach is ideal for modelling this material. In this case, a smeared approach introduced by Lisjak et al. (2015) has been commonly accepted to model shale in FDEM. It is assumed that cohesive element anisotropy explains macroscopical strength anisotropy of rock. Similarly, Li and Zhang (2019) have proposed a shale model that assigns different cohesive laws to the cohesive elements in the shale matrix and bedding planes to simulate the shale

anisotropy. Thus, this study investigates the failure mechanisms of shale under various conditions in laboratory tests and deep tunnel excavation by using the smear method to explicitly simulating bedding planes. The creation of the FDEM shale model in ABAQUS can be briefly described as follows:

1) Meshing the intra-layer shale matrix using a random triangulation method, ensuring cohesive elements are aligned along the direction of the bedding planes, as shown in Figure 3.4a.

2) Cohesive elements are inserted into adjacent elastic elements using Python code, as shown in Figure 3.4b.

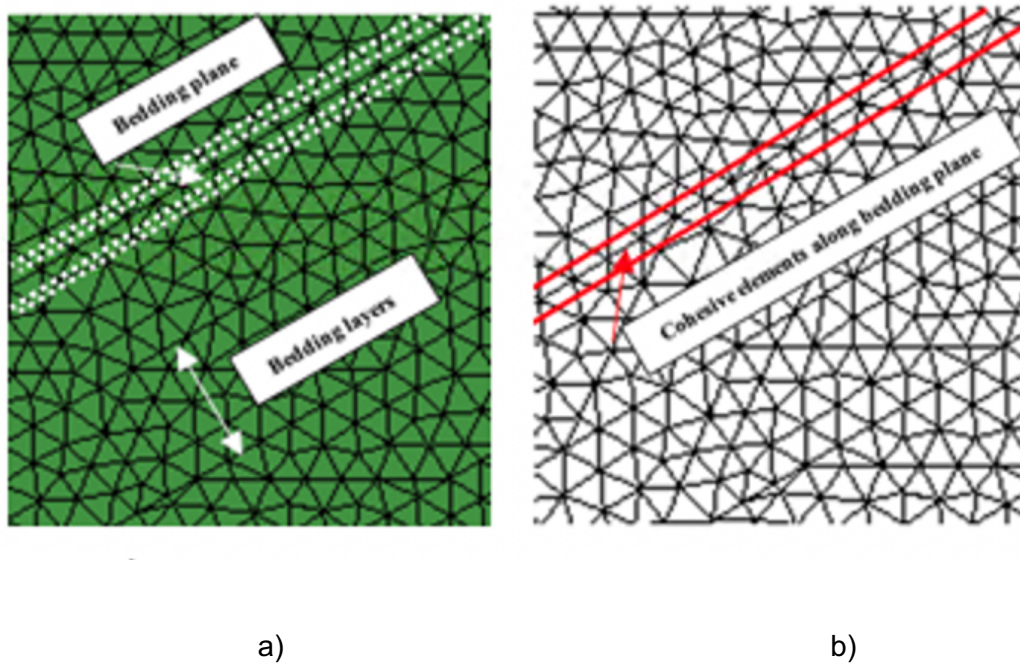


Figure 3.4 Modelling shale anisotropy in FDEM. a) Mesh topology, b) Cohesive element alignment.

3) Assigning different cohesive strength parameters to different cohesive elements. The cohesive elements inside the shale model can be divided into two different types, matrix cohesive elements and bedding plane cohesive elements. As shown in Figure

3.5, the matrix cohesive elements (COH1) are distributed inside the shale matrix with strong cohesive strength parameters, while bedding plane cohesive elements (COH2) are assigned along the bedding plane with weak cohesive strength parameters.

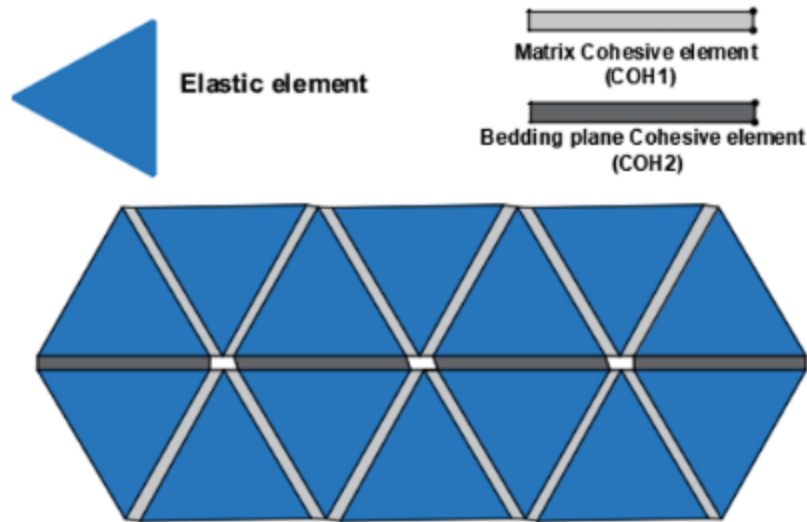


Figure 3.5 The distribution of the two different types of cohesive elements (Note: the thickness of the cohesive elements in this Figure is only representative and for better visualisation to distinguish between the two different cohesive elements. The actual/analytical thickness of the cohesive elements in FDEM model is zero).

Using this method, the shale structural characteristics can potentially be modelled in FDEM through ABAQUS.

3.3 The development of shale laboratory scale FDEM model

3.3.1 The Methodology of Hybrid Finite and Discrete Element modelling

In FDEM, the modelling domain is discretised into three-node triangular elements with four-node rectangular cohesive elements between the triangular elements, as shown

in Figure 2.19, Chapter 2. The combined FDEM has adopted continuum mechanics principles to govern small strain changes in the elastic and cohesive elements, while DEM algorithms are used to trace the interaction between the elastic bulk elements after the cohesive elements have ‘failed’ and fractures formed. The transformation of the domain from continuous to discontinuous is therefore realised by breaking and deleting the ‘failed’ cohesive elements, known as the cohesive zone model (CZM), to simulate fracture initiation and propagation (Zhou et al., 2016)

Dugdale and Barrenblatt (1961) first introduced the concept of the CZM to study the formation and propagation of fractures in materials. As illustrated in the previous chapter, this approach has been widely used to investigate the failure phenomena in a diverse range of materials (e.g., steel, concrete, and rocks) (Chandra et al., 2002, Hillerborg et al., 2007 and Ha et al., 2021). The creation of this approach is to capture the zone called Fracture Process Zone (FPZ) that formed with micro-cracks in front of the macro-crack tip inside of rocks. According to Hillerborg et al. (1976), when the stress at the fracture tip reaches its maximum level, the fracture starts to form. It is assumed that bonding stress does not drop to zero at once when the fracture opens, but rather decreases with an increase in fracture width, as shown in Figure 3.6a. When the fracture width reaches to certain value, δ_o , the bonding stress fall to zero. As shown in Figure 3.6b, FPZ in CZM was created using this model to simulate fracturing situations.

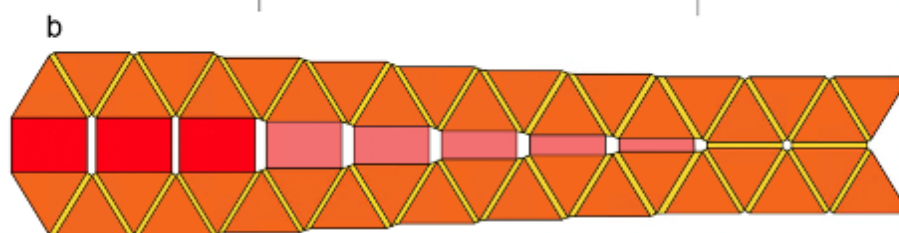
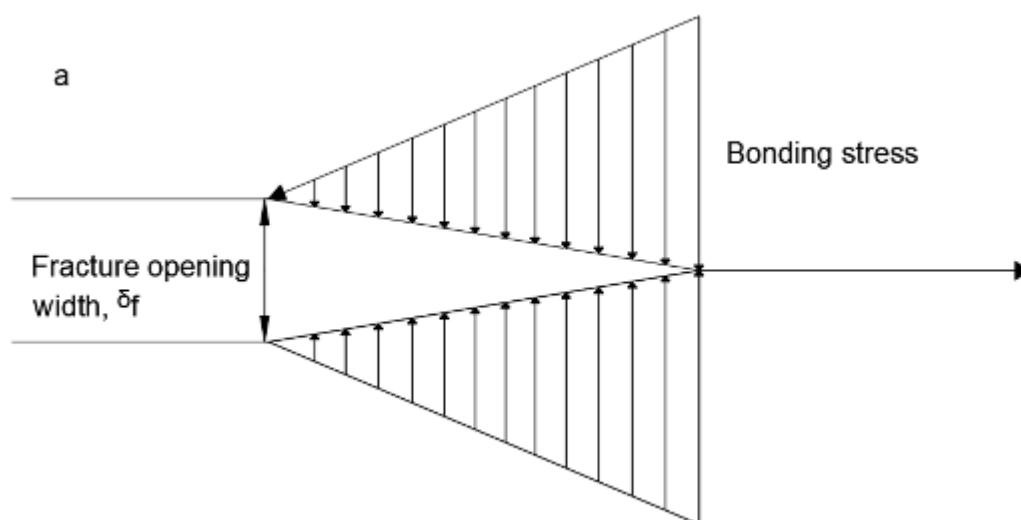


Figure 3.6 The conception of the Fracture Process Zone in rock . a) Theoretical FPZ model by Hillerborg (Hillerborg et al., 1976). b) FPZ in CZM through FDEM.

Cohesive elements are yielded when it is extended, and bonding stress appears at its interfaces in order to prevent separation. The bonding stress decreases until it drops to zero as the displacement of the cohesive element keeps increasing.

The constitutive model of the cohesive elements is represented in a traction-separation response, where the traction stress t is a linear function of the displacement δ , as shown in Figure 3.7. The stress-strain curve of the cohesive element can be divided into two parts, in terms of strain hardening and strain softening. During the strain hardening phase, the linear function between the traction t and displacement δ is given by Equation 3.2 (Zhou et al., 2016).

$$t = \begin{Bmatrix} t_n \\ t_s \end{Bmatrix} = \begin{Bmatrix} k_n \delta_n \\ k_s \delta_s \end{Bmatrix} \quad \text{Eq.3.2}$$

Where t_n , k_n and δ_n are the traction stress, cohesive element stiffness, and displacement in the normal direction, respectively, while t_s , k_s and δ_s are the equivalent quantities in the shear direction, respectively.

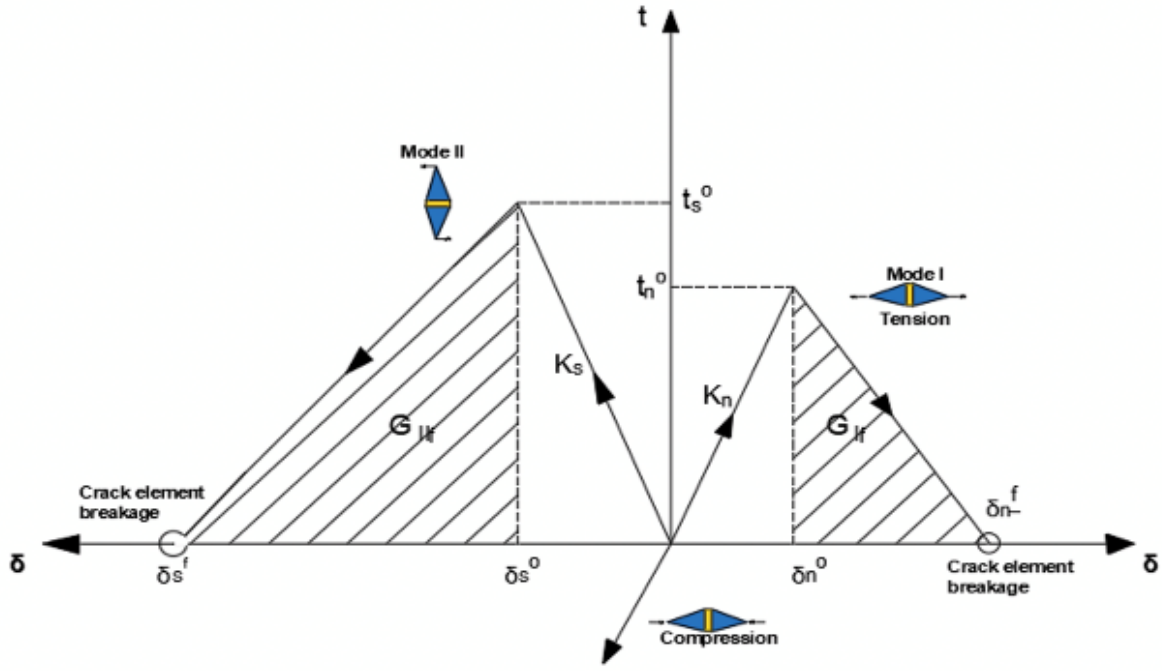


Figure 3.7 Constitutive model for the cohesive elements (k_n , δ_n^o , δ_n^f and t_n^o are the cohesive element stiffness, effective displacement at damage initiation, effective displacement at complete failure and effective traction stress at damage initiation in the normal direction, respectively; k_s , δ_s^o , δ_s^f and t_s^o are the equivalent quantities in the shear direction, respectively. Meanwhile, G_{II} and G_{III} are the cohesive elements fracturing energy in normal and shear direction, respectively).

During the strain softening part, in Mode I, a fracture starts to develop when the displacement of the cohesive element reaches the critical value, δ_n^o , which corresponds to the maximum normal traction, t_n^o . As the displacement continues to increase, the traction stress decreases gradually. When the displacement δ reaches the residual value, δ_n^f , the cohesive element between two elastic elements is broken; thus, a traction free fracture is developed (Munjiza, 2004). The formation of the fracture in Mode II is simulated through a slip-weakening model. A tangential (shear) traction stress, t_s , and a normal stress, t_n , exist between two adjacent elastic elements.

According to the Mohr-Coulomb criterion, which has been adopted by ABAQUS, the maximum shear traction stress, t_s , is calculated using Equation 3.3 (Dassault, 2014):

$$t_s = c + t_n \tan \phi \quad \text{Eq.3.3}$$

where ϕ and c are the internal friction angle and cohesion, respectively. As depicted in Figure 3.7, the traction stress, t_s , decreases gradually after the displacement reaches the critical value, δ_s^0 .

The fracture energy G_f is the external energy needed to break a unit surface area of traction separation fracture (Lisjak et al., 2014a). G_{If} and G_{IIIf} are defined as the energy needed for the break of the cohesive element in Mode I and Mode II, respectively.

The damage initiation is related to a quadratic nominal criterion. Different stresses acting in different directions were considered under this criterion. Damage is presumed to begin when a quadratic interaction function involving the nominal stress ratios reaches one (Zhou et al., 2015) :

$$\left\{ \frac{\langle t_n \rangle}{t_n^0} \right\}^2 + \left\{ \frac{t_s}{t_s^0} \right\}^2 = 1 \quad \text{Eq.3.4}$$

Where $\langle t_n \rangle$ is shown in Equation 3.5.

$$\langle t_n \rangle = \begin{cases} t_n, t_n \geq 0 \text{ (tension)} \\ 0, t_n < 0 \text{ (compression)} \end{cases} \quad \text{Eq.3.5}$$

The penalty contact algorithm and Coulomb's friction law govern the contact behaviour between adjacent elastic elements once the cohesive element has broken completely in ABAQUS (Dassault, 2014).

3.3.2 Model description

In the past years, different laboratory tests on Longmaxi shale have provided detailed parameters for quantitatively reproducing the short-term behaviour of the shale through FDEM. Hence, the capacity of FDEM to model the anisotropic mechanical and failure behaviour of shale in laboratory scale has been particularly verified through UCS and Brazilian disc (BD) tests on Longmaxi shale.

The FDEM models were calibrated against laboratory results (i.e., UCS and BD test) reported by Wang et al. (2018) and Ma et al. (2018) for the Longmaxi shale. A two-dimensional 100 mm × 50 mm rectangular model and a 50 mm diameter circular model were created for the UCS and BD tests respectively. It was assumed that the cross-section of each model would lie perpendicular to the bedding planes' strike. Hence, by changing the inclination of the bedding planes in the models, the anisotropy of the shale was achieved in different directions, as shown in Figure 3.8.

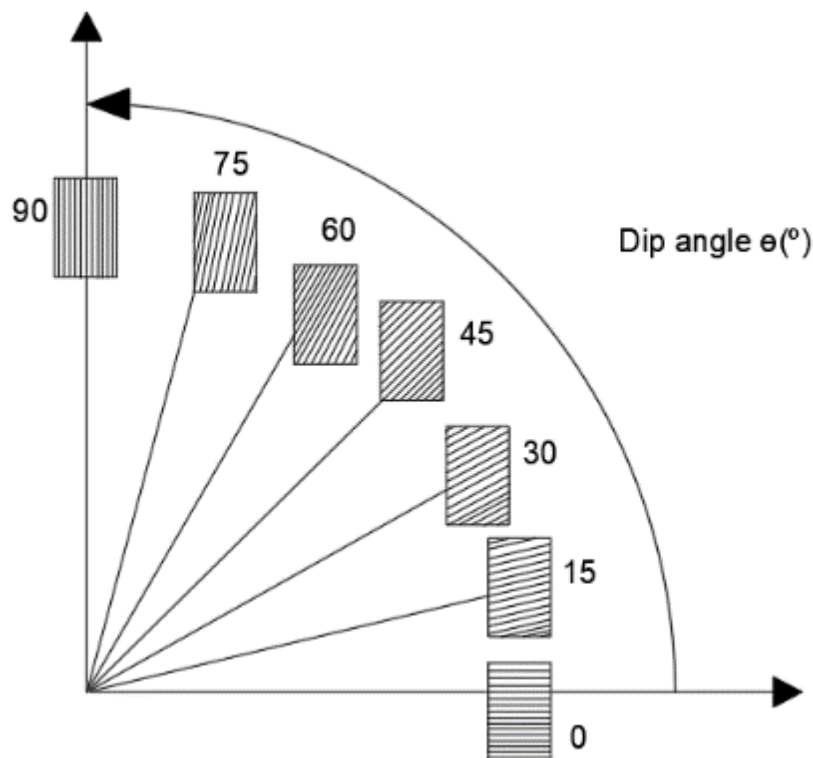


Figure 3.8 Diagram showing the various inclinations of the bedding plane of a shale FDEM model.

As discussed previously (section 3.2.3), specimens were discretised in the mesh topology described previously, and interlayers were meshed in unstructured triangular grids, whereas cohesive elements were aligned along bedding planes. The loading platens, placed on the top and bottom of the specimen, were moved in opposite directions as shown in Figure 3.9. Lower loading rates result in longer loading times and a dramatic increase in computational time in the numerical simulation. The loading rate of the two platens is 50mm/s, which is much greater than 1.8mm/min used in the experiments. However, the simulated strengths were found to approach constant values close to the experimental values when the loading rates were lower than 0.15m/s. The sensitivity studies of element size and loading rate are illustrated in the following section.

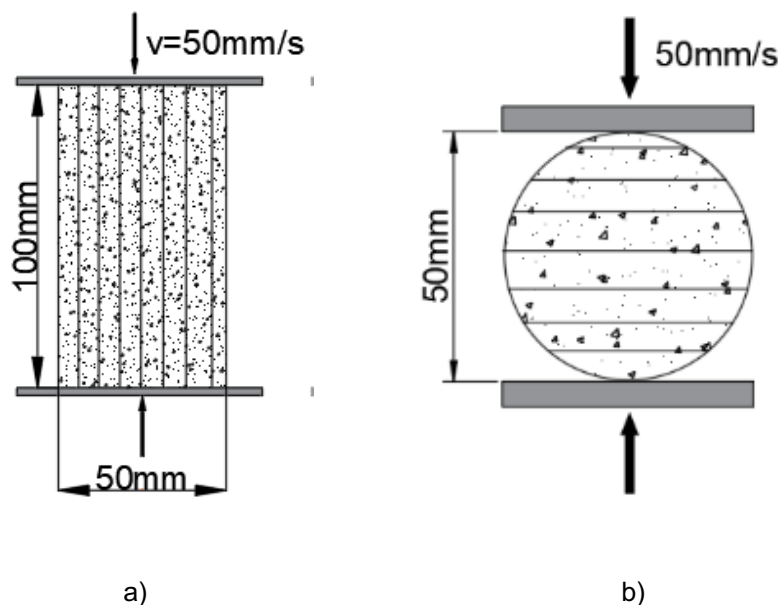


Figure 3.9 The FDEM models created in ABAQUS, a) Uniaxial compression test and b) Brazilian disc test.

3.3.3 Sensitivity study

1) Mesh sensitivity

The element size should be smaller than l_{cz} , which defines the length of the FPZ, in order to ensure the FPZ accurately processes the traction stress inside of the cohesive elements. Rice (1980) proposed a formula to analytically estimate the value of l_{cz} , as illustrated in Equation 3.6.

$$l_{cz} = \frac{9\rho G_{If}^2}{32(t_n^0)^2} \quad \text{Eq.3.6}$$

Where G_{If} is Mode I fracture energy and t_n^0 is Mode I tensile strength. When the bedding plane is orientated at 90° , the value of l_{cz} is approximately 6.5 mm by using values collected from laboratory tests (Ren et al., 2021). In the FPZ, no specific minimum number of cohesive elements is required, but several researchers have validated models with 3-10 cohesive elements (Yan et al., 2016, Turon et al., 2007 and Lisjak et al., 2014a). Mode I and Mode II fracturing are involved in the failure process inside the rock, making it more complex than Rice's (1980) simple Mode I fracturing scenario. By simulating the UCS test model at 0° inclination with element sizes ranging from 0.5 mm to 3 mm, this study investigated the element size sensitivity of the FDEM shale model. Shale uniaxial compressive strength appears to converge with decreasing element size, as shown in Figure 3.10. Despite the advantages of using submillimetre elements for capturing shale mechanical behaviour, the large number of elements can result in excessive computational costs. Figure 3.10 illustrates that shale models with 0.8 mm and 1 mm average element sizes are close to the laboratory values. According to Liu and Deng (2019), the results of the fracturing scenario model is improved with smaller elements and larger numbers of elements.

Meanwhile, it appears that the peak strength converges after 0.8mm. As a result of adopting smaller element sizes, the total element grows rapidly, while the explicit time integration scheme of FDEM also demands smaller time steps for stability. Based on this, the average element size in this study adopted 0.8mm, which reduces mesh sensitivity with a reasonable number of elements and produces a numerical model that matches the experimental uniaxial compressive strength to within 5% (Wang et al., 2020, Ma et al., 2018).

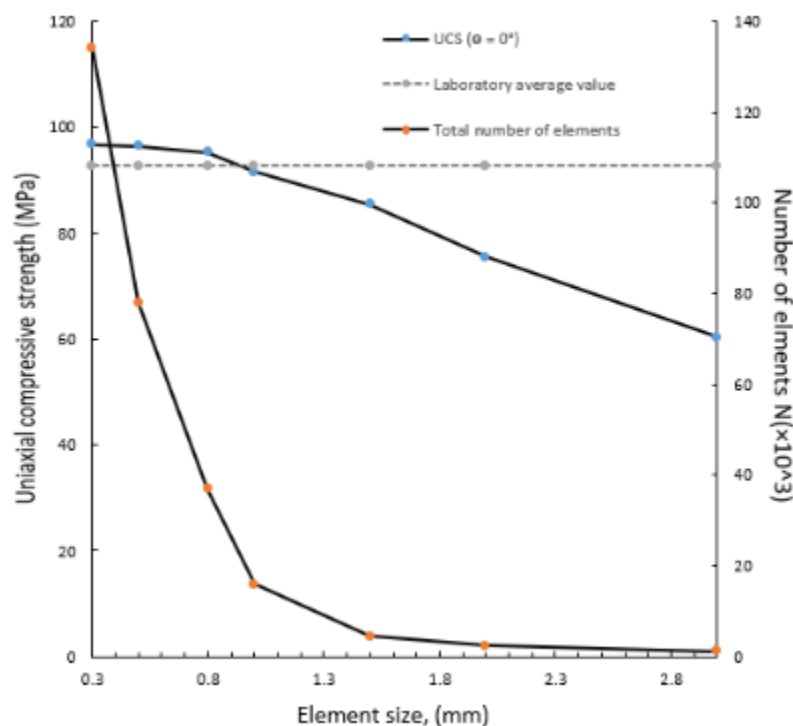


Figure 3.10 The sensitivity of element size to shale compressive strength at bedding plane inclinations of 0° and the number of elements as a function of the average element size.

2) Loading rate sensitivity

Within the numerical model, the loading rate is one of the most significant factors that affect the mechanical behaviour, and a lower loading rate results in longer

computational times. All models have the same input parameters and mesh topology in the following analysis to investigate the sensitivity to loading rate. After the loading rate dropped below 100mm/s, the values for the strength of the shale in UCS test started to converge as shown in Figure 3.11.

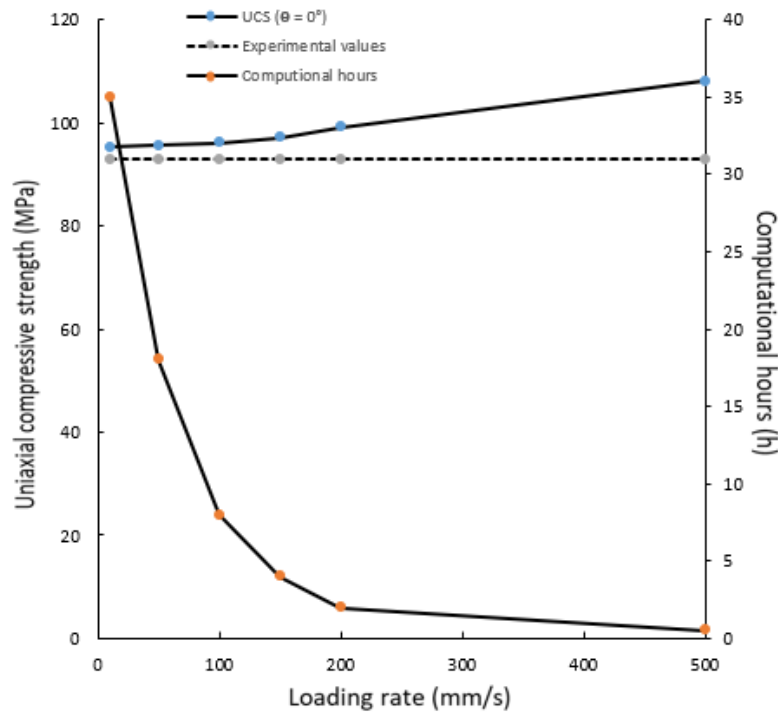


Figure 3.11 The relationship between uniaxial compressive strength and loading rate for shale with inclination of the bedding plane at 0° and computational hours as a function of the loading rate.

3) Internal elastic elements sliding friction coefficient sensitivity

As another important factor controlling the mechanical response of simulation models, the internal elastic elements sliding friction coefficient, μ , should also be considered in the sensitivity study. By simulating shale models with bedding plane inclination at 0° in the UCS test under different sliding friction coefficients, Figure 3.12 illustrates the effect of the internal elastic element sliding friction coefficient on the uniaxial compressive strength. With increasing sliding friction coefficients, the uniaxial

compressive strength increases. With a sliding friction coefficient of 0.8, the uniaxial compressive strength of the shale model is within 5% of the laboratory average value. Thus, this value was chosen for further analysis.

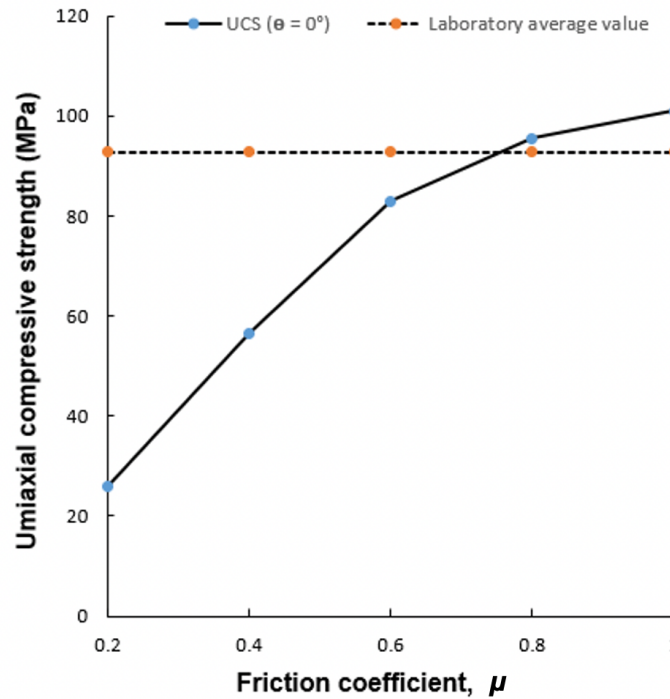


Figure 3.12 The relationship between uniaxial compressive strength and sliding friction coefficient for shale model with inclination of the bedding plane at 0° .

3.3.4 Model calibration and input parameters

Simulation of macroscopic behaviour of materials using a FDEM model relies on micromechanical interactions of elements. In general, material parameters obtained from laboratory experiments cannot be directly input into FDEM models (Lisjak et al., 2014b). A calibration process should be used to determine the final input parameters, which some target strength values are compared with those obtained from laboratory tests (Potyondy and Cundall, 2004).

The FDEM numerical models of shale were calibrated against the UCS and BD experimental test results reported by Wang et al. (2020), Wang et al. (2018) and Ma et al. (2018) for the Longmaxi shale. The critical parameters used for the calibration were uniaxial compressive strength and tensile strength. As the matrix cohesive and bedding plane cohesive elements were assigned to the micromechanical properties of shale models with bedding plane inclinations of 0° and 90° , these were evaluated first in the numerical models. Further, the macroscopic properties of shale models with 45° bedding plane inclinations were examined to validate the adopted micro parameters. The elastic constants for the elastic elements were derived directly from the laboratory tests (Wang et al., 2020 and Ma et al., 2018).

The model requires inputs of several parameters concerning the cohesive element, including fracture energy, friction angle, cohesion, stiffness and tensile strength (Mahabadi et al., 2012). The stiffness of the cohesive elements, as one of the critical parameters, can significantly affect the elastic response of the FDEM model. According to the study conducted by Yuan et al. (2014), a rock numerical model is not sensitive to the cohesive stiffness once the stiffness of the cohesive element has exceeded the Young's modulus of the rock matrix. Based on the recommendation by Mahabadi et al. (2012) and Lisjak et al. (2014b), the values of the cohesive normal and shear stiffness were set to ten times and one times the Young's modulus of the rock matrix, respectively. Meanwhile, Deng et al. (2021) have studied the sensitivity of the cohesive parameters to the FDEM. They found that the fracture energies have a significant impact on the mechanical strength and also failure mode. With increasing fracture energies, the strength of the rock model increases. While the tensile strength and cohesion increase, the value of the fracture energies increases. The friction angle has no effect on the fracture energies (Deng et al., 2021). Accordingly, Deng et al.

(2021) recommended that the cohesion and friction angle can be directly determined from laboratory tests, but the tensile strength and fracture energies must be calibrated. Based on the study by Deng et al. (2021), the cohesion and friction angle have been taken directly from the laboratory data. Some variation was made to the cohesive elements tensile strength and fracture energy in Mode I and Mode II to improve the numerical results for the UCS and BD tests. As a first estimate, the input parameters of tensile strengths and fracture energies of Mode I of the two bedding inclinations (i.e., 0° and 90°) were taken from the laboratory data from Ren et al. (2021). Due to the difficulty of obtaining the value through laboratory testing, fracture energy Mode II is not available. From the experience by Lisjak et al. (2014b), Mode II fracture energies ($G_{II\bar{f}}$) for rocks are approximately 5-10 times those for Mode I fracture energies ($G_{I\bar{f}}$). In the calibration process, the following trial-and-error processes are performed:

- 1) The tensile strengths (i.e., $f_{t\bar{p}ar}$ and $f_{t\bar{p}er}$) and fracture energies (i.e., $G_{I\bar{f}p\bar{a}r}$ and $G_{I\bar{f}p\bar{e}r}$) in Mode I were varied until the model results agreed with the laboratory indirect tensile strength values ($T_{p\bar{a}r}$ and $T_{p\bar{e}r}$) in the BD test models. The Mode II fracture energies ($G_{II\bar{f}p\bar{a}r}$ and $G_{II\bar{f}p\bar{e}r}$) in BD models used 10 times of Mode I energies obtained in the laboratory tests, based on the recommendation by Lisjak et al. (2014b).
- 2) The Mode II fracture energies ($G_{II\bar{f}p\bar{a}r}$ and $G_{II\bar{f}p\bar{e}r}$) were varied until the model results of the the uniaxial compressive strengths matched those in the UCS tests ($UCS_{P\bar{a}r}$ and $UCS_{P\bar{e}r}$).
- 3) Input the Mode II fracture energies obtained in step 2 back to BD models to validate all parameters.

The parameters adopted in this research are listed in Table 3.1. Once the cohesive element was broken, the elastic elements were governed by the contact scheme in

ABAQUS, as mentioned in section 3.2.1. The normal contact in this research has adopted a hard mode, which means there was only the normal force transferred and no penetration allowed between elements under contact. This can help reduce the computational time. The shear contact stress was calculated through the Coulomb's friction law. Deng et al. (2021) recommended using $\tan \phi_i$ (value of friction angle of shale) as the internal elements sliding friction coefficient, μ , based on the sensitivity study. This has been widely used in FDEM models by several researchers (Deng et al., 2022, Zhou et al., 2015 and Lisjak et al., 2014a). Here, an elastic elements sliding friction coefficient of 0.8 was used initially and Section 3.3.2 investigates its sensitivity on the results. The friction coefficient between the steel loading plane and rock element, f_i , was 0.1, which has been widely adopted by several researchers in several FDEM laboratory models (Zhou et al, 2015, Lisjak et al, 2014b and Lisjak et al., 2014a).

Table 3.1 Input parameters for the Longmaxi shale FDEM model (Wang et al., 2018, Wang et al., 2020, Ma et al., 2018 and Ren et al., 2021)

Parameter	Value
Elastic elements	
Density, ρ (kg/m ³)	2586
Young's modulus parallel to bedding, E_{par} (GPa)	21.5
Young's modulus perpendicular to bedding, E_{per} (GPa)	14.6
Poisson's ratio parallel to bedding, ν_{par}	0.23
Poisson's ratio perpendicular to bedding, ν_{per}	0.22
Shear modulus, G (GPa)	9.08
Cohesive elements	
Tensile strength parallel to bedding, f_{tpar} (MPa)	1
Tensile strength perpendicular to bedding, f_{tper} (MPa)	2

Cohesion parallel to bedding, c_{par} (MPa)	8.9
Cohesion perpendicular to bedding, c_{per} (MPa)	16.2
Mode I fracture energy parallel to bedding, G_{Ifpar} (J/m ²)	30
Mode I fracture energy perpendicular to bedding, G_{Ifper} (J/m ²)	45
Mode II fracture energy parallel to bedding, G_{IIpar} (J/m ²)	130
Mode II fracture energy perpendicular to bedding, G_{IIper} (J/m ²)	350
Friction angle of intact material, ϕ_i (deg)	36.27
Normal stiffness, k_n (GPa/m)	250
Shear stiffness, k_s (GPa/m)	25
Element/Loading platen friction coefficient, f_l	0.1
Elastic elements internal sliding friction coefficient, μ	0.8

Table 3.2 compares the mechanical properties of the numerical models with the values obtained from the experimental tests on Longmaxi shale. The relative errors for all values are within 5%. The adoption of 5% of relative errors as threshold value is based on the recommendation by Lisjak et al. (2014a) and Zhou et al. (2015).

Table 3.2 Comparison of the mechanical properties of the Longmaxi shale between the numerical model and experiment average results (Wang et al., 2018, Wang et al., 2020 and Ma et al., 2018) (Note: the shale model with bedding plane inclinations of 90° and 0° is illustrated parallel and perpendicular to the bedding planes in the Table).

Mechanical properties	Experimental value	Numerical value
Elastic modulus parallel to bedding, E_{Par} (GPa)	21.5±0.2	22.2
Elastic modulus perpendicular to bedding, E_{per} (GPa)	14.80±0.25	14.30

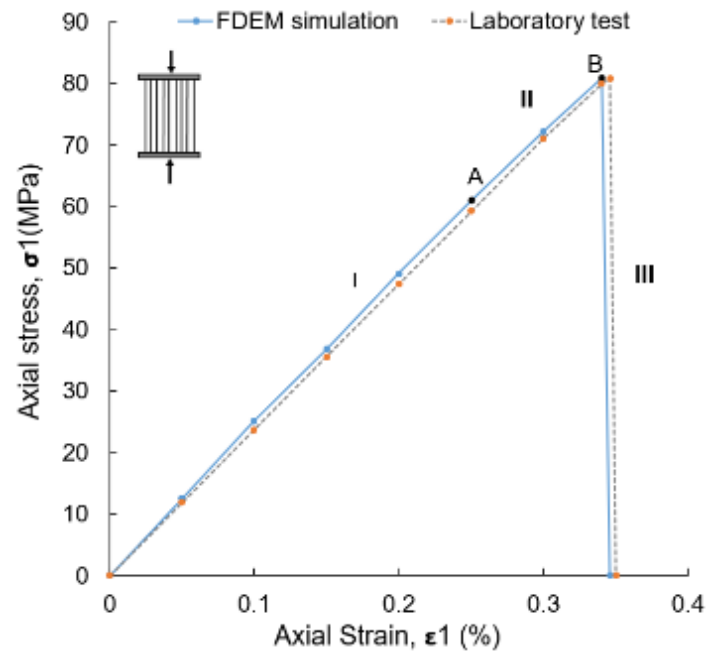
Uniaxial compressive strength parallel to bedding, σ_{uPar} (MPa)	76.80±4.00	80.93
Uniaxial compressive strength perpendicular to bedding, σ_{uPar} (MPa)	92.17±0.60	95.59
Indirect tensile strength parallel to bedding, T_{par} (MPa)	3.50±0.50	3.17
Indirect tensile strength perpendicular to bedding, T_{per} (MPa)	6.60±0.70	6.57

3.3.5 Calibration results

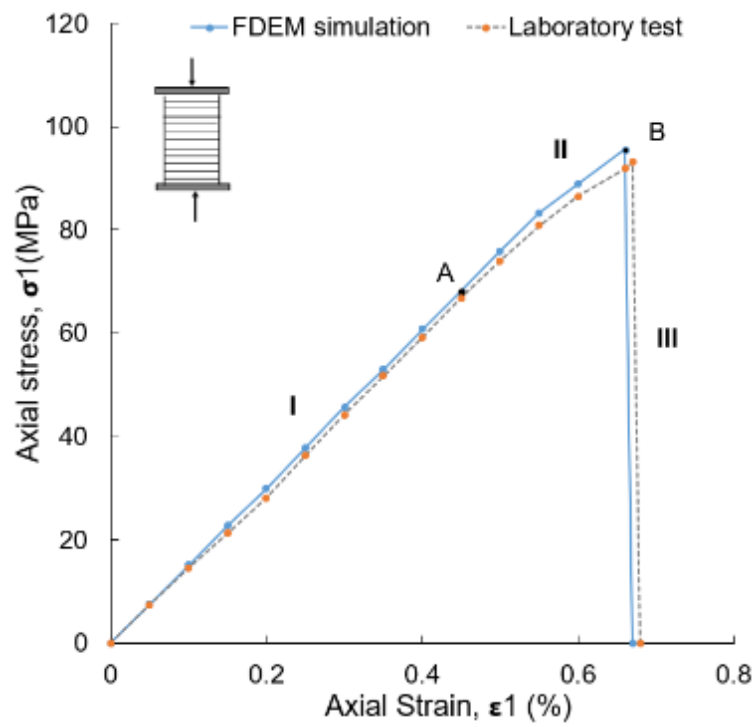
1) Stress-strain response in UCS tests through FDEM

Figure 3.13 compares laboratory tests and FDEM simulation for stress-strain curves in UCS tests on Longmaxi shale with bedding plane inclination of 0° and 90° . In both shale models, the peak strength and slope of the stress-strain curves are close to those observed in the laboratory tests with minor differences (Wang et al., 2020). The Longmaxi FDEM models exhibit few phases of stress-strain behaviour similar to that observed in several brittle rocks. Before the forming of the fractures, both stress-strain curves from point 0 to point A show a linear elastic phase. The stiffness of cohesive elements and continuum elastic elements captured the elastic response of the model. The model enters phase II after point A (crack damage threshold) when fractures are formed and coalesce within the model, resulting in macro-failure. Macroscopic fractures propagate throughout the entire model in Phase III, which occurs beyond point B. The strength of the models suddenly dropped within small strains. A uniaxial compressive strength value of 80.93 MPa is obtained for $\theta = 90^\circ$ and 95.59 MPa for θ

= 0°. These values are in reasonable agreement with those obtained by the laboratory tests, as can be seen in Table 3.2.



a)



b)

Figure 3.13 The stress-strain curves of the shale for laboratory UCS test with bedding plane inclinations of a) 90° and b) 0°, compared with FDEM simulation results (point A is the crack damage stress threshold, and point B is the peak strength) (Wang et al., 2020).

It can be seen in Figure 3.14 that the uniaxial compressive strength and elastic modulus as a function of different bedding plane inclinations from the FDEM models are within 5% of the average laboratory values (Wang et al., 2020), except for inclinations of 45° and 60° which differ by 9% and 7.3%, respectively. However, the simulation results are within 5% to the minimum experiment values at 45° and 60°, respectively. It is the same behaviour when assessing the results from the FDEM and the laboratory data for the elastic modulus. This may be a result of calibrating the the micro-parameters of cohesive elements in the FDEM model against the macro-mechanical strengths of shale samples at 0° and 90°, which causes the macro-mechanical strengths of the shale FDEM models in the shearing through the matrix (i.e., 0° and 15°) and tensile splitting (i.e., 75° and 90°) failure modes to fit better with laboratory values, as compared to bedding plane delamination failure mode (i.e., 30°, 45° and 60°). Shale failure modes in UCS tests are discussed later in Chapter 4, Section 4.2. Figure 3.14(a) shows that the uniaxial compressive strength decreases (0°-60°) and then increases as the bedding plane inclination increases, whereas Figure 3.14(b) shows that the elastic modulus increases with increasing bedding plane inclination. Under different bedding plane inclinations, the anisotropy of the uniaxial compressive strength and elastic modulus of shale are related to different failure modes, which are illustrated in section 5.1.

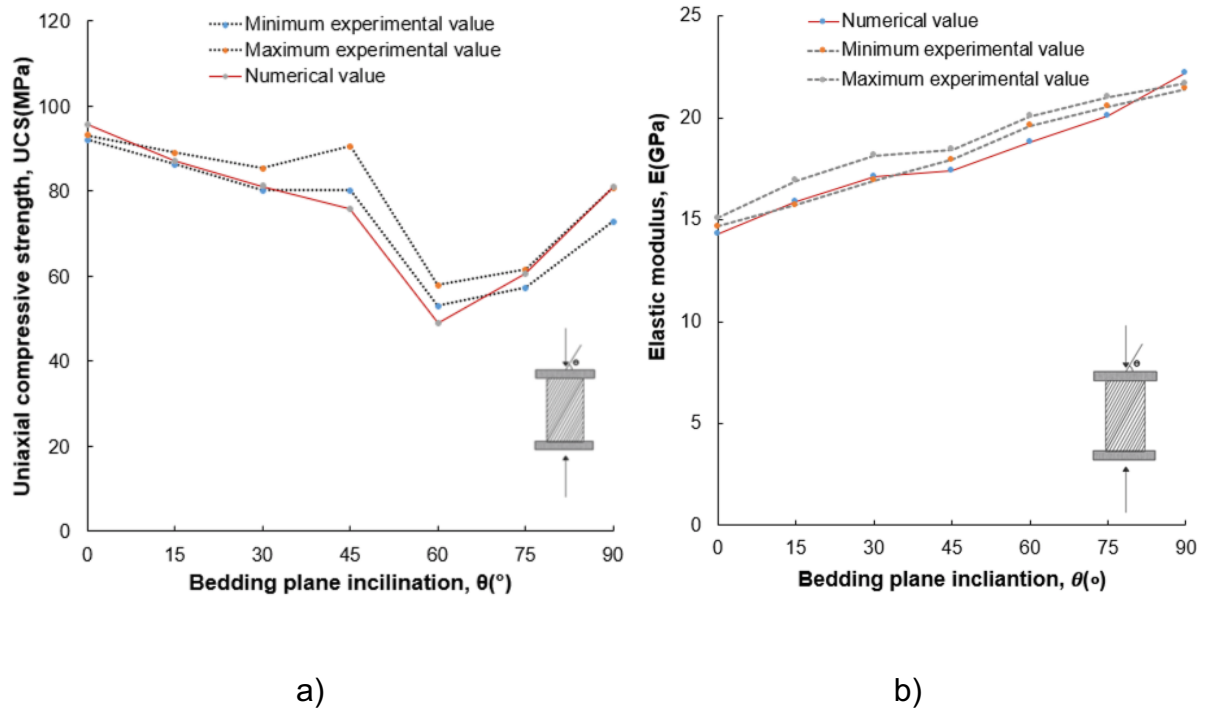


Figure 3.14 a) Variation of the uniaxial compressive strength and b) elastic modulus values for the Longmaxi shale for UCS test with different bedding plane inclinations in the FDEM models and experimental tests (Wang et al., 2020).

2) Stress-displacement response in BD tests through FDEM

Equation 3.7 is used to calculate the indirect tensile strength from the BD tests (Lisjak et al., 2014).

$$T = \frac{2P_{max}}{\pi t_m D_m} \quad \text{Eq. 3.7}$$

where P_{max} is the maximum load on the loading platen, D_m is the model diameter (50mm), and t_m represents the thickness of the model (a unit thickness is assumed in 2D).

Longmaxi shale BD test model peak strengths are 6.57 MPa and 3.17 MPa with bedding plane inclinations of 0° and 90°, respectively, as illustrated in Figure 3.15.

These values matched well with the laboratory values of 6.6 MPa and 3 MPa for shale models with bedding inclinations of 0° and 30° , respectively (Table 3.2).

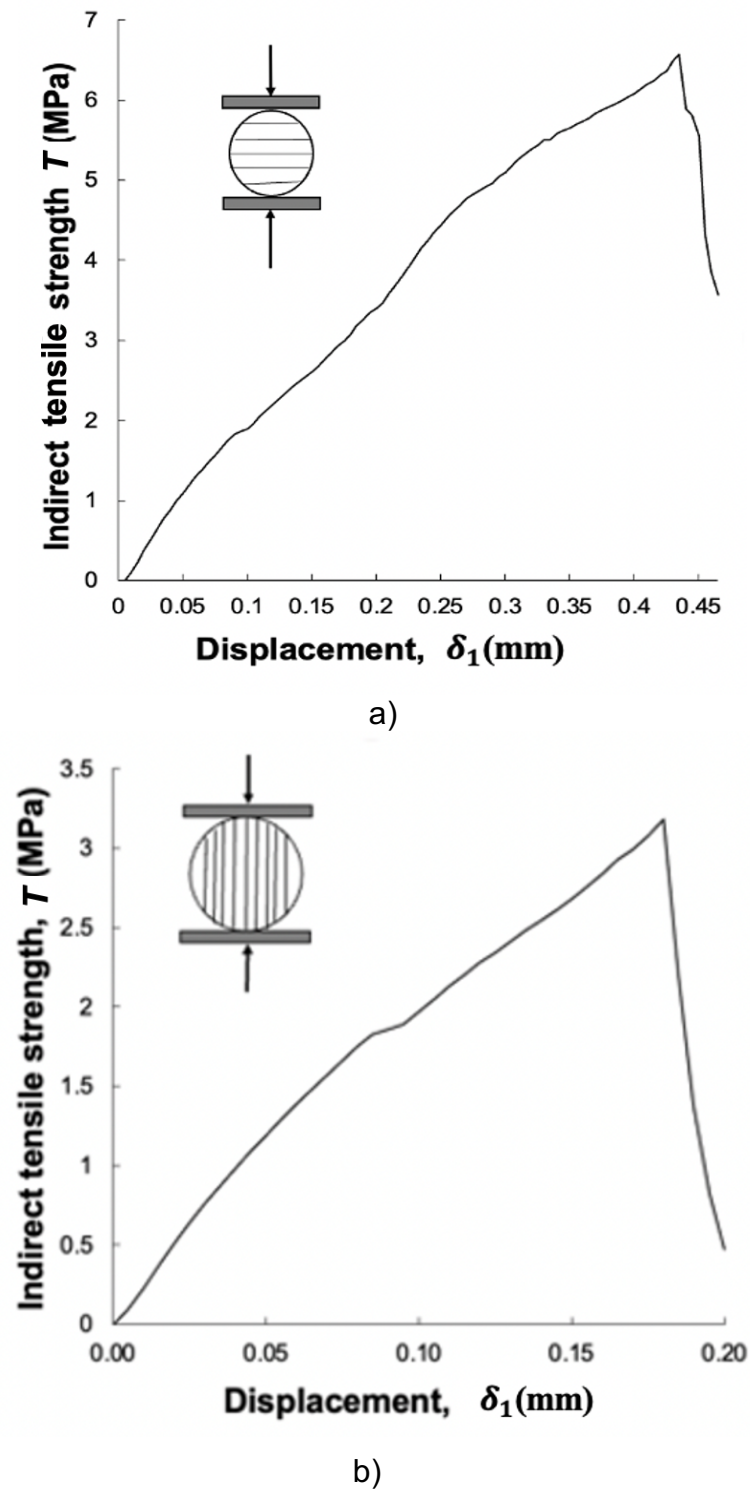


Figure 3.15 Stress-displacement response of the Longmaxi FDEM model for BD tests with bedding plane inclinations at a) 0° and b) 90° .

A comparison of the indirect tensile strength values in FDEM models and laboratory tests is shown in Figure 3.16. The FDEM models and BD tests on Longmaxi shale with different bedding planes inclination show similar indirect tensile strengths. As an indication of the variation of the laboratory values of Longmaxi shale in BD tests, the two black lines indicate the lower and upper limit values (Ma et al., 2018). Laboratory results as well as results from FDEM models indicated that the indirect tensile strength of Longmaxi shale decreases with increasing bedding plane inclination.

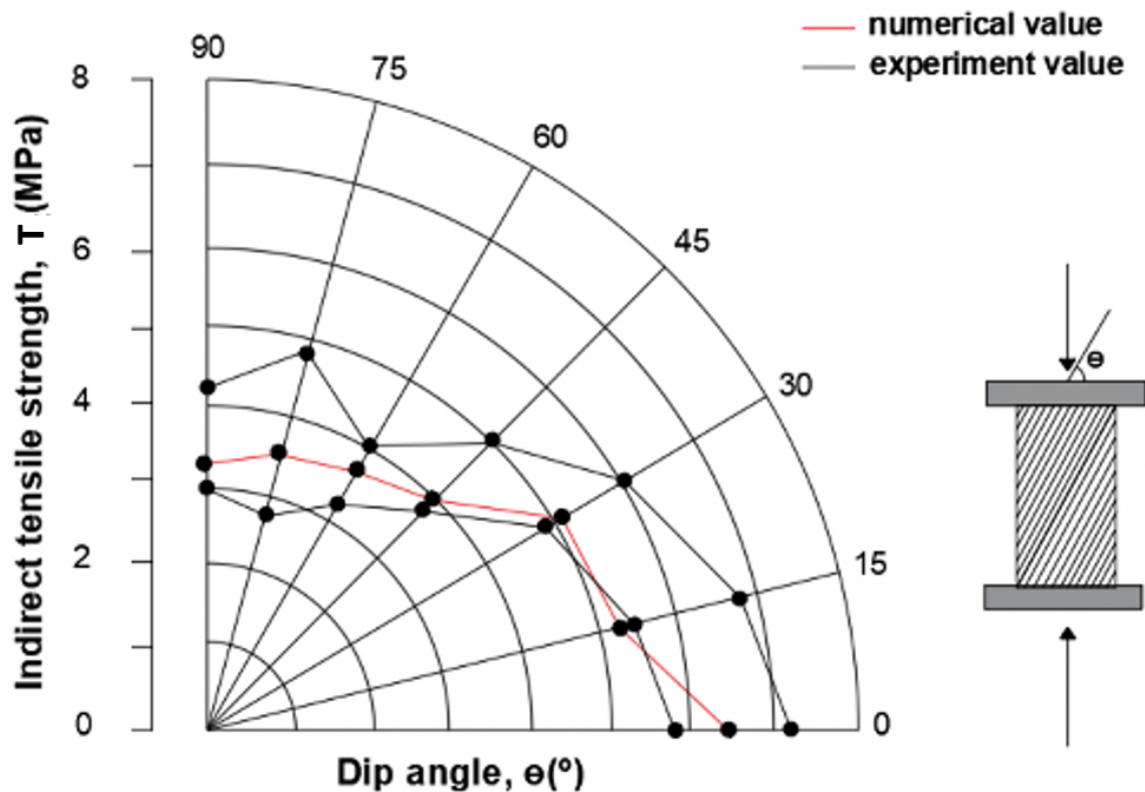


Figure 3.16 The indirect tensile strength values in the FDEM models and experimental tests for the Longmaxi shale varied with bedding plane inclinations with the two black lines indicating the upper and lower limits (Ma et al., 2018).

3.4 The development of field scale FDEM model

Previous section demonstrated the effectiveness of the FDEM in modelling shale in small laboratory scale. Field scale circular tunnel excavation in Opalinus Clay has been simulated using FDEM models to further investigate shale anisotropy effects on deep buried tunnel EDZ fracture mechanisms. Large-scale shale field tunnel model reproduces qualitatively the short-term excavation deformation fields observed in the field. This Full-scale Emplacement tunnel in Opalinus Clay was chosen because it provided detailed data and information about rock mechanical parameters as well as tunnel wall displacements in the field.

3.4.1 Project background

3.4.1.1 Geological conditions and stress field

In Canton Jura, Switzerland, the Mont Terri underground research laboratory (URL) is located northwest of the town of St-Ursanne (Lisjak, 2015). URL is located in the southeast limb of Mont Terri, with an average overburden depth of 300 meters. The URL lies entirely within the Opalinus clay formation (Nussbaum et al., 2011). Opalinus clay is a dark grey shale with transversely isotropic mechanical behaviour (Bock, 2009). A large set of data is available from the under-coring measurements by Corkum and Martin (2007a) and this is used in the current research. The maximum principal stress is vertical with values ranging between 6-7 MPa. At a depth of 250 metres, this corresponds to the lithostatic pressure values. In the meantime, the minimum principal stress is horizontal, ranging between 4-5 MPa.

3.4.1.2 Rock material

The bedding orientation of Opalinus Clay at Mont Terri, Switzerland, is 139/33 (strike/dip), resulting in the excavation axis almost parallel to the bedding plane strike (Jaeggi et al., 2013). The Opalinus Clay is a brittle shale with a transversely isotropic mechanical behaviour (Lisjak et al., 2014b).

3.4.1.3 Full-scale Emplacement tunnel construction

Full-scale Emplacement tunnel is 50m long, and the diameter of the tunnel is approximately 3 m (including shotcrete lining). The Full-scale Emplacement tunnel excavation method has adopted mechanical excavation method (i.e., pneumatic hammer and road-header). Reinforced, low pH shotcrete with a thickness of 160 to 240 mm was used to support the excavation face (Lisjak et al., 2015).

3.4.1.4 Field monitoring programme

In order to study how the tunnel excavation affected the rock mass, several monitoring programmes in the field were conducted by Lisjak et al. (2015). The monitoring included:

1) Post-support tunnel wall displacement

By using two total stations with integrated distance measurements, geodetic surveying was used to measure the tunnel wall displacement in three dimensions after the support was installed (Lisjak et al., 2015). In the Full-scale Emplacement tunnel, a total of five cross sections were monitored with an average spacing of 6 m. The optical reflectors were placed approximately 1 m - 1.5 m behind the tunnel face, before shotcrete was applied, giving five target points (M1 - M5) on each monitoring section.

The total displacements of the tunnel wall after the installation of support were obtained. Figure 3.17 shows the total displacements of the five monitoring points after installation of the sprayed concrete lining of the tunnel wall in one monitoring section, C₃. From Figure 3.17, tunnel wall deformations start to converge around 9m (3D) behind the excavation face (Lisjak et al., 2015).

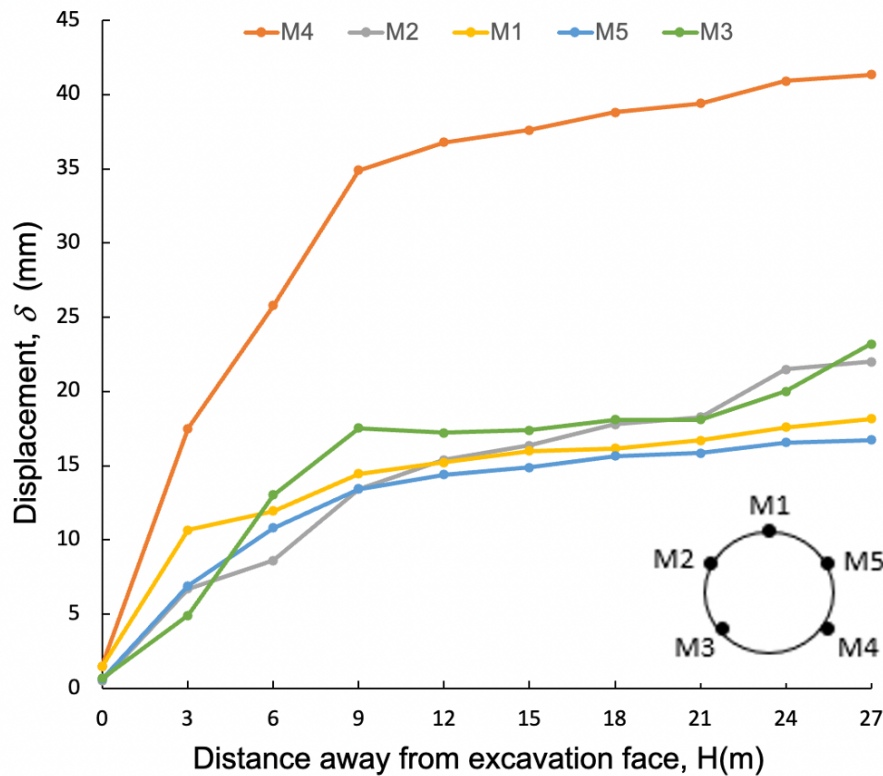


Figure 3.17 The evolution of the post-support displacements on five monitoring points at section three (Lisjak et al., 2015).

2) Inclinoimeters

Inclinometer chains were permanently installed above the tunnel crown in order to monitor the total displacement of the tunnel wall during the excavation. Two 45m long inclinometers were placed in boreholes that were drilled sub-parallel (dip = 1°) to the tunnel axis. Inclinometer probes were located between 1.4 and 2.4 metres from the

tunnel crown (Lunardi., 2008). The monitoring data showed that the averaged vertical displacement values for the two inclinometer chains were 22mm and 21mm, respectively (Lisjak et al., 2015).

3.4.2 Description of FEM and FDEM field scale model

The excavation short-term response of the Full-scale Emplacement tunnel is illustrated through field measurements in the last section. FDEM Full-scale Emplacement tunnel excavation model was calibrated using these data. The calibrated FDEM Full-scale Emplacement tunnel excavation model is then employed to present the mechanical performance of the surrounding rock deformation and fracture development as regarded in EDZ.

3.4.2.1 FEM model

To compare the deformation values monitored in the field with the following FDEM simulation, the FEM models are used. Table 3.5 in section 3.4.3 shows the properties of the linear elastic medium used in the FEM model to represent the deformability of Opalinus clay in the Full-scale Emplacement tunnel. The model geometry was chosen to minimize the boundary conditions effects on the simulation. Based on the recommendation of Lisjak et al, (2014b) and Deng et al. (2021), a 30m × 30m square domain with a 3.0 m diameter, circular tunnel located in the centre has been created. The adopted in situ stresses for the FEM models are based on the field values obtained by Corkum and Martin (2007a), as shown in Table 3.3. Meanwhile, a liner of 20 cm thickness was adopted. Based on the recommendation of Lisjak et al. (2014b), Lisjak et al. (2015), Ha et al. (2021), Ha (2017) and Vlachopoulos and Vazaios (2018), the far-field boundary conditions consist by pinned displacements in horizontal and vertical directions to maintain in situ stress conditions during excavation.

Table 3.3 In-situ stress conditions applied to the Full-scale Emplacement tunnel numerical model.

Model Scenario	Stress scenario	Vertical stress, σ_v (MPa)	Horizontal stress, σ_h (MPa)	Coefficient of lateral earth pressure, K_0
FEM and FDEM analysis	a (Field)	6.5	4.5	0.7

3.4.2.2 FDEM model

According to Figure 3.18, the FDEM model consisted of a circular Full-scale Emplacement tunnel with a diameter of 3.0 m centred within a 30 m x 30 m square domain, same as the FEM model. At least 4D on each side of the tunnel wall is recommended by Lisjak et al (2015) and Liu and Deng (2019) to make sure the excavation is not impacted by the model boundary. Bedding planes have been created in the model that are inclined at $\theta = 33^\circ$, and the layering thickness, t , has been set to 0.75m. According to the laboratory scale simulation, FDEM can effectively capture the mechanical response of shale with millimetre-sized elements. With tens of metres of elements in a two-dimensional field-scale model, such a fine spatial discretization would result in a long computation time. Based on the recommendation of Lisjak et al. (2014b), the EDZ was built with a mesh refinement zone to keep computational runtimes within practical limits while maximizing model resolution. Normally, the excavation zone extends within 1.5 times the diameter from the excavation wall, so the refinement zone was set at 4.5m away from the excavation wall (Schuster and Alheid, 2007; Paul et al., 2002 and Armand et al., 2014). Various element sizes have been adopted by researchers over the years, ranging from 0.03 m to 0.16 m (Lisjak et al., 2015; Deng et al., 2022 and Ha et al., 2021). The element size sensitivity study

conducted by Liu and Deng (2019) indicates that the depth of the EDZ starts to converge once the element size is smaller than the fracture process zone, l_{FPZ} . Using Equation 3.6, the l_{FPZ} for the Opalinus Clay was determined to be approximately 0.125 m. Within the mesh refinement zone, the elements are ranging from 0.05~0.12 m. From the refinement zone boundaries to the external boundaries, the size of the elements with an average of 0.3 m. In total, the model contains approximately 140,000 elements. The thickness of the support adopted 16 cm, same as for the FEM model (Lisjak et al., 2015). Similar to the FEM model, the far-field boundary conditions are simulated by pinned displacements in the horizontal and vertical directions.

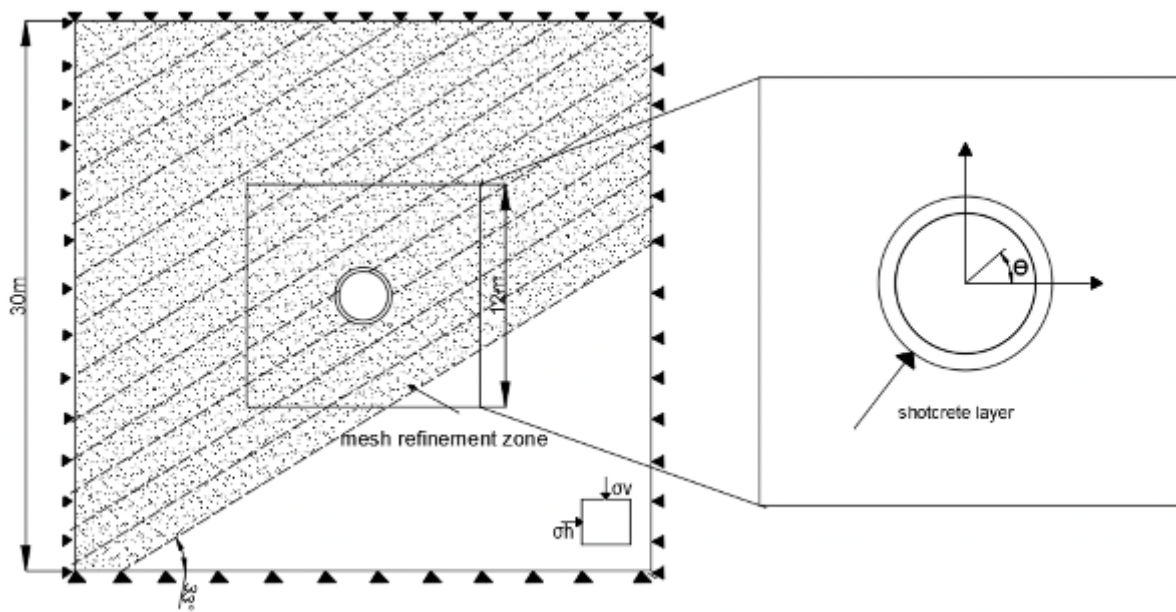


Figure 3.18 FDEM model geometry and boundary conditions

3.4.3 In-situ stress and input parameters

The adopted in-situ stress field for the FEM and FDEM model was based on the values from section 3.4.1, as shown in Table 3.3. The adopted simulation parameters were initially based on FDEM model of the Full-scale Emplacement tunnel by Lisjak et al. (2015). Based on the study of Deng et al. (2021), the strength of the rock are

significantly under the influence of the fracture energies. In this case, the fracture energies (G_I and G_{II}) of the cohesive elements were calibrated to match the average vertical displacement of the tunnel crown reported in section 3.4.1. Table 3.4 lists the input parameters resulting from the trial-and-error process.

Table 3.4 Input parameters for the Full-scale Emplacement tunnel (Lisjak et al., 2015)

Parameter	Value
Elastic elements	
Density, ρ (kg/m ³)	2330
Young's modulus parallel to bedding, E_{par} (GPa)	3.8
Young's modulus perpendicular to bedding, E_{per} (GPa)	1.3
Poisson's ratio parallel to bedding, ν_{par}	0.35
Poisson's ratio perpendicular to bedding, ν_{per}	0.25
Shear modulus, G (GPa)	0.9
Cohesive elements	
Tensile strength parallel to bedding, f_{tpar} (MPa)	0.44
Tensile strength perpendicular to bedding, f_{tper} (MPa)	1.8
Cohesion parallel to bedding, c_{par} (MPa)	2.8
Cohesion perpendicular to bedding, c_{per} (MPa)	24.8
Mode I fracture energy parallel to bedding, G_{Ifpar} (J/m ²)	1.2
Mode I fracture energy perpendicular to bedding, G_{Ifper} (J/m ²)	23.4
Mode II fracture energy parallel to bedding, G_{IIpar} (J/m ²)	33
Mode II fracture energy perpendicular to bedding, G_{IIper} (J/m ²)	116
Friction angle of intact material, ϕ_i (deg)	22
Normal stiffness, k_n (GPa/m)	38
Shear stiffness, k_s (GPa/m)	3.8

3.4.4 Modelling excavation procedure

After tunnel excavation, the rock surrounding the tunnel undergoes a three-dimensional stress redistribution. The removal of the soil causes a redistribution of the stresses around the tunnel wall. The exposed tunnel walls are supported by the core soil, which creates a pressure that enables the excavated sections to stand up until support can be installed (Karakus, 2007 and Deng et al., 2020). Figure 3.19 further illustrates that the rock mass's stress state is disturbed ahead of the tunnel face, whereas it gradually declines behind the tunnel face (Curran et al., 2003). In the case of a support system installed behind the tunnel face, there is a pre-convergence over time. Due to the three-dimensional stress distribution around the tunnel face, direct two-dimensional numerical analyses of the tunnel excavation are inaccurate. Therefore, in order to use the two-dimensional model simulation realistically, the tunnel wall displacement before the installation of the support needs to be considered.

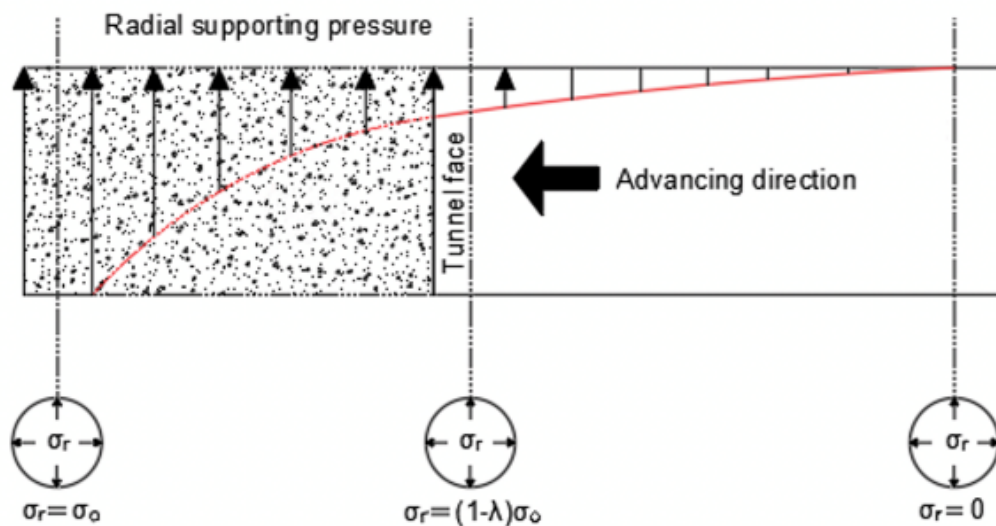


Figure 3.19 Supporting pressure around the excavation face (σ_r is radial supporting stress, σ_0 is initial radial supporting stress and λ is a function of the reduction factor).

The excavation stress relaxation method and the material softening method have been commonly adopted by researchers to simulate the supporting effect of tunnel walls in two-dimensional models (Cai, 2008 and Li et al., 2014). In contrast to the stress relaxation method, material softening reduces the impact of the transience on the material failure and provides a more static solution, which is important when considering crack propagation (Bai et al., 2016). Furthermore, a heterogeneous or even anisotropic rock mass will have different radial supporting pressures on different parts of the tunnel wall. Using the stress relaxation method, it is difficult to apply different loads to the tunnel wall. As a result of the above issues, the material softening method has been widely used for FDEM two-dimensional tunnel excavation (Ha et al., 2021, Lisjak et al., 2015 and Deng and Liu, 2020).

1) Modelling excavation processes for advancing tunnel excavation

This study has adopted the material softening method. Using a fictitious softening elastic material in the tunnel core, the three-dimensional tunnel face supporting effect is captured, which results in a progressive reduction of the radial supporting stresses (Curran et al., 2003). A two-dimensional analysis model of the tunnel excavation can only be applied realistically if the displacement before the installation of the supporting structures can be estimated (Lisjak et al., 2015). The tunnel wall deformation prior to the installation of the tunnel support has been identified as a critical factor affecting tunnel lining closure in relation to distance from the excavation face. As a result, a ratio, δ^* , has been calculated between the post-support displacement and the total displacement (including the displacement of tunnel crown occurring before the installation of supports) at the tunnel crown. The δ^* and the total displacement at the

tunnel crown, δ , from the field measurements have been adopted to calibrate the appropriate elastic modulus reduction in the FDEM model.

Figure 3.20 indicates the vertical displacement of the surrounding rocks during core soil excavation in FEM models with different reductions in Young's modulus. In the excavated tunnel crown, the total displacement is increasing with a greater reduction in Young's modulus in the core soil, but the post-support tunnel crown displacement is decreasing (Figure 3.20). The ratio δ^* gets smaller with an increase in the core soil Young's modulus reduction, as shown in Figure 3.20. The values of the ratio δ^* from the field range from 38% to 55%, which indicates the most appropriate Young's modulus deduction value for the FEM model is approximately 1E-02- 1E-01 (Lisjak et al., 2015). The maximum displacement of the surrounding rock in the model with a reduction of the Young's modulus of the core soil of 1E-03 is 8.98 mm, which is still significantly less than the 22mm of tunnel crown displacement obtained in the field. Thus, a reduction factor for the Young's modulus of 1E-01 of the core soil for the FEM model is applied leading to a bigger crown displacement value.

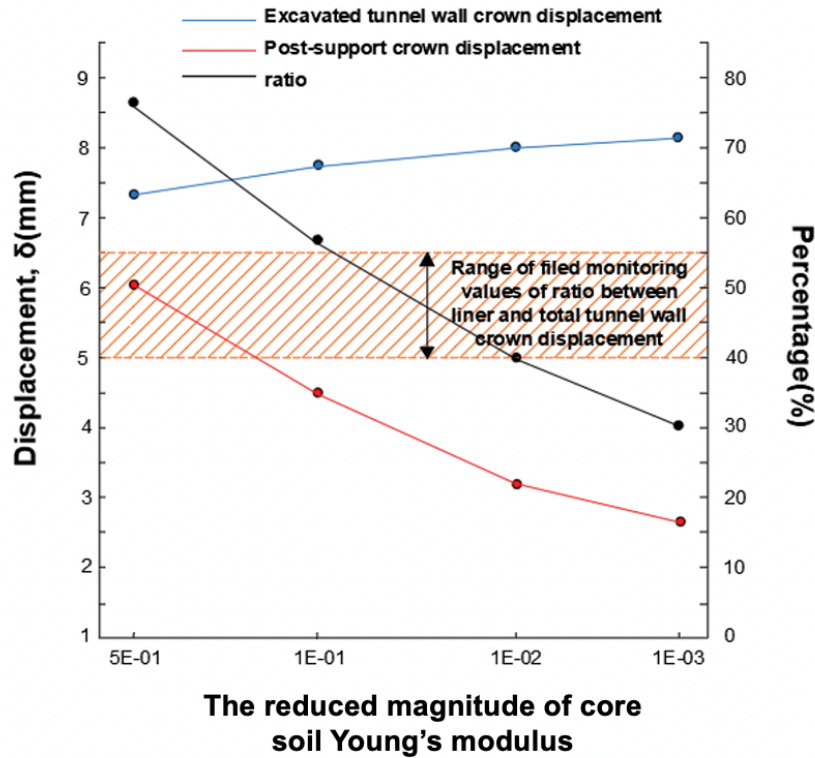


Figure 3.20 The vertical displacement of the excavated tunnel wall crown, post-support tunnel crown in the FEM models with different reduced Young's modulus magnitudes (Black line is the ratio, δ^* , between the post-support displacement of tunnel crown and total displacement of tunnel wall crown from FEM models, orange area is the range of the ratio, δ^* , between the post-support displacement of the tunnel crown and total displacement of tunnel wall crown from fields data).

Four models with different reduction of the Young's modulus in the core soil have been created through FDEM. Similar to the FEM, the total displacement of the surrounding rock is increasing with greater reduction in Young's modulus in the core soil, whereas the post-support displacement of the tunnel crown is decreasing (Figure 3.21). According to Figure 3.21, the most appropriate reduction magnitude of the Young's modulus for the FDEM model is between 1E-01 and 5E-02 based on the values of the ratio δ^* from the field. The displacement of the tunnel crown using a reduction factor

of 5E-02 for the Young's modulus is bigger than using 1E-01, and is closer to the filed values, 21-22mm. Thus, this value is adopted for the FDEM model in this thesis.

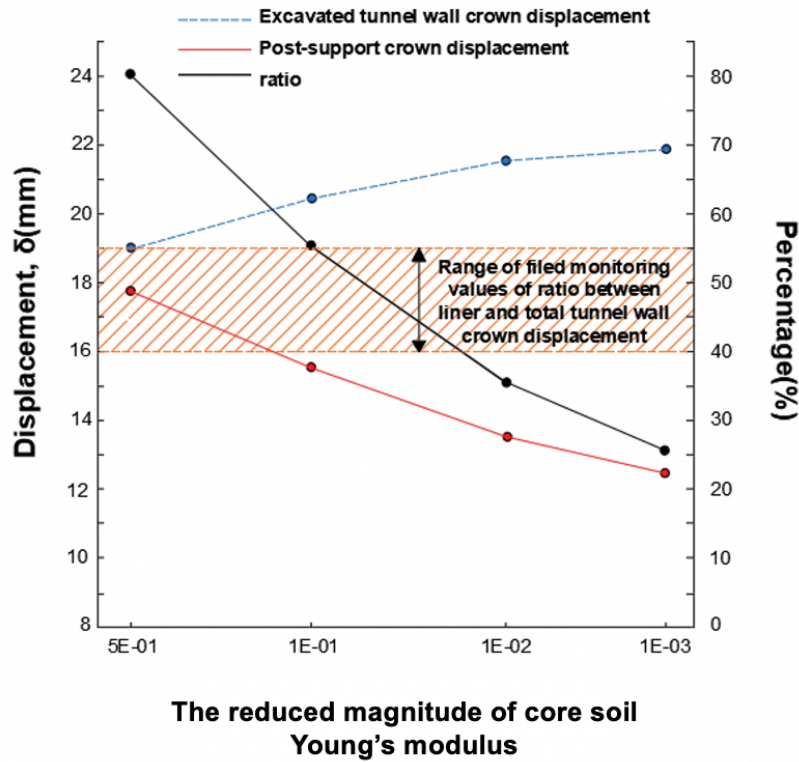


Figure 3.21 The vertical displacement of the excavated tunnel wall crown and post-support tunnel crown in the FDEM models with different reduced young's modulus magnitudes (Black line is the ratio, δ^* , between the post-support displacement of tunnel crown and total displacement of tunnel wall crown from FEM models, orange area is the range of the ratio, δ^* , between the post-support displacement of the tunnel crown and total displacement of tunnel wall crown from fields data).

2) Excavation procedure in FDEM

Following the suggestions of Lisjak et al. (2014a) and Ha et al. (2021), the simulation of the FDEM model excavation contains three steps:

1) Applying in-situ stresses: In the first step, the vertical and horizontal in-situ stresses from the field were applied to the model, and gravity is enabled. The cohesive elements have been deactivated in the FDEM model, which means that the

unexcavated model is deforming under in-situ stresses until equilibrium is reached using FEM. A revised set of nodal coordinates was obtained after the in-situ stresses were applied.

2) Reducing the soil strength of the core: Before reducing Yong's modulus of the soil core, the cohesive elements inserted between the elastic elements are activated. In the second step, the revised nodal coordinates of the model in the first step were set as the initial nodal coordinates. By using the core soil softening method, the supporting effect of the tunnel face in two dimensional has been captured. According to study by Deng and Liu (2020), similar results (i.e., depth of EDZ and failed cohesive elements) have been obtained under different softening curves. Accordingly, this study linearly reduced the core soil's Young's modulus in this step, following Ha et al. (2021).

3) Removing the soil of the tunnel core and applying a liner: In step three, the soil of the tunnel core was removed, and the elastic properties (i.e., Young's modulus and Poisson's ratio) of the liner were activated. Upon reaching one percent of the maximum total kinetic energy, the model is reaching equilibrium according to Zhou et al. (2015).

3.4.5 Validation of the FDEM model

1) FEM in-situ stress field and displacement after excavation

Due to the excavation, the in-situ stresses were redistributed. Figure 3.22 illustrates the stress and displacement field around the tunnel with the plane of anisotropy orientated at 33° . At $\theta = 110^\circ$ and 163° of the excavated tunnel wall, respectively, the minimum and maximum stresses are 3.4 MPa and 13.6 MPa. These values are similar to those obtained in the FEM simulation by Lisjak et al. (2015) where the minimum

and maximum stresses were 6.2 and 15.7 MPa respectively at $\theta = 108^\circ$ and 162° . The difference in values is a result of Lisjak et al. (2015) using a $1\text{E-}02$ reduction of the core soil and using no liner support.

The total displacement at $\theta = 110^\circ$ accounted for the largest displacement of 7.8 mm on the excavated wall due to the relatively low stiffness sub-perpendicular to the bedding. Field monitoring indicated that the magnitudes of displacement obtained from the FEM model underestimated the surrounding rock displacement.

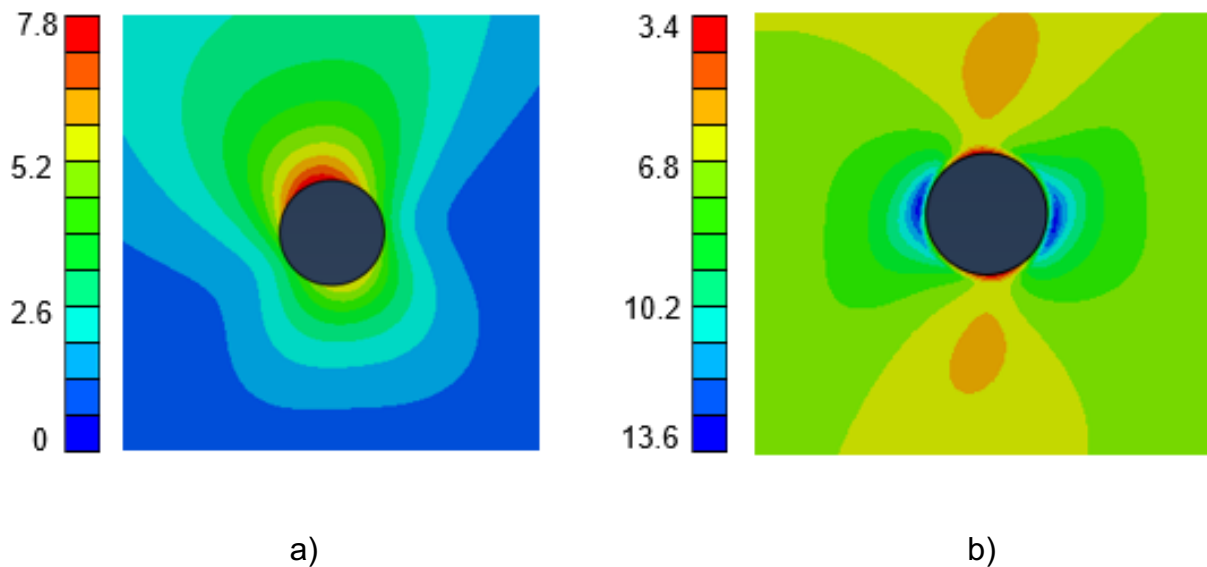


Figure 3.22 Results from the FEM model a) total displacement (mm) and b) maximum principal stress (MPa).

2) FDEM In-situ stress field and displacement after excavation

According to the total kinetic energy monitored during excavation, the excavation reached equilibrium after about 0.38s. The transversely isotropic elastic properties of the shale also affect the redistribution of stress after excavation in the FDEM model, same to FEM model. As bedding planes delaminate, the maximum principal stress is re-oriented in the direction perpendicular to bedding, suppressing the extension of the

EDZ in lateral direction. Figure 3.23 shows a fractured zone with low to moderately negative stress values in the left shoulder and right knee near the tunnel boundary as a result of bedding plane slippage at $t = 1$ s.

The total displacement field is also depicted in Figure 3.23. As a result of the stress redistribution around the tunnel after excavation, the rock mass has slipped along the bedding planes due to their lower strength. Because of the low stiffness in the direction perpendicular to the bedding planes, a local stress perturbation caused by slippage around the bedding plane causes large displacements perpendicular to the layering during the subsequent simulation process. The displacement at $\theta = 128^\circ$ obtained the largest displacement of 30.2 mm on the excavation wall.

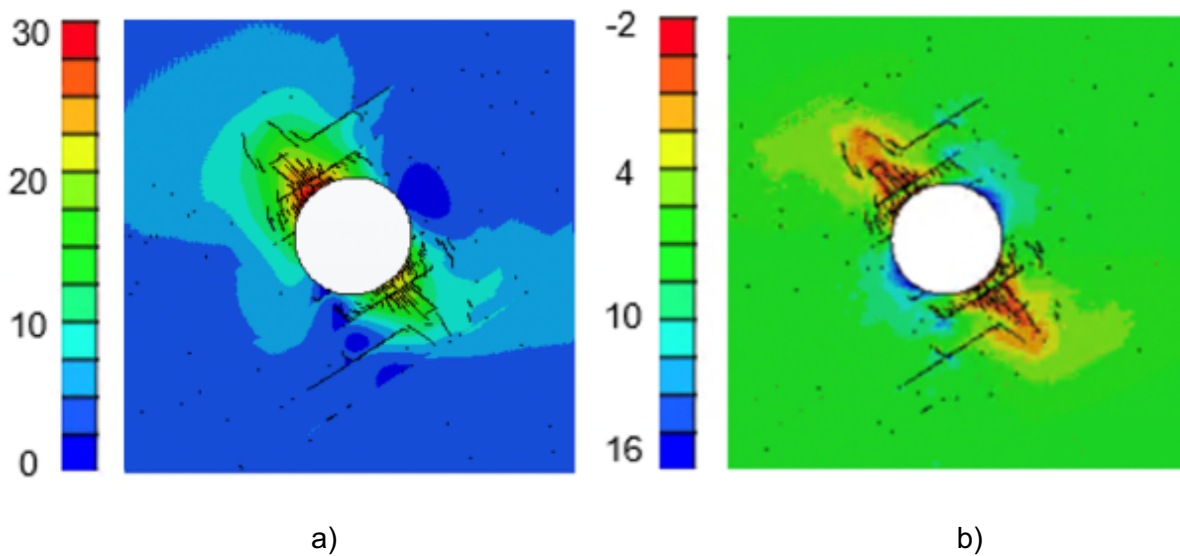


Figure 3.23 The maximum principal stress and total displacement field in FDEM model at $t = 1$ s a) Displacement (mm) b) Maximum principal stress (MPa).

3) Simulated fracturing behaviour

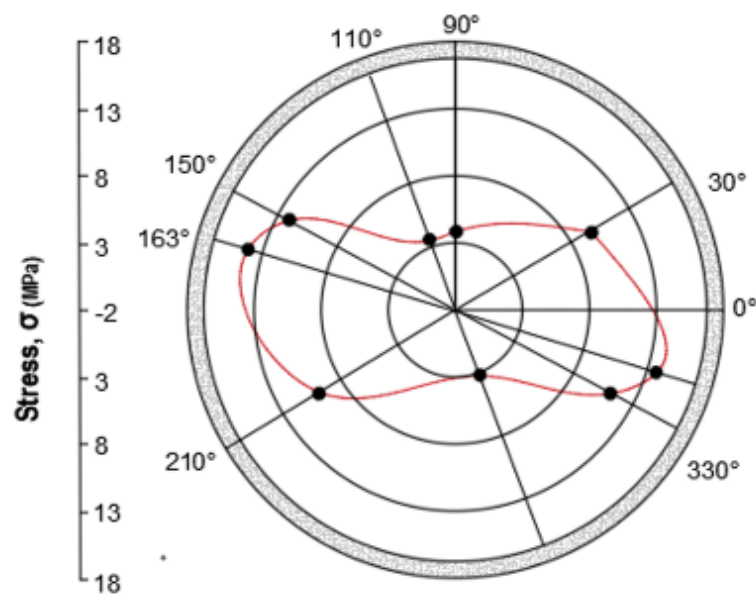
In proximity to the tunnel wall, two severe V-shape notched fractured zones are visible, as shown in Figure 3.23. One of them is located at the left shoulder of the tunnel, while

the other is at the right knee. The location for the EDZ results from a combination of compressive stress concentration around the tunnel wall and the lower strength of bedding planes. The slippage between the layers causes shear fractures forming along the bedding plane and local stress perturbation, which subsequently induces large displacements towards the tunnel in the direction perpendicular to the layering. The large displacements perpendicular to the bedding planes along the tunnel wall cause strain-driven fractures in the layers and a release of confinement stress. An inner and outer EDZs can be observed in Figure 3.23. Bossart et al. (2002) observed through boreholes that the inner zone is characterized by massive, interconnected fractures inside a notch that contains both Mode I and Mode II fractures. Meanwhile, the interconnected fracture network is connected to the tunnel. Within the outer zone, there are only a few Mode II or Mode I fractures and these fractures are generally not interconnected to the inner zone. Based on this, an inner and outer EDZs can also be observed in Figure 3.23 and the size of the inner EDZ is approximately $0.4D$ using visual inspection of Figure 3.23. The size of the EDZ is approximately $0.82D$ away from the tunnel wall. According to Garitte and Vietor (2012), the simulation value closes to the field value obtained by water pressure measurement on Full-scale Emplacement tunnel, with an EDZ distance of 2.8m ($0.92D$) away from tunnel walls.

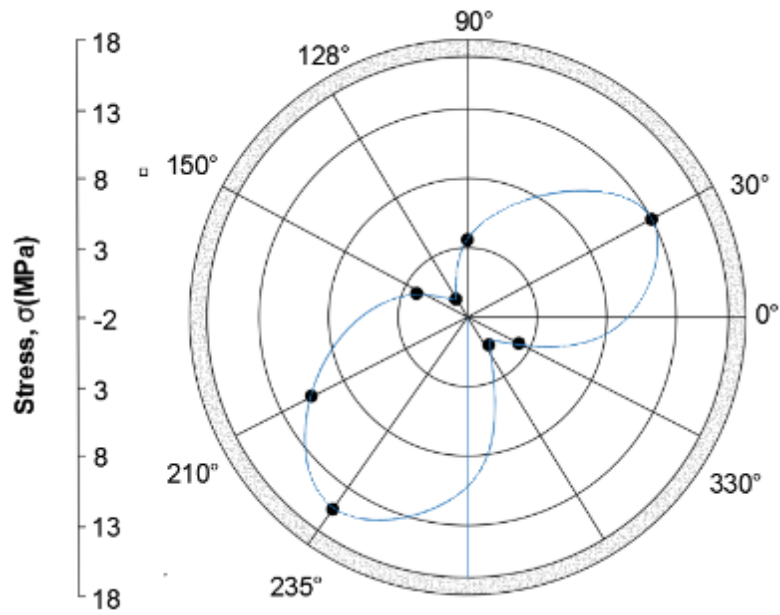
4) FEM and FDEM results comparison

Figures 3.24a and 3.24b respectively show the maximum principal stresses along the tunnel boundary in the FEM and FDEM models. In comparison, an isotropic medium created though FEM exhibits a stress distribution with minimum and maximum values of 6.5 MPa and 12.4 MPa , respectively, as depicted in Figure 3.24c. There is a significant impact of the transversely isotropic elastic properties of shale on the stress

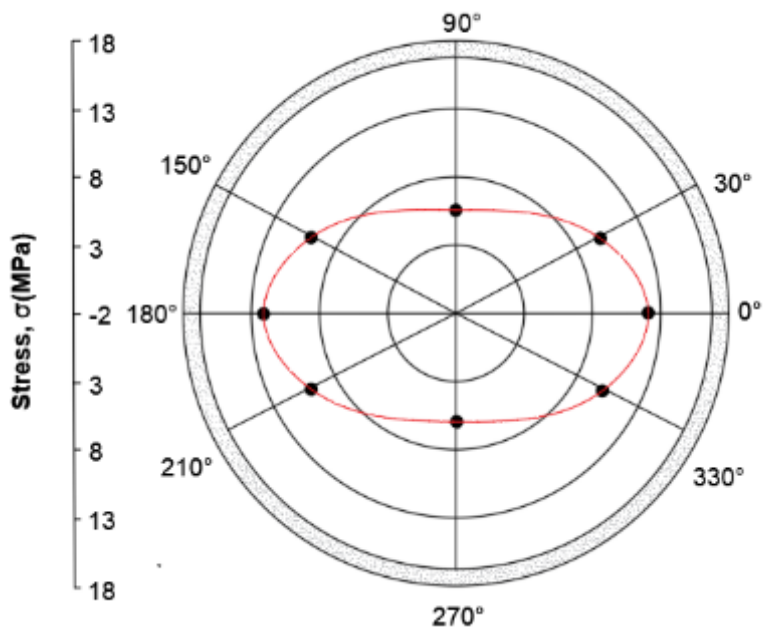
fields in both FEM and FDEM models (Figure 3.24a and 3.24b). The FDEM model, however, has a more severe redistribution of the stress field than the FEM model. Although the maximum value of principal stresses in the FDEM model is 15.6 MPa, which is slightly higher than the value in the FEM model, 14.2 MPa, the minimum value in the FDEM model is negative, -1.9 MPa, as opposed to 4 MPa in the FEM model. As a result of fracturing incorporated into the analysis using FDEM, bedding plane slippage causes a sharp reduction of stress with low to moderately negative values around the right shoulder and the left knee where bedding plane slippage occurs.



a) FEM



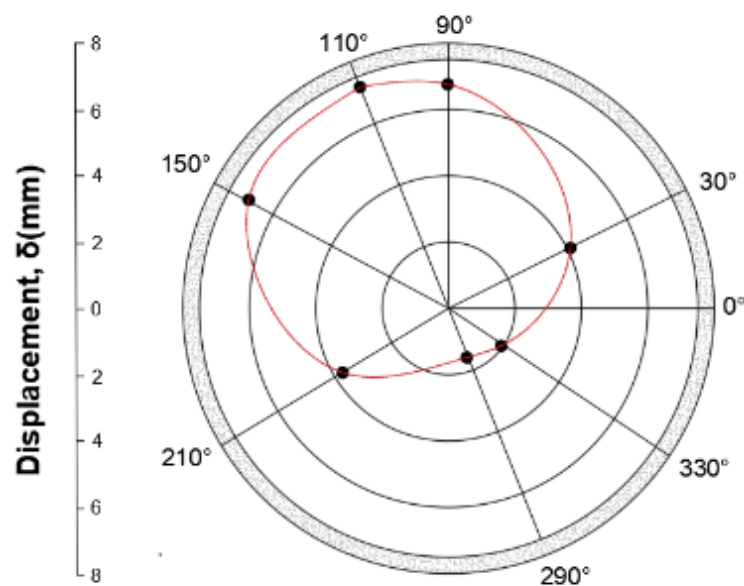
b) FDEM



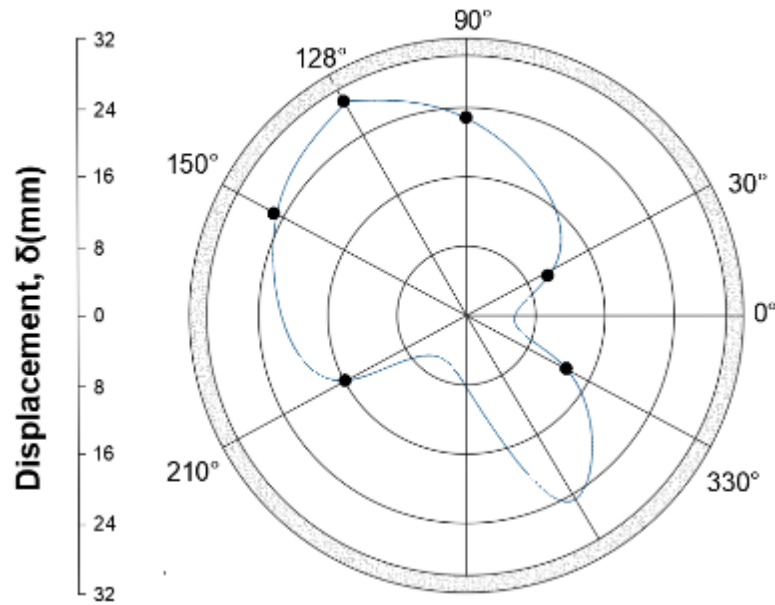
c) Isotropic medium in FEM

Figure 3.24 The FEM and FDEM Full-scale Emplacement tunnel models simulated maximum principal stresses along tunnel boundary, comparing to isotropic medium in FEM.

According to section 3.4.5, the displacement values obtained using the FEM model are significantly lower than the field values, which indicates that linear elasticity deformation isn't the primary cause of rock movement. Plastic deformation occurs near the tunnel wall during tunnel excavation in the FDEM model. The rock mass experiences large displacements as a result of slippage along the bedding planes. According to Figure 3.25, the maximum displacement in FEM is 7.7mm and in FDEM is 30.2mm. In FDEM, the total displacements around the circumference of the tunnel wall are generally three to four times bigger than those obtained in FEM. According to field data, the total displacement of the tunnel wall crown is around 21.8 mm, which is close to the value, 21-22 mm, obtained from the FDEM simulations (Lisjak et al., 2015).



a) FEM



b) FDEM

Figure 3.25 The total displacement along the tunnel boundary in FEM and FDEM models.

Post-support displacements have been determined from the FEM and FDEM models at five points across the tunnel circumference (i.e., T1 – T5) at the outside of the tunnel wall. The locations of these five points coincide with those of the field monitoring. In comparison with the post-support displacement of the tunnel crown from the field measurements, the FEM model significantly underestimates the displacement as shown in Figure 3.26. In the meantime, the FDEM model captures the response at T1 and T2 well, within an approximately error of 2 mm to the average field values. The displacement of T3 and T5 is less than the average field value by approximately 5 mm and 7 mm respectively, but is close to the lower bound of the measurements for T3 and T5, respectively. The displacement of T4 is underestimated by approximately 18 mm compared to the average value in the field. The difference between the simulated data and data obtained from field monitoring can be explained, in parts, by the

heterogeneity of the excavation environment, which cannot be captured by a homogeneous model. It is also possible that the discrepancy could be explained by a localised material weakness near T4 (such as a fault zone) in the field experiment. Meanwhile, the results of the current model match the results by Lisjak et al. (2015) for points T1 and T5, whereas T2 and T3 differ by approximately 3mm. The difference between the results for the current model and that used by Lisjak et al. (2015) for point T4 is approximately 9mm. These difference could be due to a different reduction of the magnitude of Young's modulus in the core soil during exaction in the FDEM model and different supporting parameters.

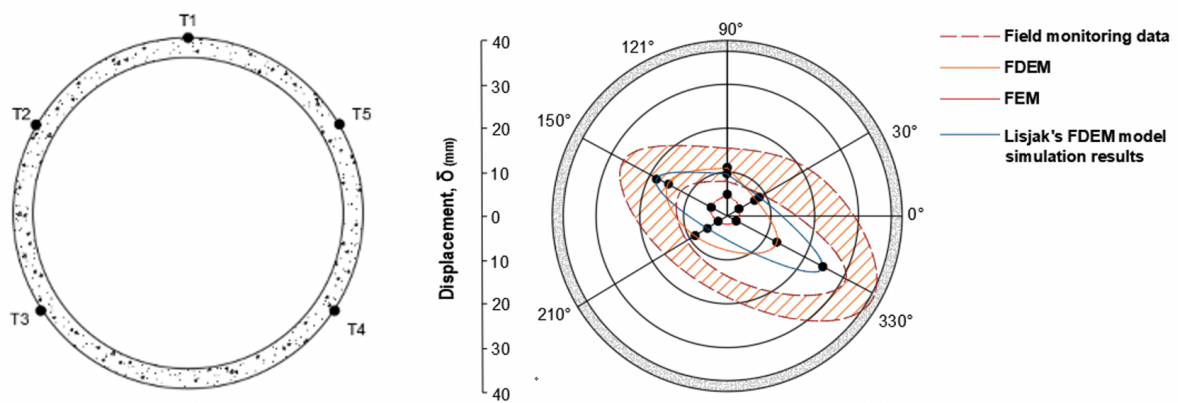


Figure 3.26 Post-support displacement around the tunnel boundary of five monitoring points in FDEM, comparing with FEM, field data and predictions from Lisjak's (Lisjak et al., 2015) (Orange area indicates the range of variation of the correspondent field measurements at the five points).

3.5 Summary

This chapter discussed the methodology applied to develop the FDEM models using both laboratory data and field data. Initial results were presented which were used to develop the appropriate properties of the material as well as model settings.

The fundamental principles of FDEM and creating shale model in ABAQUS were discussed. This research developed a code through Python to fix the problem of ABAQUS not allowing freely inserting multiples cohesive elements into the FEM domain. The conception of inserting cohesive elements in ABAQUS through Python was illustrated.

Meanwhile, both laboratory scale and field scale models were verified. Shale FDEM model mechanical strengths matched laboratory test data within a relative error of 5%. The field scale FDEM model showed it can capture the large displacements in surrounding rock caused by localized shearing fracturing failure along the bedding planes. The FDEM results of the total deformation of the tunnel crown are well-matched with the field observations. In the meantime, the post-support displacements at the crown and left shoulder of the tunnel wall match field data satisfactorily. In contrast, the displacements at the other three post-support points (left knee, right knee, right shoulder) are underpredicted, possibly due to the nonhomogeneous rock mass in the field. A FEM model was also created, but it became clear that it significantly underpredicts the deformation of the rock mass measured in the field and hence will not be taken forward.

CHAPTER 4 THE STUDY OF SHALE ANISOTROPY FROM MICRO CRACK LEVEL BASED ON FDEM SIMULATION

4.1 Introduction

In Chapter 3, small-scale shale laboratory models have validated the effectiveness of FDEM by quantitatively reproducing the short-term macro mechanical strengths of Longmaxi shale in laboratory tests (i.e., uniaxial compression strength (UCS) tests and Brazilian disc (BD) tests). Under the effects of bedding plane inclinations, Longmaxi shale's mechanical strengths (i.e., uniaxial compressive strength, Young's modulus, and tensile strength) show significant anisotropy. In Chapter 2, it is discussed that most previous studies focused on the macro mechanical properties of shale anisotropy through conventional laboratory tests, however, the understanding of macro strength from microscopic level remains an open book. Meanwhile, brittleness has been used by researchers to evaluate the failure conditions of rocks. Under shale anisotropy, shale fracturing behaviour changes, which naturally affects brittleness, but this has been overlooked. Hence, this chapter provides the results and discussion of the shale anisotropic effects on its mechanical behaviours from micro crack level, in terms of fracturing mechanism, fracturing behaviours and brittleness, based on the validated laboratory scale FDEM models in Chapter 3. The following sections (section 4.2, 4.3 and 4.4) show the results of the mechanical responses (i.e., failure mode, number of fractures and brittleness) of the validated shale UCS test models with bedding inclinations of 0° , 15° , 30° , 45° , 60° , 75° and 90° .

Meanwhile, the effects of shale layer thicknesses on shale anisotropy are also discussed in section 4.5.

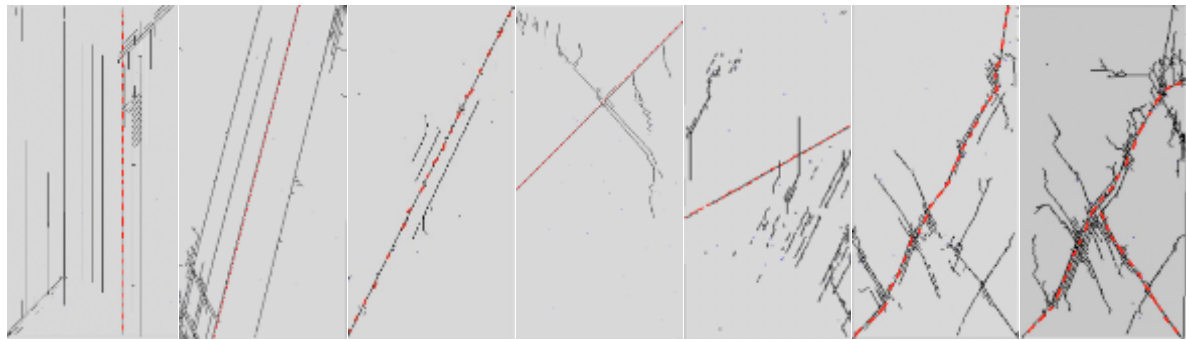
4.2 Shale failure modes with anisotropy

4.2.1 Failure behaviour of shale in Uniaxial Compression Strength (UCS) test simulations

Wang et al. (2020) collected 14 Longmaxi cylindrical specimens from Chongqing, China, with diameters of 50mm and lengths of 100mm. The specimens were prepared in seven directions to have seven different bedding inclinations (i.e., 0°, 15°, 30°, 45°, 60°, 75° and 90°). Two specimens were tested at each inclination angle. As discussed in section 3.3.1, the FDEM UCS models (i.e., two-dimensional 100 mm x 50 mm rectangular modes) with different bedding inclinations (i.e., 0°, 15°, 30°, 45°, 60°, 75° and 90°), corresponding to the laboratory test samples, are created. All models averaged elements size, loading rates, adopted elastic elements and cohesive elements parameters (see Table 3.1) were the same as used for the validated UCS shale model with bedding planes inclination of 0° and 90°.

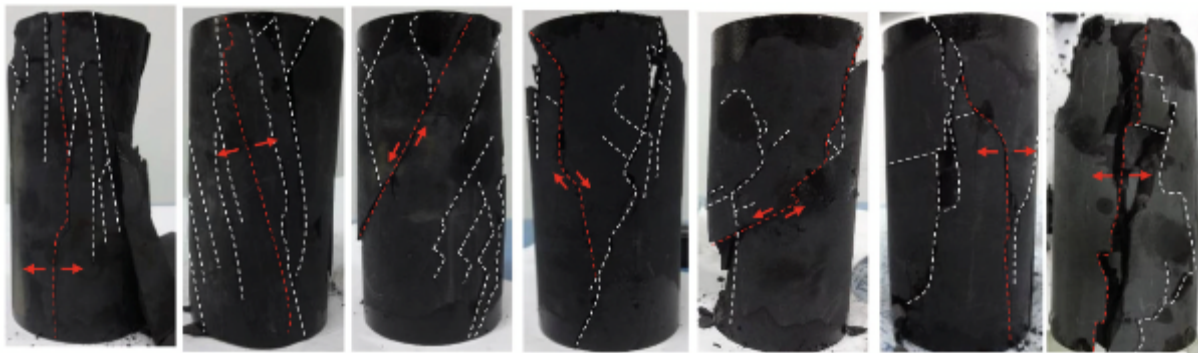
The microscopic fracturing response of the Longmaxi shale observed in the FDEM model and experimental tests (Figure 4.1.a,b) highlights a distinct variation in the failure patterns depending on the bedding plane inclination. As shown in Figure 4.1 (a and b), the failure modes of the shale with different bedding plane inclinations can be classified into three distinct modes, with transition phases between these modes. For shale with larger bedding plane inclinations (90° and 75°), the failure of the shale is caused by tensile splitting (T-S) along the bedding planes. Multiple tensile fractures developed through the bedding planes, while some shear fractures formed between the layers. For plane inclination values from 30° to 60°, the failure mode of the shale involved bedding plane delamination (B-D). This generally involved two major types of fractures: major fractures shearing along the bedding plane and tensile fractures

forming perpendicular to the shearing fractures. For shale with bedding plane inclinations from 0° to 15° , the specimens failed due to cracks shearing through the rock matrix (S-M).



$\theta=90^\circ$ $\theta=75^\circ$ $\theta=60^\circ$ $\theta=45^\circ$ $\theta=30^\circ$ $\theta=15^\circ$ $\theta=0^\circ$

a)



$\theta=90^\circ$ $\theta=75^\circ$ $\theta=60^\circ$ $\theta=45^\circ$ $\theta=30^\circ$ $\theta=15^\circ$ $\theta=0^\circ$

b)

Figure 4.1 Comparison of failure patterns during UCS test on Longmaxi shale between FDEM models and experimental samples a) model analysis and b) laboratory results (Wang et al., 2020) (the red lines highlight the main failure fractures to distinguish failure mode).

The identified failure modes among shale models with various bedding plane inclinations can assist in understanding shale mechanical anisotropy. When the shale is in the T-S mode, the fractures extend along the bedding planes. The tensile splitting of the failed shale specimen leads to circumferential expansion. In this case, there is a small deformation along the vertical axis of the specimen indicating that shale under T-S has larger elastic modulus values. For shale in the B-D failure mode, shale models tend to shear along bedding planes. This plane works as the weakest plane in the shale, which results in the lowest uniaxial compressive strength values, as shown in Figure 3.14a, section 3.3.3. This observation agrees with the conventional Coulomb-Navier theory that the weakest plane for shale under compression is approximately given by equation Equation 4.1 (Jaeger, 1960).

$$\alpha = 45^\circ - \frac{1}{2}\phi \quad \text{Eq.4.1}$$

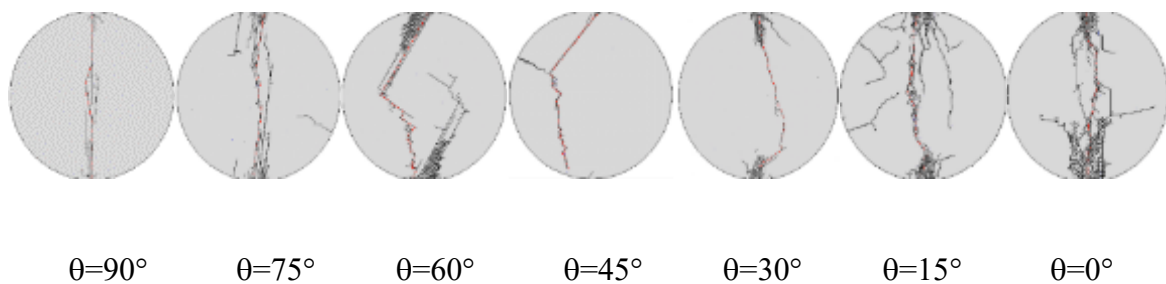
where ϕ is the rock internal friction angle and α is the angle between the failure plane and the maximum principal stress. Based on the equation and adopted parameters for Longmaxi shale, α is approximately 27° . It is close to the lowest uniaxial compressive strength measured in both the laboratory and simulation tests for shale samples with bedding plane inclinations of 30° .

Due to the change in failure mode from T-S to B-D, the shale specimens show more axial deformation, which indicates a smaller elastic modulus, as shown in Figure 3.14b, section 3.3.3. When the shale is in the S-M mode, the strength of the shale matrix plays a dominant role in controlling the failure strength of the shale specimens as the fractures form inside of the matrix. In this case, the shale failure strength in the S-M mode is larger than those for the other two modes. However, the S-M mode allows the shale specimens to have larger plastic deformation along the vertical axis of the

specimen; consequently, the S-M mode has the smallest elastic modulus, comparing with other two failure modes.

4.2.2 Failure behaviour of shale in Brazilian Disc (BD) test simulations

A set of test experiments on Longmaxi shale with different bedding planes inclinations (i.e., 0° , 15° , 30° , 45° , 60° , 75° and 90°) carried out by Ma et al., (2018), was used to validate the macroscopic strength results of the FDEM BD test model developed in Chapter 3. The failure modes of all the FDEM models' analyses and experimental tests are displayed in Figures 4.2.a, and 4.2.b, respectively. Three different modes can be distinguished from the results, which indicates that the shale bedding plane inclination significantly influence the anisotropic strength of shale. As shown in Figure 4.2 (a and b), the three different failure modes can be described as: 1) central spilt along the bedding planes (C-S) when $\theta = 90^\circ$ and 75° ; 2) inclined arch fracturing (I-A) when $\theta = 60^\circ$, 45° and 30° ; 3) central arch fracturing (C-A) with branches when $\theta = 15^\circ$ and 0° . The ranges of θ between these classified modes show transitional fracture patterns with no clear threshold between the modes.



a)

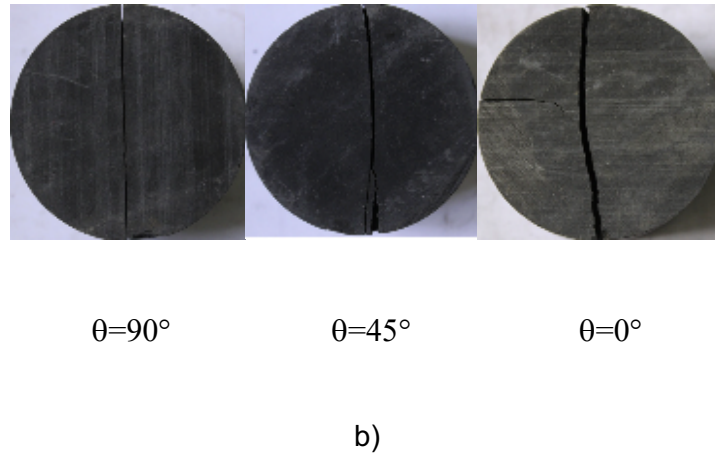


Figure 4.2 Comparison of the failure patterns during BD tests on Longmaxi shale a) FDEM model results and b) experimental test specimens (Ren et al., 2021).

Similarly, to the UCS test, the identified failure modes among the shale models with various bedding plane inclinations can assist in understanding shale mechanical anisotropy. When the shale is in the C-S failure mode, fractures are mainly formed through the shale matrix, which leads to a greater tensile strength than other modes (Figure 3.16). With an increase in bedding plane inclination, more fractures form along the bedding planes as these provide weaker pathways for the fractures to propagate. In turn, the tensile strength of the shale decreases gradually, as shown in Figure 3.16.

4.3 Shale brittleness with anisotropy

To further understand the behaviour of fracturing in shale under the influence of anisotropy, brittleness was adopted as one of the important parameters to evaluate frac-ability in rock.

4.3.1 The adopted conventional brittleness indices in this study

Researchers have proposed different BIs based on different characteristics of rock brittleness since there is no definition of brittleness. These BIs are mainly based on

rock strength, stress-strain curves, energy balances, and components analysis. Due to the fact that they only focus on some properties of brittleness, all of these BIs have their limitations. For example, strength and strain BIs only consider a few characteristics of the shale, their results can be contradictory in some cases (He et al., 2021). In the case of rock types with the same strength, different displacements would result in different rock brittleness values based on different equations for BI (Hucka et al., 1974). In this case, to evaluate the brittleness of shale, this research adopted several published BIs based on available values obtained from UCS tests and BD tests (Table 4.1).

Table 4.1 Adopted Brittleness indices in this research (Hucka and Das, 1974)

Approaches	Formulae	Notes
Strength parameters	$BI_1 = \sigma_u / \sigma_t$	σ_u = uniaxial compressive strength, σ_t = Brazilian tensile strength
Stress-strain curves	$BI_2 = \varepsilon_e / \varepsilon_t$	ε_e = elastic strain, ε_t = total strain at failure
Energy balance analysis	$BI_3 = U_{et} / (U_{et} + U_p)$	U_{et} = total elastic energy, U_p = plastic energy

Two phases can be distinguished in the evolution of the energy in a stress-strain curve: the pre-peak phase and the post-peak phase, as mentioned in section 2.2.4. Fractures within a shale model before macro-failure is discussed in this research, which is

essential in understanding fracture formation and propagation during the pre-peak phase in UCS test. Through the stress-strain curve (and more specifically the area under the stress-strain curve), Figure 4.3 illustrates the pre-peak phase of the rock's energy evolution. Two parts of energy evolution can be distinguished before reaching the uniaxial compressive strength of rock (point C). During elastic deformation, rock materials absorb external energy and store it as elastic energy. Upon reaching point A (Figure 4.3), where fractures are starting to yield in the rock, some of the energy absorbed dissipates because of internal damage. The stress-strain curve reflects the detectable plastic deformation due to internal damage such as fracture formation, propagation, and friction between particles. As illustrated in Figure 4.3, the black area represents the elastic energy stored in the rock before macro failure, which would be the source of energy for the post-peak rock failure. Meanwhile, the grey area indicates the plastic energy that has been consumed by internal damage.

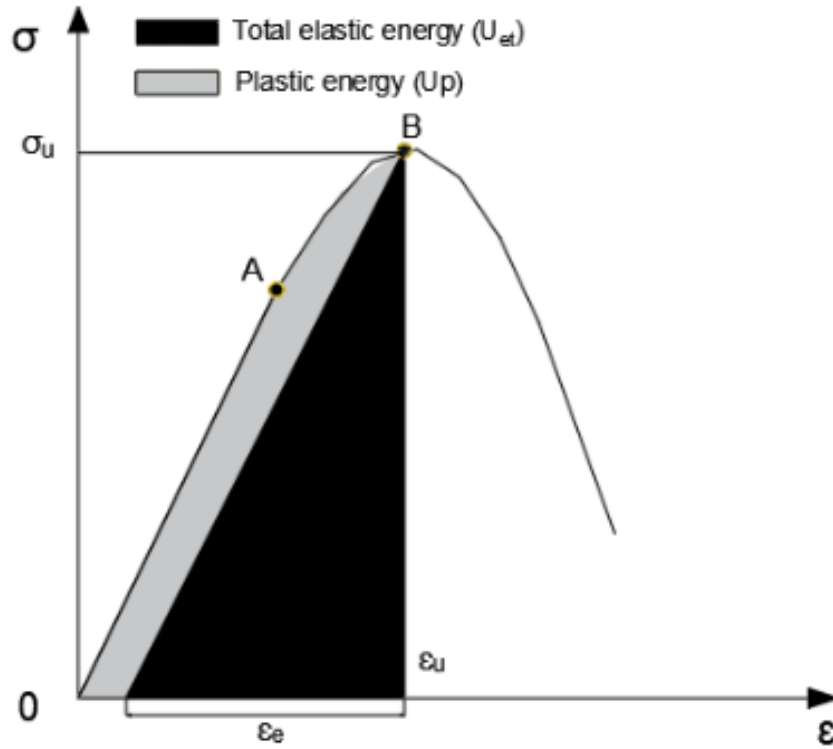


Figure 4.3 The energy evolution of rock during UCS test (Point A: crack damage stress (CD), Point B: uniaxial compressive strength, ε_e is the elastic displacement before peak strength, ε_u is the total displacement at peak strength and σ_u is the peak strength).

Equation 4.2 calculates the elastic energy U_{et} based on Figure 4.3.

$$U_{et} = \frac{1}{2E} \sigma_u^2 \quad \text{Eq.4.2}$$

Where E is the Young's modulus of the rock, and σ_u is the uniaxial compressive strength.

In addition, Equation 4.3 gives the total energy U_t based on Figure 4.3.

$$U_t = \int_0^{\varepsilon_u} \sigma d\varepsilon \quad \text{Eq.4.3}$$

Hence, the equation of brittleness index Bl_3 from Table 4.1 can also be written as:

$$Bl_3 = \frac{\sigma_u^2}{2E \int_0^{\varepsilon_u} \sigma d\varepsilon} \quad \text{Eq.4.4}$$

4.3.2 Analysis of conventional brittleness indices for Longmaxi shale

Brittleness indexes have been commonly used in previous research to characterize the relative behaviour of materials based on the stress-strain curve obtained from a conventional UCS test or triaxial compression test (Hucka and Das, 1974 and Li et al., 2017). To evaluate the brittleness of Longmaxi shale, Bl_2 and Bl_3 (from Table 4.1), based on the stress-strain curve before the pre-peak phase, have been applied.

According to Equations 4.2 and 4.4, the value of energy absorption can be derived from the stress-strain curves of different shale models' analyses with different bedding plane inclinations as shown in Figure 4.4. Figure 4.4 depicts the absorbed pre-failure energies for each shale UCS test model with different bedding plane inclinations. Figure 4.4 indicates that the energy absorption in shale shows anisotropic properties with bedding plane inclination. The shape of the curve between the energy absorption and the bedding plane inclination is the same as the uniaxial compressive strength (i.e., Figure 3.14a) , which is a 'U' shape. According to Equations 4.2 and 4.4, the uniaxial compressive strength significantly affects energy absorption. Initially, the absorbed energy decreases as the bedding plane inclination increases from 0° to 60° which is expected because the failure mode changes from S-M to B-D. As discussed in the previous section, the failure of a shale model in S-M is shearing through the rock matrix, while B-D is shearing along bedding planes. Due to the low mechanical properties of the bedding planes, the energy required in B-D failure mode is smaller than that in S-M. Once damage occurs along the bedding plane, fractures form and propagate quickly, which leads to smaller plastic deformations and lower

energy dissipation. After the value of the absorbed energy reaches a minimum value at 60°, it starts to increase with increasing bedding plane inclination as the results of the failure mode changed from B-D to T-S. In comparison to shale models that shear along a single bedding plane in B-D mode, shale models are experiencing multiple tensile cracks fracturing along bedding planes. The significant increased number of fractures in T-S mode naturally need more energies to fracturing, comparing to B-D.

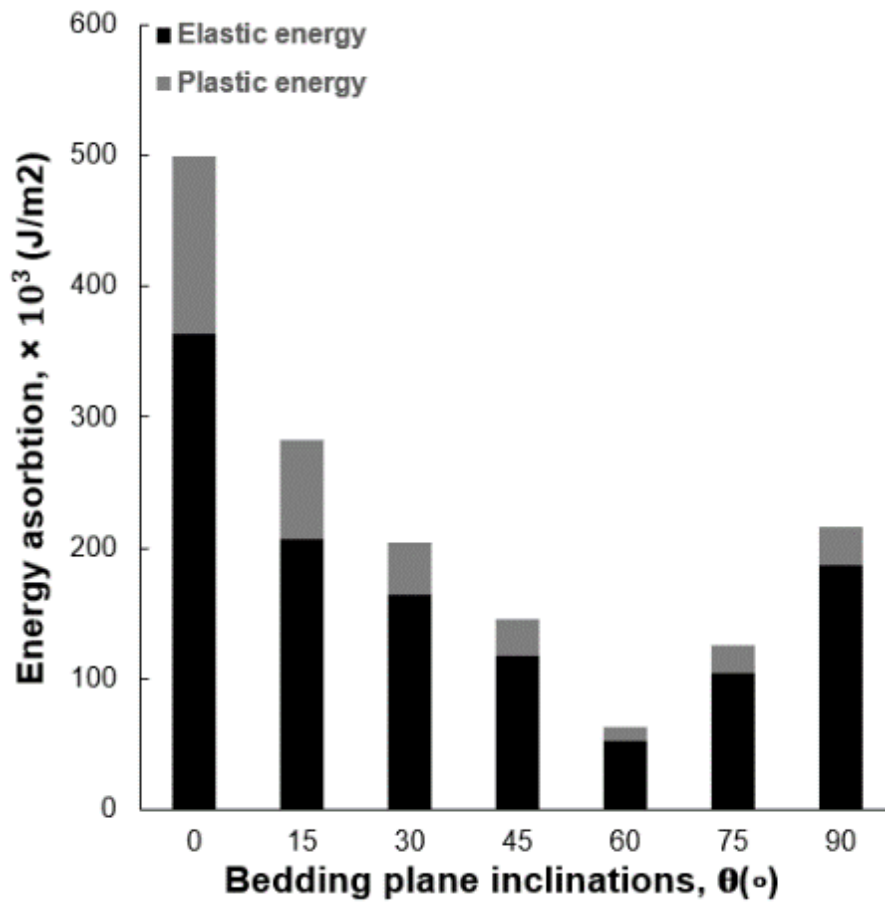


Figure 4.4 The absorption of energy pre-failure.

Figure 4.5 shows the variation of conventional brittleness indices, in terms of Bl_{2-S} , Bl_{2-E} , Bl_{3-S} and Bl_{3-E} , with different bedding plane inclinations. Simulation-derived Bl_{2-S} and Bl_{3-S} brittleness indices for Bl_2 and Bl_3 are compared with experimental-derived Bl_{2-E} and Bl_{3-E} brittleness indices for Bl_2 and Bl_3 (Wang et al., 2009 and Wang et al., 2020).

As shown in Figure 4.5, Bl_2 and Bl_3 show similar experimental and simulation results. The curves of Bl_2 and Bl_3 indicate that the bedding plane inclinations have a large influence on the brittleness of shale. For Bl_2 and Bl_3 , the brittleness index of the three modes in magnitude order is: T-S > B-D > S-M. When the inclination of the bedding increases from 0° to 30° , the failure mode changes from shearing through the shale matrix (S-M) to bedding plane delamination (B-D). As the shale matrix mechanical property is stronger than bedding plane, shale in the S-M mode can provide enough plastic deformation, which leads to more energy dissipation. As the fractures propagate more easily along the bedding planes, the shale will become more brittle. Therefore, the brittleness in the B-D mode is larger than in the S-M mode. In contrast, compared to splitting, shear failure tends to occur by slippage along the bedding plane, which allows for larger plastic deformation and lower brittleness. Overall, the brittleness values of the three failure modes of shale with different bedding plane inclinations are in the order of: T-S > B-D > S-M.

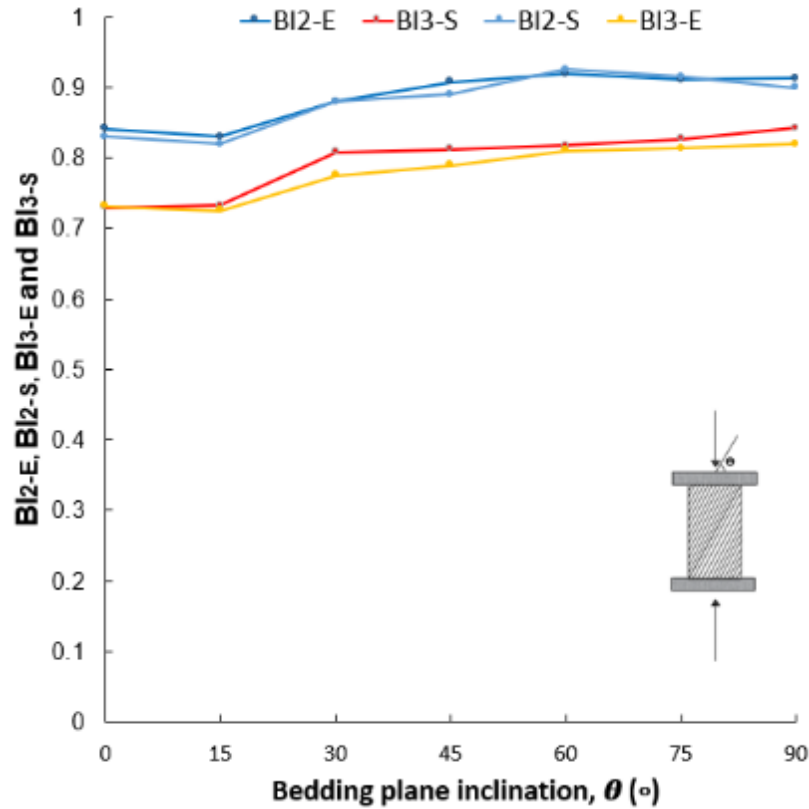


Figure 4.5 Variation in brittleness indices (BI_{2-E} , BI_{2-S} , BI_{3-E} and BI_{3-S}) with bedding plane inclination (Subscripts S and E refer to simulation and experiment respectively).

4.3.2 New proposed brittleness indices

1) A new brittleness index based on fracture numbers (BI_f)

During the energy dissipation of the pre-peak phase, a proportion of the energy is consumed by fractures forming and propagating. According to previous research, it is assumed that rock materials with higher values of brittleness are more prone to form fractures (Cotterell and Rice, 1980). The number of fractures generated inside the FDEM models before macro-failure for different bedding plane inclinations are shown in Figure 4.6. In ABAQUS FDEM models, fracture counts are derived from field output data on the status of cohesive elements.

The largest number of fractures formed in the shale with a bedding plane inclination of 90° , while the shale with a bedding plane inclination of 60° has the smallest value. From the brittleness index, shale with a bedding plane inclination of 0° has the smallest index, however it has formed large number of fractures. This can be explained by the energy dissipation. From Figure 4.4, the shale with a 0° bedding plane inclination has consumed the largest energy due to the internal damage, which is due to the large plastic deformation. However, even though the value of energy dissipation at 0° is approximately 4 times larger than at 90° , the number of fractures that are formed is similar. It is understood that fracturing within the matrix needs more energy than failure along bedding planes, and multiple fractures tend to form at the same time along the bedding planes in the T-S failure mode. Thus, although the shale with plane inclinations of 0° and 15° have larger plastic energy compared to 75° and 90° , the number of fractures is smaller. Meanwhile, shale in the B-D failure mode tends to form and propagate along one or limited number of bedding planes, which leads to a smaller number of fractures. Overall, the number of total fractures formed inside the shale for the three failure modes are in the order: T-S > S-M > B-D. Meanwhile, the number of fractures forming along the bedding plane (COH2) is bigger than fractures in the shale matrix (COH1) in T-S failure mode, as shown in Figure 4.6. As the fractures mainly form and propagate along the bedding plane in shale with bedding plane inclinations of 60° , COH2 occurs most frequently compared to other bedding plane inclinations. Fractures tend to form inside the matrix as the bedding plane inclinations decrease, which leads to an increasing frequency of COH1. As a result, the S-M failure mode consumes more energy than the other two failure modes.

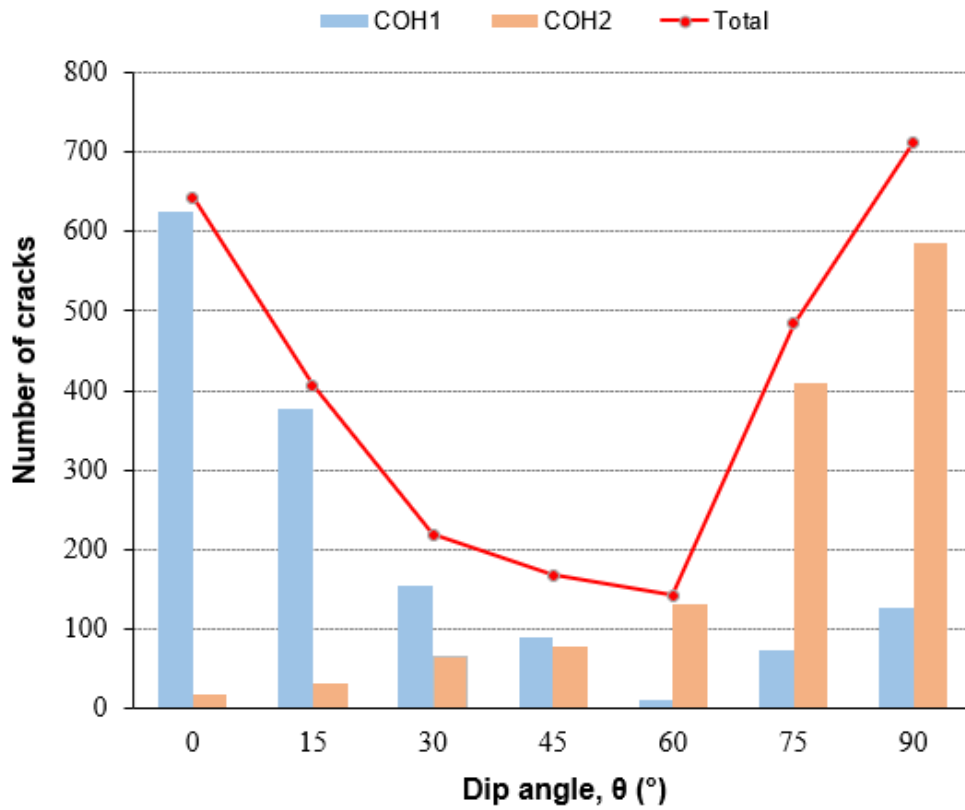


Figure 4.6 Failed cohesive elements inside the shale with bedding plane inclination.

Shale gas exploration industry have widely evaluated rock frac-ability to assess the ability of reservoirs to form fractures (Lu et al., 2022). However, there still is no general evaluation method to quantitative shale frac-ability. The brittleness of rocks is one of the properties that have been used to evaluate the fracturing ability of shale (Hucka and Das, 1974). Generally, it is believed that shale with a high brittleness is more easy to fracture (Sui et al., 2019). Yuan et al. (2013) proposed using rock fracture toughness to evaluate the frac-ability. On the other hand, Guo et al. (2013) assessed the fracture-ability of shale by examining multiple rock properties, including brittleness indices, fracture toughness, and mechanical parameters. However, fracture numbers in shale and fracture energies used to produce fractures were not considered when evaluating rock frac-ability in previous studies. Therefore, a new brittleness index BI_f is proposed in this study as defined in Equation 4.5:

$$Bl_f = \frac{M}{U_p} \quad \text{Eq.4.5}$$

where M is the total number of the fractures formed in the pre-peak phase, and U_p is the plastic energy. The details of the crack formation (e.g., fracture numbers) in the laboratory tests can be gained from X-ray computed tomography (CT) images and acoustic emission (AE) (Wang et al., 2016 and Zhai et al., 2020). This brittleness index indicates the number of fractures formed per unit of energy dissipation and the ability of the shale to transform energy into fractures. With a higher brittleness index indicating the shale is more likely to form fractures. Based on the total fracture numbers from Figure 4.6 and plastic energy from Figure 4.4, the Bl_f for different shale models with different bedding plane inclinations are obtained from Equation 4.5.

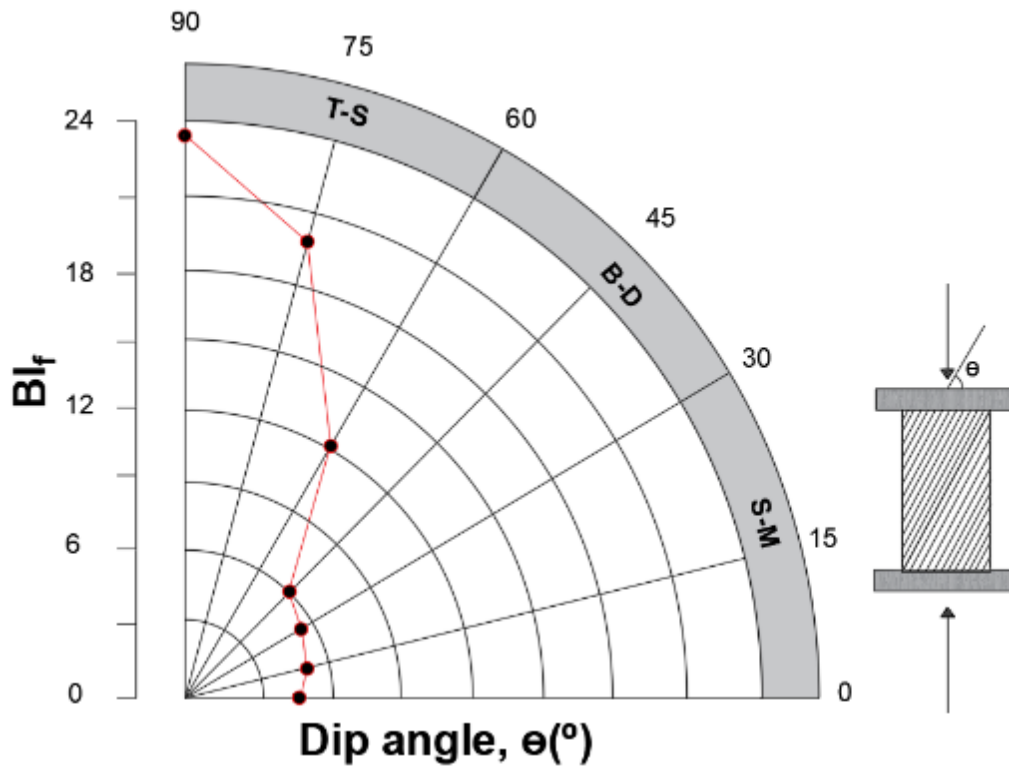


Figure 4.7 The variation in Bl_f with different bedding plane inclinations.

Figure 4.7 shows that as the bedding plane inclination increases, the Bl_f increases, and hence the number of the fractures formed per unit energy dissipation increases. The transfer of energy to fractures in the three failure modes of shale are in the order of: T-S > B-D > S-M.

In the three failure modes of the shale under different bedding plane inclination, the brittleness indexes Bl_2 , Bl_3 and Bl_f have revealed that the order of the brittleness for the three failure modes is T-S > B-D > S-M. Bl_f 's formula directly incorporates the number of fractures formed, which provides a more accurate analysis of the rocks' frac-ability than other conventional brittleness indices. In projects that are concerned about fractures after excavation, it can be used as an important parameter to evaluate rock frac-ability.

2) New brittleness index Bl_{CD} based on crack damage stress (CD)

The crack initiation stress (CI) is defined as the stress threshold at which cracks start forming and propagating, whereas the crack damage stress (CD) is defined as the stress level where cracks start to form unstably and coalesce into a major fracture. CI and CD have been accepted as significant parameters to evaluate the fracturing behaviour of rocks. As mentioned in section 2.2.2, Li et al. (2020) have found that the CD of shale is significantly affected by shale anisotropy. To continue investigating the fracturing behaviours of shale under the influence of anisotropy, the research has gathered CD of all shale models with different bedding plane inclinations based on the stress-strain curves of different shale models' analyses with different bedding plane inclinations as shown in Figure 4.8.

Figure 4.8 depicts that the CD for different bedding plane inclinations show a large variation, which indicates the CD is also sensitive to the bedding plane inclination. The

shape of the curve between the *CD* and the bedding plane inclination is the same as the uniaxial compressive strength (i.e., Figure 3.14a) , which is a 'U' shape. When the stress inside the shale reaches the *CD* under the UCS test, cracks begin to propagate inside the shale. They may propagate along the bedding planes, cross the bedding plane, or even stop propagating, which depends on the bedding plane inclination. Different crack paths lead to different strains and stresses within the shale. As a result, the failure modes of shale models with different bedding plane inclinations may affect the final emergent strength (i.e., uniaxial compressive strength).

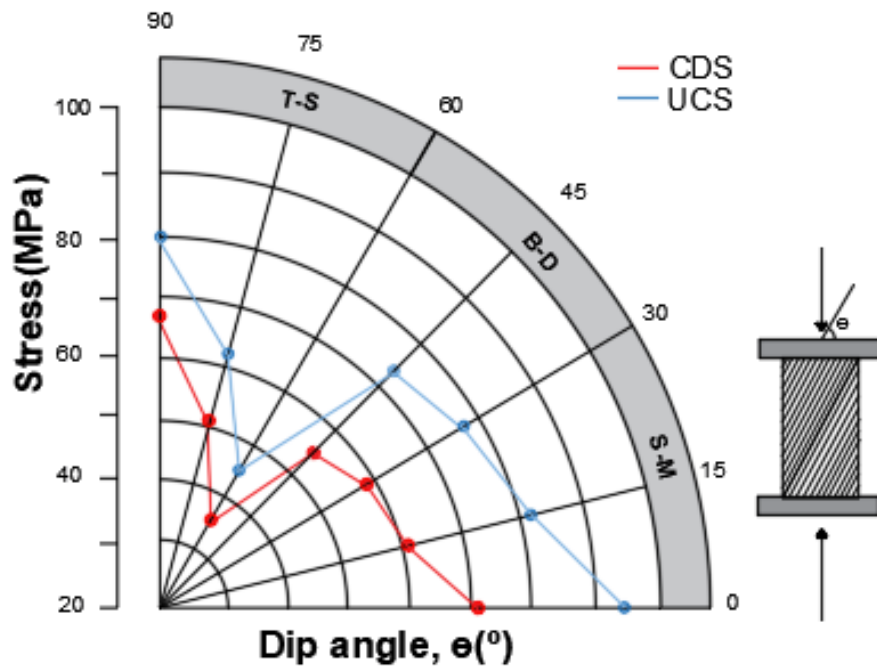


Figure 4.8 Uniaxial compressive strength and *CD* variation with different bedding plane inclinations.

Based on this observation, a new brittleness index, Bl_{CD} is proposed in this study as shown in Equation. 4.6.

$$Bl_{CD} = CD/\sigma_u \quad \text{Eq.4.6}$$

As with the other brittleness indices, the higher the value of Bl_{CD} , the more brittle the shale. The variation of Bl_{CD} based on the Longmaxi shale FDEM modelling with different bedding plane inclinations is shown in Figure 4.9. The order in which the failure takes place in the shale is T-S > B-D > S-M according to Bl_{CD} . With increasing bedding plane inclination, the Bl_{CD} increases, which agrees with Bl_2 , Bl_3 and Bl_f . This behaviour is due to brittle rocks having a smaller plastic deformation (Gong et al., 2022). The higher the value of Bl_{CD} , the quicker the rock reaches the σ_c after the threshold of CD with smaller plastic strains.

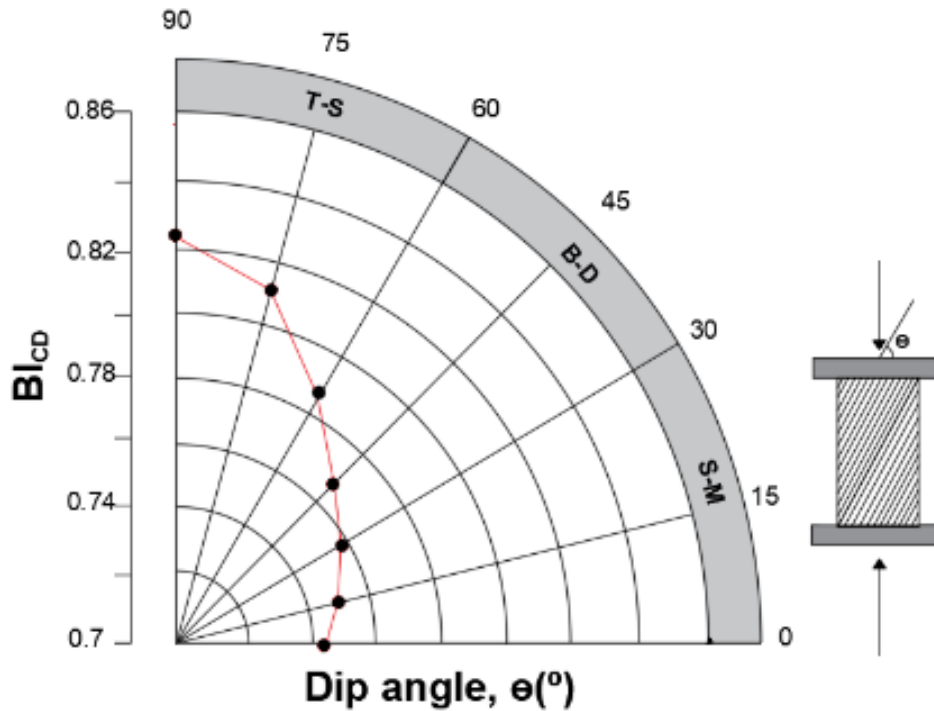


Figure 4.9 Variation of Bl_{CD} based on the Longmaxi shale FDEM models with different bedding plane inclinations.

4.4 New empirical relationship to predict minimum and maximum tensile stresses based on UCS test

Compared to the conventional brittleness index Bl_1 , which is based on the σ_u and σ_t ratio, Bl_{CD} is easier to obtain as it only requires the UCS test to be performed. To validate the accuracy of Bl_{CD} , values of Bl_{CD} collected from different rock types are plotted in Figure 4.10. The Bl_{CD} of different rocks illustrated in Figure 4.10 are obtained using Equation 4.6 with published values of CD and σ_u from the literature. It can be seen from Figure 4.10 that there is an apparent trend between Bl_{CD} and Bl_2 . Based on the rock data presented in Figure 4.10, there are minimum values of Bl_{CD} and Bl_2 of 0.58 and 6.47, respectively. Due to the ease of obtaining Bl_{CD} compared to other brittleness indices, it can be a useful way of predicting the brittleness of different rocks, including shales.

According to Figure 4.10, there is a relationship between the Bl_2 and Bl_{CD} . Bl_2 is the ratio between the σ_u and σ_t , while Bl_{CD} is the ratio between the CD and σ_u , which indicate that there is a relationship between the tensile strength and CD. As the data set contains 26 samples, it is a small sample size and thus should fit a t-distribution. The t-distribution confidence interval (CI) for the data set can be calculated using Equation 4.7.

$$CI = X_{mean} \pm t_c \bullet \frac{SD}{\sqrt{n}} \quad \text{Eq.4.7}$$

Where X_{mean} is the mean value of the data set, t_c value is the critical value of the data set, SD is the standard deviation of the data set, and n is the sample size. According to Figure 4.10, the mean value of the confidence interval (CI) for the data set is 0.52. and the standard deviation is 0.1. This project adopted a standard 99% probability as

the confidence level for the data set to ensure a high probability of the parameters' values. Using the t-value table, the t-value for 26 samples is 2.485 (Beyer, 2019). Based on Equation 4.7, the CI for the data set with a probability of 99% should be in the range of (0.47, 0.57). Hence, the relationship between the tensile strength and CD can be determined by:

$$\sigma_{tmin} = \frac{0.016\sigma_u}{\frac{CD}{\sigma_u} - 0.47} < \sigma_t < \sigma_{tmax} = \frac{0.016\sigma_u}{\frac{CD}{\sigma_u} - 0.57} \quad \text{Eq.4.8}$$

However, this empirical equation is based only on limited data collected in this paper and requires further improvement (e.g., experiments on various types of rocks, broader range of tensile strengths) to achieve a greater prediction accuracy and hence care is needed when using it outside the range.

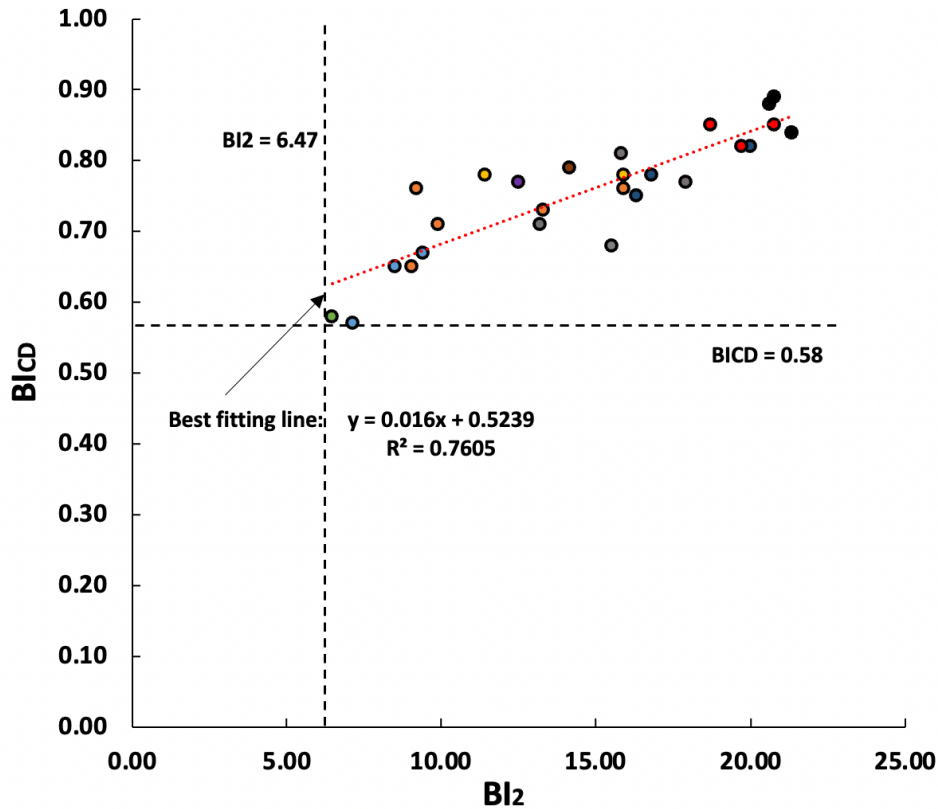


Figure 4.10 BI_{CD} vs. BI_2 for different rocks, including granite (red), shale (grey), limestone (orange), diorite (dark blue), siltstone (green), sandstone (blue), coal (yellow), marble (black) and quartzites (brown) (Xue et al., 2014, Cai et al., 2004, Ghasemi et al., 2020, Palchik and Hatzor, 2002, Li et al., 2020, Zhao et al., 2013, Modiriasari et al., 2017, Gatelier et al., 2002, Palchik, 2010, Wu et al., 2021, Taheri et al., 2020, Song et al., 2020a, Song et al., 2020b and Wang et al., 2016).

In Figure 4.11, the predicted tensile strength for the Longmaxi shale with different bedding inclinations using Equation 4.8 based on the average uniaxial compressive strength are compared with the experimental values, which shows that these are in line with the predicted range of tensile strength values, except for an inclination of 60° . Using the maximum experimental UCS value of the Longmaxi shale, with bedding planes inclined by 60° , Equation 4.8 predicts an upper limit tensile strength of 3.74 MPa, higher than the experimental value. Hence, the proposed empirical equation

works well in predicting the tensile strength of the rock using the uniaxial compressive strength. Considering that testing the tensile strength of rocks may be difficult under certain conditions, using an empirical relationship (Equation 4.7) to predict the range of the tensile strength of the rock may provide a useful alternative method.

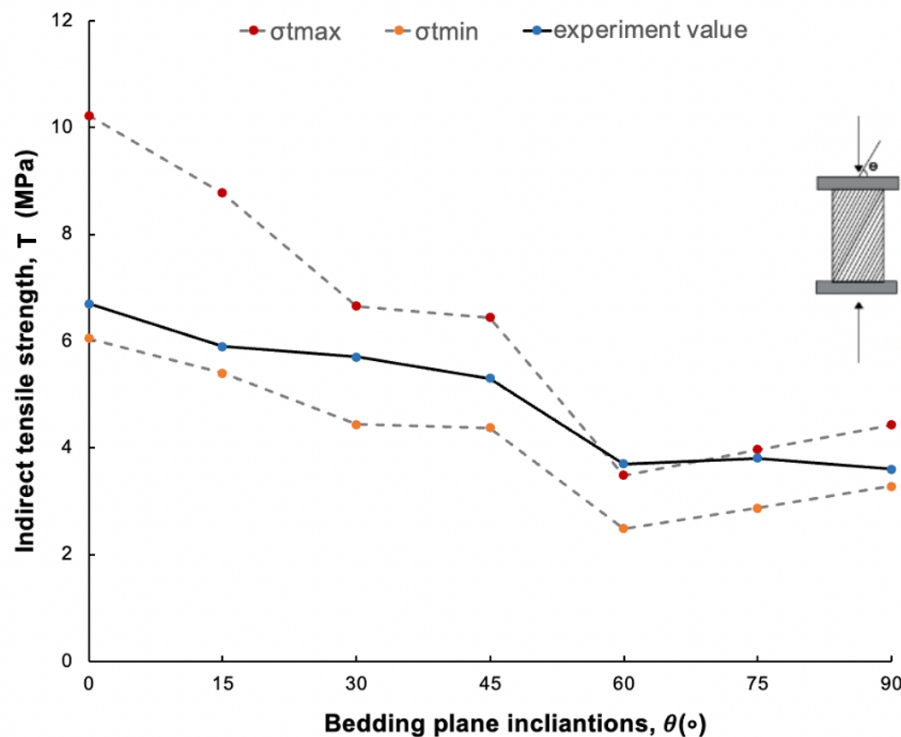


Figure 4.11 The comparisons between the predicted tensile strength for shale with different bedding plane inclinations using the empirical relationships and the experiment values (Ma et al., 2018).

4.5 Layer thickness effects on shale anisotropy

It is important to understand bedding layer thickness for the design and stability of underground constructions, such as mining, tunnelling, hydraulic fracturing, and nuclear waste disposal (Price and Cosgrove, 1990). The shale's mechanical properties and fracture mechanism are greatly affected by the presence of bedding planes. The effects of the fracturing behaviour on the mechanical strength of shale samples have

been discussed in section 4.2. Therefore, the number of bedding planes in the shale samples may affect the fracture mechanism by affecting the fracture paths during compression, which affects the mechanical properties. Lisjak et al., (2014b) have studied the layer thickness effects on the macro mechanical strength of shale through FDEM simulation. There is, however, no literature study that examines the effect of bedding layer thickness on its fracture mechanisms. To fulfil this knowledge, this research has created shale FDEM UCS test model with bedding plane inclinations of 0° , 45° and 90° in different layer thickness (i.e., 2.5mm, 5mm, 10mm, 17.5mm). These three angles are chosen to specifically represent three different failure modes (i.e., T-S, B-D and S-M). The average element size (0.8 mm) and loading rates for the model are same to the validated UCS shale model with bedding planes inclination of 0° and 90° . To ensure each layer is big enough for meshing elements, the smallest layer thickness adopted was 2.5mm. The adopted parameters for the elastic and cohesive elements are same to the UCS shale model with bedding planes inclination of 0° and 90° , as listed in Table 3.1, section 3.3.3. Figure 4.12 illustrates shale UCS model with bedding planes inclinations of 90° in different layer thicknesses.

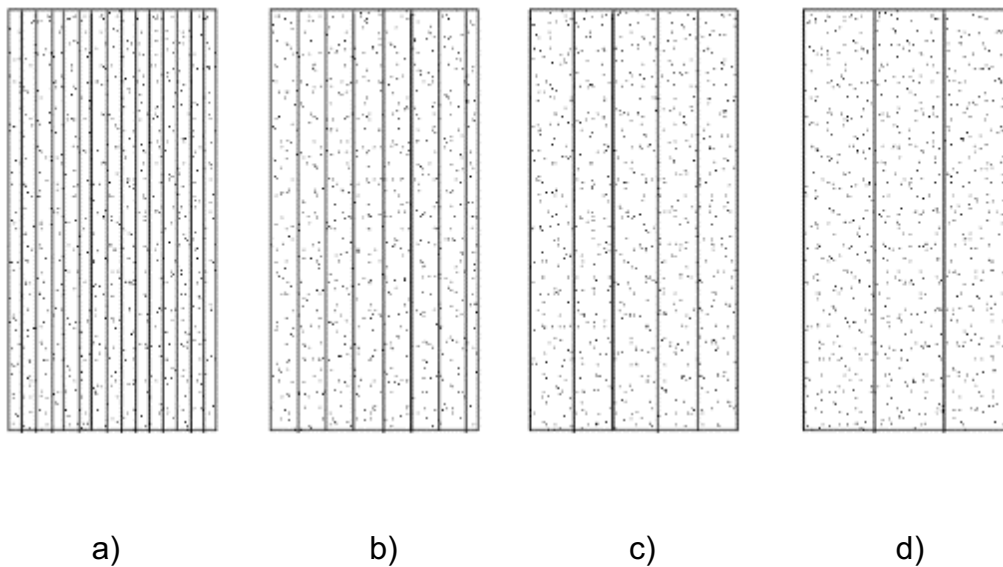
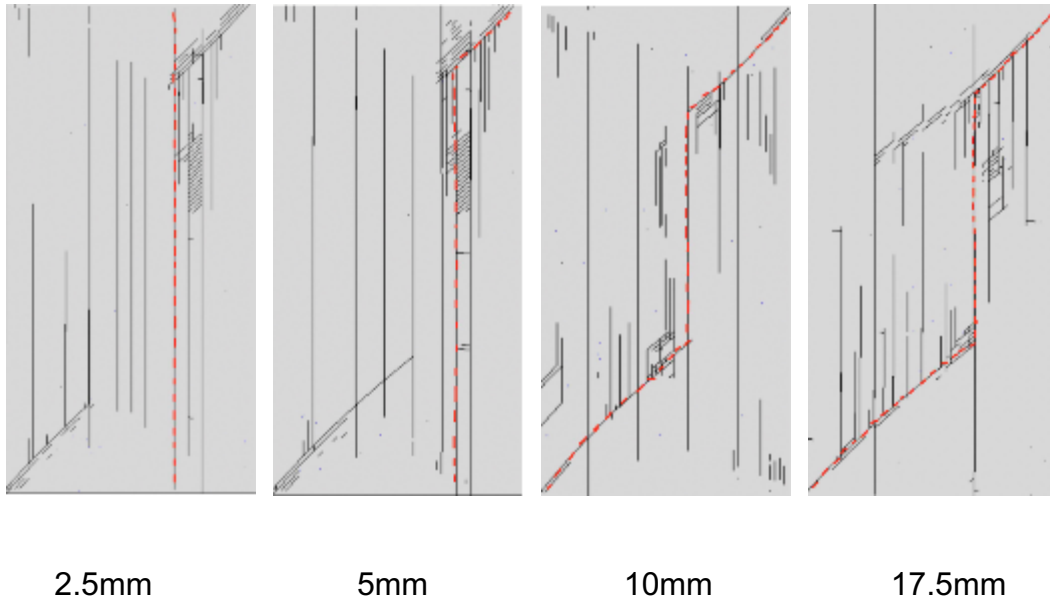


Figure 4.12 FDEM shale model with bedding planes inclination 90° bedding layer thickness of a) 2.5mm, b) 5mm, c) 10mm and d) 17.5mm.

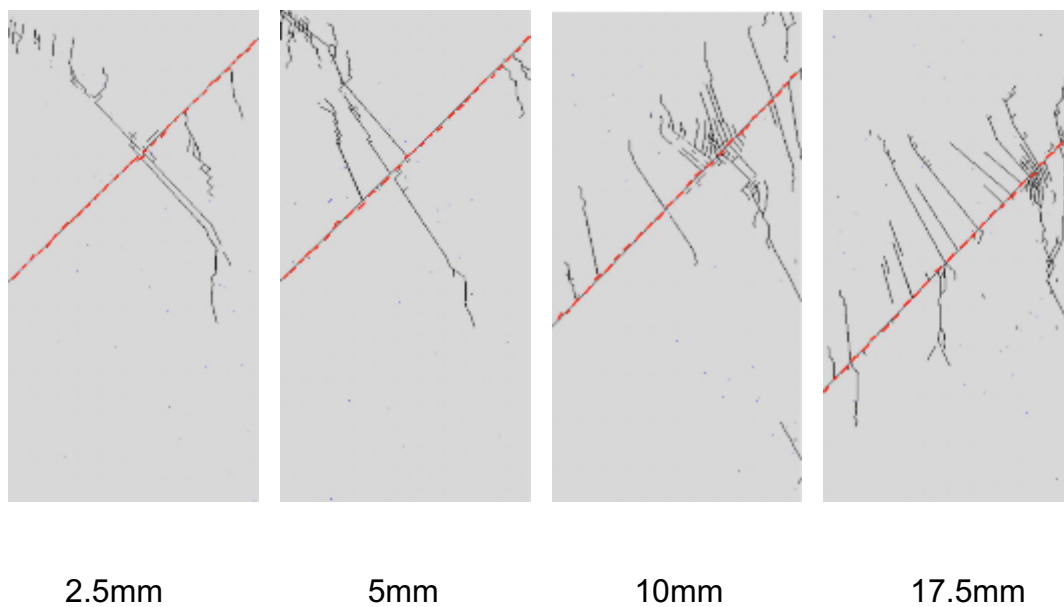
4.5.1 Failure modes

Figure 4.13 illustrates the effects of the bedding plane thickness on the failure modes of shale. Figure 4.13a shows that failure modes of shale with bedding plane inclinations at 90° differed from tensile splitting (T-S) to tensile splitting with shearing (T-S-S) as bedding plane thickness increased from 2.5mm to 17.5mm. With the increase of layer thickness, failure modes of shale with bedding plane inclinations of 0° and 45° remained unchanged, according to Figures 4.13b and 4.13c. With respect to shale with bedding plane inclinations of 0° and 45°, failure modes of shale with a bedding plane inclination of 90° are sensitive to the thickness of the bedding planes. As a result of the reduction of bedding planes, shale models in thick layers (10mm and 17.5mm) require shearing through the layers to cause macro-fractures until failure, whereas shale in thin layers (2.5mm and 5mm) loses its strength with multiple tensile fractures forming along the bedding planes. The figure illustrates the number of failed cohesive elements in shale models with bedding plane inclinations of 0°, 45°, and 90° at different thicknesses of bedding layers. In the shale models with an inclination of 0°, the number of failed cohesive elements did not change noticeably with layer thickness. When the layer thickness increased, the number of fractures in the shale models with 90° inclinations decreased steadily. As a result of changing failure modes from T-S to T-S-S, shearing fractures through the layers have replaced the multiple tensile splitting along bedding planes. The number of fractures increased with increasing layer thickness for shale models with 45° bedding plane inclinations. Modelling a shale with bedding planes inclined at 45° demonstrated that it undergoes B-D failure mode during compression, so decreasing the number of bedding planes in the model increases the

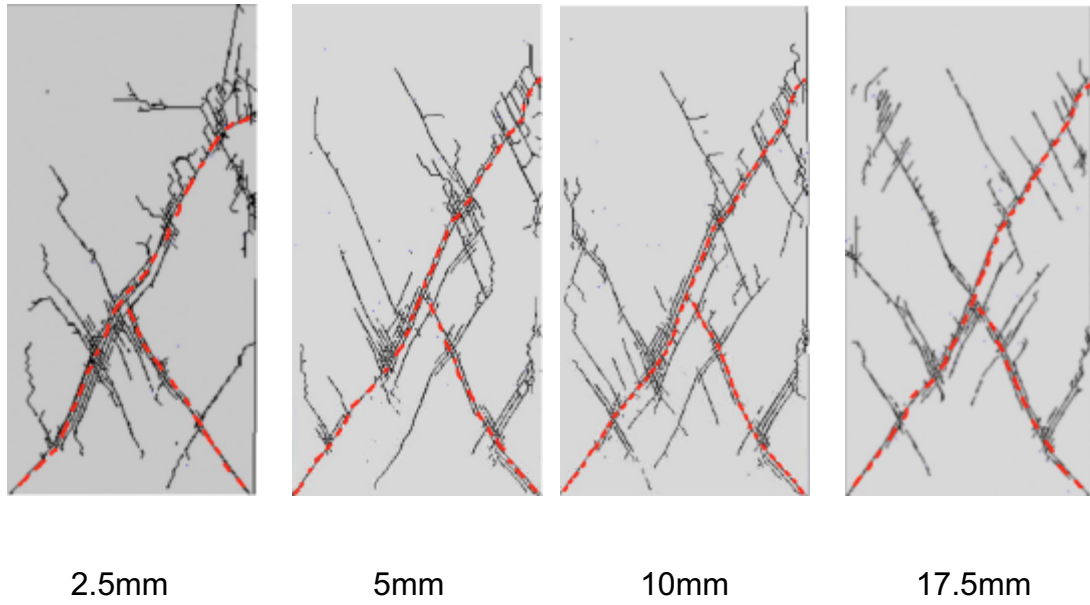
energy needed for shearing along the potential least-energy failure path. Shearing along the bedding plane required more energy, resulting in more fractures.



a)



b)



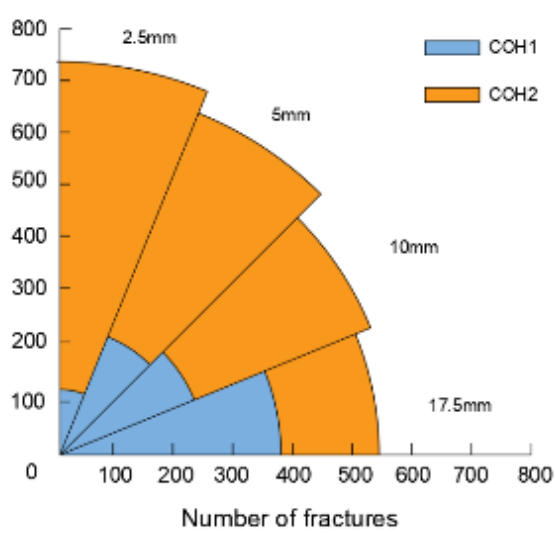
c)

Figure 4.13 Failure modes of FDEM shale model with different bedding planes inclination in different bedding layer thicknesses of a) 90°, b) 45° and c) 0° (the red lines highlight the main failure fractures to distinguish failure modes).

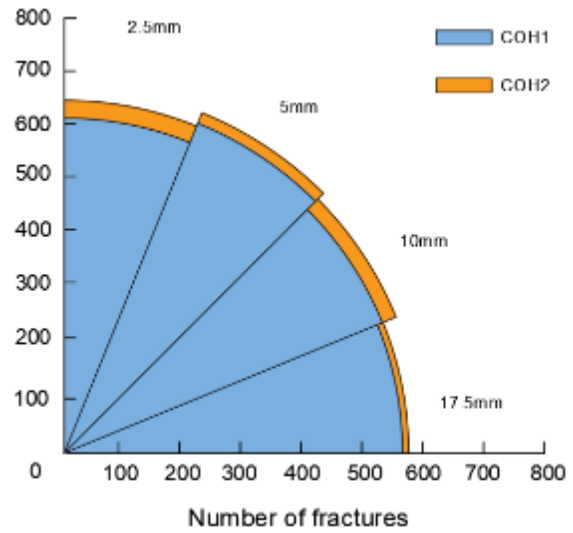
4.5.2 Fracturing conditions

The number of failed cohesive elements in shale model with bedding plane inclinations of 0°, 45° and 90° in different bedding layer thicknesses are depicted in Figure 4.14, separately for COH1 (shale matrix cohesive elements) and COH2 (bedding planes cohesive elements). The number of failed cohesive elements decreased in shale models with bedding plane inclinations of 90° as the bedding layer thickness increased due to the dramatic decrease in failed number of COH2. The failed number of COH1 and COH2 in shale models with bedding planes inclination of 0° varied slightly according to the layer thickness. The total number of fractures in the shale model with bedding plane inclinations of 45° increases with increasing layer thickness due to the increase in COH1. As the shale models with bedding plane inclinations of 45° tends

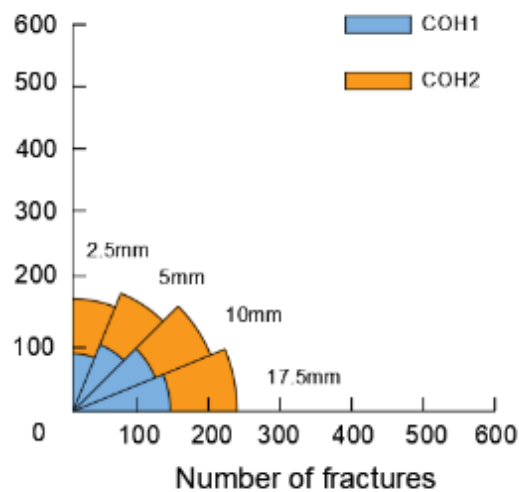
to shearing along the bedding planes, the decreasing of the number of bedding planes in the model increases the energy needed for shearing along the potential least-energy failure path. Along the bedding plane, the increased energies were released by generating more tensile fractures next to the shearing fractures.



a)



b)



c)

Figure 4.14 Two types of failed cohesive elements in shale models with bedding planes inclinations of a) 90°, b) 0° and c) 45° in different bedding layer thicknesses.

4.5.3 Mechanical strengths

According to Figure 4.15, uniaxial compressive strength values vary for shale models with bedding planes inclined at 0°, 45°, and 90° in different bedding layer thicknesses. The uniaxial compressive strength of shale models with bedding planes inclined 0° remained stable as the layers thickness changed. This also showed in the number of fractures. The shale model with bedding plane inclination of 0° showed no effect of layer thickness on its mechanical strength and fracturing mechanism. Conversely, the values of shale models with bedding planes inclined at 45° and 90° increased with layer thickness. This agrees with the simulation results by Lisjak et al. (2014b). This can be understood from the fracturing mechanism. As shown in Figure 4.14a and c, the number of COH1 increased with the increasing layer thickness in the shale model with bedding plane inclinations of 45° and 90°, which indicates it needs more fracturing energies until failure. When the layer thickness is modified for the shale models with a bedding plane inclination of 0°, the fracturing numbers of COH1 and COH2 remain approximately constant.

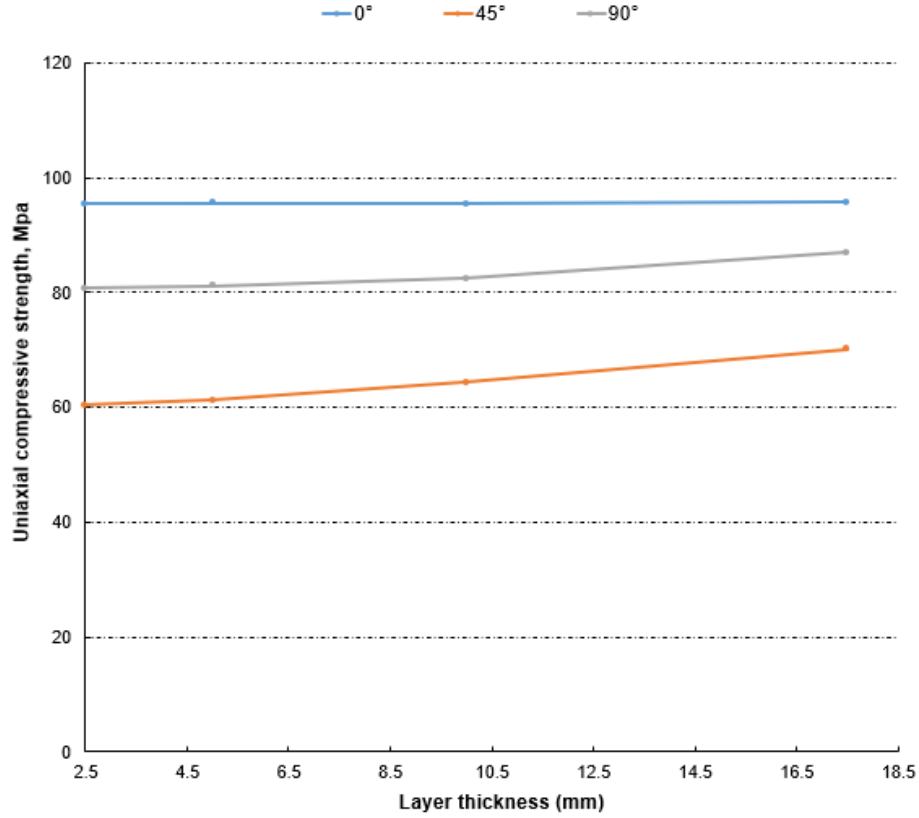


Figure 4.15 Variations of uniaxial compressive strength values in shale models with bedding planes inclinations of 0°, 45° and 90° in different bedding layer thicknesses.

4.5.4 brittleness index Bl_f

The brittleness of shale is strongly influenced by its layer thickness, as shown in Figure 4.16. However, the impact of the layer thickness on the Bl_f varies among shale models with different bedding plane inclinations. With different layer thicknesses, Bl_f of shale models remained stable with a bedding plane inclination of 0°. This can be understood that the layer thickness has no effect on the failure mode and behaviour of the shale models with 0° bedding plane inclination. The value of Bl_f for shale models with bedding planes inclined at 45° and 90° decreased as layer thickness increased, indicating that the brittleness of shale with these bedding planes decreases with increasing layer thickness. As the layer thickness increases, the fracturing number in

shale models with bedding planes inclined at 90° drops, resulting in smaller Bl_f . Meanwhile, the number of fractures in the shale models with bedding planes inclined at 45° increases with thicker layer thicknesses, though most of the fractures were shale matrix fractures (COH1). Failure at COH2 needs more fracturing energies than COH1, which leads to smaller Bl_f .

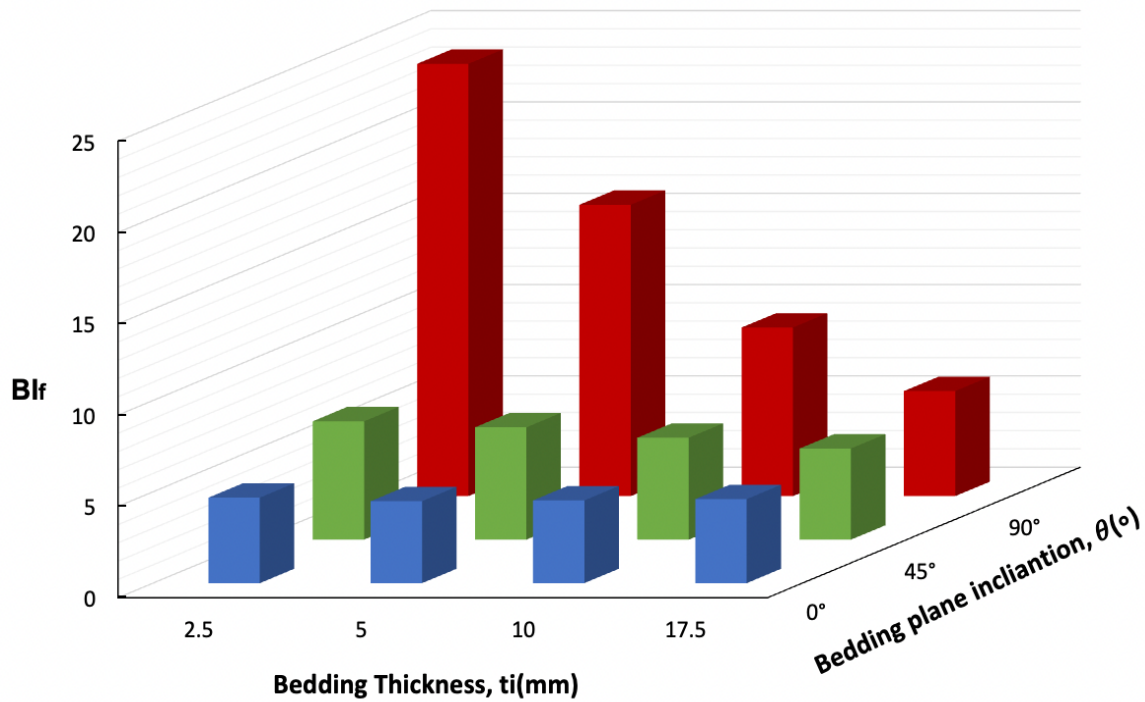


Figure 16 Variations of Bl_f in shale models with bedding planes inclinations of 0°, 45° and 90° in different bedding layer thicknesses.

4.6 Discussions and Findings

This chapter has modelled the shale anisotropy effects on the shale fracturing mechanism and also brittleness. In the UCS tests with shale models with different inclined bedding planes, three failure modes have been identified: S-M, T-S, and B-D, which are similar to the failure modes of shale samples (i.e., tensile splitting, shear through bedding planes and shear along bedding planes) with different bedding plane

inclinations identified by Yang et al. (2020) through UCS tests. This research has found that there is a tendency of T-S mode to tensile fracturing along multiple bedding planes, resulting in the largest number of fractures of all three failure modes, as shown in Figure 4.16. In addition, shale models tend to shear fracture along one or limited bedding planes in B-D, and shear fracture through shale matrix in S-M.

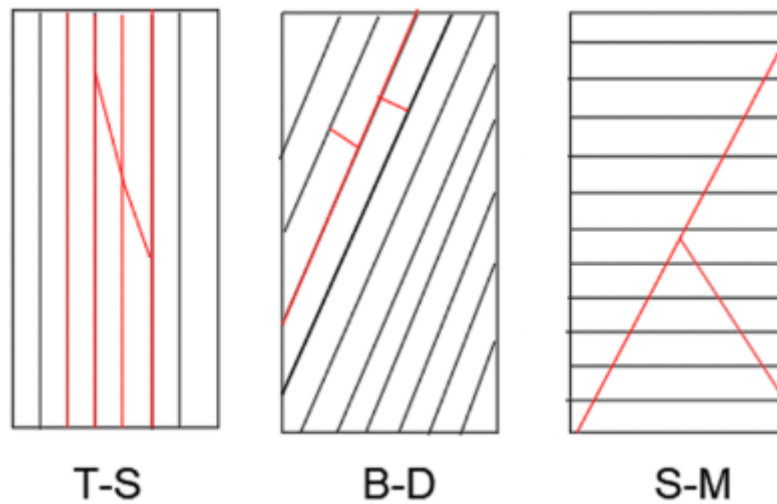


Figure 17 The diagram of three failure modes of shale under compression.

As fractures cause the rock to fail during compression, shale's mechanical strength is determined by its failure modes. The more fractures formed in rocks during compression, the more energy is absorbed and released, leading to higher mechanical strengths. As shown in Figure 4.6, the total number of fractures formed in the three modes are in the order: T-S > S-M > B-D. As a result of the low strength of the bedding planes, numerous tensile fractures formed along bedding planes in the T-S model when the shale model failed. Meanwhile, failures occur as a result of shearing for the B-D and S-M failure models. The shale in S-M mode needs more energy to reach macro failure comparing to B-D, which causes more fractures during compression. This can be attributed to the strength of the bedding plane being weaker than the matrix. When damage occurs along the bedding plane, fractures form quickly, resulting

in smaller plastic deformations and reduced energy dissipation. Shale anisotropy has a significant influence on the fracturing mechanism due to the presence of bedding planes. Due to the preferential path of least energy failure during fracture propagation, the lower strength of bedding planes affects fracturing paths (Lisjak et al., 2015).

Meanwhile, the anisotropy of shale significantly affects the mechanical strength at the crack level. The CD threshold obtained from UCS tests on shale with different bedding plane inclinations show that it is sensitive to the shale's anisotropic properties, which agrees with Li et al. (2020) laboratory results. When the stress inside the shale reaches the CD under the UCS test, fractures begin to form and propagate inside the shale. They may propagate along the bedding plane, cross the bedding plane, or even stop propagating, which depends on the bedding plane inclination. Different fracture paths lead to different strains and stresses within the shale. Based on this, a new brittleness index, Bl_{CD} is proposed in this study. The more efficiently the shale reaches the CD , the smaller the plastic strains. The higher the value of Bl_{CD} , the more brittle the shale. The order of the Bl_{CD} for the three failure modes is T-S> B-D> S-M.

Based on the various data collected from previous literatures, it was found that there is a relationship between Bl_2 and Bl_{CD} . Bl_2 represents the ratio between uniaxial compressive strength, σ_u , and tensile strength, σ_t , and Bl_{CD} represents the ratio between crack damage stress (CD) and σ_u , which indicates there is a relationship between σ_t and CD . An empirical relationship has been proposed to predict the tensile strength based on the CD and σ_t . This empirical relationship can be used for researchers and engineers to roughly predict the tensile strength based only on UCS tests in the future. In some situations, this can be helpful when it is difficult to conduct a BD test to determine the tensile strength for some materials.

The layers thickness has been proven to have a significant influence on the mechanical strength and fracturing mechanical of shale. The influence of the layer thickness of the shale models with a bedding plane inclination of 0° on its mechanical response is limited. Fractures in the S-M failure mode are mainly matrix fractures. A limited number of fractures occur along the bedding planes in the S-M failure mode. The deduction of the bedding planes in the model has no noticeable effect on its number of fractures and fracturing mode. While, for the T-S failure mode, the mechanical strength and failure mode have changed due to a changing fracturing mechanism. The deduction of the number of bedding planes in the shale model with bedding plane inclinations of 90° changed the failure mode from T-S to T-S-S. Shearing fractures through the layers have replaced multiple tensile splitting along the bedding planes. The total number of fractures decreased, but matrix fractures required much more energy to form than bedding plane tensile fractures, which led to a bigger mechanical strength. Due to the existing bedding planes working as weakening planes in the shale model, the deduction of number of bedding planes would not change the B-D failure mode. However, decreasing the number of bedding planes in the model increases the energy needed for shearing along the potential least-energy failure path. This leads to more fractures and bigger mechanical strength.

4.7 Summary

This chapter has studied shale anisotropy effects on its mechanical behaviours from micro crack level based on FDEM model created through ABAQUS. FDEM has shown it can well capture the failure mode of the rocks by simulating fracture formation and propagation, which has brought new insight into the behaviour of the shale anisotropy properties. The key conclusions are:

1) Three failure modes identified from both the numerical models and published experimental results in UCS test were the S-M ($\theta = 0^\circ$ and 15°), B-D ($\theta = 30^\circ$, 45° and 60°) and T-S ($\theta = 75^\circ$ and 90°), with transitioning phases between these. Meanwhile, the failure modes of the shale in the BD test can be recognised into three different modes: C-S ($\theta = 75^\circ$ and 90°), I-A ($\theta = 30^\circ$, 45° and 60°) and C-A ($\theta = 0^\circ$ and 15°).

2) The brittleness of shale is greatly affected by shale anisotropy. Based on conventional brittleness indices obtained from the ratio between the uniaxial compressive strength and tensile strength, the brittleness for the three failure modes of shale with different bedding plane inclinations are in the order: T-S > B-D > S-M.

3) The total number fractures of shale under stress in UCS test is not only related to the brittleness or frac-ability of shale, but also shale structures. High brittleness in shale means it is more easily fractured, as it has greater frac-ability. However, the total number of fractures formed inside the shale for the three failure modes are in the order: T-S > S-M > B-D. The total fracturing numbers of shale under stress is related to the shale structure, as it significantly affects fracturing paths.

4) The anisotropic property of shale significantly affects the mechanical strength and failure mechanism at the micro crack level. The *CD* threshold obtained from UCS tests on shale with different bedding plane inclinations are sensitive to shale anisotropic properties. The reason is that the *CD* corresponds closely to crack propagation, and different bedding layer orientations will affect crack propagation paths.

5) Two new brittleness indices are proposed in this study to improve the brittleness evaluation of shale. Bl_f , based on rock energy evolution, to predict the fracture formation inside the shale is proposed. The Bl_f describes the efficiency of shale to transform plastic energy into fractures under compression. Bl_f 's formula directly

incorporates the number of fractures formed, which provides a more accurate analysis of the rocks' frac-ability than other conventional brittleness indices. The parameter may be useful for evaluating rock frac-ability after excavation for projects that are concerned with fractures. Reservoirs can be evaluated for frac-ability using this brittleness index. In hydraulic fracturing, using less energy to produce large fractures is the priority in the shale gas exploration industry. Engineers can use it to locate an exploration site with a higher Bl_f value and optimize the exploration method to produce more fractures with lower energies. In addition, this brittleness index can be useful for locating more suitable locations for underground excavation (such as tunnels and nuclear waste disposal repositories) that are sensitive to excavation-induced fractures. In addition, Bl_{CD} , based on the ratio between the CD and the uniaxial compressive strength, has been proven by both experimental data and numerical simulation data to be able to accurately evaluate shale brittleness. Comparing Bl_{CD} to conventional brittleness indices, based on the ratio between uniaxial compressive strength and tensile strength, Bl_{CD} can be easily obtained from UCS tests, which makes it more convenient for evaluating the brittleness of rocks. Bl_{CD} and Bl_f for the three modes are in the same order: T-S > B-D > S-M.

6) An empirical relationship has been proposed to predict the tensile strength based on the UCS tests. It has been shown that there is a relationship between the tensile strength and CD . Considering that obtaining the tensile strength of rocks directly may be difficult under certain conditions, using this empirical relationship based only on the UCS test can provide an alternative. However, this empirical relationship needs further improvement (e.g., more experimental data on different types of rocks) to give greater confidence in its accuracy.

7) Shale's mechanical strength, fracturing conditions, and brittleness are influenced significantly by the layer thickness. However, it varies among shale models with different bedding plane inclinations. For S-M failure mode, the influence of the layer thickness on shale's mechanical strength, fracturing conditions and brittleness is limited. On the other hand, the reduction in layer thickness of shale has resulted in a reduction in mechanical strength and greater brittleness for T-S and B-D failures.

CHAPTER 5 FDEM simulation of the fracturing behaviour of EDZ under anisotropic shale formation

5.1 Introduction

As mentioned in section 2.4, Chapter 2, the rock mass strength and in-situ stress are two key factors affecting the fracturing conditions and fracturing mechanisms of the EDZ during excavation. Previously, in Chapter 4, it was demonstrated that the mechanical strengths of shale are affected by bedding plane inclinations and layer thicknesses from micro crack level. In the previous studies, Lisjak et al (2015) used the FDEM model for the first time to simulate failure mechanisms of surrounding rock of Full-scale Emplacement tunnel in Opalinus clay and investigated in-situ stress effects. Deng et al (2022) have further studied the failure mechanisms of anisotropic surrounding rock mass under different environment environmental conditions (e.g., dip angle of rock layers and layer thickness). Nevertheless, they did not further examine how environmental conditions (i.e., in-situ stress, dip angle of layers and layer thickness) affect EDZ properties (i.e., EDZ location, depth, fracturing number, and frequency) during tunnel excavation in anisotropic shale formation. Therefore, this chapter aims to use the developed FDEM large-scale tunnel model in the Chapter 3 to reveal the in-situ stress, shale anisotropy and layer thickness effect on the fracturing mechanisms and fracturing conditions (i.e., location, depth, fracturing number, and frequency) of the excavation damage zone (EDZ) in shale formation.

All scenarios and FDEM models created in this chapter are illustrated in Section 5.2. The following sections (section 5.3, 5.4 and 5.5) show the results of the fracturing mechanism (i.e., EDZ depth and number of fractures).

5.2 Field tunnel FDEM models for different scenarios

The field Full-scale Emplacement tunnel FDEM model has been verified in section 3.4, Chapter 3, by qualitative comparison of the deformation fields with field monitored values. A total of 13 field tunnel models (i.e., $A_1 - A_{13}$) have been created, as shown in Table 5.1, which lists the different scenarios and objectives.

Table 5.1 Field tunnel FDEM models for different scenarios

Model	Scenario			Objective
	Coefficient of lateral earth pressure, K_0	Bedding planes inclinations ($^\circ$)	Layer thickness (m)	
Full-scale Emplacement tunnel	A_1 (Field)	0.7	33	In-situ stress effects on the fracturing mechanism of EDZ in anisotropy shale formation
	A_2	0.4	33	
	A_3	1	33	
	A_4	1.3	33	
	A_5	0.7	0	Bedding plane inclinations effects on the fracturing mechanism of EDZ in anisotropy shale formation
	A_6	0.7	15	
	A_7	0.7	45	
	A_8	0.7	60	
	A_9	0.7	75	
	A_{10}	0.7	90	
	A_{11}	0.7	33	Layer thickness effects on the fracturing mechanism of EDZ in
	A_{12}	0.7	33	

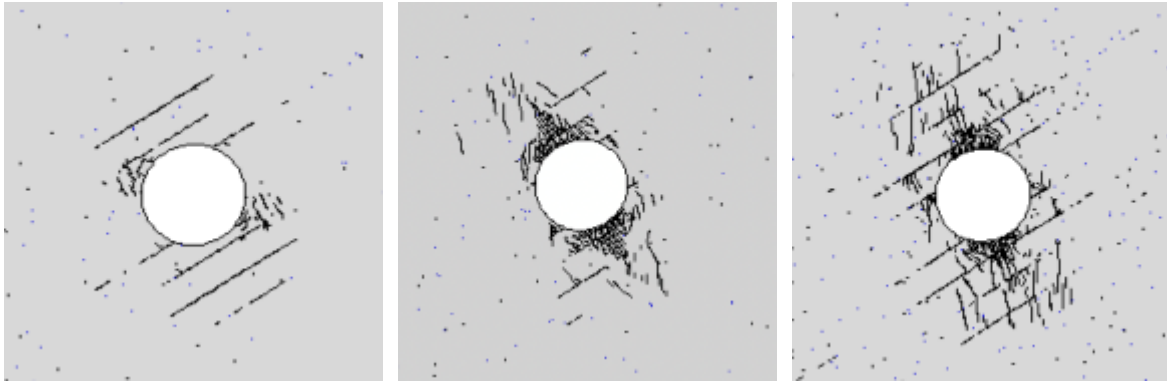
A_{13}	0.7	33	3.0	anisotropy shale formation
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To study the effect of anisotropy on the in-situ stress on the EDZ, four models (i.e., A_1 – A_4) with different in-situ stresses were created. With the initial field coefficient of lateral earth pressure, K_0 (i.e., 0.7), values of 0.4, 1.0 and 1.3, leading to four models, were tested to evaluate the sensitivity of the results to K_0 . With a value of $K_0 = 1$, isotropic field stresses with can be obtained. Static equilibrium cannot be achieved if K_0 is raised to 1.6. In addition, seven models (i.e., A_1 , A_5 – A_{10}) in seven directions (i.e., 0° , 15° , 30° , 45° , 60° , 75° and 90°) were created to study bedding plane inclinations effects on fracturing mechanism of the EDZ in an anisotropy shale formation. These reflect the seven bedding inclinations used in the laboratory tests on Opalinus clay conducted by Lisjak et al. (2014b). The layer thickness was chosen to ensure the smallest layer thickness is big enough for the meshing elements. The elements are ranging from 0.05 ~ 0.12 m in Full-scale Emplacement tunnel FDEM model, as illustrated in section 3.4.2, Chapter 3. Hence, the smallest layer thickness adopted was 0.3 m. Four models (i.e., A_1 , A_{11} – A_{13}) with different layer thickness (i.e., 0.3m, 0.75m, 1.5m and 3m) were created. The adopted elastic elements and cohesive elements parameters for all models are the same as the ones used in the Full-scale Emplacement tunnel FDEM model, shown in Table 3.5, Chapter 3.

5.3 Different in-situ stress

Simulations were performed for the four different lateral stress, K_0 cases presented in Table 5.1 to assess how in-situ stress affect fracture evolution around the tunnel, as shown in Figure 5.1. With the decreasing of the horizontal stress to a high anisotropic in-situ stress ($K_0 = 0.4$) conditions, it causes shear fractures more frequently along the bedding planes at the upper left shoulder and right knee of the tunnel. Under isotropic

stress conditions ($K_0 = 1$), the increased lateral stress decreased the sliding forces that cause shearing of the rock mass along the bedding planes. Due to the high concentration of stress in the EDZ, the rock mass is heavily fragmented. The in-situ stress field of the rock mass with a $K_0 = 1.3$ not only causes the rock mass to experience increased sliding forces for shearing along the bedding planes, but it also results in intensive fractures among the layers. It can be noted that all four modes have notches next to the tunnel wall formed by tensile and shear fractures inside of their EDZ, and the location of the notches is moved from the sidewalls of the tunnel ($K_0 = 0.4$) to the left shoulder and right knee of the tunnel ($K_0 = 0.7$ and 0.1), and to the crown and invert in the last ($K_0 = 1.3$). This kind of notch failure have been spotted in several research as shown in Figure 5.2 (Blümling et al., 2007 and Read, 2004). The fracturing mechanism of all EDZ between $K_0 = 0.4$ and 1.3 is caused by bedding plane delamination, which results in a same fracturing mode of bedding plane delamination notches (BD-N). The change in lateral stress has no effect on the fracturing mode of EDZ. This agrees with the simulation results of Lisjak et al (2015) and Deng et al (2022). On the other hand, as shown in Figure 5.3, both the depth of the EDZ, and the total number of fractures inside of EDZ are increasing with bigger lateral stress. The depth of the EDZ are normalized to the tunnel diameter, D . EDZ fracturing conditions (i.e., location, depth, and number of fractures) are significantly affected by lateral stress.

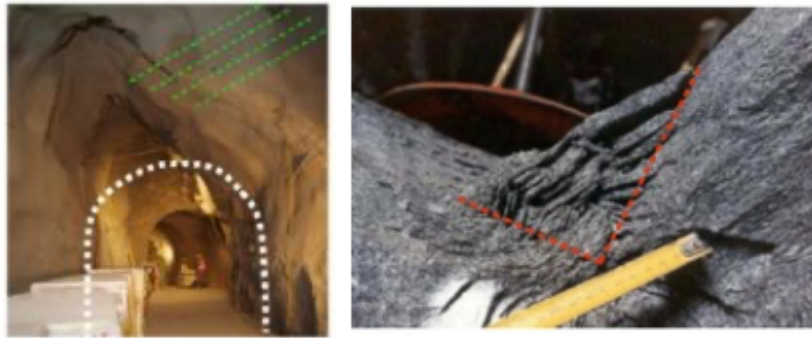


a)

b)

c)

Figure 5.1 Effect of in-situ stress conditions on the EDZ around the Full-scale Emplacement tunnel a) 0.4, b) 1.0 and c) 1.3 (The case of $K_0 = 0.7$ fracture pattern is shown in Figure 3.24, Chapter 3).



a)

b)

Figure 5.2 Notch fracturing failures of shale rock mass in the field, as shown in a) by Blümling et al. (2007), and b) by Read (2004) (the green line in the figure indicates the bedding planes, the white line indicates the formerly horseshoe shape tunnel and the red line draws out the notch shape of failure).

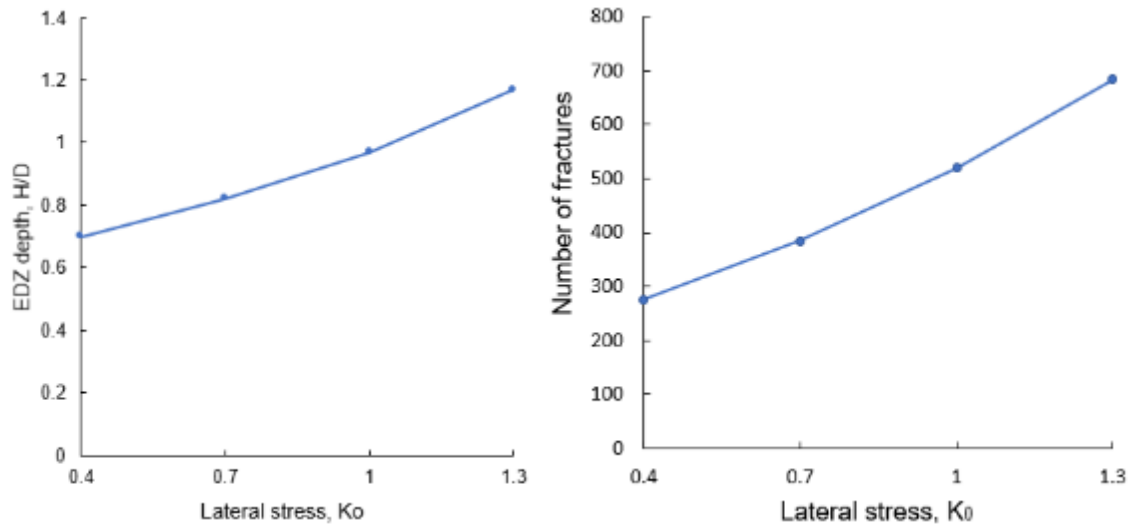


Figure 5.3 a) The depth of the inner and outer zone of EDZ (normalized to tunnel diameter, D) and b) number of fractures with different lateral stress, K_0 .

5.4 Shale anisotropy

5.4.1 Simulated stress fields and fracturing behaviour

To study the effect of the shale anisotropy on the EDZ of a tunnel, different dip angles of bedding planes were realised by changing the inclination of the bedding planes in the models as illustrated in Figure 5.4.

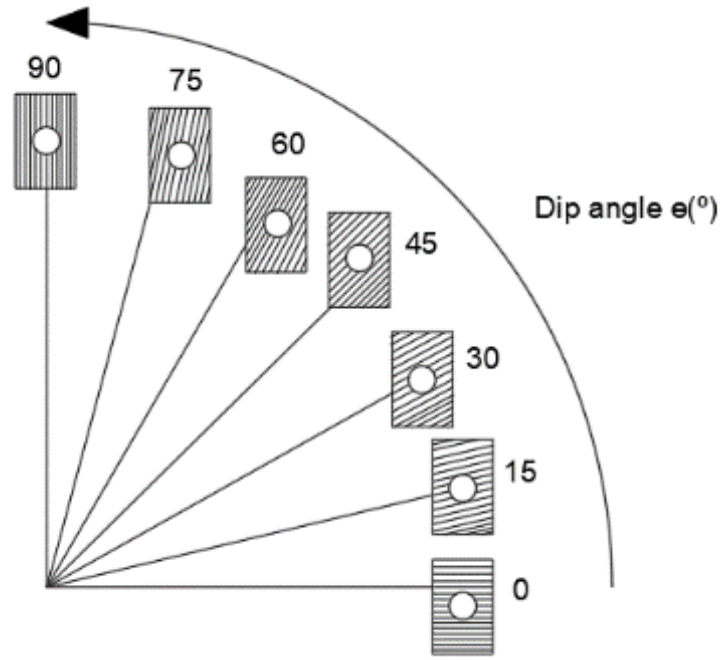


Figure 5.4 Different bedding plane inclinations in the FDEM tunnel models.

Figure 5.6 shows the results of the different models for the EDZ indicating that the bedding plane inclinations have a great effect on the fracturing mode of the surrounding rock. Simulation results indicate three types of EDZ around the tunnel: tensile-splitting spalling (TS-S) (75° and 90°), bedding plane delamination notches (BD-N) (33°, 45° and 60°) and shearing through layers notches (SL-N) (15° and 0°).

For steep dip angles (75° and 90°), the EDZ is located at the crown and invert of the tunnel which is the same failure mode found by Perras and Diederichs (2014), and Deng et al. (2022), as shown in Figure 5.5. The spalling failure near the tunnel is caused by the tensile fractures in rocks (Fairhurst and Cook, 1966, and Perras and Diederichs, 2014). Due to the low tensile strength of the bedding planes, layers at the crown and invert tend to experience tensile splitting along the bedding planes. It is noted that tensile fractures formed parallel to the maximum principal stress, which

agrees with the observations from several researchers (Read, 2004, Martin and Christiansson, 2009).

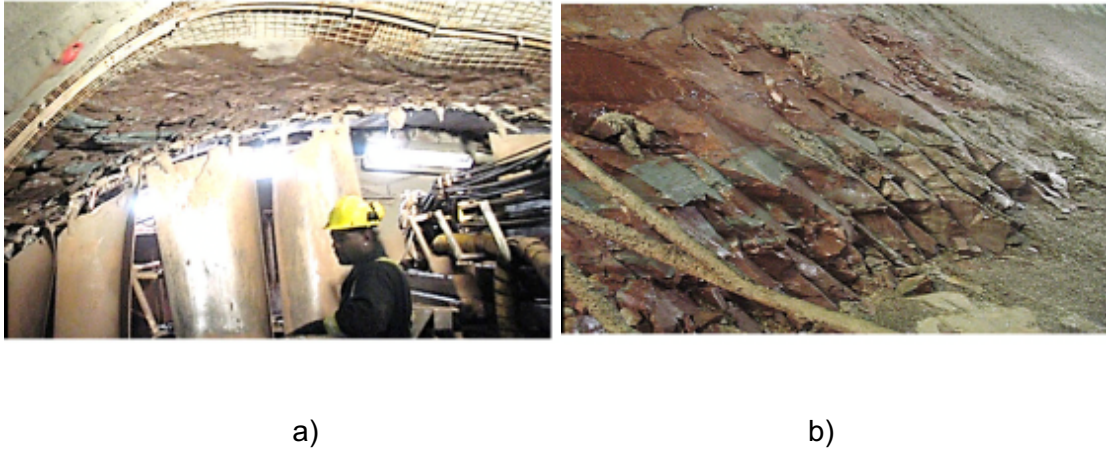


Figure 5.5 Onion spalling of surrounding rocks observed in the crown and invert of Niagara Tunnel in sedimentary rocks with approximately 85° bedding plane inclinations; a) Crown, b) Invert (Perras and Diederichs, 2014).

Two notches next to the tunnel wall can be identified in the other models with smaller bedding plane inclinations (60°, 45° and 33°). The EDZs are observed to be generally perpendicular to the bedding plane in all of the models, which agrees with the results of the FEM simulations by Fortaskis et al. (2012) of the transversely isotropic rock mass. As outlined in section 3.3, the location of the excavation failure around tunnels is caused both by the excavation-induced stress redistribution and the lower strength of the bedding planes oriented towards the slip. When the bedding planes slip, the stress field is perturbed locally, resulting in a few tensile fractures next to the bedding planes. As the inclination of the bedding planes gets much smaller ($\theta=15^\circ$ and 0°), the sliding force between the layers induced by the excavation is difficult to overcome due to the cohesion of the bedding planes. Similar to the failure of shale with horizontal bedding planes under a uniaxial compressive test, shear fractures through the layers start to occur. These shear and tensile fractures at the crown and invert of the tunnel

obliquely intersect with the tunnel boundary, which leads to V-shape notches at those locations. The SL-N failure mode can be also noticed in the FDEM studies by Deng et al. (2022) and Bradley (2015) with horizontal bedding planes shale formation. This fracturing mode has also been observed by Grunicke et al. (2013) in field observation.

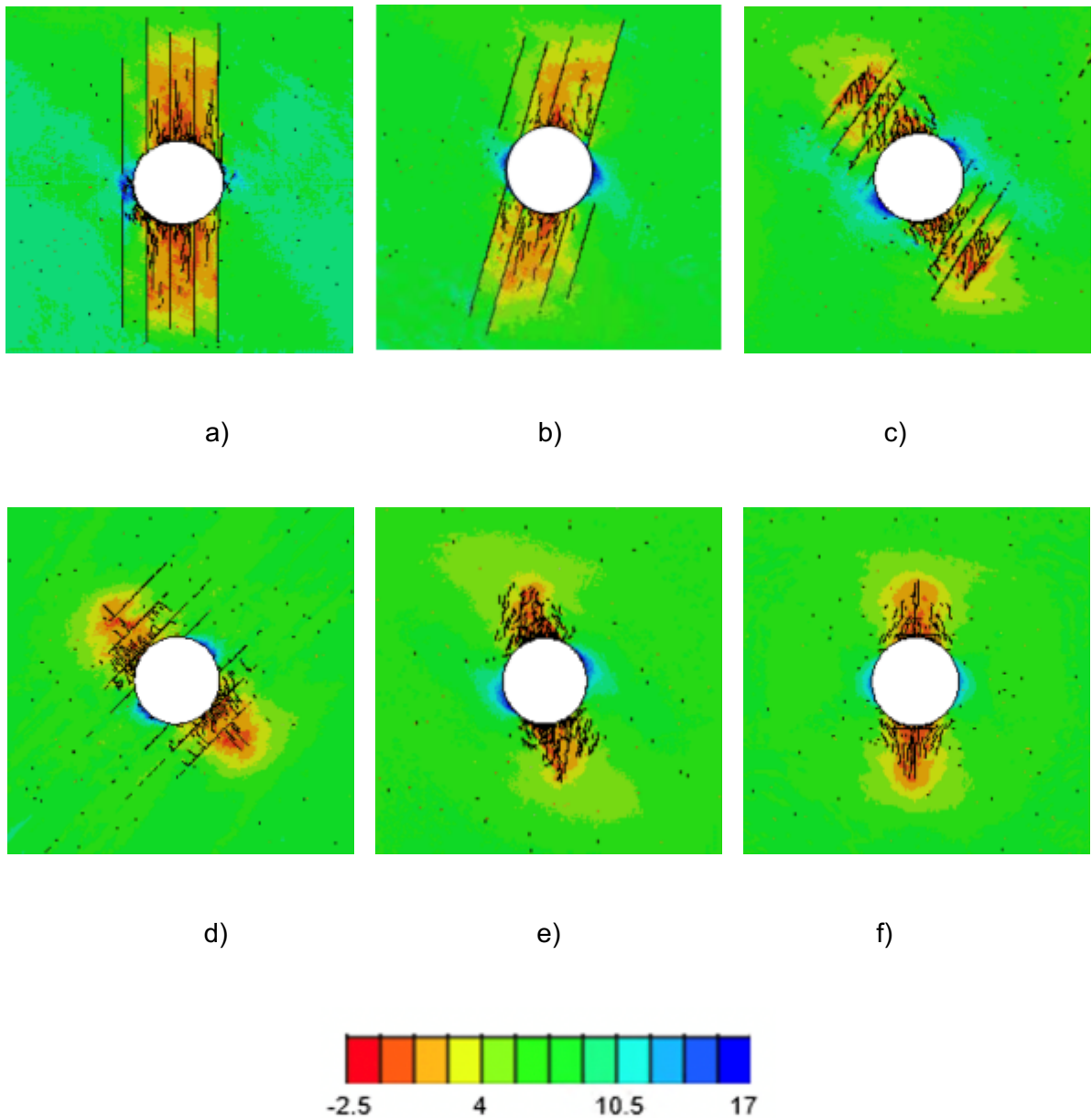


Figure 5.6 Maximum principal stress field of the tunnel models with different dip angles of rock layer for a) 90°, b) 75°, c) 60°, d) 45°, e) 15° and f) 0°).

Figure 5.7 shows that the depth of the EDZ increases as the inclination of the bedding plane increases. The largest of the EDZ is around $1.41D$, which can be obtained when $\theta = 90^\circ$, while the smallest EDZ with $0.5D$ can be spotted in the model with a bedding plane inclination of 0° . When the bedding planes have steep inclinations ($\theta \geq 75^\circ$), the EDZ is formed in the surrounding rock in the TS-S fracturing mode. Based on the results of the uniaxial compressive test, the weak cohesion strength of the bedding planes leads to the least amount of energy needed for fracturing, resulting in the largest EDZ depth and fracturing numbers. With the decreasing of the bedding plane inclinations, the EDZ failure mode changes from TS-S to BD-N, which requires more energy to fracture. As the bedding planes reach smaller inclinations ($\theta = 15^\circ$ and 0°), the sliding force between the layers induced by the excavation is difficult to overcome due to the cohesion of the bedding planes. It is difficult for fractures to form and propagate in the surrounding rock since it tends to fracture through the layers, which leads to a small EDZ depth and also fewer number of fractures. It is noted that when the EDZ is in the TS-S failure mode ($\theta \geq 75^\circ$), the EDZ depth is around $1.4D$ within 5% difference. Meanwhile, for the BD-N failure mode ($\theta = 60^\circ, 45^\circ$ and 33°), the EDZ depth is approximately $0.9D$ within 7% difference. For the SL-N failure ($\theta = 15^\circ$ and 0°), the EDZ depth is approximately $0.5D$ within 5% difference.

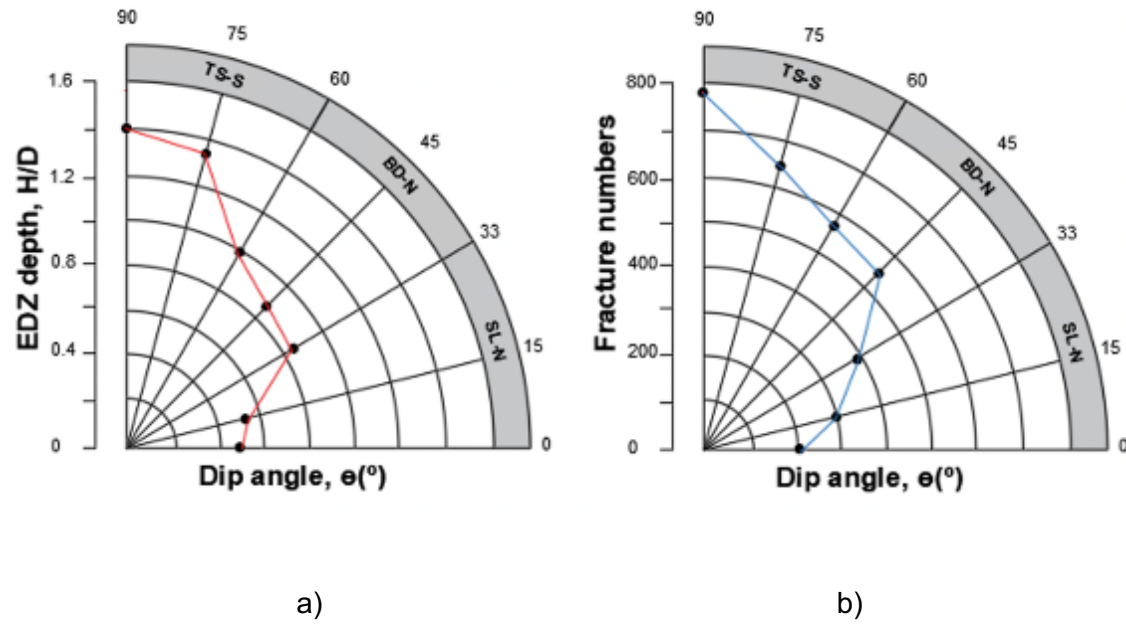


Figure 5.7 a) Variation of the EDZ depth (normalized to tunnel diameter) and b) fracture numbers with different bedding plane inclinations in the FDEM tunnel models.

5.4.2 Displacement fields

The displacement field is also strongly affected by the dip angle inclinations of the layers in a shale formation, as shown in Figure 5.8. With increasing dip angle inclinations, maximum displacement increases. The biggest displacement is approximately 39.1mm at 90° , while the smallest displacement is approximately 25.7mm at 0° . With different bedding plane inclinations, the location of maximum displacement varies. The polar angle of maximum displacement point increased from approximately 92° to 137° in the first, and then decreased to 89° with decreasing bedding plane inclinations, as shown in Figure 5.8. The locations of the maximum displacement in models with different bedding plane inclinations agree with He et al. (2012) study. It has been found that the largest displacements in the models with bedding plane inclinations of 0° and 90° are located at the crown of the tunnel, while

the largest displacements in the models with bedding plane inclinations of 30° and 60° are located at the right shoulder through DEM simulation.

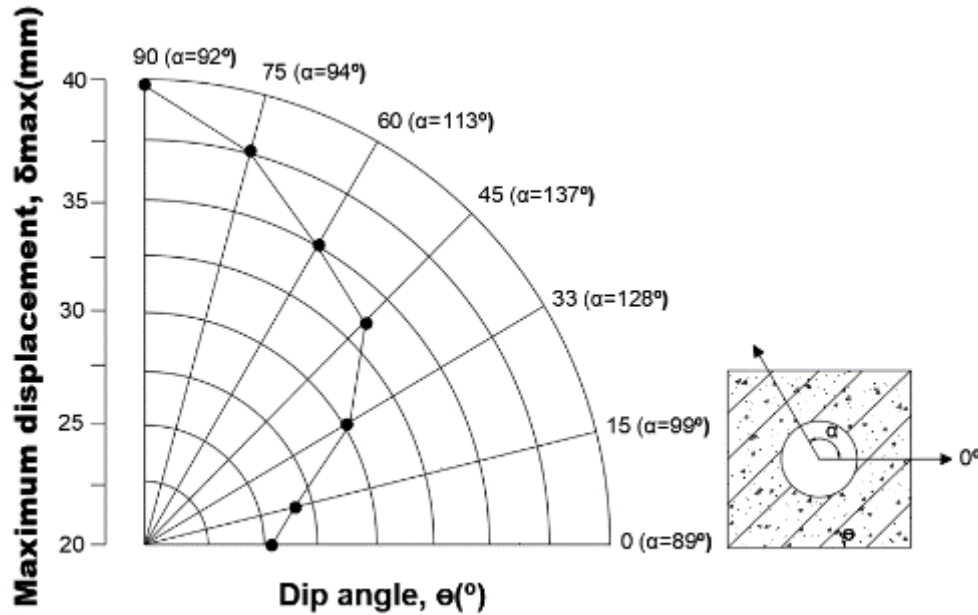


Figure 5.8 Variation of maximum total displacement along tunnel boundary with different bedding plane inclinations (θ is the bedding plane dip angle, and α is the polar angle of the maximum displacement point in the model).

As a result of the location of the maximum displacement in the models changing with bedding plane inclinations, the tunnel crown displacement initially decreases from 0° to 45°, then increases until it reaches 90°, as shown in Figure 5.9. As the bedding planes are horizontal or vertical, the maximum displacement occurs around the tunnel crown, so the displacement values at tunnel crown are close to the largest displacement in the two models. With the bedding plane inclinations decreasing from 90° to 45°, the location of maximum displacement in the model moved from tunnel crown to right shoulder. The localised large deformations caused by bedding plane sliding in the model moved away from the tunnel crown to side walls, which leads to relatively small displacement at the crown. The biggest tunnel crown displacement is

approximately 37.8 mm at 90°, while the smallest tunnel crown displacement is approximately 19.4mm at 45°.

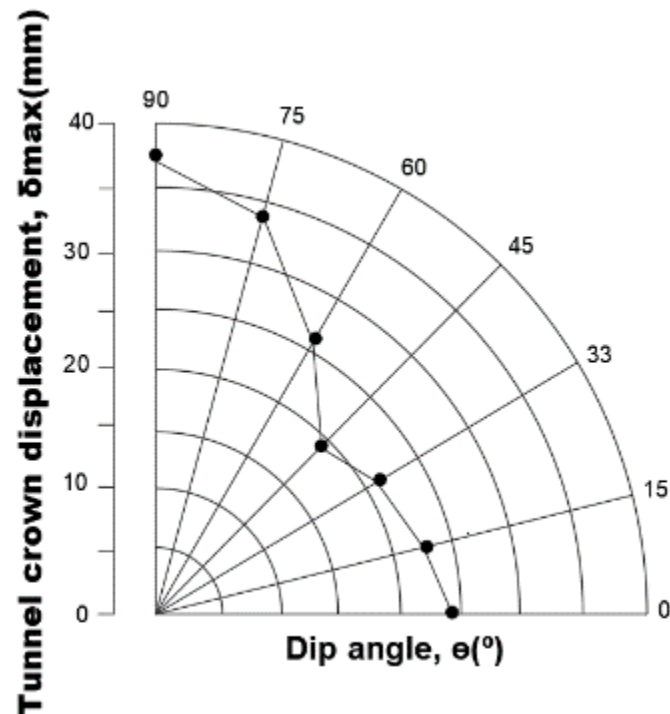


Figure 5.9 Tunnel crown displacement with different bedding plane inclinations in the FDEM tunnel models.

5.5 Layer thickness

5.5.1 Displacement fields

A total of four Full-scale Emplacement tunnel FDEM models with different layer thicknesses, in terms of 0.3m, 0.75m, 1.5m and 3m have been created to understand the effect of thickness on the EDZ, as shown in Figure 5.10.

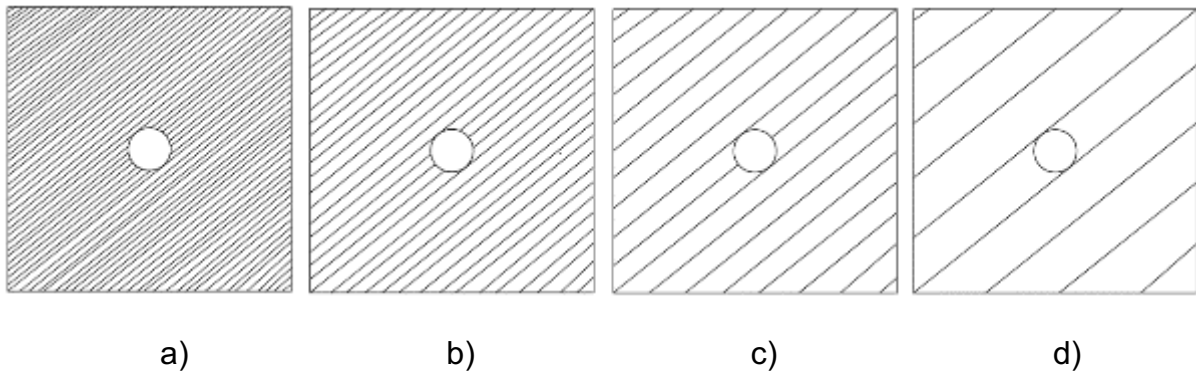
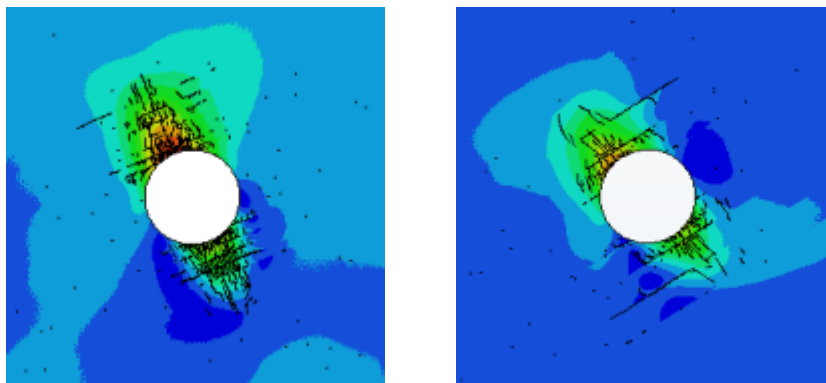


Figure 5.10 Diagram of different layer thickness in the Full-scale Emplacement tunnel FDEM model a) 0.3m b) 0.75m c) 1.5m d) 3m.

Figure 5.11 shows the simulation results of the displacement fields in the surrounding rock mass when the thickness of the layer λ changes ($\lambda = 0.3\text{m}$, 0.75m , 1.5m and 3m). The 0.75m (Full-scale Emplacement tunnel) results are depicted in Figure 3.24, section 3.3.1. As the layer thickness increases, the simulated maximum displacement in the surrounding rock decreases from 35.8mm to 21.3mm . When the layer thickness decreases, the number of low cohesion bedding planes increases in the surrounding rock mass, enabling the rock mass to more easily shear-slip along the bedding plane, which causes larger displacements. The field monitoring data of the Full-scale Emplacement tunnel from section 3.4.1.4 (Chapter 3) suggested a total displacement of the tunnel crown of approximately $21\text{-}22\text{mm}$, which is close to the simulation results of layers with a thickness of 0.75m .



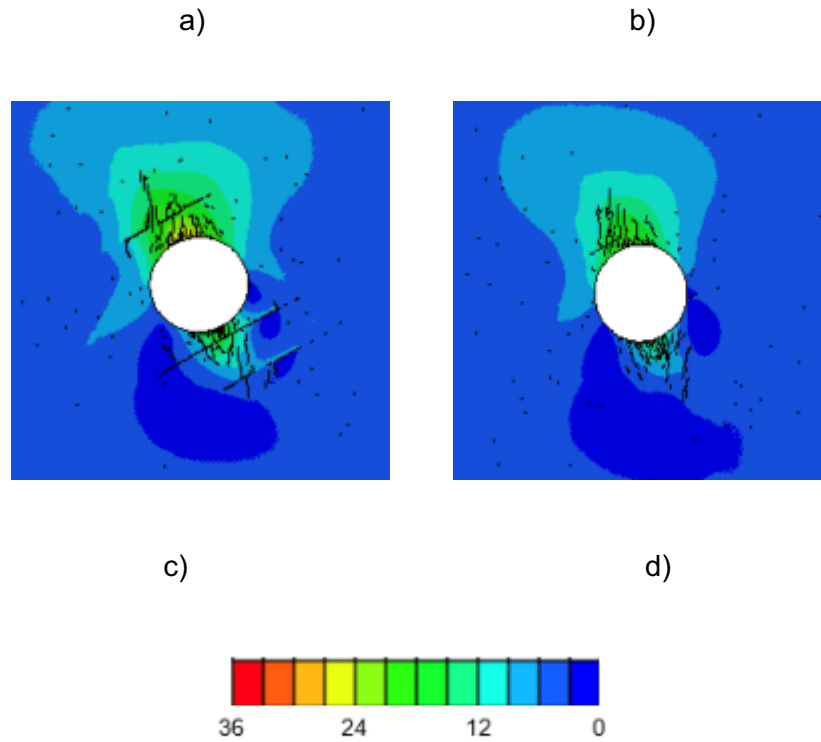
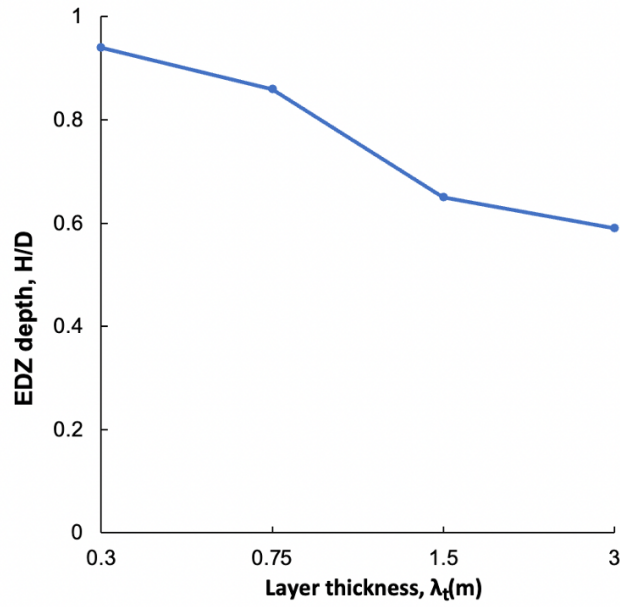


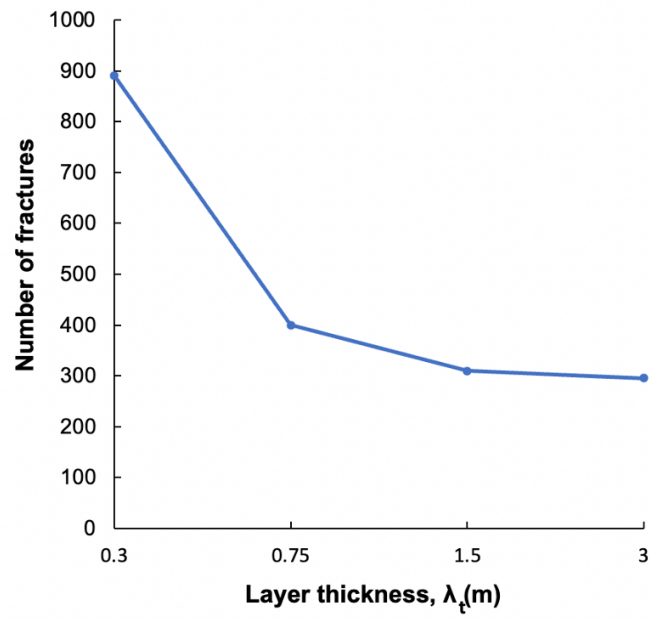
Figure 5.11 Effect of layer thickness on the total displacement fields around the Full-scale Emplacement tunnel for a) 0.3m, b) 0.75m,c) 1.5m and d) 3m.

5.5.2 Simulated fracturing behaviour

As shown in Figure 5.11, the EDZ fracturing mode in the simulated models with different layer thicknesses, λ_t , has gradually changed from BD-N with a $\lambda_t = 0.3\text{m}$ to SL-N with a $\lambda_t = 3\text{m}$. As the layer thickness increases, the surrounding rock mass becomes more difficult to shear-slip along the bedding plane. This leads to shearing failure through the layers due to excavation. With increasing layer thickness, the EDZ depth decreases from $0.98D$ to $0.6D$, as depicted in Figure 5.12. Additionally, the fracture numbers decrease from 882 to 236 with a thickness of 0.3m and 3m respectively. The EDZ fracturing mechanism is greatly affected by the presence of bedding planes in the surrounding rock.



a)



b)

Figure 5.12 a) Depth of the EDZ (normalized to tunnel diameter) and b) fracture numbers with different layer thickness, λ_t .

5.6 Opalinus clay's BI_f

In order to validate the use of BI_f on the field projects to predict fracturing conditions in the EDZ, this study have modelled laboratory-scale FDEM Opalinus clay UCS model to obtain BI_f values.

5.6.1 Model description and input parameters

As with the Longmaxi UCS model illustrated in Chapter 3, the Opalinus clay UCS model is developed in the same way. The FDEM UCS models were calibrated against laboratory results reported by Bock (2009) for the Opalinus clay. A two-dimensional 35 mm × 17.5 mm rectangular model was created for the UCS tests. Same to the Longmaxi UCS model, it was assumed that the cross section of each model would lie perpendicular to the bedding planes strike. In the shale model, three different bedding plane inclinations have been created at 0°, 45°, and 90° to represent the three different failure modes (i.e., tensile splitting, bedding plane delamination, and shearing through matrix). As shown in Figure 5.13(a), Shale uniaxial compressive strength appears to converge with decreasing element size after 0.25mm. As a result of adopting smaller element sizes, the total number of elements grows rapidly, while the explicit time integration scheme of FDEM also demands smaller time steps for stability. Based on this, the average element size in this study adopted 0.25mm, which reduces mesh sensitivity with a reasonable number of elements and produces a numerical model that matches the experimental uniaxial compressive strength to within 5% (Bock, 2009). Meanwhile, After the loading rate dropped below 150mm/s, the values for the strength of the shale in UCS test started to converge as shown in Figure 5.13(b). Based on the sensitivity studies, the average element size and loading rate in the model were 0.25mm and 0.1m/s, respectively. The Opalinus clay FDEM model was

calibrated with the data from the experiments through the trial-and-error process as illustrated in Chapter 3, section 3.3.4. The final parameters used for the model are listed in Table 5.2.

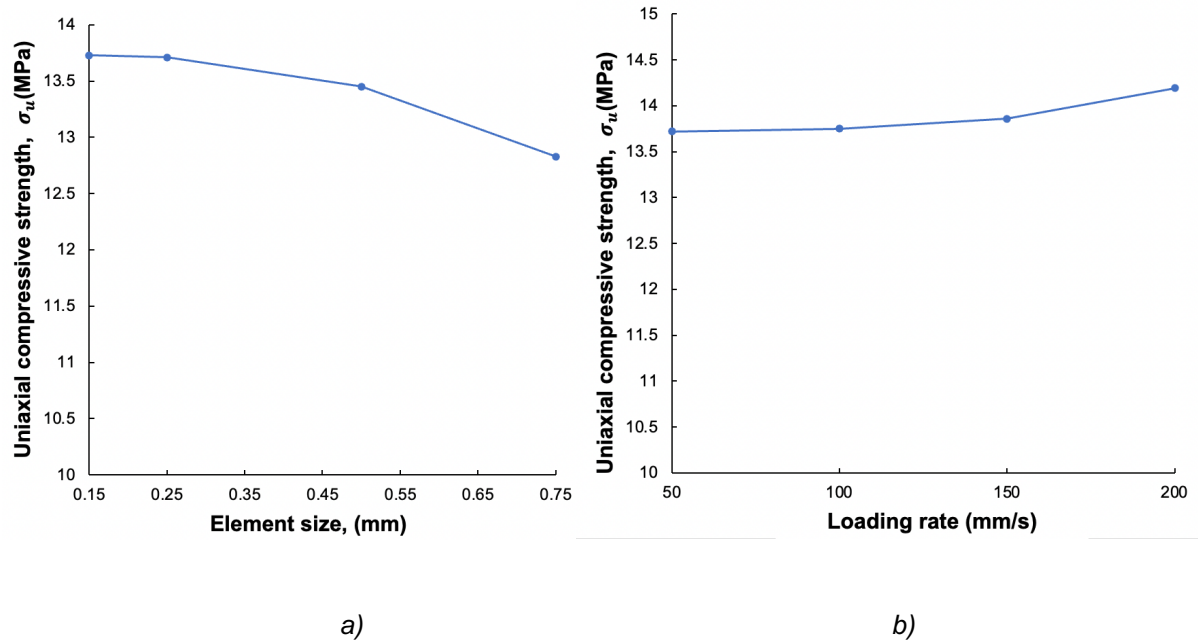


Figure 13 The sensitivity studies of Element size and loading rate: shale compressive strength at bedding plane inclinations of 0° as a function of the average element size and loading rate, respectively. a) element size, b) loading rate.

Table 2 Input parameters for the Opalinus clay model

Parameter	Value
Elastic elements	
Density, ρ (kg/m ³)	2330
Young's modulus parallel to bedding, E_{par} (GPa)	3.8
Young's modulus perpendicular to bedding, E_{per} (GPa)	1.3
Poisson's ratio parallel to bedding, ν_{par}	0.35
Poisson's ratio perpendicular to bedding, ν_{per}	0.25
Shear modulus, G (GPa)	0.9

Cohesive elements	
Tensile strength parallel to bedding, f_{tpar} (MPa)	0.6
Tensile strength perpendicular to bedding, f_{tper} (MPa)	0.15
Cohesion parallel to bedding, c_{par} (MPa)	1
Cohesion perpendicular to bedding, c_{per} (MPa)	9
Mode I fracture energy parallel to bedding, G_{Ifpar} (J/m ²)	0.2
Mode I fracture energy perpendicular to bedding, G_{Ifper} (J/m ²)	5
Mode II fracture energy parallel to bedding, G_{IIpar} (J/m ²)	10
Mode II fracture energy perpendicular to bedding, G_{IIper} (J/m ²)	25
Friction angle of intact material, ϕ_i (deg)	22
Normal stiffness, k_n (GPa/m)	38
Shear stiffness, k_s (GPa/m)	3.8
Element/Loading platen friction coefficient, f_l	0.1
Elastic elements internal sliding friction coefficient, μ	0.4

The mechanical properties of the numerical models are compared with the experimental values for Opalinus clay in Table 5.3. The relative errors for all values are within 5%.

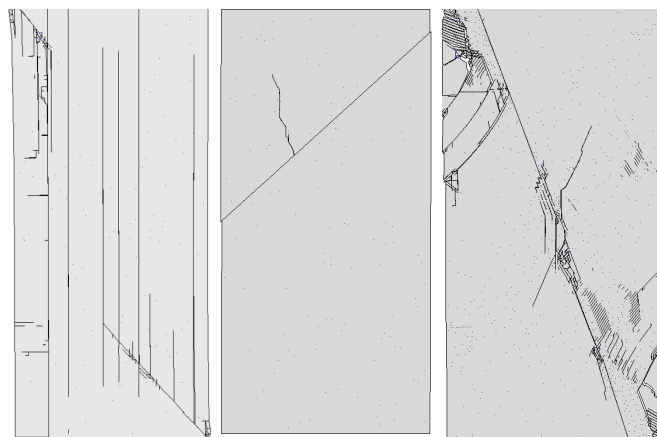
Table 3 Comparison of the mechanical properties of the Opalinus clay between the numerical model and experiment average results (Bock, 2009) (Note: the shale model with bedding plane inclinations of 90° and 0° is illustrated parallel and perpendicular to the bedding planes in the Table).

Mechanical properties	Experimental value	Numerical value
Elastic modulus parallel to bedding, E_{par} (GPa)	3.8±1.5	3.26
Elastic modulus perpendicular to bedding, E_{per} (GPa)	1.3±0.7	0.94

Uniaxial compressive strength parallel to bedding, σ_{uPar} (MPa)	11.6±3.9	10.68
Uniaxial compressive strength perpendicular to bedding, σ_{uPar} (MPa)	14.9±5.1	13.71

5.6.2 Fracturing behaviours

Figure 5.14 illustrates the microscopic fracturing response of the Opalinus clay observed in the FDEM model and experimental tests. Same to the Longmaxi shale, the failure patterns of Opalinus clay can also be classified into three distinct modes, in terms of tensile splitting, bedding planes delamination and shearing through matrix. These failure modes match the observation in the experiment tests (Popp et al., 2008).

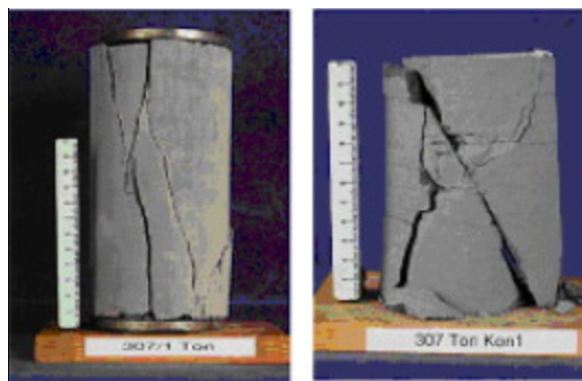


$\theta=90^\circ$

$\theta=45^\circ$

$\theta=0^\circ$

a)



$\theta=90^\circ$

$\theta=0^\circ$

b)

Figure 14 Comparison of failure patterns during UCS test on Opalinus clay between FDEM models and experimental samples a) model analysis and b) laboratory results (Popp et al., 2008)

Figure 5.15 shows the failed cohesive elements inside the shale model with different bedding planes inclinations. The largest number of fractures formed in the shale with a bedding plane inclination of 90° , while the shale with a bedding plane inclination of 45° has the smallest value. This phenomenon has been explained early in Section 4.3.2, Chapter 4.

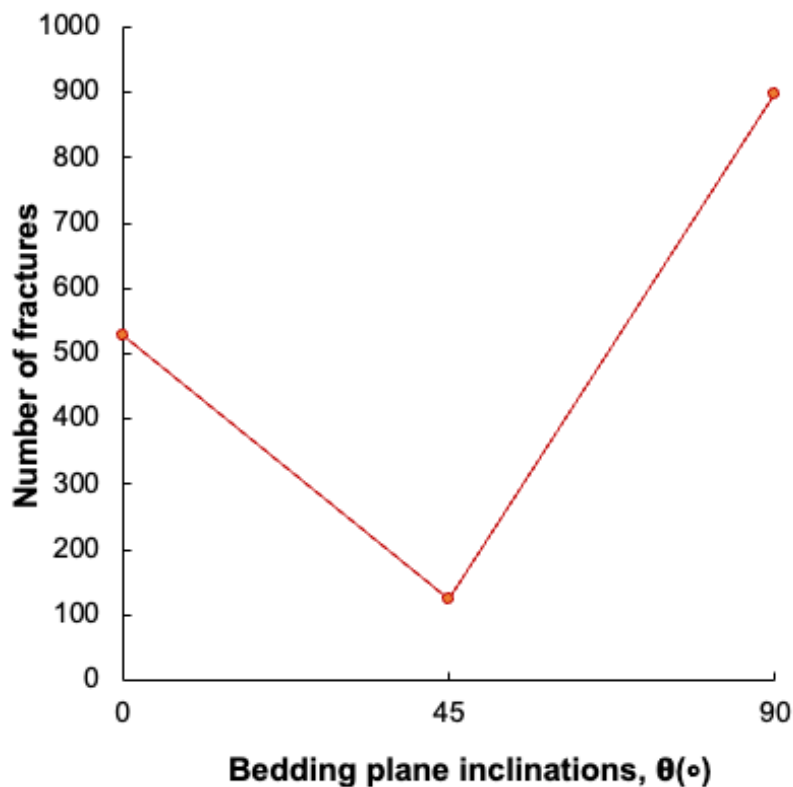


Figure 15 Failed cohesive elements inside the shale model with different bedding planes inclinations.

5.6.3 Brittleness index BI_f

Based on the Equation 4.5, the BI_f for Opalinus clay model with different bedding plane inclinations are illustrated in Figure 5.16. Figure 5.16 shows that as the bedding plane inclination increases, the BI_f increases, and hence the number of the fractures formed per unit energy dissipation increases. The transfer of energy to fractures in the three failure modes of shale are in the order of: T-S > B-D > S-M, which is same to Longmaxi shale. Rock with a higher BI_f value has a bigger frac-ability, leading to more severe fracturing conditions in the EDZ. Field-scale FDEM Opalinus clay models have demonstrated this early in Section 5.4.1. As shown in Figure 5.7, field-scale FDEM Opalinus clay model with a bedding plane inclination of 90° have a much more severe fracturing conditions (i.e., EDZ depth and fracture number) than 45° and 0° .

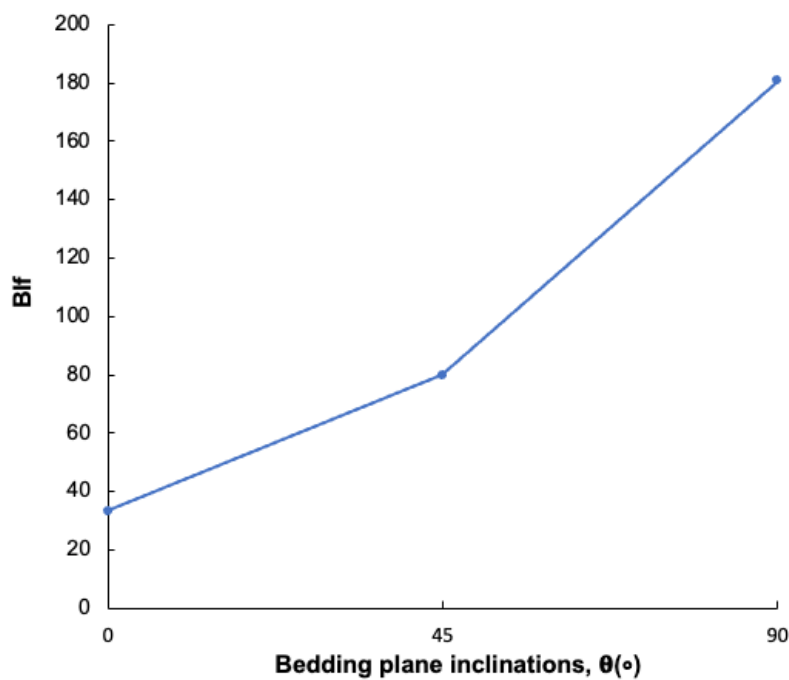


Figure 16 The variation in BI_f with different bedding plane inclinations.

5.7 Discussions

The fracturing mode of anisotropic surrounding rock masses (layered rock masses) after excavation is significantly affected by the underground environmental conditions (i.e., in-situ stress, layer thickness and bedding plane inclinations), as discussed in the previous sections. Section 5.4 showed that the fracturing modes can be generally divided into three categories: 1) tensile splitting spalling (TS-S), 2) bedding plane delamination notches (BD-N), and 3) shearing through layers notches (SL-N), as shown in Figure 5.17.

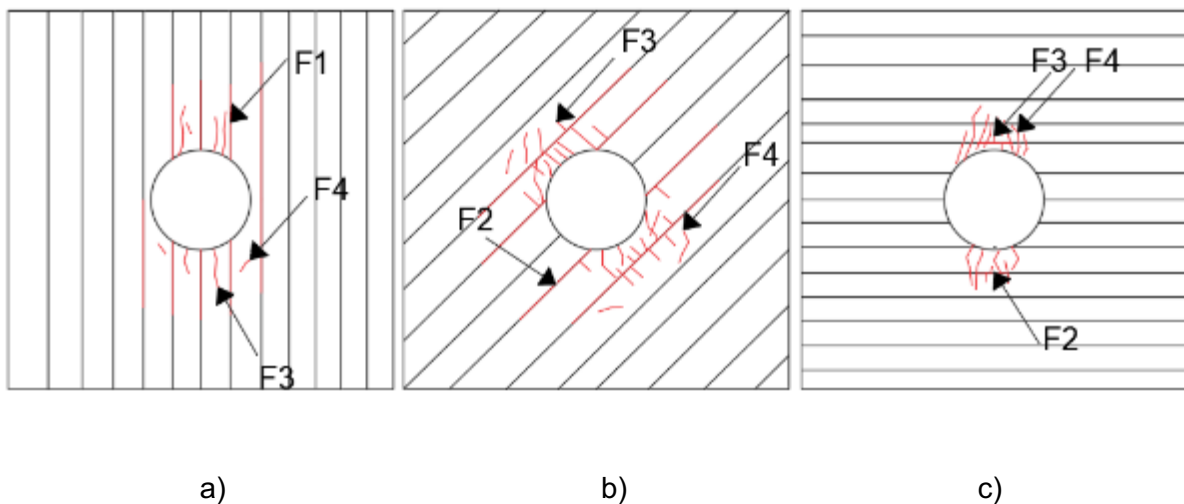
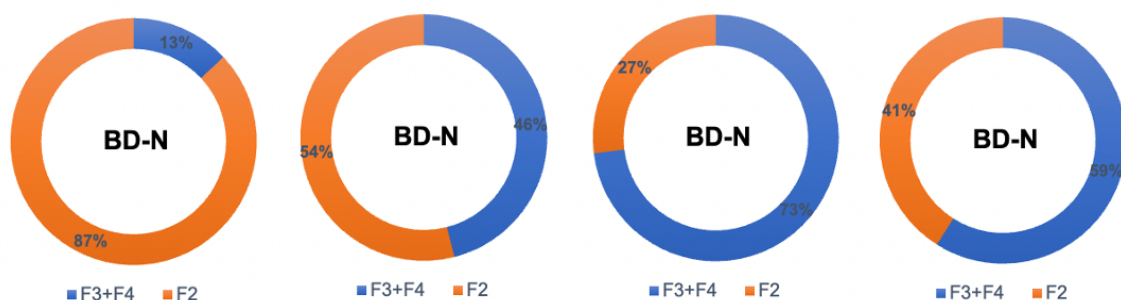


Figure 17 The diagram of three fracturing modes of tunnel excavation in shale formation with different type of fractures for a) TS-S, b) BD-N, c) SL-N.

These three fracturing modes are all combinations of bedding plane tensile fractures (F1), bedding plane shear-slip fractures (F2), shale matrix tensile fractures (F3), and shale matrix shear fractures (F4), similar to the classified fractures in Deng et al., (2022). Based on cohesive element types (i.e., matrix cohesive element and bedding plane cohesive element) and fracturing mechanism of each fracturing mode, F1 and F2 fractures are associated with the bedding planes of the cohesive elements (COH2)

that formed along the bedding planes in the models, while F3 and F4 fractures are associated with matrix cohesive elements that developed inside of the shale matrix, as illustrated in section 3.2.4, Chapter 3. The number of broken cohesive elements, in terms of COH1 and COH2 are collected from each failure model (i.e., A1 – A13). The distinguishing of F1 and F3 fractures is based on the fracturing mechanism of the model and also fracture propagating behaviours (Shen et al., 1995). As illustrated in Figure 5.17, F3 and F4 fractures in the fracturing model are hard to distinguish, since they are normally both present. Hence, the number of F3 and F4 (i.e., COH1) are counted together. Figures 5.18-5.20 illustrate the fracturing modes of the surrounding rock mass showing the frequency of the different fracture types under different conditions.

As depicted in Figure 5.18, the BD-N fracturing mode is mainly consisting of F2, F3 and F4 fractures. This is due to the failure mode caused by the shear-slip of the layers along the bedding planes. With increasing the lateral stress coefficient K_0 , the frequency of F2 drops initially until $K_0 = 1$. After that, the frequency of F2 increased when the lateral stress continued to increase. A highly anisotropic in-situ stress condition promotes the slippage of the bedding planes in the EDZ in the BD-N fracturing mode, whereas an isotropic in-situ stress condition limits the bedding plane slippages.



d)

Figure 18 Fracturing modes of the surrounding rock masses with the frequency of varying fracture types under different in-situ stress conditions a) $K_0 = 0.4$, b) $K_0 = 0.7$, c) $K_0 = 1.0$ and d) $K_0 = 1.3$.

As shown in Figures 5.1 and 5.18, changes in the in-situ stress in the surrounding rock have no impact on the fracturing mechanism of the shale tunnel, except the fracture frequency. Slippage of the bedding plane causes fracturing of the EDZ of the Full-scale Emplacement tunnel models with varying coefficients of lateral earth pressure. However, the in-situ stress greatly influences the EDZ fracturing conditions (e.g., EDZ depth, fracture numbers, and frequency of fracture types). The EDZ depth and fracture number increase as the lateral stress increases. Meanwhile, a highly anisotropic in-situ stress conditions promotes fracturing along the bedding planes.

According to Figure 5.19, the TS-S fracturing mode is mainly made up of F1, F3, and F4 fractures, and it is dominated by bedding plane tensile fractures F1. Meanwhile, SL-N is the same as BD-N and mainly formed by F2, F3 and F4 fractures. With bedding plane inclinations at 15° and 0°, SL-N fracturing mode cause by shearing through layers, so F3 and F4 dominate the fracturing mode with a contribution of 83% and 86%, respectively.





Figure 19 Fracturing modes of the surrounding rock masses with the frequency of varying fracture types under different bedding plane inclinations.

Based on Figures 5.7, 5.8 and 5.19, the bedding plane inclinations have a great impact on shale tunnel fracturing mechanism and fracturing conditions. The fracturing mode is significantly related to the bedding plane inclinations. With small bedding plane inclinations (i.e., 0° and 15°), the fracturing conditions of the surrounding rock mass is stable with a small EDZ and low fracturing numbers in the SL-N fracturing mode compared to the other two failure modes due to the fact that most of the fracture events happened inside of the shale matrix. With increasing bedding plane inclinations, the fracturing mode changes from SL-N to TS-S. The contribution of the F2 (COH2)

fractures are increasing. Hence, the depth and fracture numbers of the EDZ are also increasing due to the low strength of the bedding planes.

With the thickness of the layers increasing, the fracturing mode of the EDZ changes from BD-N to SL-N. While the frequency of F3 and F4 for layer thicknesses of 30mm, 75mm, and 150mm is 60%, 46%, and 62% respectively, the frequency of the F3 and F4 for a thickness of 300mm is increased to 91%, as shown in Figure 5.20. In the BD-N fracturing mode, the surrounding rock of the tunnel has a small layer thickness with many bedding planes, so the EDZ tends to slip along the bedding planes, resulting in a large number of F2 fractures. Due to the large layer thickness, the EDZ is in SL-N failure mode, resulting in fracturing inside the matrix with large numbers of COH1 (F3+F4) fractures.

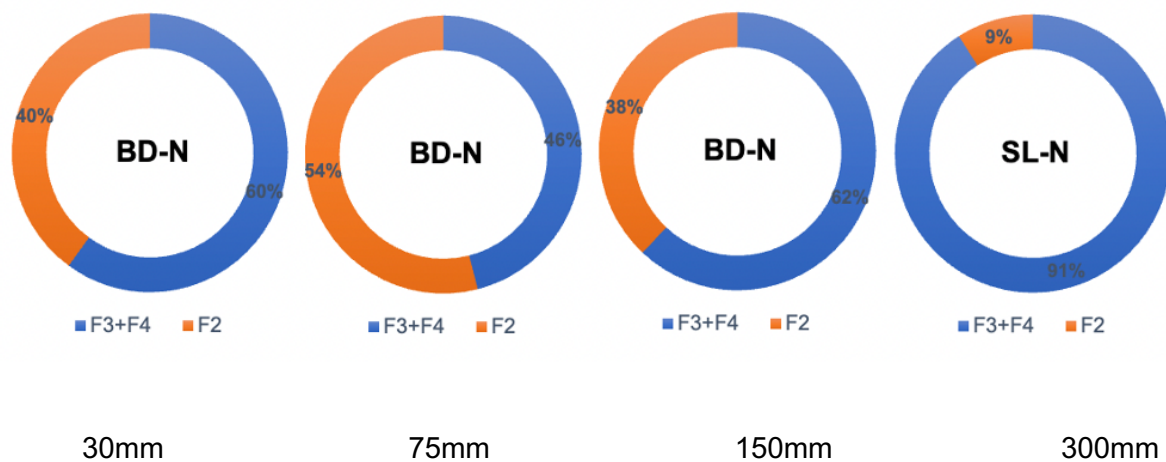


Figure 20 Fracturing modes of the surrounding rock masses with the frequency of varying fracture types under different layer thickness.

As shown in Figures 5.11, 5.12, and 5.20, the layer thickness in shale has a notable influence on shale tunnel fracturing mechanisms and fracturing conditions. With increasing layer thickness, the fracturing mode changes from BD-N to SL-N. With the reducing of bedding planes inside of the surrounding rock mass, it is harder for

fractures to form and propagate along the bedding planes. Hence, the displacements caused by the slippage of the bedding planes are limited, which leads to smaller EDZ depth and small fracture numbers.

As discussed above, the EDZ fracturing mechanisms and fracturing conditions (i.e., EDZ depth, fracture numbers, fracture frequencies) are significantly affected by layer thickness, and bedding plane inclinations. In-situ stress only affects the fracturing conditions in the EDZ, however. The fracturing mechanism of the EDZ is not related to in-situ stress. Three fracturing modes of EDZ have been picked up from the 13 models, in terms of BD-N, SL-N and TS-S. The failure mode of the TS-S only exists in situations when excavating in rocks with steep bedding plane inclinations. It is not related to other environmental conditions (i.e., in-situ stress and layer thickness).

Figure 5.21 shows three failure modes with the number of fractures and the depth of the EDZ under various environmental conditions. The number of fractures and EDZ depth in the three fracturing modes are generally in the following order: TS-S > BD-N > SL-N. As discussed in section 5.3.1, the weak cohesive strength of the bedding planes leads to the least amount of energy needed for fracturing based on the results of the uniaxial compressive test. As the TS-S fracturing mode results from tensile splitting of bedding planes, the EDZ depth and fracturing numbers tends to be the larger than other fracturing modes. In SL-N fracturing mode, shearing inside a shale matrix requires more energy than fracturing along bedding planes to form fractures and propagate them. Hence, SL-N fracturing mode tends to have the smallest number of fractures and depth of the EDZ. Compared to other scenarios, scenario A₁₁ (i.e., layer thickness of 0.3m) in BD-N fracturing mode has the most fractures in the EDZ. Based on the study of layer thickness effects on shale mechanical strength in section

4.5.1, the strength of shale model with inclinations is greatly affected by the layer thickness. In the model, low cohesion bedding planes are increased as layer thickness decreases, resulting in lower mechanical strength and severe fracturing conditions. This phenomenon indicates the layer thickness has a great impact on the fracturing conditions in the EDZ. The layer thickness effect on the fracturing mechanism of EDZ has been studied in previous studies, but its effect on the EDZ properties still remains unexplored (Deng et al., 2022). Future tunnel excavations should consider layer thickness through FDEM model to understand the fracturing laws of EDZ in anisotropic rock formations.

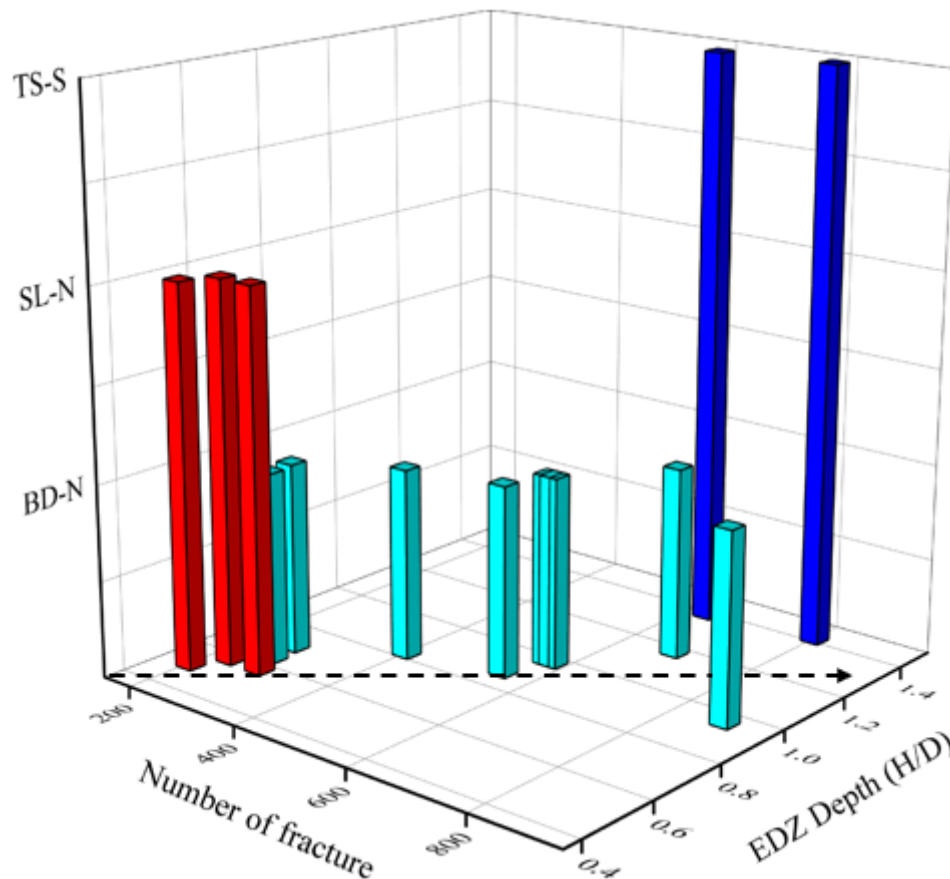


Figure 21 The number of fractures and EDZ depth in each model with corresponding fracturing modes (red bars indicate SL-N fracturing mode, light blue bars indicate BD-N fracturing mode, and dark blue bars indicate TS-S fracturing mode).

The depth of the EDZ is also greatly affected by the fracturing mode. The EDZ depth in the TS-S fracturing mode is approximately 1.4D. Meanwhile, the BD-N fracturing mode, the EDZ depth is approximately 0.9D. For the SL-N fracturing mode, the EDZ depth is approximately 0.5D.

5.8 Summary

One of the most challenging aspects of underground space excavation is the stability of underground cavities under shale formations. The anisotropic property of shale makes it difficult to predict the fracturing mode inside of the EDZ and its depth. The excavation response of the Full-scale Emplacement tunnel under Opalinus clay is simulated through FEM and FDEM, and the results are compared with field measurements in Chapter 3 . The validated Full-scale Emplacement tunnel FDEM model was then used to simulate the fracturing modes of the tunnel excavated in different conditions (i.e., in-situ stress, layer thickness and bedding plane inclinations). The key conclusions are:

- 1) Fracturing modes and fracturing conditions (i.e., EDZ locations, depth, fracture numbers and fracture frequencies) of the EDZ are significantly affected by the angle of the bedding plane, and the layer thickness. In-situ stress, however, only affects fracturing conditions in the EDZ. The fracturing mechanism of the EDZ is not related to in-situ stress.

- 2) The fracturing modes of tunnels excavated in shale under different conditions can be generally classified into three types: tensile-splitting spalling (TS-S), bedding plane delamination notches (BD-N) and shearing through layers notches (SL-N). The failure mode of TS-S only exists in situations when excavating in rocks with steep bedding

plane inclinations. It is not related to other environmental conditions (i.e, in-situ stress and layer thickness).

3) The fracturing mode affects where EDZs are located. In TS-S and SL-N fracturing modes, EDZs are located around the tunnel crown and invert, while in BD-N, it are approximately located at the left shoulder and right knee of the tunnel.

4) The displacement field is strongly affected by the dip angles of the layers in shale formation after excavation. With increasing dip angles, maximum displacement increases. However, the location of the largest displacement in each model is corresponding to the location of EDZs. As a result of the location of the maximum displacement in the models changing with bedding plane inclinations, the tunnel crown displacement initially decreases from 0° to 45° , then increases until it reaches 90° .

5) It has been approved that Bl_f is capable of predicting the fracturing conditions in EDZ. The greater the Bl_f , the more severe fracturing conditions in EDZ (e.g., fracture number and depth of EDZ).

6) The number of fractures in the three fracturing modes are generally in the following order: TS-S > BD-N > SL-N. The three fracturing modes are all combinations of bedding plane tensile fractures (F1), bedding plane shear-slip fractures (F2), shale matrix tensile fractures (F3), and shale matrix shear fractures (F4). TS-S fracturing mode is made up by F1, F3, and F4 fractures, and it is dominated by bedding plane tensile fractures F1. Meanwhile, the SL-N is the same to the BD-N formed by F2, F3 and F4 fractures. The failure of the EDZ in the BD-N is caused by the bedding planes sliding, while the failure in the SL-N is caused by shearing through the layers. Comparing to BD-N, SL-N have a higher frequency of F3 and F4. Having a higher frequency of F3 + F4 fractures indicates that the most fractures are formed and

propagated in the shale layers. Due to its higher mechanical strength, fracturing inside layers is more difficult than cracking along the bedding planes, which leads to a smaller EDZ depth.

7) The depth of the EDZ is related to the fracturing modes. With different bedding plane inclinations, the EDZ depth in the TS-S fracturing mode is approximately $1.4D$. Meanwhile, the BD-N fracturing mode, the EDZ depth is approximately $0.9D$. For the SL-N fracturing mode, the EDZ depth is approximately $0.5D$. Under different environmental conditions (i.e., layer thickness, in-situ stress and bedding plane inclinations), the extent of the EDZ in each fracturing mode varies. Generally, the depth of EDZ is in the order (from large to small): $TS-S > BD-N > SL-N$.

CHAPTER 6 CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

6.1. Introduction

In this research, two-dimensional FDEM models, developed in ABAQUS, were used to improve the understanding of shale anisotropy (i.e., mechanical properties, fracturing mechanism and brittleness) and its effect on the fracturing mechanisms and fracturing conditions of the EDZ in deep buried tunnels. Both laboratory experiments and full-scale tunnel excavations were used to evaluate the mechanisms.

The laboratory scale FDEM models were calibrated against mechanical values observed in laboratory tests on Longmaxi shale. By changing the bedding plane inclination in the shale model, the shale fracturing mechanics, the fracturing behaviours and the brittleness of the shale under shale anisotropy were studied from micro crack level. Two novel brittleness indices for shale and an empirical relationship to predict the tensile strength of shale, based only on uniaxial compression test results, have been proposed using the data gained from the FDEM simulation of the laboratory Brazilian disc tests.

The FDEM model was then extended to field scale to study the forming and propagation of the fractures inside of the EDZ during tunnel excavation under anisotropy shale formation. The ability of FDEM in modelling tunnel excavation is validated by comparing the surrounding rock mass constituting of Opalinus Clay with FEM model and field monitoring results. Furthermore, the short-term response of the anisotropic surrounding rock mass after tunnel excavation under different environment conditions (i.e., in-situ stress, layer thickness and bedding plane inclinations) were studied to gain new insights into the EDZ fracturing laws in shale. A summary of the

key findings from the studies conducted in this research is presented in this chapter, along with suggestions for future research.

6.2. Key findings and contributions to the field of knowledge

In comparison to conventional continuum methods, it was shown that FDEM models in ABAQUS can capture the fracturing behaviours of rocks by simulating fracture formation and propagation, which has been further used to bring new insights into the anisotropic behaviours of shale and its effects on deep buried tunnel EDZ properties and fracture mechanisms from a micro crack level of the deep buried tunnel EDZ.

Based on this, the key findings of this research are:

- 1) The literature review revealed that most studies investigating shale anisotropy have focused on macro mechanical strengths, but there is still a gap in understanding the mechanical behaviour under shale anisotropy at the micro crack level. The failure of rocks under stress is related to the propagation and coalescence of fractures, as addressed in previous studies. Moreover, the literature review has highlighted that fractures are one of the most prominent characteristics in the EDZ, but general conclusions and laws are lacking to understand the fracturing mechanism and fracturing conditions in shale formation. Several researchers had used numerical simulation for studying the shale anisotropy, but currently used numerical simulation approaches, such as finite element method (FEM) and discrete element method (DEM), have limitations when simulating anisotropic shale. They fail to accurately simulate the discontinuous features of the rock (e.g., joint and fractures) because of the continuum assumptions, and also the most significant post-excavation properties of fracture forming, and growth cannot explicitly be represented in

the model, as it lacks an internal fracturing mechanism. From the literature review it was shown that FDEM can model the transition of domains from continuums to discontinuum while requiring a reasonable amount of computation time for field scale simulations with explicitly simulating brittle fractures. This addressed objective 1.

2) Based on the identified gap in a literature, a FDEM modelling approach was developed by freely inserting cohesive elements into adjacent elastic elements in ABAQUS based on Python-code in this study to simulate shale anisotropy. Published data on Longmaxi shale laboratory tests and tunnel excavation in Opalinus clay shale was used to validate the new models. The FDEM model predicted well the short-term response of the surrounding rock with explicit show the fracturing behaviours inside rocks, which was a significant improvement over the FEM results which drastically underpredicted the deformation response of the rock mass. After the validation, addressing objectives 2 and 3, the model was used extensively to provide an in-depth insight of the failure mechanisms.

3) To address objective 4, this study investigated the shale failure modes, fracturing behaviours and brittleness from a microscopic viewpoint taking the shale anisotropy into account through FDEM simulation based on the calibrated shale laboratory scale model. The following are the key conclusions based on the results:

- Three failure modes were identified from the numerical model based on UCS data. This demonstrated that the failure process of anisotropic shale occurs in the order of shearing through the shale matrix (S-M) ($\theta = 0^\circ$ and 15°), bedding plane delamination (B-D) ($\theta = 30^\circ$, 45° and 60°) and tensile splitting (T-S) ($\theta = 75^\circ$ and 90°), with transitioning phases between these. At the same time, three different modes, in terms of central split along bedding planes (C-S) ($\theta = 75^\circ$

and 90°), inclined arch fracturing (I-A) ($\theta = 30^\circ, 45^\circ$ and 60°), central arch fracturing (C-A) ($\theta = 0^\circ$ and 15°) were identified in the BD test, with transitioning phases between these. These results agree with the published literature.

- Based on conventional brittleness indices obtained from both experimental and simulation results, the brittleness for the three failure modes of shale with different bedding plane inclinations are in the order: T-S > B-D > S-M. In rocks, bigger brittleness normally indicates greater frac-ability to fracture. However, based on the modelling, it was shown that the total fracturing numbers for the three failure modes is in the following order: T-S > S-M > B-D. This indicates the total fracturing numbers of shale under stress is not just related to the brittleness or frac-ability, but also shale structures. Shale in B-D failure mode tends to fracture along one bedding plane, which results in a small number of fractures.
- Shale frac-ability has been widely used in shale gas exploration industry to assess the ability of reservoirs to form fractures. However, there is still no general method for evaluating shale frac-ability quantitatively. Previous studies have proposed using different rock properties (e.g., conventional brittleness indices, fracture toughness and mechanical strengths) to assess the frac-ability. However, fracture numbers and fracture energies used to produce fractures were not considered. Therefore, a new brittleness index, Bl_f , has been proposed in this study. Bl_f is the ratio between the fracture numbers and plastic energy during UCS test which describes the efficiency of shale to transform plastic energy into fractures under compression. By better understanding the rock's frac-ability during tunnelling projects constructed in highly anisotropic shale, practitioners can make better decisions about the lining and support

requirements. The proposed brittleness indices, Bl_r , has the potential to provide the fracturing conditions of the surrounding rock due to underground excavation.

- The anisotropic property of shale significantly affects the mechanical strength and failure mechanism at the crack level. The crack damage stress (CD) threshold of shale is sensitive to shale anisotropic properties. Based on the observations, the shape of the curve between the CD and the bedding plane inclination is the same as the uniaxial compressive strength, which is a 'U' shape. When the stress inside the shale reaches the CD under the UCS test, cracks begin to propagate inside the shale. They may propagate along the bedding planes, cross the bedding plane, or even stop propagating, which are strongly affected by the bedding plane inclination. As a result, the failure modes of shale models with different bedding plane inclinations may affect the final emergent strength (i.e., uniaxial compressive strength). According to this phenomenon, this research proposed another novel brittleness index, Bl_{CD} , based on the ratio between the CD and the uniaxial compressive strength, σ_c . The higher the value of Bl_{CD} , the quicker the rock reaches the σ_c after the threshold of CD with smaller plastic strains. Comparing Bl_{CD} to conventional brittleness indices, based on the ratio between uniaxial compressive strength and tensile strength, Bl_{CD} can be easily obtained from UCS tests, which makes it easier for evaluating the brittleness of rocks.
- Based on the experimental data collected from literature, it has been shown that there is a relationship between the tensile strength, σ_t and CD . An empirical relationship has been proposed in this study to predict the σ_t based on the UCS tests. By comparing the predicted tensile strength for the Longmaxi shale with different bedding inclinations using the empirical equation with the experimental

values, the empirical equation is verified. Considering that obtaining the tensile strength of rocks directly may be difficult under certain conditions, using this empirical relationship based only on the UCS test can provide an alternative. However, this empirical relationship needs further improvement (e.g., more experimental data on different types of rocks) to give greater confidence in its accuracy.

- The thickness of anisotropic rock layers plays a significant role in its mechanical strength, fracturing conditions, and brittleness. However, it varies among anisotropic rock with different bedding plane inclinations. For S-M failure mode, the influence of the layer thickness on anisotropic rock's mechanical strength, fracturing conditions and brittleness is limited due to its failure mostly happened inside of rock matrix. In the meantime, the reduction of layer thickness in anisotropic rock has resulted in reduced mechanical strength and greater brittleness for T-S and B-D failures, since rock failure occurs along bedding planes in the two failure modes.

4) In regard to objectives 5 and 6, the verified field scale tunnel excavation model was exposed to 13 different scenarios in order to study the effects of in-situ stress, bedding plane inclination, and layer thickness on the EDZ properties in anisotropic shale formation. As a result of analysing the EDZs' locations, depth, fracturing mode and fracturing conditions of each scenario, the following conclusions can be drawn:

- The fracturing modes of a tunnel excavated in shale under different conditions can be generally classified into three types: tensile-splitting spalling (TS-S), bedding plane delamination notches (BD-N) and shearing through layers notches (SL-N). These modes were all confirmed by other researchers previously.

- EDZ properties are greatly affected by in-situ stress, bedding plane inclination, and layer thickness. Fracturing modes and fracturing conditions (i.e., EDZ locations, depth, fracture numbers and fracture frequencies) are significantly affected by the dip angle of the bedding plane, and the layer thickness. In-situ stress, however, only affects fracturing conditions in the EDZ. The fracturing mode of the EDZ is not related to in-situ stress. Meanwhile, the failure mode of TS-S only exists in situations when excavating in rocks with steep bedding plane inclinations. It is not related to other environmental conditions (i.e., in-situ stress and layer thickness). These findings can help improving the understanding of the shale fracturing mechanism and behaviours during excavation under complicated geo-environments.
- This study provided the first analysis of EDZ's fracturing modes from fracturing numbers and frequencies of fractures. The number of fractures in the three fracturing modes are generally in the following order: TS-S > BD-N > SL-N. The three fracturing modes are all combinations of bedding plane tensile fractures (F1), bedding plane shear-slip fractures (F2), shale matrix tensile fractures (F3), and shale matrix shear fractures (F4). TS-S fracturing mode is made up by F1, F3, and F4 fractures, and it is dominated by bedding plane tensile fractures F1. Meanwhile, the SL-N is the same to the BD-N formed by F2, F3 and F4 fractures. The failure of the EDZ in the BD-N is caused by the bedding planes sliding, while the failure in the SL-N is caused by shearing through the layers. Comparing to BD-N, SL-N have a higher frequency of F3 and F4. Having a higher frequency of F3 + F4 fractures indicates that the most fractures are formed and propagated in the shale layers. Due to its higher mechanical

strength, fracturing inside layers is more difficult than cracking along the bedding planes, which leads to a smaller EDZ depth.

- The locations and depth of EDZ is related to the fracturing modes. In TS-S and SL-N fracturing modes, EDZs are located around the tunnel crown and invert, while in BD-N, is approximately located at the left shoulder and right knee of the tunnel. With different bedding plane inclinations, the EDZ depth in the TS-S fracturing mode is approximately 1.4D. Meanwhile, the BD-N fracturing mode, the EDZ depth is approximately 0.9D. For the SL-N fracturing mode, the EDZ depth is approximately 0.5D. Under different environmental conditions (i.e., layer thickness, in-situ stress and bedding plane inclinations), the extent of the EDZ in each fracturing mode varies. Generally, the depth of EDZ is in the order (from large to small): TS-S > BD-N > SL-N. These new finding can help researchers and engineers in future to predict the depth of the EDZ, optimize the supporting methods and parameters and access to the stability of the tunnel.
- The Bl_f has been used to validate its application to the field tunnel projects. It has been approved that Bl_f is capable of predicting the fracturing conditions in EDZ. The greater the Bl_f , the more severe fracturing conditions in EDZ (e.g., fracture number and depth of EDZ).

6.3. Recommendations for future research

While this research has significantly advanced the understanding of shale failure mechanisms taking into account its anisotropic behaviour, there are some aspects which require further work to provide further confidence in the findings.

- 1) The improvement of the proposed empirical relationship

In Chapter 4, an empirical relationship has been proposed to predict the tensile strength based on the UCS tests. In order to give greater confidence in its accuracy, the empirical relationship needs further improvement (e.g., more experimental data on different types of rocks).

2) Excavation method influence on the EDZ

The FDEM model developed in this thesis can be used to model different excavation methods thereby helping to understand the contributions of the anisotropy of shale to the fracturing conditions of the EDZ (e.g., the depth of the EDZ and fracturing numbers), which will help researcher and engineers in the future to choose appropriate excavation methods and optimize the supporting parameters.

3) The study of the long-term stability of the tunnel using FDEM

This research only focused on the short-term response of the surrounding rock during the excavation through FDEM. Several hydro-mechanically coupled processes seem to influence the long-term response of the surrounding rock in shale formations (e.g., rock mass desaturation, swelling, fracture self-healing etc). Future work focusing on the long-term stability of the tunnel in shale should consider those important processes in numerical simulation.

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Appendix A Source code

Following is a list of the code implementations used in this thesis. This algorithm helps to inserting cohesive elements into ABAQUS 2D models' domains. A description of the basic logic of this code can be found in Chapter 3, Section 3.2.2. The adopted programming language is Python. After the symbol of #, the essential inline source codes are commented to help reviewers understand.

Source Code:

```
Ori_file=open("/file_directions/Hongtao_Li_ABAQUS_fdem.inp",'r') #open inp file
filelines=Ori_file.readlines() #create a list with lines from inp file
a=0
b=0
Ori_node_dic={} #create a dictionary of original nodes information from inp file
for i in range(len(filelines)): #looking for lines start with *node in list
    if filelines[i].startswith('*Node'):
        a=a+1
    if filelines[i].startswith('*Element'):
        a=0
        break
    if a==1:
        b+=1
        if b>1:
            NL=filelines[i].replace(' ','').replace('\n','').split(',')#create a new list
            with node information
            Ori_node_dic[NL[0]]=NL[1:]#append keys information in the node
            dictionary
```

```

        else:

            pass

Max_number=b-1

for i in range(len(filelines)): #find element set start and end numbers

    if filelines[i].startswith('*Elset, elset=Set-1, generate'):

        ele_start=int(filelines[i+1].replace(' ',').replace('\n','').split(',')[0])

        ele_end=int(filelines[i+1].replace(' ',').replace('\n','').split(',')[1])

a=0

b=0

Ori_ele_dic={}#create a dictionary of original elements information

for i in range(len(filelines)):

    if filelines[i].startswith('*Element'):

        a=a+1

    if filelines[i].startswith('*Nset'):

        a=0

        break

    if a==1:

        b+=1

        if b>1:

            EL=filelines[i].replace(' ',').replace('\n','').split(',')#create a list with
element information

            if int(EL[0]) in range(ele_start,ele_end+1):

                Ori_ele_dic[EL[0]]=EL[1:4] #append keys information in the
element dictionary

        else:

            pass

```

```
Node_Number_L=[NL[0]]#create a list of node number
```

```
Ori_Node_appeartimes=dict.fromkeys(Node_Number_L,0)#count each original node  
appeartimes in all element list
```

```
for i in Ori_ele_dic:
```

```
    for j in Ori_ele_dic[i]:
```

```
        if j in Node_Number_L:
```

```
            Ori_Node_appeartimes[j]+=1
```

```
New_node_dic={}#create a list of new node number
```

```
for i in Ori_node_dic:
```

```
    if i in Node_Number_L:
```

```
        for j in range(Ori_Node_appeartimes[i]+1):
```

```
            New_node_dic[str(j*(10**(len(str(Max_number))))+int(i))]=New_node_dic[i]
```

```
New_node_dic_sort=sorted([int(i) for i in New_node_dic.keys()])#write new nodes in new  
file
```

```
New_file=open("/newfile.txt",'w')
```

```
for i in range(len(filelines)):
```

```
    New_file.write(filelines[i])
```

```
    if filelines[i].startswith('*Node'):
```

```
        break
```

```
for i in New_node_dic_sort:
```

```
    New_file.write(str(i))
```

```
    New_file.write(',')
```

```
    New_file.write(New_node_dic[str(i)][0])
```

```
    New_file.write(',')
```

```
    New_file.write(New_node_dic[str(i)][1])
```

```

        New_file.write('\n')

New_file.write('*Element, type=CPS3\n')

Element_nodes_assign=dict.fromkeys(New_node_dic,1)#assign elements with new nodes

def f(x):#Recognise new nodes number

    if len(x)<=len(str(Max_number)):

        return x

    if len(x)>len(str(Max_number)):

        return str(int(x[-len(str(Max_number))]))

for i in Ori_ele_dic:

    for j in range(3):

        for k in Element_nodes_assign:

            if Element_nodes_assign[k]!=0 and f(k)==Ori_ele_dic[i][j]:

                Ori_ele_dic[i][j]=k

                Element_nodes_assign[k]=0

New_ele_dic_sort=sorted([int(i) for i in Ori_ele_dic.keys()])

for i in New_ele_dic_sort:

    New_file.write(str(i))

    New_file.write(', ')

    New_file.write(New_node_dic[str(i)][0])

    New_file.write(', ')

    New_file.write(New_node_dic[str(i)][1])

    New_file.write(', ')

    New_file.write(New_node_dic[str(i)][2])

    New_file.write('\n')

```

```
New_file.write('*Element, type=COH2D4\n')#write the type of cohesive elements in  
ABAQUS
```

```
Coh_ele_dic={} #create a dictionary of cohesive element
```

```
m=ele_end+1
```

```
ela_ele=sorted([int(i) for i in Ori_ele_dic.keys()])
```

```
for i in ela_ele: #assign the cohesive elements with nodes
```

```
    for j in range(i+1,ele_end+1):
```

```
        c=[]
```

```
        for k in ela_ele[str(i)]:
```

```
            for l in ela_ele[str(j)]:
```

```
                if f(k)==f(l):
```

```
                    c.append([k,l])
```

```
            if len(c)==2:
```

```
                Coh_ele_dic[str(m)]=[c[0][0],c[0][1],c[1][0],c[1][1]]
```

```
                m+=1
```

```
#write cohesive elements with assigned nodes in new file
```

```
for i in Coh_ele_dic:
```

```
    New_file.write(str(i))
```

```
    New_file.write(',')
```

```
    New_file.write(Coh_ele_dic[str(i)][0])
```

```
    New_file.write(',')
```

```
    New_file.write(Coh_ele_dic[str(i)][1])
```

```
    New_file.write(',')
```

```
    New_file.write(Coh_ele_dic[str(i)][2])
```

```
    New_file.write(',')
```

```
    New_file.write(Coh_ele_dic[str(i)][3])
```

```
New_file.write('\n')
```

```
New_file.close()
```

Appendix B Publications and conference

HT, Li., D, Chapman., A, Faramarzi., N, Metje., 2023. FDEM analysis of the fracturing mechanism and brittleness characteristics of anisotropic shale – *Rock Mechanical and Rock Engineering*.

HT, Li., D, Chapman., A, Faramarzi., N, Metje., 2023. Numerical simulation of the EDZ of shale around tunnel excavation using the FDEM – *Tunnel and Underground Space Technology* (Under review).

HT, Li., A, Faramarzi., D, Chapman., N, Metje., 2023. FDEM analysis of the thickness of bedding layers effects on the fracturing mechanism and brittleness characteristics of anisotropic shale – Finished writing and plan to submit to *Computers and Geotechnics*.

Attended UKACM 2021 Conference, Presented 'The effect of anisotropic characteristics of shale on its mechanical properties and failure patterns'.