



Analysis of Permeability Evolution due to Compaction Localisation in Porous Reservoir Rocks

A Thesis submitted for the Degree of Master of Philosophy

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by

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HDR THESIS DECLARATION

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THESIS ABSTRACT

Constitutive modelling of geomaterials that can both describe the field-scale behaviour and microscopic details while dealing with hydro-mechanical coupling problems is crucial for predicting the failure of petroleum reservoirs. Highly porous rocks like sandstone, which are typically found in petroleum and gas reservoirs, have been observed to exhibit localised deformation both in experiments and in the field. This phenomenon occurs when stress concentration in weak zones at the grain scale triggers localised deformation, leading to the formation of narrow zones called compaction bands and hence bifurcation of behaviour from homogeneous to strongly localised. Breakage mechanics has been successfully used to describe the mechanisms of grain crushing, a key factor constituting the formation of compaction bands. This theory provides the capability of linking stress with evolving grain size distribution and hence permeability for a homogeneous volume element. However, as a continuum model that relies on the assumption of homogeneous deformation, it fails to correctly describe the post-localisation stage of behaviour where the assumption of homogeneous deformation is no longer valid.

This study aimed to develop a model, based on breakage mechanics, that could correctly capture both pre- and post-localisation stages of behaviour. In addition, the progressive characteristics of compaction bands should be taken into account as they have been observed to develop successively until the whole volume is compacted. It should be noted that the current breakage model cannot efficiently cope with the material behaviour under low confining pressure, and thus the high-pressure regime is the primary focus in this study. The key innovation is exploring the macro permeability evolution of porous rocks by using this enhanced model to track the stress-permeability behaviours at a lower scale corresponding with the compaction band and its surrounding mass.

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LIST OF SYMBOLS

Latin symbols

B	breakage variable
C_{ij}	localisation acoustic tensor
D	grain diameter
D_H	harmonic grain size
$\langle D^2 \rangle_0$	second-order moments of the initial grain size distribution
$\langle D^2 \rangle_u$	second-order moments of the ultimate grain size distribution
D_{ijkl}^e	elastic stiffness tensor of the material
D_{ijkl}	tangent stiffness tensor of the material
D_{ijkl}^i	tangent stiffness tensor of the region inside of a localisation band
D_{ijkl}^o	tangent stiffness tensor of the region outside of a localisation band
E_B	breakage energy
E_c	breakage critical energy threshold
f	volume fraction of a localisation band
F_0	initial cumulative function of grain size distribution
F_u	ultimate cumulative function of grain size distribution
g	plastic potential
g_j	directional vector of the relative velocity between the regions inside and outside of a localisation band
G	shear modulus
h	thickness of a localisation band
H	characteristic length of the volume element containing a localisation band
$\mathcal{H}$	hydraulic head
K	bulk modulus (in the calculation of material stiffness)
K	isotropic permeability (in the calculation of permeability)
$\mathbf{K}$	macroscopic permeability (matrix form)
K_i	permeability component of the region inside of a localisation band
K_o	permeability component of the region outside of a localisation band
M	ratio of the ultimate shear and volumetric stress
$\mathbf{n}$	orientation vector of a localisation band (matrix form)
n_l	orientation vector of a localisation band (tensorial form)
p	effective mean stress

p_c	confining pressure in triaxial experiment
p_{cr}	critical crushing pressure
p_u	ultimate grain size distribution
p_0	initial grain size distribution
∇p	hydraulic pressure gradient
q	deviatoric shear stress
r_i	residual traction
R_K	permeability reduction
s_{ij}	deviatoric stress tensors
S	surface area of a localisation band (in the calculation of localisation volume fraction)
S	surface area of a particle-shape grain (in the calculation of permeability)
t_i	traction tensor
T	hydraulic tortuosity
$\dot{u}_k$	relative velocity jump between two faces of the localisation band
V	volume of a volume element
$\mathbf{v}$	Darcy relative flow velocity (matrix form)
$\mathbf{v}^f$	fluid velocity (matrix form)
$\mathbf{v}^s$	solid velocity (matrix form)
v_i	fluid velocity in the region inside of a localisation band
v_i	fluid velocity in the region outside of a localisation band
y	yield function

Greek symbols

ε_a	axial strain
ε_s	total shear strain
ε_s^e	elastic shear strain
ε_v	total volumetric strain
ε_v^e	elastic volumetric strain
ε_{kl}	total strain tensor
ε_{kl}^e	elastic strain tensor
$\dot{\varepsilon}_{kl}$	incremental total strain tensor
$\dot{\varepsilon}_{kl}^p$	incremental plastic strain tensor
$\dot{\varepsilon}_{kl}^e$	incremental elastic strain tensor
ε_{kl}^i	strain tensor of the region inside of a localisation band
ε_{kl}^o	strain tensor of the region outside of a localisation band
ϑ	breakage grading index
λ	the non-negative plastic multiplier
σ_{ij}	total stress tensor

σ_{ij}^i	stress tensor of the region inside of a localisation band
σ_{ij}^o	stress tensor of the region outside of a localisation band
ϕ	porosity
Φ	breakage dissipation potential
ψ	breakage energy potential
ω	plastic-breakage coupling angle

Chapter 1

THESIS OUTLINE

Porous reservoir rocks have been addressed as vital sources of oil and gas extraction while featuring complex behaviour and damage related to their vulnerability to the fluid flow. Two vital characteristics of reservoir rocks are porosity and permeability which permit petroleum storage and flow communication, respectively. However, these properties can vary significantly during the extraction procedure when boreholes are drilled down to the earth's crust and perforate it, creating petroleum pathways to connect reservoirs with production wells (Papamichos et al., 1993; Torabi et al., 2015; Liu et al., 2021; Sawa et al., 2021). These artificial operations, alongside tectonic movements (burial and uplift), can induce overburden stress and confining pressure which causes compressive deformation, and thus, reduces permeability. Hence, an accurate assessment of the performance of reservoirs requires understanding their behaviour and how it affects fluid flow under different loading conditions. Moreover, feasible prediction of permeability evolution during exploration and production is only possible if the mechanisms affecting its evolution are understood.

The study of reservoir rock can be conducted on samples in lab experiments after being harvested from outcrops. To obtain trustworthy responses similar to in-situ reservoir rocks, these cores should be chosen adequately. Sandstone is often considered to be a replicate of reservoir rocks based on the fact that the original formation of reservoir rocks primarily involves sand deposition, which explains why 60% of all petroleum reserves today are made of sandstone (Bjørlykke and Jahren, 2010). Moreover, among the main sedimentary components including arkose, sandstone, limestone, and dolomite, sandstone exhibits the most similar micromechanical behaviours to that of the reservoir rock. In order to understand and predict the failure of large scale structures composed of porous rock, some critical questions related to the underlying deformation mechanisms should be addressed: what types of micro-mechanisms of reservoir rocks should be chosen in numerical simulation to ensure the accurate calculations of macroscopic deformation? How small should they be so that the micro-macro link is still maintained and the cost of computational analysis is relatively low? What theory and computational technique will allow us to do that?

The non-linear inelastic behaviour of porous rocks is usually associated with the formation of localized deformation zones. They are usually in the form of dilation bands at low confining pressures and compaction bands at high confining pressures (Olsson, 1999; Fossen et al., 2007; Kolyukhin et al., 2010; Renard et al., 2019; Makhnenko et al., 2020; Baud et al., 2021) as observed in many conventional triaxial tests. It is intrinsically governed by the interaction

between crushing, grain sliding/rotation of grains and pore collapse inside the localisation band at the micro-scale (Menéndez et al., 1996; Fossen et al., 2007; Barnicoat et al., 2009; Sufian and Russell, 2013; Ecay et al., 2020). Previous studies have found this phenomenon occurring in sandstone samples as shear bands under low confining pressure controlled by cement debonding or compaction bands induced by grain crushing under high confining pressure. This localised deformation holds great potential for governing the inelastic failure, with a strong gradient or discontinuity of kinematic quantities, of the whole host rock. **Chapter 2** discusses the fundamentals of localised deformation and the effect of deformation on the behaviour of sandstone as well as permeability change. In addition, the particular compaction mode of localisation is addressed because this is quite common in sandstone reservoirs during field observations, which is also in agreement with the findings in triaxial compressive experiments.

Grain crushing, cement debonding and pore collapse are three competing micro-mechanisms that govern the formation of localisation bands in different modes. The initiation and evolution of these mechanisms depend on the magnitude of confining pressure. The behaviour of a compaction band is strongly dictated by the effects of grain crushing under high confining pressure where the grains are crushed and rearranged, resulting in a change in grain size distribution. The theory of breakage mechanics, deriving from the original work of Einav (2007a,b) can take into account this grain crushing phenomenon to track the evolving grain size distribution that associates with the macro continuum stress-strain response through an internal variable. The first section of **Chapter 3** explains the fundamentals of breakage mechanics as well as the implementation of breakage mechanics into a constitutive model to analyse the behaviour of the sandstone specimen under high-confining pressure in triaxial tests.

It is well known that compaction localisation leads to strong inhomogeneous deformation which models based on the classical continuum approach are not able to describe correctly. Field observations, experimental studies, as well as computational assumptions, have recognised that the width h of a localisation band has a connection with the microstructure and inelastic microstructural changes of the material inside the band (Mühlhaus and Vardoulakis, 1987; Fossen et al., 2011; Cheung et al., 2012; Baud et al., 2015; Farquharson et al., 2017; Leuthold et al., 2021b). In contrast, the problem boundary for the numerical technique often takes into account another length scale H , representing the spatial discretisation over the domain where the constitutive response of the material is defined. The second section of **Chapter 3** discusses the so-called dual-scale framework (Nguyen et al., 2012; Nguyen et al., 2014; Nguyen et al., 2016b; Nguyen and Bui, 2020) that can connect these two length scales in correspondence with the material behaviour inside and outside the localisation zone. The key idea of this framework is to enhance the description of the constitutive behaviour in numerical analysis to account for strong inhomogeneous deformation due to compaction localisation. The application of this framework to correctly describe and capture both pre- and post-localisation behaviour at the constitutive level will enable physically meaningful solutions to be obtained in large-scale failure analysis.

Within the framework of breakage mechanics theory, the importance of localisation characteristics has been investigated using different models (Das et al., 2011, 2013; Das et al.,

2014; Tengattini et al., 2016; Nguyen et al., 2017), all of which employ the classical discontinuous bifurcation criterion (Rudnicki and Rice, 1975) to detect the onset of localisation and orientation of localisation band. Other models based on damage mechanics and plasticity theory have also been employed to capture both the onset of localisation and post-localisation behaviour (Mir, 2017; Mir et al., 2018). However, these models cannot capture localised modes of failure in conventional triaxial tests under low confining pressures due to the lack of appropriate constraints for describing the symmetry properties of the applied confining stresses under conventional triaxial conditions.

In **Chapter 4**, an approach to analysing bifurcation using a breakage mechanics model (Einav, 2007a, b) is developed to better predict the onset of localisation bands in conventional triaxial tests. The number of stress-strain tensor components is reduced from six to five based on an extra constraint on the symmetry of confining stress in conventional triaxial conditions, resulting in a more appropriate matrix form of tangent stiffness and normal vector. This allows the breakage model to correctly detect localisation in a wide range of confining pressures at the onset of yielding. The promising features of this approach are elucidated, and the results validated with experimental counterparts.

Based on the available experimental results, the analysis in this research was conducted using the enriched dual-scale framework based on the theory of breakage mechanics to describe the constitutive behaviour of porous reservoir rocks. The general approach involves a Representative Volume Element (RVE) with a composite skeleton comprising the macroscale volume outside and the mesoscale volume inside the localisation band which possess distinct responses (Figure 1.1). The analysis revealed the relationship between compaction localisation in reservoir sandstone and effective permeability. The findings of this project address the gaps in the current literature concerning how the permeability quantitatively changes when compaction localisation occurs.

Chapter 5 demonstrates the validation of the macro stress-strain response from the dual-scale constitutive model based on the theory of breakage mechanics as well as discussing localisation mechanisms behind the curve which the model can correctly describe and capture. Once the constitutive structure is correctly described, the stress-permeability relationship, taking into account compaction localisation and post-localisation behaviour, can be obtained to demonstrate the importance of compaction localisation in capturing the evolution of permeability.

Chapter 6 summarises the research findings in this thesis and considers future directions including (i) improving the capability of the breakage model in describing behaviour in a low-confining pressure regime, (ii) addressing the calibration of the experimental results to obtain a better set of parameters for numerical modelling, and (iii) identifying/investigating the fluid flow characteristics in a volume element with an embedded localisation band.

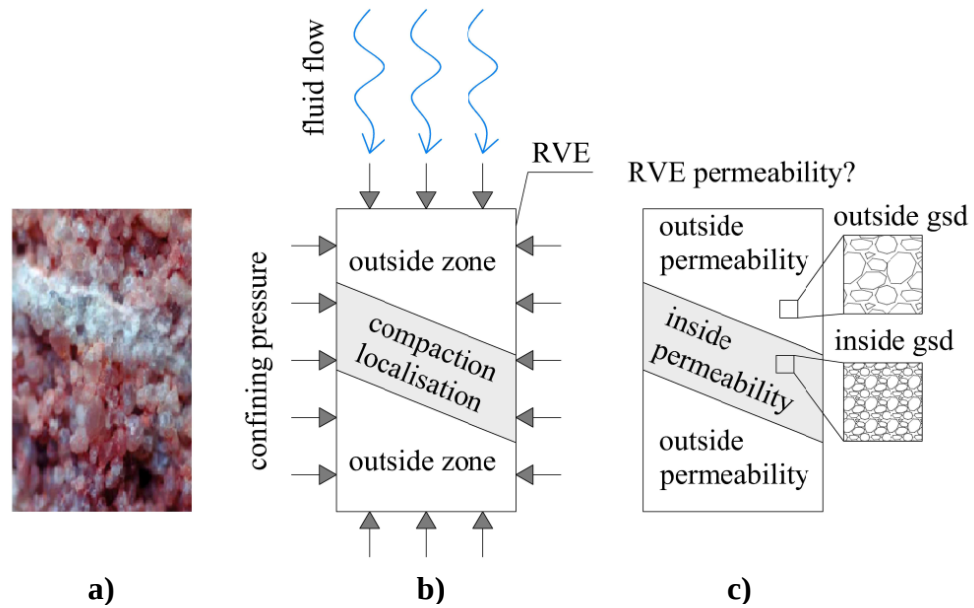


Figure 1.1. a) A compaction band found in Nubian Sandstone, Tayiba Red Beds, Sinai (Fossen et al., 2007); b) an RVE embedded with a localisation band under triaxial confining pressure while being exposed to the fluid flow; and c) a constitutive model based on the theory of breakage mechanics, which captures the involving gsd due to grain crushing, is implemented into a dual-scale framework, which is capable of describing a set of three separate constitutive relationships (macro-inside-outside) as well as the corresponding permeability evolution of porous reservoir rocks exhibiting compaction localisation.

Chapter 2

THE BEHAVIOUR OF POROUS RESERVOIR ROCKS AT DIFFERENT LENGTH SCALES

2.1 Overview of porous rock behaviour from micro- to macro-scale

Porous rocks are identified with many different microstructural features such as grain and pore size, the spatial distribution of pores, cracks, etc. The behaviour and failure of rocks from the macroscopic continuum perspective have been extensively explored alongside their underlying mechanisms occurring at the microscopic scale. Over the last few decades, observational studies on deformed rock samples have indicated that different types of porous rocks, implying different microstructural characteristics, undergo distinctive damage development. The macroscopic inelastic behaviour is often categorised by two distinct modes called “brittle” and “ductile”. The main difference between brittle and ductile behaviour lies in the rocks’ tendency to endure inelastic strain without forming fractures (Paterson and Wong, 2005). Brittle and ductile behaviour, as well as their transitioning phase, in granular material are associated with different levels of pressure, loading rate, temperature and most important of all, their microstructural mechanism.

The link between brittle-ductile response and the evolution of microscale mechanism of porous rocks have been investigated, especially on the outside of the elastic region. In the brittle faulting state, the mechanical response of the rock involves microcracking and frictional sliding (Evans et al., 1990) which allows the grain to debond, rotate and slip, resulting in the granular flow and shear stress drop (Wong et al., 1997; Zhu and Wong, 1997). In contrast, rocks may exhibit cataclastic (ductile) flow under high confining pressure where the grains are crushed and rearranged into the pore space, causing the material to harden (Zhang et al., 1990; Menéndez et al., 1996; Wu et al., 2000).

Questions have been raised regarding whether there is a bridge that brings these grain-scale processes to the field-scale behaviour. Studies on that mesoscopic connection have introduced the definition of strain localisation where the effect of micro-mechanisms strongly exhibits in a region observable as a thin band with inhomogeneous deformation inside an elastic bulk volume (Borja, 2000). In porous rocks sheared under high confining pressure, a link has also been observed between the phenomenon of compaction localisation and the stress states in the brittle-ductile transition, as documented by Wong et al. (2001).

Through a systematic classification, strain localisation in porous reservoir rocks is categorised into different modes which commonly include shear, compaction and dilation bands (Figure 2.1). Shear bands are predominated by shearing in the host rock while compaction and dilation bands are related to volumetric deformation (Aydin et al., 2006). Furthermore, hybrid bands have been categorised where compaction and dilation bands feature shear offset and become the compactional-shear and dilatant-shear bands (Figure 2.2). The mode differences governing the physical properties may lead to distinct non-uniform failure along with the heterogeneity of permeability and the behaviour of pore fluid flow (Fossen et al., 2007).

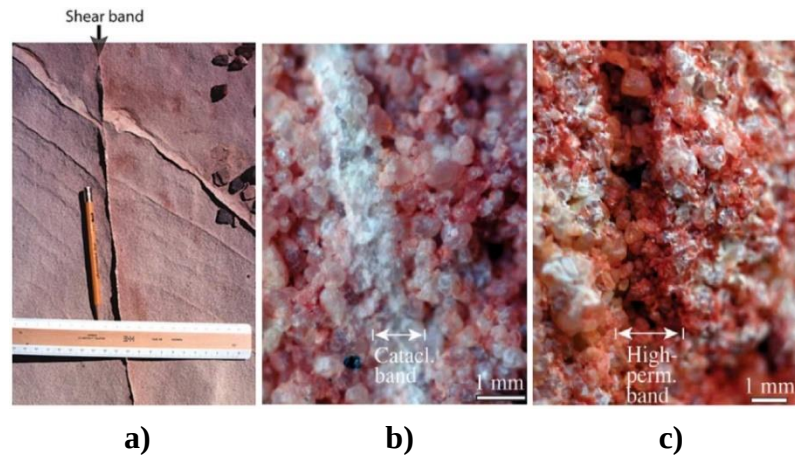


Figure 2.1. a) Shear band in Entrada sandstone (Aydin et al., 2006); b) compaction band featuring lower porosity than the surrounding; and c) Dilation band where higher porosity is observed (Fossen et al., 2007).

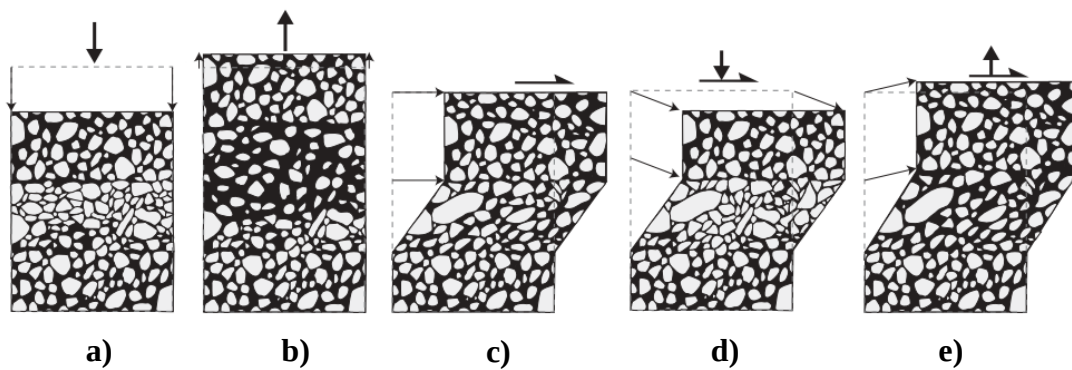


Figure 2.2. Kinematics classification of localisation band a) Compaction band; b) Dilation band; c) Shear band; d) Compaction shear band; and e) Dilation shear band (Fossen et al., 2007).

Observational studies of strain localisation on macroscopic stress-strain behaviour have identified a link between brittle-ductile responses with the mode of failure (Antonellini et al., 1994; Wong et al., 1997; Wong et al., 2001). Specifically, brittle shear and dilation bands are usually formed under low confining pressure. Conversely, high confining pressure leads to ductile deformation with volumetric compaction and cataclastic failure with the formation of

compaction bands. As highlighted by Fossen et al. (2007), low porous rocks are more likely to form tension fractures. Thus, it could be inferred that the high porosity level of reservoir rocks makes them more susceptible to compaction band formation, where grain crushing and pore collapse dominate.

2.2 Compaction localisation in porous rocks

2.2.1 Field-scale observations of compaction bands

Aydin and Johnson (1978) observed the failure of sandstones through formations of localized deformation bands in Entrada and Navajo sandstones, but these were not categorized as compaction or shear bands at the time. The term “pure compaction band” (PCB) was introduced after the exploration of localisation bands in Aeolian sandstones (Mollema and Antonellini, 1996) formed under compacting mode without any involvement of shear deformation. The grain size lying in the zone of compaction bands was noted to reduce one order of magnitude. On the other hand, a compaction band can refer to shear-enhanced compaction bands (SECB) with small shear offset or a compaction-shear band with a high degree of shear.

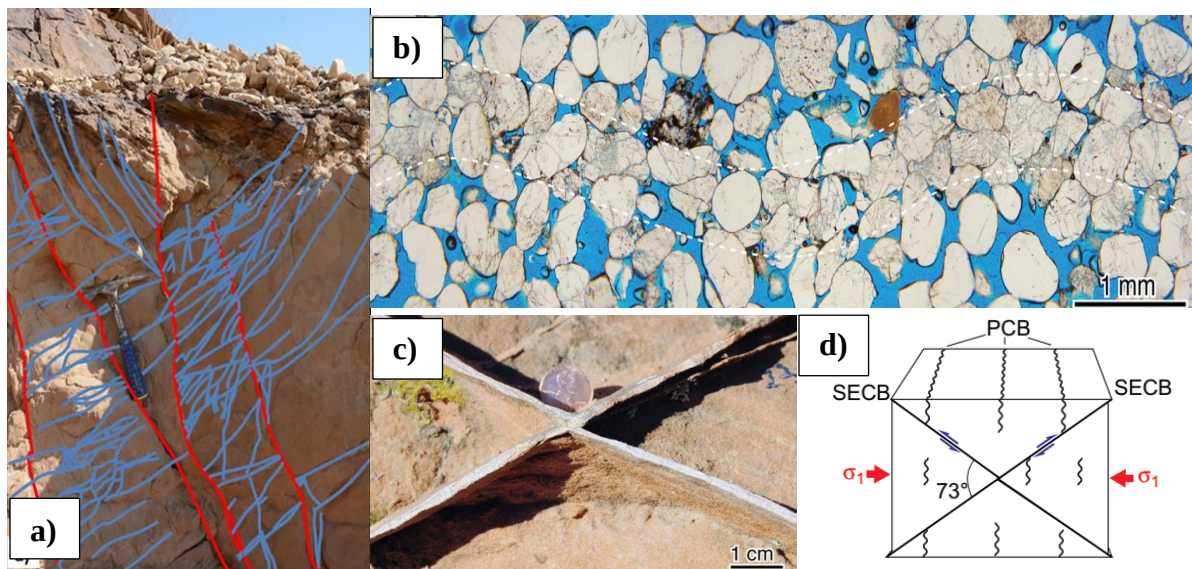


Figure 2.3. a) The occurrence of compaction bands (blue lines) as subparallel subarrays intersected with shear bands (red lines) which were found in the outcrop of Lower Cretaceous porous sandstone (Gajst et al., 2018). Geological observation of b) pure compaction bands and c) Shear-enhanced compaction bands in Navajo sandstone, Utah where their formation corresponds to the principal stress direction (Fossen et al., 2011).

Figure 2.3a-c show the continuum observations of compaction bands forming as a wavy band with around 1 mm thickness, while shear-enhanced compaction bands are thicker (Mollema and Antonellini, 1996). This geometry is a possible result of pore collapse clusters (Fortin et al., 2009; Fossen et al., 2011). Figure 2.3d demonstrates the conceptual difference in orientation between pure and shear-enhanced compaction bands within a sandstone cross-section. The

plane of pure compaction bands occurs perpendicular to the maximum compressive stress whereas a formation of crossing conjugate planes with a large dihedral angle can be detected with shear-enhanced compaction bands as reported by Eichhubl et al. (2010).

Recent field studies (Rotevatn et al., 2013; Rotevatn et al., 2016; Gajst et al., 2018) of shear-enhanced compaction bands and pure compaction bands have similarly concluded that they both form in highly porous rocks with large grains and that their occurrence tends to drastically reduce the rock porosity and grain sizes on their occurrence.

2.2.2 Compaction bands observed in laboratory-scale experiments

Laboratory-scale experiments on localisation bands are required since it is time-consuming to monitor these bands from the initiation to the propagation stage in the outcrops and also difficult because of their arbitrary occurrence. In fact, field studies conducted on existing localisation bands have missed the details of favourable stress conditions for the onset of localisation. Conducting a compressive triaxial test is a common technique that mimics the tectonic loading to obtain compaction bands. In order to obtain compaction bands inside the porous rock specimen, pure isotropic confinement was first applied without forming any kind of strain localisation. Afterwards, triaxial shearing was conducted once the stress condition had reached the required level at very high confining pressure, resulting in a progressive expansion of intense grain sliding/rotating and crushing zones all over the specimen volume. The microstructural process inside compaction bands during the deformation of porous rocks has been observed by many techniques including Acoustic Emission (AE) activity (Zhang et al., 1990; Wong et al., 1997; Baud et al., 2004; Fortin et al., 2006; Charalampidou et al., 2014), electron microscope scanning (Baud et al., 2004; Vajdova et al., 2004) and X-Ray CT-imaging (Antonellini et al., 1994; Charalampidou et al., 2010; Fonseca et al., 2013; Sufian and Russell, 2013; Shahin et al., 2019; Chen et al., 2020; Wu et al., 2020).

The modes of inelastic deformation are altered with different levels of confining pressure (Wong and Baud, 2012). Shearing at very low confining pressure induces softening behaviour with dilation failure as the porosity increases. While in the intermediate stress level regime, the mixed-mode localisation can be observed as shear-enhanced compaction bands forming an angle with maximum principal stress, the high to very high confining pressure will create pure compaction localisation with parallel arrays with respect to the bedding plane. In terms of the macroscopic response of highly porous sandstone, samples with low confining pressure often exhibit strain softening behaviour with increasing porosity which indicates dilatant deformation and the formation of shear bands (Figure 2.4a,b). It can be seen that the occurrence of localisation always induces the global strain softening of the specimen at the first stage of the post-yield phase. However, under high confining pressure and above, a switch from softening to hardening response takes place after reaching a large enough strain. In this case, the deviatoric stress promotes the formation and inelastic evolution of localised compaction. This is a consequence of significant compaction since increasing confining pressure leads to the reorganisation of the crushed grain structure inside the compaction bands. The local hardening

response propagates gradually until dominating the entire sample volume, resulting in a global strain hardening response (Figure 2.4c).

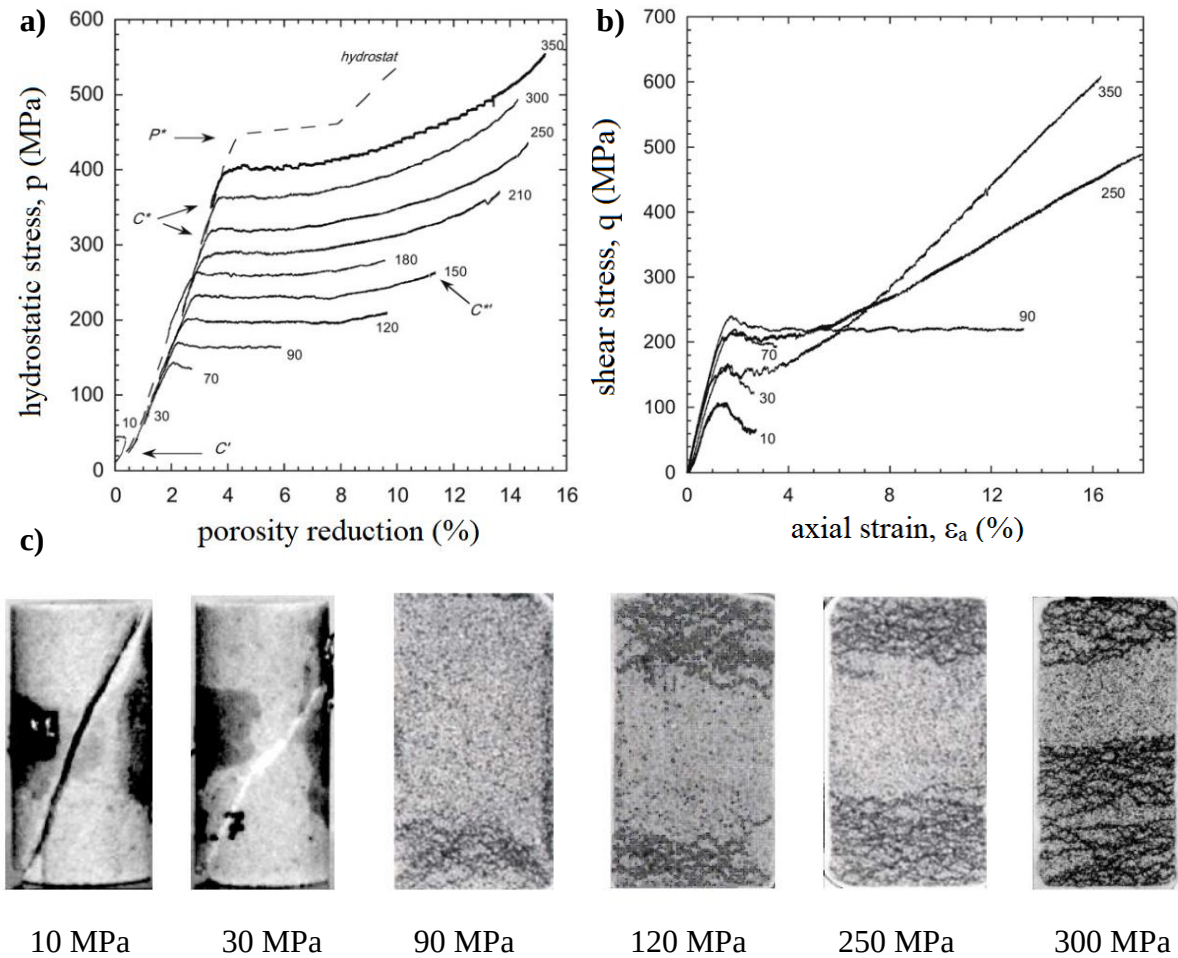


Figure 2.4. The macroscopic behaviour of drained triaxial test on highly porous rock (Bentheim sandstone) under different levels of confinement; a) the volumetric behaviour; b) the shear behaviour (Wong and Baud, 2012). c) Different failure modes of localisation in Bentheim sandstone samples from low to high confining pressure (Wong et al., 2001; Klein and Reuschlé, 2003; Baud et al., 2004).

From the above microstructural analysis, the onset of compaction bands can be triggered by an increasing stress concentration at weak points induced by local microstructural heterogeneity. Compaction localisation has been noticed to occur as a cluster of bands at the two ends of the triaxial specimen and propagate toward the centre during shearing under high confining pressure. This formation of localisation can also be detected through the stress-strain curves where episodic stress drops are located (Baud et al., 2004). Besides, the favourable stress condition where strain localisation initiates may relate to the yield stress and the peak stress which establishes the initial yield envelope. Specifically, peak stress indicates the development of conjugate shear failure induced by brittle faulting under low confining pressure, whereas the yield stress, detected by a surge in acoustic emissions, marks the formation of compaction bands in the high-pressure regime (Figure 2.5).

In addition, the degree of porosity in sandstones strongly governs the development of compaction bands. Baud et al. (2004) showed that the low-porous Darley sandstone failed with brittle deformation of the shear band at 10 MPa confining pressure and at 110 MPa displayed cataclastic flow failure, with no prior form of compaction localisation detected. However, Bentheim sandstone, known for its highly porous structure, has been documented to form subparallel arrays, perpendicular to the axial loading direction, of discrete compaction bands under a wide range of confining pressure (90 – 395 MPa).

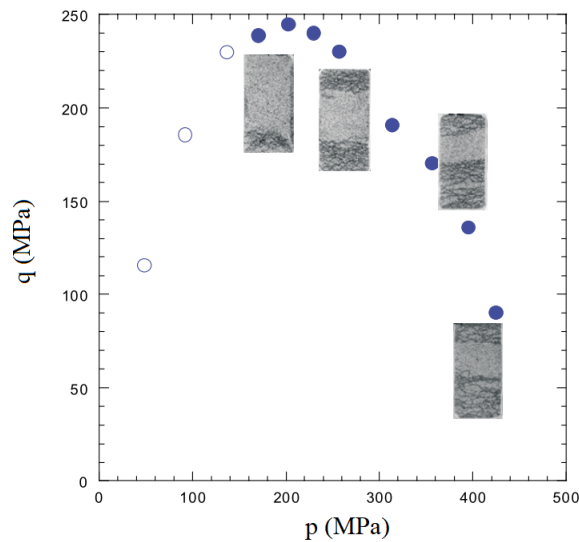


Figure 2.5. The peak stresses (open circle) for sample failing at brittle faulting and the compactive yield stresses (dark circle) at the onset of compaction localisation for Bentheim sandstones (Baud et al., 2004).

Inside the compaction band, the grain is crushed into very small fragments which appears as a dark area of intense comminution observable to the naked eye. (Figure 2.6a). This zone possesses micro-cracking within the cement/grain matrix which results in grain fragmentation and leads to a large strain-jump, referred to as cataclastic flow, compared to the surrounding volume (Zhang et al., 1990; Wu et al., 2000). Whereas on the outside, the crushing damage is negligible as very few cracks were detected. AE activity along with the recorded shear response were the shreds of evidence for compaction bands where their formation occurs at locations of episodic stress drops and surging AE levels (Figure 2.6b). Regarding the macroscopic behaviour under high pressure, the material undergoes accumulation of compacting damage which induces the compacting and hardening mechanism to progressively proceed all over the sample volume.

Despite the achievement of capturing the compaction bands in the specimen, these experiments still lack some features of the localisation conditions in the field. For instance, the strain rate in the field is much smaller than in the experiments during the band formation process (Fortin et al., 2006). This argument has also been mentioned by Fossen et al. (2011), specifically that undrained laboratory conditions under abnormally high pressure for well-cemented rock, like Berea sandstone, have resulted in different kinds of compaction bands as compared with the compaction bands found in outcrops. As a consequence, the degree of grain crushing, and the

length and the thickness of compaction bands in the field were much less than those in laboratory works.

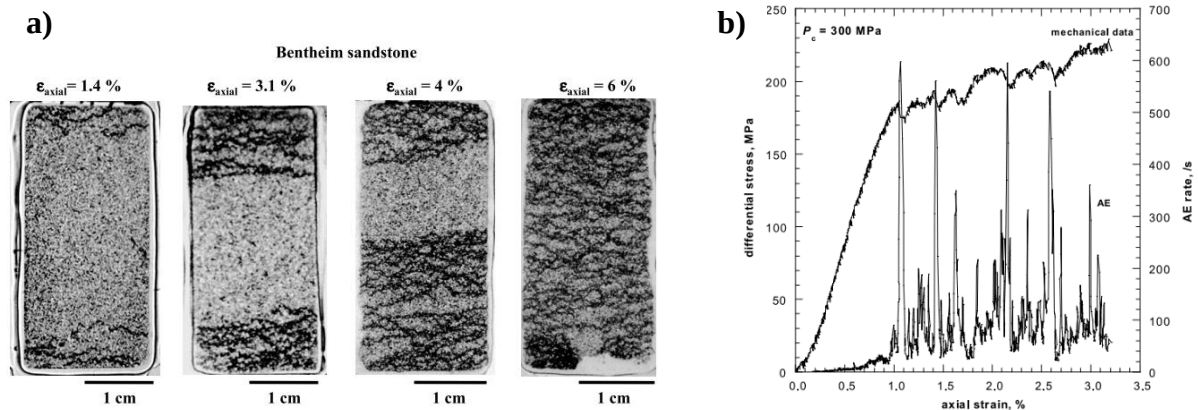


Figure 2.6. A typical experimental study (Baud et al., 2004) using AE detection to observe the mechanical behaviour of porous sandstone obtained from Bentheim, Germany. a) The propagation of compaction bands with increasing levels of axial strain. The dark area indicates grain breakage comminution; and b) shear response of Bentheim sandstone under high confining pressure showing that episodic stress drops imply the initiation of a compaction band.

2.3 The evolution of the permeability in porous rocks under compaction localisation

2.3.1 Effects on the permeability of microstructural mechanisms induced by compaction bands on permeability

The complex correlation between the petrophysical properties in reservoirs and mechanical deformation has challenged studies of permeability in porous rocks. There have been many investigations into the evolution of permeability using experimental, theoretical and computational approaches (Vajdova et al., 2004; Zhu et al., 2010; Fossen et al., 2011; Baud et al., 2012; Farquharson et al., 2017; Gajst et al., 2018; Gholami et al., 2019; Nanda et al., 2020). Regardless of any measurement technique or simulation, the fluctuation of permeability invariably involves changes in porosity, thermal variation, mass movement, mechanical deformation, and failure mechanisms of the host material. In this research, the focus is on how the overall permeability evolves in porous reservoir rock as a function of microstructural changes where compaction localisation occurs.

Under controlled loading in laboratory experiments, the porosity and permeability of the sample holding compaction bands may experience remarkable reduction by changes in the internal pore structure inside the localised zone due to being vulnerable to grain crushing and pore collapse (Chen et al., 2020). As also indicated by Torabi et al. (2015), localisation bands predominantly form in sandstone layers that exhibit a certain range of properties including cementation, porosity, permeability and grain size. These properties tend to change as a function of stress

and temperature over the lifespan of sandstone. Inside the cataclastic deformation bands, internal changes like grain reorganization, grain size reduction or grain fracturing can lead to permeability reduction (Fossen et al., 2007). Microstructural deformation, such as pore collapse inside the localised zone, has been proven to be the cause of alterations to the porosity and permeability of the host rock as it may induce a surge of inelastic strain which can imply the formation of compaction bands (Farquharson et al., 2017) (Figure 2.7).

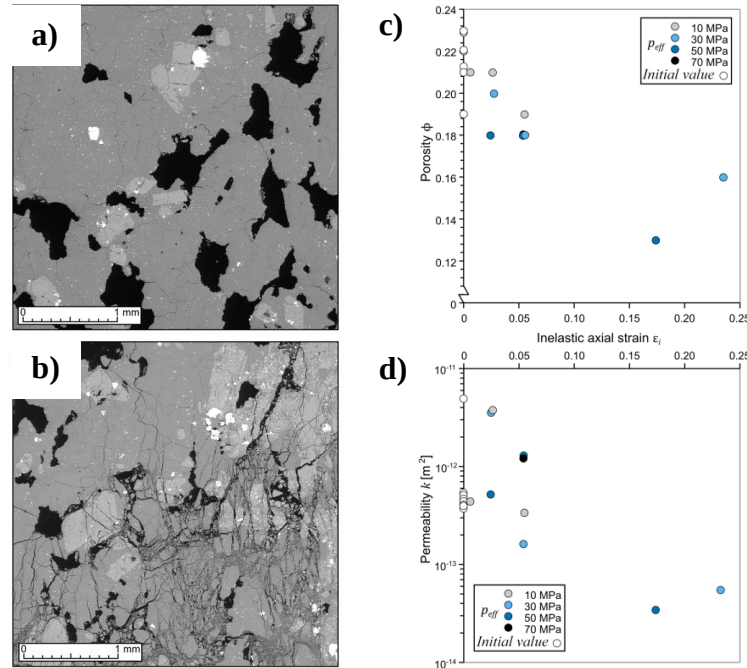


Figure 2.7. Electron microscope scanning images showing pore collapse of porous rock from Volcán de Colima. Two phases were demonstrated with a) undamaged state; and b) post-deformed state as associated with a compaction band where the void space is depicted by the black area; c-d) the relationship between different levels of confining pressure and permeability/porosity reduction as plotted against axial strain in the post-deformation stage (Farquharson et al., 2017).

The occurrence of porosity loss in porous rocks leading to the change in grain size/shape and strain hardening of deformation bands may cause local stress concentrations which allow the nucleation of a compaction band in the centre of the specimen (Gajst et al., 2018) (Figure 2.8a-b). This hypothesis has been reinforced by mapping and describing the porosity and stress-strain growth for sandstone through a visco-poroelastic damage model where the compaction regime possesses intense damage accumulation leading to a high reduction in porosity (Shalev et al., 2016) (Figure 2.8c). Permeability reduction could be inferred from this porosity observation as Baud et al. (2012) stated that in compacted cataclastic flow, porosity and permeability often decrease proportionally together, in contrast to dilatancy where porosity increases while permeability decreases. Furthermore, from drained triaxial tests and oedometer experiments, it was concluded that permeability reduction can also be a consequence of an increase in axial strain and volumetric strain where slipping and closing of fractures occur, resulting in the filling of friction grains (Yu et al., 2019; Leuthold et al., 2021a).

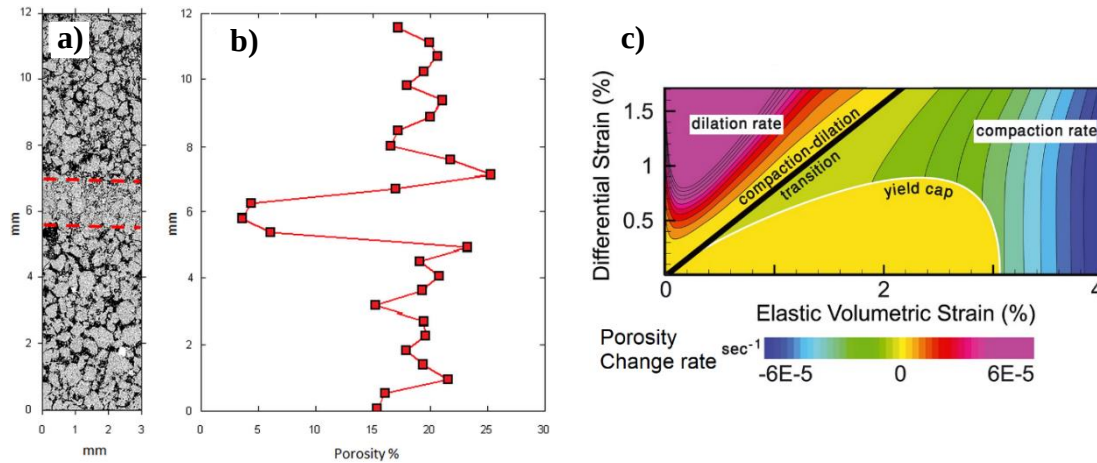


Figure 2.8. a-b) Scanning electron microscope image of Hatira sandstone showing the correspondence between porosity reduction with the area of grain crushing inside compaction localisation zone (dash red line). The black area indicates void space while Quartz grains are shown in grey (Gajst et al., 2018); and c) The map of porosity change rate expressed in triaxial strain space corresponding with dilation and compaction deformation from a visco-poroelastic damage model for sandstone (Shalev et al., 2016).

A qualitative description of the relationship between micro-deformation and permeability has been introduced as a conceptual model for the evolution of permeability in porous siliciclastic rocks (Zhu and Wong, 1997). Accordingly, grain crushing has been identified as the cause of the reduction in the overall permeability of sandstone, reducing it by approximately three orders of magnitude after reaching critical hydrostatic pressure. This is supported in Vajdova et al. (2004) where a significant decrease of more than one order of magnitude was observed under compacted deformation in both low and high confining pressure regimes. In these experiments, grain crushing and pore collapse intensify the reduction in void space which lowers the hydraulic conductivity and the tortuosity inside the affected zone. Consequently, the flow rate and the flux through the sample were diminished, leading to the conclusion that there had been a reduction in permeability.

However, lab-scale experiments can only measure the effective permeability of the whole sample volume and qualitative descriptions of different hydraulic behaviours due to the varying microstructural attributes inside and outside the localisation band. Furthermore, permeability can only be measured at relaxed states instead of stress states with continuous loading. Therefore, a proper numerical model is required to predict the permeability based on the evolving microstructures.

Compressive cataclastic deformation with minor shear under very high confining pressure may be recognised as pure compaction bands which appear as an accumulation of subparallel arrays. Tracking the propagation of these pure compaction bands via the increasing axial strain in triaxial tests may provide crucial insights into the relationship between the evolution of permeability and microstructure. A common trend identified in experimental studies on compacted rocks is that both porosity and permeability are likely to gradually reduce under

continuous loading, whereas a rapid drop can be observed once compaction localisation is detected (Vajdova et al., 2004). In addition, the modes of inelastic failure, whether homogenous or heterogeneous (localised), can also be very different in terms of their effect on permeability reduction (Baud et al., 2012).

The degree of anisotropy in the host material and the direction in which permeability is measured can also provide insight into the connection between compaction localisation and permeability evolution. Homogenous rocks like Bentheim, Diemelstadt, or Bleurwiller sandstone often exhibit discrete compaction bands, whereas diffuse compaction bands have been found in heterogeneous rocks like Darley Dale or Rothbach sandstone (Baud et al., 2012). In homogenous sandstone, intense permeability reduction has been observed in discrete compaction bands appearing as tabular, parallel, or subparallel to the bedding plane. In contrast, diffuse compaction bands, which grow at an oblique angle, close to the sample end, are shorter, more tortuous, and less efficient at restricting fluid flow. In conjunction with these observations, it has also been observed that the permeability measured in the band-parallel pattern is only marginally affected by compaction bands while band-normal effective permeability is extremely sensitive to compaction bands (Sternlof et al., 2004; Baud et al., 2012). Furthermore, studies have revealed that the sample cored in the normal direction to the bedding is turned from a high permeability rock into a low permeability one just when the first compaction band normal to the maximum principal stress was detected, even in a narrow thickness. Nevertheless, a minor and gradual reduction in permeability was observed in the rock sample that deformed in parallel to the bedding (Baud et al., 2012).

In the recent study on the anisotropy of permeability evolution under the effect of compaction band, Gerolymatou and Leuthold (2021) tried to evaluate the validity of the isotropic assumption in a constitutive-level analysis. This research went against the majority of the literature in being based on the argument that under the influence of compaction localisation, the horizontal permeability shows more intense permeability reduction than the permeability measured in a vertical direction. Although the permeability from their numerical model agrees with a few experimental results, more comprehensive evaluation of the model with a wider range of data sets should be addressed. A feature of their model, conspicuous in its absence, is the lack of consideration for the grain crushing process and the evolution of grain size distribution when analysing the effect of compaction bands on global permeability.

2.3.2 Numerical models on permeability evolution considering compaction localisation

There is a vital need for the development of an economical approach and one that uses computational resources efficiently which is capable of scaling the permeability inside the localisation band to the permeability of the macrostructure. The up-scaling equivalent/effective permeability method (Renard and de Marsily, 1997; Durlofsky, 2005; Rotevatn et al., 2013) has been developed but explicit links between the permeability with mechanical responses of localisation band are still missing. Several other available methods when being used for field-

scale simulations that involve strain localisation has produced invalid results due to the improper description of localised deformation.

There are currently four large groups of permeability evolution models which have been classified Ma (2015):

- The permeability-porosity methods,
- The stress/damage-permeability methods,
- The equivalent channel concept,
- The network model.

The first group strongly relies on the porosity-permeability relation and consists of two widely used models; the exponential law and power law Kozeny-Carman functions. Although this method is popular in engineering practice due to its simplicity, it does not take mechanical properties into account and is unsuited for materials with a large pore-size range (Marshall, 1957). The stress/damage-permeability methods link (David et al., 1994; Zhu and Wong, 1997), is inherently limited because real in-situ stress condition and mechanical parameters inside the localisation band are impossible to identify with the current measurement technology. Despite these weaknesses, these two methods have great potential for evaluating permeability evolution due to the grain crushing in discrete crushable granular sandstone.

Some approaches concentrated on the effect of the compaction band by embedding it into a volume element for the determination of equivalent permeability estimation developed from flow across a layered medium (Vajdova et al., 2004; Fortin et al., 2005; Farquharson et al., 2017). This approach takes into account the number of localisation bands, the permeability of the band and the host rock, the domain length and the thickness of an individual band. Although the expression is simple and straightforward, the permeability of the band is not trivial because the ratio between the two permeability factors are heavily based on empirical results (i.e. $K_{\text{host}}/K_{\text{band}}$ equals 20 to 400 for Bentheim sandstone). This expression also completely neglects vital microstructural evolutions inside the localisation just like many other classical methods. Following a similar path to continuum models, Farquharson et al. (2017) modelled a layered medium embedded with an idealised compaction band composed of packed spheres holding the grain size and band porosity (Figure 2.9). Although the global permeability was successfully described through deformation and porosity change by accounting for the characteristics of grain size and band thickness, the medium failed to mimic the growing characteristics of compaction bands. This was because the porous network was not well captured due to the particle size distribution and particle shape being fixed with idealisation.

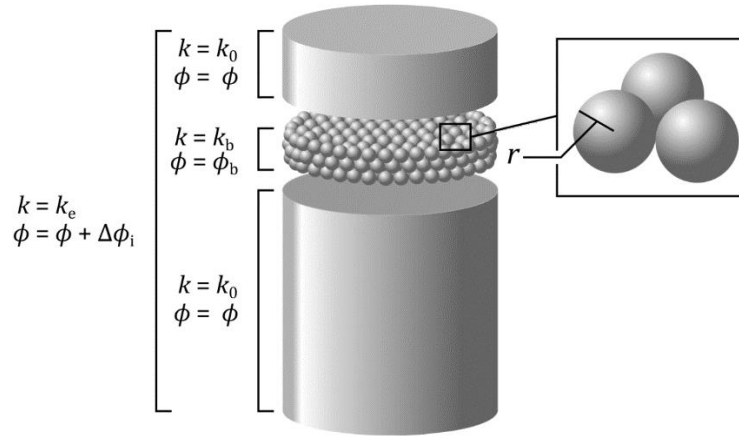


Figure 2.9. Model of a layered medium to predict post-deformation permeability k_e . The compaction band with thickness ω_b is embedded in a medium of permeability k_0 as a granular bed, considering the grain size as monodisperse particle radius r , which holds the band permeability k_b and band porosity ϕ_b (Farquharson et al., 2017).

There have also been approaches that consider the microstructure of porous rocks but ignore the effect of localisation, such as the capillary bundle model, to predict permeability from pore size distribution (Ecay et al., 2020). Furthermore, other techniques use the initial-current permeability ratio with enrichment to adapt the characteristics of compaction bands. For example, Leuthold et al. (2021b) calculated permeability in a constitutive description formulated by the nonlocal regularisation function of plastic axial strain inserted in the ratio between the thickness of the compacted and uncompacted material. However, the grain crushing factor in this model is still a fitted parameter relating to a specific surface.

The implementation in the grid-based family for permeability approximation is also popular, such as the dual-permeability model (Aguilar-López et al., 2020) or the coupled finite-difference/finite-element based on the homogenisation theory for a two-dimensional analysis (Sternlof et al., 2004). However, the grid-based method most likely suffers from modelling the complex system of compaction localisation without pre-configuration.

The breakage mechanics theory (Einav, 2007a, b) has opened a new promising approach that enables the constitutive model to continuously track the grain size distribution associated with the grain crushing process. This method stands out from other conventional plasticity theories because it can map the internal variable breakage B to the macro stress-strain response. The detailed formulation of breakage mechanics is addressed in Chapter 3. Using the advantage of this concept, an explicit relationship between inelastic behaviour and the permeability of the material was developed by Nguyen and Einav (2009), where a modified Kozeny-Carman's formula is applied with the use of the evolving harmonic mean grain size D_H . Similarly, Nanda et al. (2020) implemented the breakage mechanics into Finite Element analysis to predict permeability in a laboratory-scale specimen. Their outcomes also include a permeability evolution map in a stress plane which shows that permeability is lower in the inelastic region, as seen in Figure 2.10. Nevertheless, after obtaining the numerical result for macro and meso

behaviour, there was no extended development, nor was the evolution for an explicit link between meso and macro permeabilities investigated.

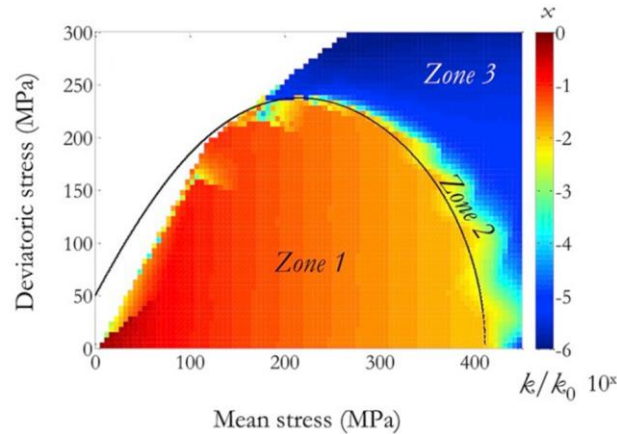


Figure 2.10. Stress-Permeability map (Nanda et al., 2020).

In general, a clear qualitative description of different hydraulic behaviours due to the varying permeability inside and outside the localisation band has been concluded from the literature. This description instigated the discovery of the quantitative governing relationship that explicitly describes how permeability evolves in between the localisation band and the surrounding porous rock. This is the most valuable key point that supports the concept of this research due to the capability of either directly or indirectly implementing or analysing the hydro-mechanical coupling relationship in the scale below the localisation band. Following this path, this study aims to link the permeability inside and outside the localisation band to discover their quantitative relationship so that the mesoscale feature of a localisation band can be bridged to a continuum presentation at a larger scale.

Chapter 3

NUMERICAL MODELLING FOR THE BEHAVIOUR OF POROUS ROCK CONSIDERING COMPACTION LOCALISATION

3.1 Development of numerical models to deal with compaction localisation

As discussed in the previous chapter, it is essential to consider the effect of strain localisation in predicting mechanical and hydraulic behaviour in geomechanics regarding problems like fluid flow in reservoirs, rock faults and geotechnical interaction. This localised deformation is widely accepted as a phenomenon of behaviour bifurcation from homogenous to inhomogeneous with an inelastic response. A well-developed numerical model should be able to capture the global deformation and failure induced by strain localisation including shear, compaction, dilation and their mix-mode.

Granular material is often vulnerable to grain crushing which will be intensified inside the compaction localisation zone and result in a macroscopic softening behaviour. In the Boundary Value Problems (BVPs), this softening response may cause stability-related issues for any constitutive description. By dealing with the material instability from non-associated plastic flow, the onset of localisation can be detected via the discontinuous bifurcation criterion originally proposed by Rudnicki and Rice (1975). After passing the bifurcation point, the uniformly deformed continuum matrix is converted into a post-localisation problem with the bifurcated constitutive description. Classical continuum models (Calhoun and Yuster, 1946; Borja and Alarcón, 1995) are incapable of capturing post-localisation behaviour due to the assumption of homogeneity which becomes invalid when strain localisation occurs. In particular, the missing component of classic continuum models during post-localisation analyses is the nonlinear deformation inside the band that dominates the macroscopic inelastic behaviour, whereas they can only produce the outside zone exhibits elastic or negligible inelastic responses.

Rate-dependent regularisation and the use of higher-order continuum such as theories of the second gradient, non-local (Chen and Schreyer, 1987; Pijaudier-Cabot and Bažant, 1987; Bazant and Pijaudier-Cabot, 1988; Bažant and Pijaudier-Cabot, 1989; Nguyen and Einav, 2010; Darabi et al., 2018) or phase-field (Francfort and Marigo, 1998; Bourdin et al., 2000; Ambati

et al., 2015) are also some leading methods to solve this problem in continuum models where the internal length scale may be introduced as a material parameter equal to the average grain size. Their problems come right from their advantage where the higher-order theory can describe the localisation behaviour despite the spatial discretisation being smoothed out below the band size for sufficient regularisation effects. A limitation is that enormous computational resource is required and even worse when the location of the localisation band is unknown beforehand. This means resolution at the sub-RVE scale has to be applied all over the field scale region.

Several other approaches using Finite Element based methods (FEM), such as the Enhanced Assumed Strain (Foster et al., 2007), Extended FEM (Sanborn and Prévost, 2011) and the Strong Discontinuity Approach (Jin and Zoback, 2017), have successfully solved the mesoscale problem in macro continuum models but still faced a serious problem. Despite correctly capturing the coupled behaviour of the localisation band and the surrounding bulk, their enhancement considered the band as a zero-thickness element based on the discretisation scheme. However, this enhanced FEM is too complicated when applied to complex crack patterns in 2D or 3D problems, thus, implying that it only works well with small deformation and/or problems involving a few localisation bands.

Besides, numerical simulations using modern approaches such as the Smoothed Particle Hydrodynamics-Lattice Boltzmann method for a mechanical-hydraulic coupling (Cleary et al., 2016) or the FEM-DEM-Deep Learning method (Wang and Sun, 2018) have been conducted on multi-scale models and were able to predict the internal properties and permeability. However, their works only focussed on simulations and behaviour inside the rock fracture whereas an explicit analytical expression for the link between the inside and outside was not developed.

Although strain localisation has been extensively researched over a few decades, the context of modelling compaction localisation with arrays of parallel tabular bands has received less attention. Some typical research on simulating the behaviour of compaction bands can be referred to a multiscale enriched Finite Element framework (Shahin et al., 2020; Wu et al., 2020; Gerolymatou and Leuthold, 2021), plasticity-based constitutive model (Buscarnera et al., 2014; Buscarnera and Laverack, 2014); Lattice Discrete Particle Models (Esna Ashari et al., 2015), material point simulation (Shahin et al., 2021), and a continuum framework based on breakage mechanics theories (Das et al., 2011, 2013; Nguyen et al., 2016a; Marinelli et al., 2017; Buscarnera et al., 2020). Given the exploration of experimental works on the mechanical response of compaction bands, these numerical models should cover some essential features of compaction localisation including:

1. Detection for the onset of compaction bands as well as some properties defining the tabular localisation-element (e.g. orientation vector, thickness);
2. Access to the evolving micro-mechanism, thus leading to the expansion and development of compaction localisation over the sample volume; and

3. Bringing the details from the microstructure to the mesoscale zone, and their governing effect on the macroscopic behaviour.

The limitation in localisation analysis of existing models, along with the requirements for modelling compaction bands, has led to a proposed hypothesis of a Representative Volume Element (RVE) crossed by a localisation band which is an advantage over the classic continuum models. In contrast to the higher order-continuum theories where discretisation needs to be smaller than the localisation band, this technique possesses an embedded finite-thickness band element which is very small compared to the host RVE. The key point of this assumption is to consider the length scale effect related to the size and orientation of the band. The numerical description of localisation behaviour relies on treatments of the mesoscopic length scale in the constitutive approach (Collins-Craft, 2019). In other words, post-localisation analysis cannot be correctly achieved without the length-scale detail at the meso level which is a common issue in classical continuum models.

Overall, in the current literature, there have been fundamental approaches to map the meso- and macro-scales together without neglecting the crucial effect that occurs in each zone. However, there is no such strong evidence to support the link between what happens inside the band and the macro properties, as well as how the permeability corresponds at these different scales. Furthermore, describing the localised fault behaviour in numerical models would require taking into account the evolving grain size distribution which has strong governance and dependence on the hydraulic conductivity and the mechanical properties. For this reason, it is necessary to assign physical meaning to this length scale which, in the case of compaction localisation, is the evolving grain size distribution. Therefore, in this chapter, a constitutive model is proposed that deals with strain localisation in porous rocks under confining conditions. The model provides a solution to two major issues in this problem where the evolving micro-mechanism of crushable granular material is captured based on the theory of breakage mechanics and connects the length scale effect of compaction localisation into the macroscopic response via a so-called dual-scale framework.

3.2 The meso-micro link based on the theory of breakage mechanics

3.2.1 Formulation of the breakage model

Granular materials, like porous reservoir rocks, have a complex multiphase microstructure that governs the entire material behaviour during the deformation and failure stages. For a volume element under continuous loading, the composing grain particles are crushed into small fragments, leading to the collapse of the pore structure and abrupt displacement of the neighbouring grains inside the affected zone. So far, there has been no experimental technique that allows access to the micro-structural processes occurring inside localisation bands. As a result, an appropriate constitutive model for porous rock is expected to record the effects of the

evolving microstructures; detect the initiation of compaction localisation in the brittle-ductile transitional regime; and capture the dissipative behaviour of compaction bands in the post-localisation stage. Nevertheless, traditional plasticity models (e.g. Mohr-Coulomb, Drucker-Prager, Hoek-Brown, Modified Cam-Clay) are incapable of satisfying the above requirements since they misrepresent the connection between the only internal variable (plasticity strain) and the underlying micro-mechanisms of porous rocks.

The breakage mechanics theory (Einav, 2007a, b) introduced an approach that enables the constitutive model to link the granular micromechanics with the macroscopic continuum model by upscaling the grain-scale energy potential via statistical homogenisation. This theory enables the tracking of grain size distribution through a scalar internal variable, B , that represents the grain crushing process in compacted porous rocks. The physical meaning of B , which ranges from zero to one, where $B = 0$, indicates an unbroken state in the material volume, while $B = 1$, demonstrates that the material has passed the crushable capacity.

During the compacting process on porous rocks, the grains are crushed and rearranged, leading to a shift in the initial grain size distribution, p_0 , toward the ultimate one, p_u , which follows a fractal law as suggested in field observations by (Sammis et al., 1987). Accordingly, the current grain size distribution corresponding with any grain size, D , can be extracted from the initial-ultimate grain size distribution and the variable, B , obtained from the breakage model via linear interpolation:

$$p(D, B) = (1 - B)p_0(D) + Bp_u(D) \quad (3.1)$$

The breakage theory is also based on the assumption that the elastic strain energy, stored within the grains, can be scaled with their surface areas to obtain the macro energy potential of the continuum model. The grading index, ϑ , ranging from 0 to 1, is the representation of this scheme. The crushing potential of the grains reduces as ϑ gets smaller, where the initial grain size distribution is closed to the ultimate grain size distribution. The index ϑ can be obtained from taking the second-order moments $\langle D^2 \rangle_0$ and $\langle D^2 \rangle_u$ of the initial and ultimate grain size distribution, respectively:

$$\vartheta = 1 - \frac{\langle D^2 \rangle_u}{\langle D^2 \rangle_0} \quad (3.2)$$

Considering the isothermal conditions, the changing grain size distribution may induce the inter-particle transmission of elastically stored and kinetic energy within a certain material volume (Nguyen and Einav, 2009). The rate of energy change in the microstructure can be averaged and scaled across the whole RVE. From the formulation of the Helmholtz free energy potential in terms of elastic strains (Nguyen and Einav, 2010), the energy scaling technique is based on the statistical homogenisation via the link between the breakage variable, B , and the grain size distribution. The change in grain size distribution during crushing comminution is considered similar to the change of stored energy within grains. In this sense, we may apply the statistical homogenisation on the microscopic variables, $A(D)$, where the grain size distribution is treated as a weighting average function (Einav, 2007a). The representative average quantity $\langle A \rangle$ for all of the grains with diameter, D is determined by:

$$\langle A \rangle = \int_{D_m}^{D_M} A(D)p(D)dD \quad (3.3)$$

By the fact that any microscopic variable $A(D)$ of grains with diameter D may be implemented in Eq. (3.3), we can assume this variable to be the grain diameter, $A(D) = D$, which leads to:

$$\langle D \rangle = \int_{D_m}^{D_M} Dp(D)dD \quad (3.4)$$

Eq. (3.4) is the form of first-order moment J_1 of the corresponding grain size distribution $p(D)$. Subsequently, the second order moment, which demonstrates the distribution of the grains about the mean grain size $\bar{D}$, can be written as:

$$\langle D^2 \rangle = \int_{D_m}^{D_M} D^2p(D)dD \quad (3.5)$$

The following notations are used: K and G are the bulk and shear modulus, respectively; p is the effective mean stress while q is the deviatoric shear stress; ε_v and ε_v^e are the total and elastic volumetric strain, respectively; ε_s and ε_s^e are the total and elastic shear strain, respectively; and σ_{ij} and s_{ij} are the total and deviatoric stress tensors, respectively.

Based on the original work by Einav (2007a, 2007b, 2007c, 2007d), the energy potential, ψ , and dissipation potential, Φ , takes the following forms:

$$\Psi = \frac{1}{2} (1 - \vartheta B) (K \varepsilon_v^{e2} + 3G \varepsilon_s^{e2}) \quad (3.6)$$

$$\Phi = \sqrt{\Phi_B^2 + \Phi_p^{v2} + \Phi_p^{s2}} \quad (3.7)$$

A more comprehensive formulation of the energy potential which considers the pressure-dependency of elastic behaviour can be referred to (Nguyen and Einav, 2009).

It can be seen in the above expression that the Helmholtz free energy potential is formulated using the elastic strains instead of the subtraction result of the total strain and the plastic strain. This implies the physical meaning of the model that relies on the determination of state variables without any given deformation history of the material. Accordingly, the total strain and plastic strain are not state variables because they are measured based on an arbitrary reference configuration. As a consequence of this proposition, the cumulative value of plastic strain should be replaced by the rate function of itself in order to define the dissipation potential.

In Eq. (3.7), the dissipation potential Φ is decomposed into three components including: the breakage dissipation Φ_B , plastic volumetric dissipation Φ_p^v , and plastic shear dissipation Φ_p^s .

$$\Phi_B = \frac{\sqrt{E_c E_B}}{(1 - B) \cos \omega} \dot{B} \quad (3.8)$$

$$\Phi_p^v = \frac{p}{(1 - B) \sin \omega} \sqrt{\frac{E_c}{E_B}} \dot{\varepsilon}_v^p \quad (3.9)$$

$$\Phi_p^s = Mp|\varepsilon_s^p| \quad (3.10)$$

where $M = q_u/p_u$ is the ratio of the ultimate shear and volumetric stress, representing the slope of the critical state line in the p - q stress space. The breakage energy threshold E_c is obtained from the critical crushing pressure, $p_{cr} = \sqrt{\frac{2KE_c}{\vartheta}}$, under isotropic loading conditions.

The constitutive model based on breakage mechanics follows the thermo-mechanical scheme for rate-independent elastoplastic models. From the energy potential, the triaxial stress-strain-breakage relationship and breakage energy, E_B (the conjugated thermodynamic forces of the breakage variable B and the axial strains, ε_v^e and ε_s^e), are obtained:

$$p = \frac{\partial \Psi}{\partial \varepsilon_v^e} = (1 - \vartheta B)K\varepsilon_v^e \quad (3.11)$$

$$q = \frac{\partial \Psi}{\partial \varepsilon_s^e} = 3(1 - \vartheta B)G\varepsilon_s^e \quad (3.12)$$

$$E_B = \frac{\partial \Psi}{\partial B} = \frac{\vartheta}{2}(K\varepsilon_v^{e2} + 3G\varepsilon_s^{e2}) \quad (3.13)$$

The same procedure is applied to obtain the dissipative triaxial stress and breakage energy from the dissipation potential:

$$\bar{p} = \frac{\partial \Phi}{\partial \dot{\varepsilon}_v^p} = \frac{\partial \Phi}{\partial \Phi_p^v} \frac{\partial \Phi_p^v}{\partial \dot{\varepsilon}_v^p} = \frac{\Phi_p^v}{\sqrt{\Phi_B^2 + \Phi_p^{v2} + \Phi_p^{s2}}} \frac{\partial \Phi_p^v}{\partial \dot{\varepsilon}_v^p} \quad (3.14)$$

$$\bar{q} = \frac{\partial \Phi}{\partial \dot{\varepsilon}_s^p} = \frac{\partial \Phi}{\partial \Phi_p^s} \frac{\partial \Phi_p^s}{\partial \dot{\varepsilon}_s^p} = \frac{\Phi_p^s}{\sqrt{\Phi_B^2 + \Phi_p^{v2} + \Phi_p^{s2}}} \frac{\partial \Phi_p^s}{\partial \dot{\varepsilon}_s^p} \quad (3.15)$$

$$\bar{E}_B = \frac{\partial \Phi}{\partial \dot{B}} \frac{\partial \Phi_B}{\partial \dot{B}} = \frac{\Phi_B}{\sqrt{\Phi_B^2 + \Phi_p^{v2} + \Phi_p^{s2}}} \frac{\partial \Phi_B}{\partial \dot{B}} \quad (3.16)$$

In the process of rate-independence, the yield function in generalised stress space, y^* , can be obtained from the degenerate Legendre transformation of dissipation potential:

$$y^* = \left(\frac{\bar{E}_B}{\partial \Phi_B / \partial \dot{B}} \right)^2 + \left(\frac{\bar{p}}{\partial \Phi_p^v / \partial \dot{\varepsilon}_v^p} \right)^2 + \left(\frac{\bar{q}}{\partial \Phi_p^s / \partial \dot{\varepsilon}_s^p} \right)^2 - 1 \leq 0 \quad (3.17)$$

The flow rules are obtained from the above yield function in generalised stress space. This yield function in generalised stress space plays the roles of the plastic potential, g , in classical plasticity theory and hence the use of g or y^* is interchangeable, $g = y^*$:

$$\dot{\varepsilon}_v^p = \lambda \frac{\partial g}{\partial p} = 2\lambda \frac{\bar{p}}{(\partial \Phi_p^v / \partial \dot{\varepsilon}_v^p)^2} = 2\lambda \frac{\bar{p}(1 - B)^2 E_B \sin^2 \omega}{p^2 E_c} \quad (3.18)$$

$$\dot{\varepsilon}_s^p = \lambda \frac{\partial g}{\partial q} = 2\lambda \frac{\bar{q}}{(\partial \Phi_p^s / \partial \dot{\varepsilon}_s^p)^2} = 2\lambda \frac{\bar{q}}{(Mp)^2} \quad (3.19)$$

$$\dot{B} = \lambda \frac{\partial g}{\partial E_B} = 2\lambda \frac{\bar{E}_B}{(\partial \Phi_B / \partial \dot{B})^2} = 2\lambda \frac{\bar{E}_B (1-B)^2 \cos^2 \omega}{E_B E_c} \quad (3.20)$$

The orthogonality condition in the form $p = \bar{p}$, $q = \bar{q}$ and $E_B = \bar{E}_B$ transforms the flow rules into:

$$\dot{\varepsilon}_v^p = 2\lambda \frac{(1-B)^2 E_B \sin^2 \omega}{p E_c} \quad (3.21)$$

$$\dot{\varepsilon}_s^p = 2\lambda \frac{q}{(Mp)^2} \quad (3.22)$$

$$\dot{B} = 2\lambda \frac{(1-B)^2 \cos^2 \omega}{E_c} \quad (3.23)$$

In the above expressions, g plays the role of a plastic potential in classical plasticity theory, which is the yield surface in mixed stress-energy space in breakage mechanics theory, while λ is the non-negative plastic multiplier; the plastic-breakage coupling angle ω governs the effect of pore collapse on the material behaviour due to fragment rearrangement and intergranular contact friction (Einav, 2007b).

The flow rules of breakage evolution, $\dot{B}$ and plastic strains, $\dot{\varepsilon}_{ij}^p$ can take the following forms (assuming the decomposition of total incremental strain, $\dot{\varepsilon}_{ij}$ into elastic and plastic components, $\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p$):

$$\dot{\varepsilon}_{ij}^p = \lambda \frac{\partial g}{\partial \sigma_{ij}} = \lambda \left[-\frac{2(1-B)^2 E_B \sin^2 \omega}{p E_c} \frac{\delta_{ij}}{3} + \frac{3s_{ij}}{(Mp)^2} \right] \quad (3.24)$$

where δ_{ij} is the Kronecker delta.

The breakage yield function in mixed stress-strain energy space can be expressed using the orthogonality condition by using Eqs. (3.8) to (3.10):

$$y = \frac{(1-B)^2 E_B}{E_c} + \left(\frac{q}{Mp} \right)^2 - 1 \leq 0 \quad (3.25)$$

In true stress space, the breakage energy E_B in terms of stress can be rewritten by using Eqs. (3.11) to (3.13), as:

$$E_B = \frac{\vartheta}{2(1-\vartheta B)^2} \left(\frac{p^2}{K} + \frac{q^2}{3G} \right) \quad (3.26)$$

The yield function expressed in triaxial stress spaces as:

$$y = \frac{\vartheta}{2E_c} \left(\frac{p^2}{K} + \frac{q^2}{3G} \right) \left(\frac{1-B}{1-\vartheta B} \right)^2 + \left(\frac{q}{Mp} \right)^2 - 1 \leq 0 \quad (3.27)$$

3.2.2 Numerical implementation of breakage models with the semi-implicit stress return algorithm and the tangent stiffness

In this section, the numerical implementation of the above breakage model will be briefly demonstrated for the localisation analysis. We obtain the relationship between stress-strain-breakage in tensorial form as:

$$\sigma_{ij} = (1 - \vartheta B) D_{ijkl}^e \varepsilon_{kl}^e \quad (3.28)$$

where D_{ijkl}^e is the elastic stiffness of the material; the term $(1 - \vartheta B) D_{ijkl}$ serves as the elastic-secant stiffness; ε_{kl}^e is the elastic strain.

Given that the incremental total strain can be treated as a summation of the incremental plastic strain and the incremental elastic strain, $\dot{\varepsilon}_{kl} = \dot{\varepsilon}_{kl}^e + \dot{\varepsilon}_{kl}^p$, we obtain the incremental constitutive relationship by expanding Eq. (3.28) using the partial differential operations with respect to the incremental macro strain, incremental plastic strain and breakage increment:

$$\dot{\sigma}_{ij} = (1 - \vartheta B) D_{ijkl}^e (\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^p) - \frac{\vartheta \sigma_{ij}}{1 - \vartheta B} \dot{B} \quad (3.29)$$

Expanding Eq. (3.29) with the breakage flow rules, then rearranging the formulation, we obtain:

$$\dot{\sigma}_{ij} = (1 - \vartheta B) D_{ijkl}^e \dot{\varepsilon}_{kl} - \underbrace{\left[(1 - \vartheta B) D_{ijkl}^e \frac{\partial g}{\partial \sigma_{ij}} + \frac{\vartheta \sigma_{ij}}{1 - \vartheta B} \frac{\partial g}{\partial E_B} \right]}_{M_{ij}} \dot{\lambda} \quad (3.30)$$

By performing a Taylor expansion of the yield function, and at the same time enforcing the consistency condition, $\dot{y} = 0$, we get:

$$\dot{y} = \frac{\partial y}{\partial B} \dot{B} + \frac{\partial y}{\partial p} \dot{p} + \frac{\partial y}{\partial q} \dot{q} = 0 \quad (3.31)$$

Rearranging the above expression with the chain rule $\frac{\partial y}{\partial \sigma_{ij}} = \frac{\partial y}{\partial p} \frac{\partial p}{\partial \sigma_{ij}} + \frac{\partial y}{\partial q} \frac{\partial q}{\partial \sigma_{ij}}$, and then substituting Eq. (3.29) into Eq. (3.31), results in:

$$\dot{y} = \frac{\partial y}{\partial B} \dot{B} + \frac{\partial y}{\partial \sigma_{ij}} (1 - \vartheta B) D_{ijkl}^e (\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^p) - \frac{\partial y}{\partial \sigma_{ij}} \frac{\vartheta \sigma_{ij}}{1 - \vartheta B} \dot{B} = 0 \quad (3.32)$$

By using the breakage flow rules, we can expand and then rearrange Eq. (3.32) in terms of the formulation for the plastic multiplier, $\dot{\lambda}$:

$$\dot{\lambda} = \frac{(1 - \vartheta B) \frac{\partial y}{\partial \sigma_{mn}} D_{mnpq}^e \dot{\varepsilon}_{pq}}{(1 - \vartheta B) \frac{\partial y}{\partial \sigma_{ij}} D_{ijkl}^e \frac{\partial g}{\partial \sigma_{kl}} - \left(\frac{\partial y}{\partial B} - \frac{\partial y}{\partial \sigma_{ij}} \frac{\vartheta \sigma_{ij}}{1 - \vartheta B} \right) \left(\frac{\partial g}{\partial E_B} \right)} \quad (3.33)$$

Back-substituting Eq. (3.36) into the constitutive relationship in incremental form, Eq. (3.30), we obtain the explicit stress driving relationships with the tangent stiffness, D_{ijkl} :

$$\dot{\sigma}_{ij} = \left[\underbrace{(1 - \vartheta B) D_{ijkl}^e - M_{ij} \frac{(1 - \vartheta B) D_{mnkl}^e \frac{\partial y}{\partial \sigma_{mn}}}{(1 - \vartheta B) D_{pqrs}^e \frac{\partial y}{\partial \sigma_{pq}} \frac{\partial g}{\partial \sigma_{rs}} - \left(\frac{\partial y}{\partial B} - \frac{\vartheta \sigma_{pq}}{1 - \vartheta B} \frac{\partial y}{\partial \sigma_{pq}} \right) \frac{\partial g}{\partial E_B}}}_{D_{ijkl}} \right] \dot{\epsilon}_{kl} \quad (3.34)$$

The semi-implicit stress return algorithm of the breakage model is hereby demonstrated using the above formulations. From a stress state that is still inside the elastic zone, we perform a trial stress increment until it passes the initial yield surface envelope (Figure 3.1). This trial stress increment is assumed to follow the elastic evolution inheriting the form of Eq. (3.28):

$$\dot{\sigma}_{ij}^{trial} = (1 - \vartheta B) D_{ijkl}^e \dot{\epsilon}_{kl} \quad (3.35)$$

Once the trial yield criterion has been detected to be larger than zero, the corrector stress increment is used to drive the stress state back onto the expanded yield surface that maintains the yield criterion. The corrector stress has the following form:

$$\dot{\sigma}_{ij}^{cor} = -(1 - \vartheta B) D_{ijkl}^e \dot{\epsilon}_{kl}^p - \frac{\vartheta \sigma_{ij}^{trial}}{1 - \vartheta B} \dot{B} \quad (3.36)$$

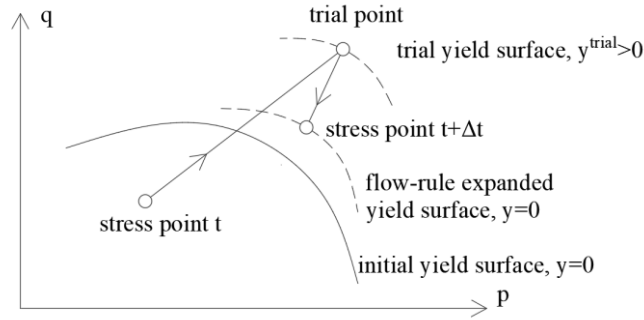


Figure 3.1. The conceptual stress return algorithm.

Conducting the Taylor expansion of the yield function about the trial stress state, similar to the procedure for obtaining Eq. (3.32), we have the function of the expanded yield surface:

$$y = y^{trial} - \lambda \left[- \left(\frac{\partial y}{\partial B} \right)^{trial} - \frac{\partial y}{\partial \sigma_{ij}} \left(\frac{\vartheta \sigma_{ij}^{trial}}{1 - \vartheta B} \right) \frac{\partial g}{\partial E_B} + \frac{\partial y}{\partial \sigma_{ij}} \left((1 - \vartheta B) D_{ijkl}^e \frac{\partial g}{\partial \sigma_{kl}} \right) \right] = 0 \quad (3.37)$$

By rearranging the above expression, we obtain the formulation of the plastic multiplier in terms of the trial stress state:

$$\lambda = \frac{y^{trial}}{(1 - \vartheta B) \frac{\partial y}{\partial \sigma_{ij}} \left(D_{ijkl}^e \frac{\partial g}{\partial \sigma_{ij}} \right)^{trial} - \left(\frac{\partial y}{\partial B} \right)^{trial} - \frac{\vartheta \sigma_{ij}^{trial}}{1 - \vartheta B} \frac{\partial y}{\partial \sigma_{ij}} \left(\frac{\partial g}{\partial E_B} \right)^{trial}} \quad (3.38)$$

This plastic multiplier is used to update the plastic strain, the breakage increment and the corrector stress. The stress increment for the new stress state is then calculated by:

$$\dot{\sigma}_{ij} = \dot{\sigma}_{ij}^{trial} + \dot{\sigma}_{ij}^{cor} \quad (3.39)$$

Figure 3.2 summarises, in the form of a flow chart, a clear concept of the stress return algorithm for the proposed breakage model.

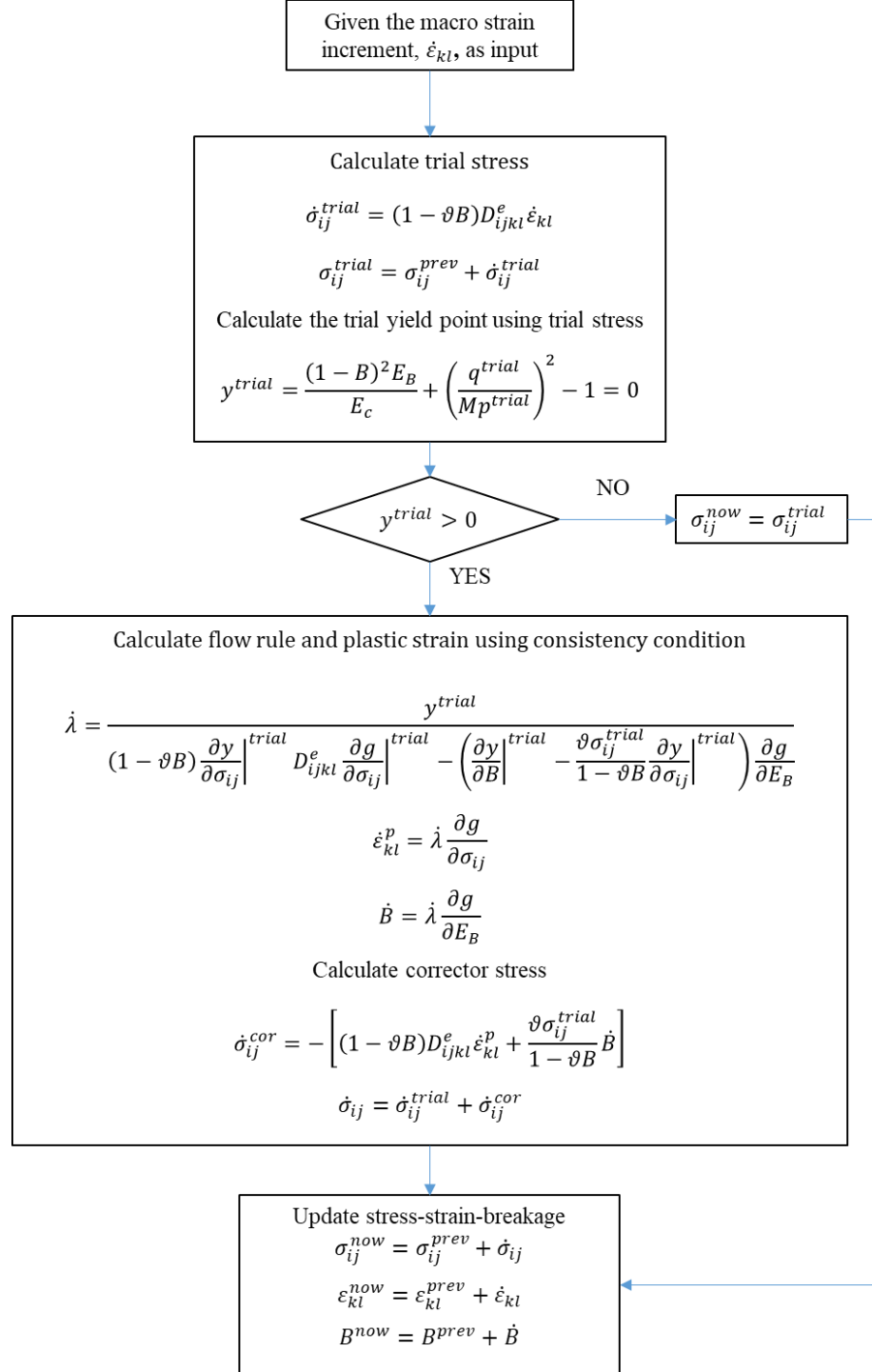


Figure 3.2. A flow chart for the semi-implicit stress return algorithm for the breakage model.

3.3 Dual-scale framework: constitutive relationships for the coupled macro-meso behaviour

The dual-scale framework is a generic and systematic enrichment taking account of the meso-scale mechanism of strain localisation that has been developed that can be implemented with any constitutive models (Nguyen et al., 2012; Nguyen et al., 2014; Nguyen et al., 2016b; Nguyen and Bui, 2020). The principal feature of the dual-scale framework is the connection between the averaged stress-strain over the domain of a RVE which can be considered as the macroscopic behaviour and the coupling response of the material inside and outside of the localisation zone. In this study, a generic constitutive framework is used for post-localisation analysis that involves a RVE with only a single localisation band embedded inside. This localisation band has two characteristics including the thickness h and orientation vector $\mathbf{n}$ that will be incorporated into the constitutive model. The thickness h depends on material microstructures and the loading paths. A more comprehensive discussion and parametric studies on the band thickness h will be addressed in Chapter 5. The orientation vector $\mathbf{n}$ can be determined from the bifurcation analysis of which detailed operations will be addressed in Chapter 4.

The volume fraction f of the localisation band can be expressed as the ratio between the thickness h of this band and the characteristic length $H = V/S$ of the volume element containing it, where S is the surface area of the localisation zone, assuming it takes the form of a planar band; and V is the volume of the RVE (Figure 3.3):

$$f = \frac{Sh}{V} = \frac{Sh}{SH} = \frac{h}{H} \quad (3.40)$$

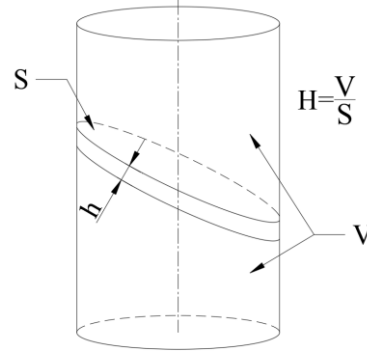


Figure 3.3. A finite thickness h localisation band embedded in a volume element with volume V , surface area S and size H .

In the generic constitutive dual-scale framework, the stress-strain response in the post-localisation stage can be expressed by two distinct stress-strain relations that reflects the behaviour inside ($\sigma_{ij}^i - \varepsilon_{kl}^i$) and outside ($\sigma_{ij}^o - \varepsilon_{kl}^o$) of the localisation zone. The homogeneous assumption is applied to each zone of which behaviour follows its own constitutive relationships. With the assumption of traction continuity across the boundary of the localisation

band, the macro stress-strain $(\sigma_{ij} - \varepsilon_{kl})$ is obtained as a result of coupling these two constitutive relationships. Consequently, the macro strain rate representing the macro behaviour of a volume element consisting of a localisation band can be considered as a volume-averaged quantity and has the form of a linear combination of the inside and outside strain rate as:

$$\dot{\varepsilon}_{kl} = (1 - f)\dot{\varepsilon}_{kl}^o + f\dot{\varepsilon}_{kl}^i \quad (3.41)$$

Due to localisation and the high gradient of strain rate across the boundary of the localisation zone, the strain rate across the boundary of the localisation zone $\dot{\varepsilon}_{ij}^i$ can be assumed to be in the following form (Neilsen and Schreyer, 1993; Oliver, 1996; Borja, 2000):

$$\dot{\varepsilon}_{kl}^i = \dot{\varepsilon}_{kl}^o + \frac{1}{h}(\dot{u}_k n_l)^s \quad (3.42)$$

The superscript “s” in Eq. (3.42) stands for symmetrisation. The relative velocity jump $\dot{u}_k$ between two faces of the localisation band, and the orientation vector n_l are taken into account in the above equation. Note that in the previous works (Nguyen et al., 2012; Nguyen et al., 2016a), Eq. (3.42) did not include the outside strain rate implying that the homogenous term is ignored which was based on the assumption of perpetual elastic behaviour for the zone outside and a band with negligible small width h . As a consequence from this assumption, the macro stress will coincide with the outside stress. However, this assumption is invalid for the behaviour of porous rocks under compaction localisation as the behaviour inside and outside of the band is allowed to be erratic. More specifically, the experimental observations have shown that the propagation of compaction localisation involves new discrete compaction bands additively developing close to the old one, thus expanding the accumulated zone of localised compaction until the entire sample is fully compacted. Based on this feature, the outside zone of the band can exhibit inelastic behaviour, where the localisation band in the model represents a localised zone of compaction which can expand, with increasing f , in correspondence to the loading condition. It should be emphasised that the condition for inelastic behaviour is only permitted to occur in the outside zone instead of implementing the enrichment of multiple bands, as demonstrated by Nguyen et al. (2017).

The basis highlighting the constitutive development of the mechanical behaviour in the coupled macro-meso length scale can be obtained from Eqs. (3.41) and (3.42) where the strain rate outside $\dot{\varepsilon}_{ij}^o$, and inside $\dot{\varepsilon}_{ij}^i$ of the localisation band are expressed as:

$$\dot{\varepsilon}_{kl}^o = \dot{\varepsilon}_{kl} - \frac{f}{h}(\dot{u}_k n_l)^s \quad (3.43)$$

$$\dot{\varepsilon}_{kl}^i = \dot{\varepsilon}_{kl} + \frac{1-f}{h}(\dot{u}_k n_l)^s \quad (3.44)$$

Given the enrichment, a connection between the behaviour of the macro volume and the inside-outside zones needs to be provided as a base formulation for the stress return algorithm.

According to the Hill-Mandel condition (Hill, 1963), the work produced by the stress-strain rate of the volume element should be in equilibrium with the work from the composing components (inside-outside) following a volume fraction rule, which leads to the expression:

$$(1 - f)\sigma_{ij}^o \dot{\epsilon}_{kl}^o + f\sigma_{ij}^i \dot{\epsilon}_{kl}^i = \sigma_{ij} \dot{\epsilon}_{kl} \quad (3.45)$$

Substituting the strain rates $\dot{\epsilon}_{kl}^i$ and $\dot{\epsilon}_{kl}^o$ in equations (3.43) and (3.44) in the above expression, we obtain:

$$(1 - f)\sigma_{ij}^o \left[\dot{\epsilon}_{kl} - \frac{f}{h} (\dot{u}_k n_l)^s \right] + f\sigma_{ij}^i \left[\dot{\epsilon}_{kl} + \frac{1-f}{h} (\dot{u}_k n_l)^s \right] = \sigma_{ij} \dot{\epsilon}_{kl} \quad (3.46)$$

The above expression can be rearranged in the following form:

$$[(1 - f)\sigma_{ij}^o + f\sigma_{ij}^i - \sigma_{ij}] \dot{\epsilon}_{kl} + f \frac{1-f}{h} (\sigma_{ij}^i n_l - \sigma_{ij}^o n_l) \dot{u}_k = 0 \quad (3.47)$$

Since the validity of Eq. (3.47) needs to be retained with arbitrary $\dot{\epsilon}_{kl}$, and $\dot{u}_k$, the following conditions, which accounts for the continuity of traction ($t_i = \sigma_{ij} n_j$) across the whole volume element containing a localisation band, are required:

$$\sigma_{ij} = (1 - f)\sigma_{ij}^o + f\sigma_{ij}^i \quad (3.48)$$

$$\sigma_{ij}^i n_j = \sigma_{ij}^o n_j = \sigma_{ij} n_j \quad (3.49)$$

From the above equations, the volume averaged form of the macro stress-strain, Eq. (3.48), is enhanced by the traction continuity, Eq. (3.49), while maintaining the Hill-Mandel condition, Eq. (3.45). The tangent stiffness for the macro stress-strain response will be different from the averaged form because of this enhancement. The implementation of a constitutive model based on breakage mechanics showing the breakage tangent stiffness using the dual-scale relationship will be demonstrated in Chapter 5.

In the field of computational geomechanics, the localisation phenomenon has always been an issue that must not be ignored due to its influence on the inelastic failure of the entire material volume. Existing numerical techniques, as well as experimental methods, often struggle in measuring the quantities lying inside this localised zone. By considering the length scale of the localisation zone as being much smaller than the host RVE, rather than discretisation below the localisation band level, the dual-scale framework has enabled the capability of accessing the details inside of the localisation zone and scaling them onto the macro response in a straightforward and computational resource-effective way. This enhancement has been introduced in some previous research work including implementation in the SPH method (Wang et al., 2019; Bui and Nguyen, 2021) and SPH model based on mixed-mode cohesive fracture law (Wang et al., 2020); cohesive model for a jointed rock mass (Le et al., 2017); extracting macro test data from localisation experiment (Le et al., 2021) and breakage models (Nguyen et al., 2016a; Nguyen et al., 2017). However, no such work has addressed the coupled mechanical-hydraulic behaviour where the link from micro mechanisms to macroscale is emphasised via a mesoscale element. For this reason, the novelty of the constitutive framework proposed in this study, that tracks permeability based on mechanical response, can be a firm foundation for further access into bridging the hydraulic quantities when there is flow through porous media and crossing the localisation band.

Chapter 4

BIFURCATION ANALYSIS AT THE ONSET OF LOCALISATION

4.1 Introduction

Due to continuous loading on the material skeleton, diffuse failure will develop with homogenous deformation occurring throughout the whole volume. Until reaching a certain stress point that causes the onset of the localised stage, two distinct regions corresponding to the outside and inside regions of the localisation band may be observed. An experimental study by Wong et al. (1997) indicated that strain localisation could develop during compaction-induced micro-mechanisms, such as grain crushing and pore collapse, resulting in a zero tangent modulus of the material, following by the formation of a non-homogenous strain field (Olsson, 1999). In order to capture this phenomenon in a numerical model, the discontinuous bifurcation criterion proposed by Rudnicki and Rice (1975) could be applied as a classical approach for determining the theoretical formulation of a localisation band. This theory works on the assumption that the localisation phenomenon may be treated as an instability of the constitutive response resulting in a non-uniform deformed planar band and homogeneous deformation bifurcates outside of the localised zone. Furthermore, this theory is capable of integrating the orientation of a localisation band as an improvement from the general bifurcation criteria (Drucker, 1950; Hill, 1958).

The constitutive model based on breakage mechanics (Einav, 2007a, b) was built to capture the macroscopic behaviours of crushable granular material by tracking the micromechanics of grain crushing and pore collapse. By using this technique, Das et al. (2011) assessed the onset of a localisation band in compacted porous rocks under high confining pressure while neglecting the low-confining regime. In this study, along with the implementation of the original breakage model, a modification to the condition is proposed, originating from the bifurcation criterion (Rudnicki and Rice, 1975; Chambon et al., 2000) that activates the formation of a localisation band at lower confining pressure zones on the breakage yield surface. The result of this prediction is verified with experimental observations on the aspect of the localisation band angle.

4.2 The formulation of bifurcation criterion

Discontinuous bifurcation is considered as a strain-jump that exhibits over the tabular localisation band while maintaining the kinematic compatibility with the surrounding material. The classical discontinuous bifurcation criterion (Rudnicki and Rice, 1975) sets a point during the continuous loading phase where the strain rate or velocity gradient becomes discontinuous across a plane of localised deformation. The geometry of a planar localisation band was defined using a normal vector $\mathbf{n}$ implying the orientation of the band and vector $\mathbf{g}$ representing the direction of the relative velocity of the regions inside and outside of a localisation band (Rudnicki, 2002) (Figure 4.1).

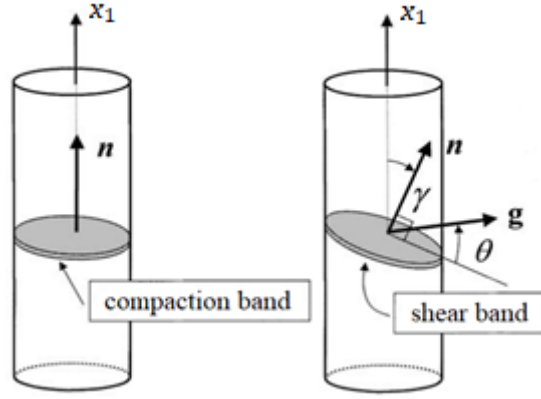


Figure 4.1. Localisation zone geometry (Rudnicki, 2002).

Regarding the compatibility condition for the localisation zone with the surrounding volume, the strain rate difference between the inside and outside regions should be in the form as:

$$\dot{\epsilon}_{ij}^i - \dot{\epsilon}_{ij}^o = n_i g_j \quad (4.1)$$

where the superscript “i” and “o” stand for inside and outside, respectively. The constitutive relationship of incremental stress-strain for the two zones are expressed accordingly:

$$\begin{cases} \dot{\sigma}_{ij}^i = D_{ijkl}^i \dot{\epsilon}_{kl}^i \\ \dot{\sigma}_{ij}^o = D_{ijkl}^o \dot{\epsilon}_{kl}^o \end{cases} \quad (4.2)$$

where D_{ijkl}^i and D_{ijkl}^o are the tangent stiffness tensors inside and outside of the localisation zone, respectively. The equilibrium at the onset of localisation is maintained by continuous traction rates across the boundary of the localisation band:

$$\dot{t}_i^i = \dot{t}_i^o \text{ or } n_i \dot{\sigma}_{ij}^i = n_i \dot{\sigma}_{ij}^o \quad (4.3)$$

By combining and rearranging Eqs. (4.1), (4.2) and (4.3), it can be written that:

$$(L_{ijkl}^i - L_{ijkl}^o) \dot{\epsilon}_{kl}^o n_i + C_{ij} g_j = 0 \quad (4.4)$$

where $C_{ij} = n_k D_{ijkl}^i n_l$ is the localisation acoustic tensor. In any case where the tangent stiffness of the inside and outside zone are identical (e.g. the outside strain rate is constrained to continuously evolve), then the condition for a discontinuous bifurcation can be derived from Eq. (4.4) as:

$$C_{ij}g_j = 0 \text{ or } \det(C_{ij}) = 0 \quad (4.5)$$

The instability of material, thus, will only occur when the acoustic tensor obtains zero. It is worthy to note that this acoustic tensor corresponds to the material properties and the orientation of localisation band. However, the assumption on identical tangent stiffness between the inside and outside zone is only valid for linear models (Chambon et al., 2000) or the strain rates are provided with additional constraints (Nielsen and Schreyer, 1993). Therefore, in the case of different tangent stiffnesses for the two zones within the breakage model, the discontinuous bifurcation criterion can also be negative (Rudnicki and Rice, 1975; Chambon et al., 2000):

$$\min_{\vec{n}} [\det(C_{ik})] \leq 0 \quad (4.6)$$

The components of the normal vector n_j of the localisation band are demonstrated in Figure 4.2, which have the following form:

$$n_j = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} = \begin{pmatrix} \cos \gamma \\ \sin \gamma \sin \beta \\ \sin \gamma \cos \beta \end{pmatrix} \quad (4.7)$$

Due to the axisymmetric geometry of the conventional cylindrical sample in triaxial tests, the angle γ between the normal vector n_j and the longitudinal axis is only required to range from 0° to 90° in the bifurcation analysis. Furthermore, because of this characteristic, the determinant of the acoustic tensor should be unaffected by the rotation of angle β . Accordingly, the general matrix form, $\mathbf{n}$, of the orientation vector in the three-dimensional space can be written as:

$$\mathbf{n} = \begin{pmatrix} n_1 & 0 & 0 & n_2 & 0 & n_3 \\ 0 & n_2 & 0 & n_1 & n_3 & 0 \\ 0 & 0 & n_3 & 0 & n_2 & n_1 \end{pmatrix} \quad (4.8)$$

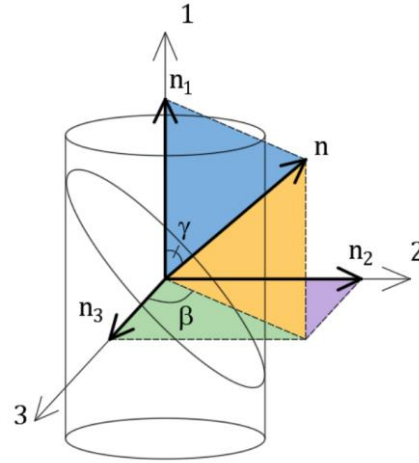


Figure 4.2. Components of the band orientation in a cylindrical sample.

Furthermore, the tangent stiffness D_{ijkl} expressed in Voigt notations has the following form:

$$\begin{pmatrix} \dot{\sigma}_{11} \\ \dot{\sigma}_{22} \\ \dot{\sigma}_{33} \\ \dot{\sigma}_{12} \\ \dot{\sigma}_{23} \\ \dot{\sigma}_{31} \end{pmatrix} = \begin{pmatrix} D_{1111} & D_{1122} & D_{1133} & D_{1112} & D_{1123} & D_{1131} \\ D_{2211} & D_{2222} & D_{2233} & D_{2212} & D_{2223} & D_{2231} \\ D_{3311} & D_{3322} & D_{3333} & D_{3312} & D_{3323} & D_{3331} \\ D_{1211} & D_{1222} & D_{1233} & D_{1212} & D_{1223} & D_{1231} \\ D_{2311} & D_{2322} & D_{2333} & D_{2312} & D_{2323} & D_{2331} \\ D_{3111} & D_{3122} & D_{3133} & D_{3112} & D_{3123} & D_{3131} \end{pmatrix} \begin{pmatrix} \dot{\epsilon}_{11} \\ \dot{\epsilon}_{22} \\ \dot{\epsilon}_{33} \\ \dot{\gamma}_{12} \\ \dot{\gamma}_{23} \\ \dot{\gamma}_{31} \end{pmatrix} \quad (4.9)$$

where $\dot{\gamma}_{12} = 2\dot{\epsilon}_{12}$; $\dot{\gamma}_{23} = 2\dot{\epsilon}_{23}$ and $\dot{\gamma}_{31} = 2\dot{\epsilon}_{31}$ are the rates of engineering shear strains.

4.3 A modified bifurcation criterion

The bifurcation analysis technique has been applied in various studies on compacted porous sandstones (Das et al., 2011; Tengattini et al., 2014; Nguyen et al., 2016a; Nguyen et al., 2017). Overall, it demonstrated great capability in detecting the activation of strain localisation on the breakage yield surface in the case of high-confining pressure regimes where grain crushing and pore collapse dominates the inelastic behaviour. However, the lack of covering lower-pressure regimes of the bifurcation criterion has restricted the model to capture other scenarios of localisation, such as shear band and dilation bands in which cement debonding has taken over. Therefore, a new approach is hereby proposed that improves the accuracy of the bifurcation condition based on the symmetry characteristics of the triaxial test specimen.

In a conventional triaxial compression test, specimen behaviour only occurs along two axes: radial and axial, where the plane of localisation band at the onset of localisation can symmetrically rotate around the axial (vertical) axis due to the horizontal symmetry of applied stress. At this stage, the localisation band has an equal chance to develop in any orientation around the longitudinal axis of the cylindrical specimen (Figure 4.3).

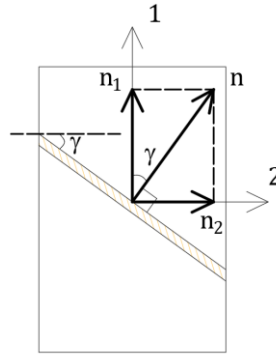


Figure 4.3. Orientation of localisation band in 2-dimensional space.

From Eq. (4.9), the components of the tangent stiffness matrix acknowledging the cylindrical symmetric constraint can be treated as $D_{1122} = D_{1133} = D_{2211} = D_{3311}$. This results in a constitutive relationship based on five stress-strain tensor components as follows:

$$\begin{pmatrix} \dot{\sigma}_{11} \\ \dot{\sigma}_{22} = \dot{\sigma}_{33} \\ \dot{\sigma}_{12} \\ \dot{\sigma}_{23} \\ \dot{\sigma}_{31} \end{pmatrix} = \begin{pmatrix} D_{1111} & 2D_{1122} & D_{1112} & D_{1123} & D_{1131} \\ D_{2211} & D_{2222} + D_{2233} & D_{2212} & D_{2223} & D_{2231} \\ D_{1211} & D_{1222} & D_{1212} & D_{1223} & D_{1231} \\ D_{2311} & D_{2322} & D_{2312} & D_{2323} & D_{2331} \\ D_{3111} & D_{3122} & D_{3112} & D_{3123} & D_{3131} \end{pmatrix} \begin{pmatrix} \dot{\epsilon}_{11} \\ \dot{\epsilon}_{22} = \dot{\epsilon}_{33} \\ \dot{\gamma}_{12} \\ \dot{\gamma}_{23} \\ \dot{\gamma}_{31} \end{pmatrix} \quad (4.10)$$

Accordingly, the compatible orientation vector to this constraint will have its three components reduced to two, thus Eq. (4.7) can be rewritten as

$$\mathbf{n} = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix} = \begin{pmatrix} \cos\gamma \\ \sin\gamma \end{pmatrix} \quad (4.11)$$

and a corresponding matrix form of a normal matrix as:

$$\mathbf{n} = \begin{pmatrix} n_1 & 0 & n_2 & 0 & 0 \\ 0 & n_2 & n_1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \cos\gamma & 0 & \sin\gamma & 0 & 0 \\ 0 & \sin\gamma & \cos\gamma & 0 & 0 \end{pmatrix} \quad (4.12)$$

4.4 Bifurcation analysis result

A parametric study is carried out to explore the onset of a localisation band using the modified version of the bifurcation condition. The model parameters are obtained by calibrating the experimental results given by Baud et al. (2004) and Baud et al. (2006). The detailed procedure for approximating ϑ can be found in Chapter 5. The calibrated parameters are given in Table 4.1.

Table 4.1. Calibrated set of parameters for selected sandstones in bifurcation analysis from the experiment data of Baud et al. (2004) and Baud et al. (2006).

	K (MPa)	G (MPa)	ϑ	p_{cr}	M	ω (°)
Bentheim	11,000	7,000	0.72	423.6	1.7	80
Berea	9,000	5,000	0.6	360	1.6	80

The proposed constitutive model is validated using these parameters with the experimental stress-strain response from Bentheim and Berea sandstone (Baud et al., 2004; Baud et al., 2006). It should be noted that the volumetric behaviour was calibrated based on the hydrostatic pressure against porosity reduction given by Baud et al. (2006) because the data under isotropic compression are only available in this document. Besides, their method of calculating porosity change is in fact equivalent to the incremental volumetric strain. In contrast, the experimental data of shear behaviour can only be found in the work of Baud et al. (2004). The experimental yield surface was taken based on the critical stress points obtained from Baud et al. (2004).

Figure 4.4 illustrates the capacity of the model in predicting the macroscopic behaviour of porous rocks. The numerical results was extracted from the Fortran self-code using the continuum model of breakage mechanics without the implementation of the dual-scale framework. Good agreement between the numerical prediction and experimental data is

observed which confirms the accuracy of the calibrated parameters. However, the model still encounters some limitations as it was built for dealing with high confining pressure behaviour in relation to the grain crushing mechanisms. It can be seen from Figure 4.4d that the low-pressure response could not match well with the experimental data where the cement debonding effect is dominating. The solution requires adding the micromechanics of bonded grains to the breakage constitutive framework rather than recalibrating any parameters. Another restriction of the current model can be seen in Figure 4.4b where the softening (downward) effect in the inelastic curve of the 75 MPa case is not well reflected, which is also a shortcoming of the current breakage mechanics framework. It is recognised that these are the limitations of the current breakage mechanics framework and the proposed constitutive models will need to address these in the future. It is noted that the nonlinear elastic behaviour observed experimentally is also neglected in this model. As shown in Figure 4.4, the model can reasonably reproduce the experimental stress-strain responses, indicating the appropriateness of the calibrated set of parameters. However, the limitation of this breakage model is acknowledged in capturing the softening response at the low confining pressure of 75 MPa.

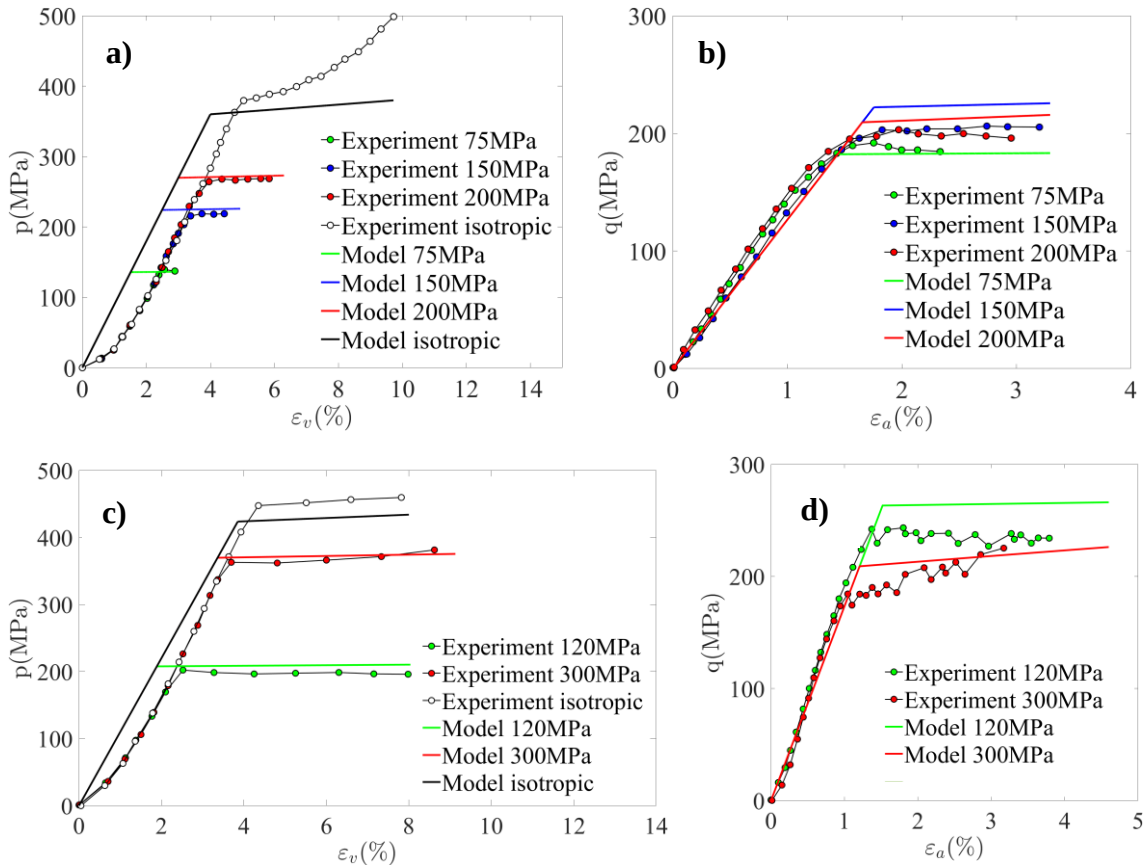


Figure 4.4. Comparisons between numerical and experimental results (Baud et al., 2004; Baud et al., 2006) for Berea sandstone with a) volumetric behaviour and b) shear behaviour of Bentheim sandstone under drained triaxial loading; for Bentheim with c) volumetric behaviour and d) shear behaviour under drained triaxial loading.

The prediction of the localisation zone using appropriate constraints for triaxial loading conditions is illustrated in Figure 4.5. It can be seen that the proposed approach, using a 5×5

tangent stiffness matrix, can predict a much wider range of stress states at the initial yield over which localisation can happen. As compared with the previous bifurcation, the modified version extends the coverage of the bifurcation zone to the low-confining pressure regime. This result has demonstrated the capability of the bifurcation analysis in detecting the activation of not only the compaction band but also shear and dilation bands when shearing at low pressure. In the very high confining pressure region, the bifurcation condition does not detect the onset of localisation which may be explained by the diffuse compaction band formation that has taken over the entire volume sample instead of any occurrence of localised compaction bands. Similar failure distribution has been observed in very high confining pressure tests by Wong et al. (2001) and Baud et al. (2004). It is clear that this is an improvement, given previous attempts using the same breakage model without appropriate constraints for conventional triaxial loading conditions (resulting in full 6×6 tangent stiffness matrix) cannot capture bifurcation at low confining pressures.

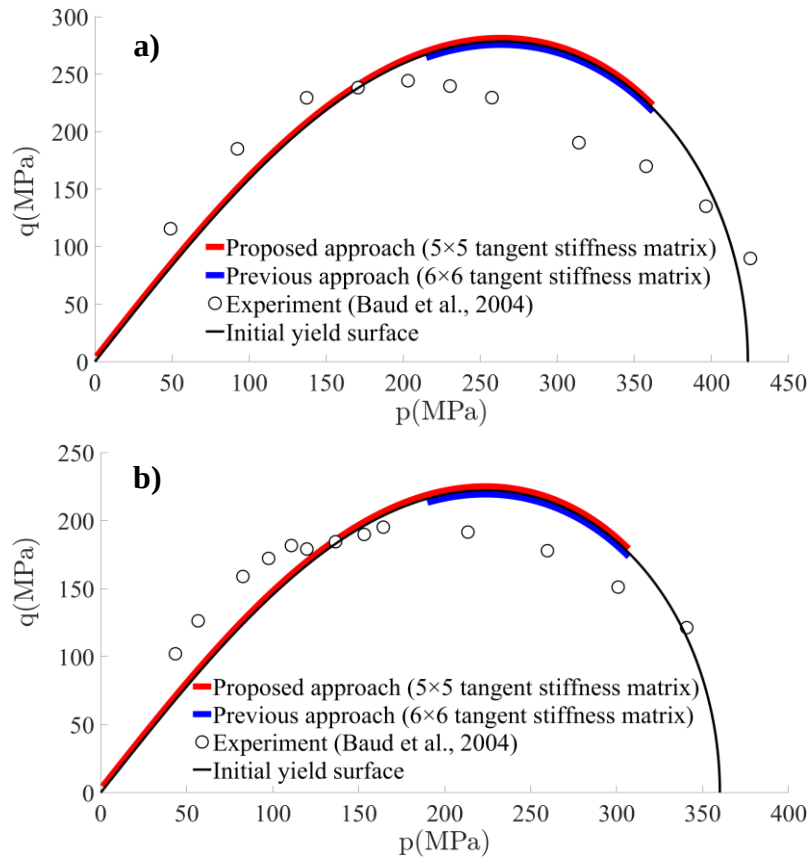


Figure 4.5. Comparisons of bifurcation zone on the initial yield surface between experimental data and numerical analyses with the cylindrical symmetry modification using 5×5 tangent stiffness for a) Bentheim sandstone; and b) Berea sandstone.

A parametric study is performed to investigate the effects of ω on the onset of localisation. The bifurcation zone at the initial yielding state is plotted in Figures 4.6 and 4.7 at different $\omega = 70^\circ, 80^\circ$ and 90° . The plastic-breakage coupling angle ω governs the effect of pore collapse on the material behaviour due to fragment rearrangement and intergranular contact friction. When $\omega = 0^\circ$, the material behaviour is purely elastic-breakage while $\omega = 90^\circ$ results in the elastic-

perfectly plastic stress path with a zero breakage increment. It can be found that an increase in ω leads to an expansion in the bifurcation zone. This feature is closely related to responses in Figure 4.6 that the hardening response is more profound when ω increases. Nevertheless, it is noted that no localization failure is observed at a much higher pressure regime.

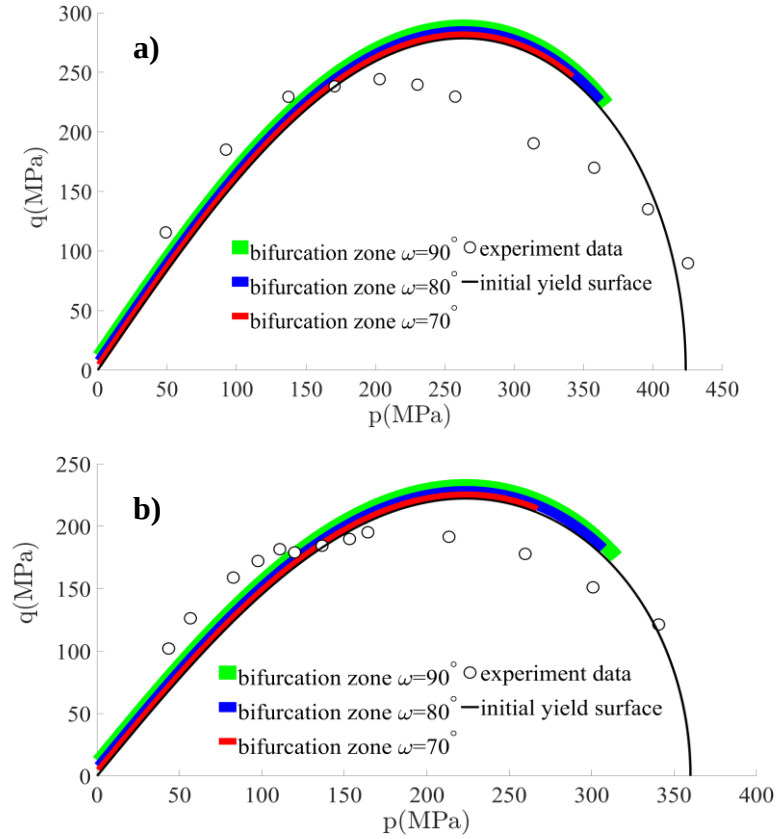


Figure 4.6. Comparisons of bifurcation zone on the initial yield surface between experimental data (Baud et al., 2004) and numerical analyses with the cylindrical symmetry modification using the 5×5 tangent stiffness and the effect of evolving coupling angle for a) Bentheim sandstone; and b) Berea sandstone.

Figure 4.8 depicts the prediction of the orientation of the localisation band by selecting the angle corresponding with the minimum negative determinant of the acoustic tensor in the bifurcation analysis where localisation bands are most likely to occur. The predicted angles are relatively close to those that have been observed in existing drained triaxial experiments (Wong et al., 2001; Klein and Reuschlé, 2003; Baud et al., 2004) which demonstrates the reliable accuracy of the predictions. The analysis can describe the relationship between the confining pressure and the localisation orientation as in the experimental observations. The increase of confining pressure from a low to high regime can lead to a more steep inclination of the band until reaching a high enough point, where a perfectly horizontal band can be observed, indicating a pure compaction mode. The restriction of this prediction is the slight difference of

angles compared with the experiment which may be a consequence from the simplified assumption of the localised phenomenon descriptions of the numerical framework.

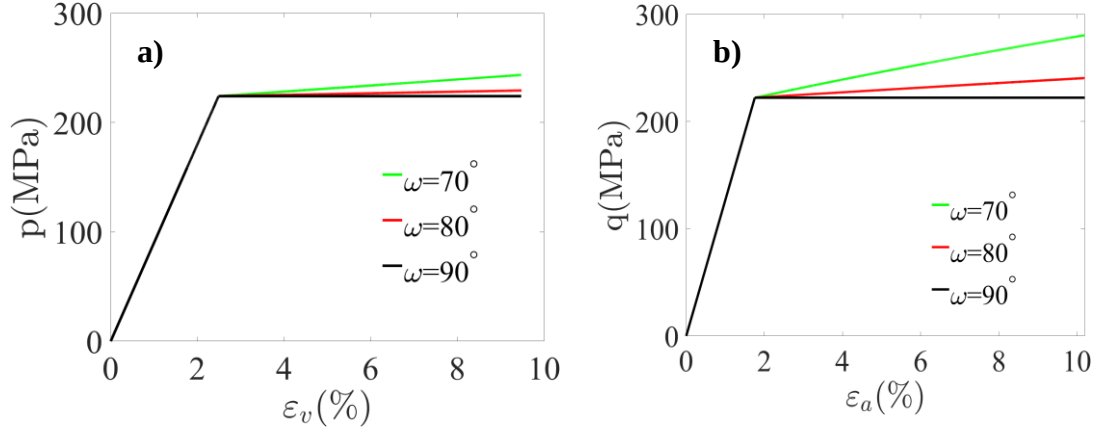


Figure 4.7. The inelastic response corresponding with varying degrees of the plastic-breakage coupling angle, ω , in the triaxial test under $p_c = 150 \text{ MPa}$ on Berea sandstone; (a) hydrostatic stress against volumetric strain response ($p - \varepsilon_v$); (b) deviatoric stress against axial strain response ($q - \varepsilon_a$).

In conclusion, the focus of this study is to provide a correct bifurcation condition in the breakage model (Einav, 2007a, b) in modelling the onset of a localisation band in porous rocks under the conventional triaxial test. An approach based on a 5×5 stiffness matrix is proposed by applying an appropriate constraint related to the symmetry of applied lateral confining stresses about the vertical axis. This allows the breakage model to correctly capture bifurcation at the onset of the yielding state from very low to high confining pressures, which was not the case before. The ability of the present approach is indicated through a good agreement between the numerical and experimental results. Some limitations of the breakage model are acknowledged for further developments in future research, such as dilation behaviour and softening under low confining pressures. It should be noted that the 5×5 matrix is indeed restricted on cylindrical samples in triaxial tests. It is used to validate the model, given the availability of both stress conditions and the orientation of the localisation band in triaxial tests. Otherwise, the general bifurcation condition using a full 6×6 matrix can be used.

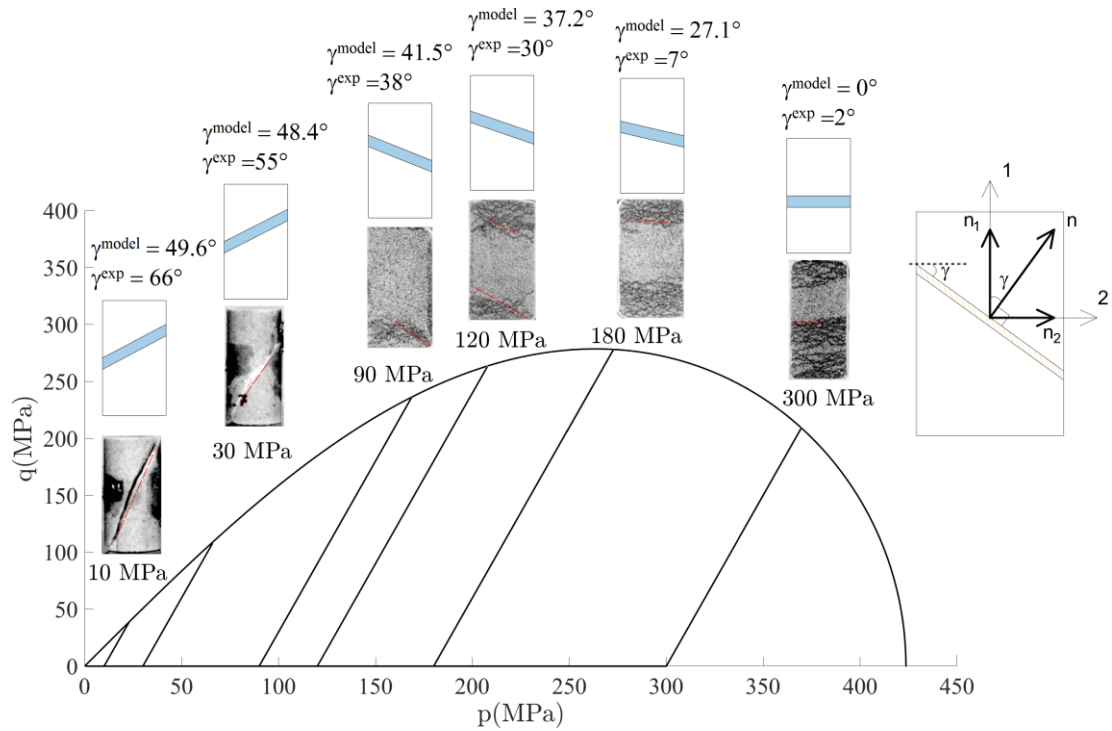


Figure 4.8. Orientation of the localisation band in Bentheim sandstone from experimental data (Wong et al., 2001; Klein and Reuschlé, 2003; Baud et al., 2004) and the modified bifurcation analysis.

Chapter 5

POST-LOCALISATION ANALYSIS AND PERMEABILITY EVOLUTION

5.1 The constitutive model based on breakage mechanics in the dual-scale framework

In Chapter 2, the behaviour of sandstones has been reviewed and discussed extensively to provide sufficient background on compaction localisation due to grain crushing in porous reservoir rocks. In the theory of breakage mechanics, the evolution of grain size distribution due to grain crushing is the emphasis of the constitutive model where a single scalar internal variable can be employed to link with the macro response, enabling tracking continuous evolution of the grain size distribution and stress path. Localised deformation takes place at a certain stage of the deformation process, with the onset and propagation of the localisation band, where inelastic response occurs. This leads to an incorrect representation of the deformation if a single homogeneous strain is used for the whole material volume as defined in traditional constitutive models in general, and the original breakage model, in specific.

In the context of analysing the mechanical behaviour and permeability evolution in porous rocks where strain localisation occurs, an accurate constitutive model should reflect the rock crushing mechanism as well as capture the physics at the initiation of localisation and the post-localisation regime. In this study, the proposed constitutive model will be an implementation between the original breakage model (Einav, 2007a, b) acting as a bridge between micro-macro behaviour, and the dual-scale framework (Nguyen et al., 2014) which connects the meso-macro response. In addition, the condition that triggers the post-localisation analysis in the constitutive operation follows the bifurcation criterion which considers the cylindrical symmetry as proposed in Chapter 4.

In the computational analysis, the triaxial experiment is replicated for a constitutive volume with a loading control procedure. The algorithms presented in this chapter are based on earlier publications that provide completeness to the formulation (Nguyen et al, 2016; Nguyen & Bui, 2020). The constitutive behaviour is initiated with isotropic loading conditions until the normal stresses in all three principal directions are equal to the expected confining pressure. Following this is the shearing phase in which two of the lateral stresses are forced constant while the incremental axial strain is continuously applied. An iterative Newton-Raphson algorithm is used for this mixed stress-strain control at the constitutive level.

5.1.1 The explicit stress driving algorithm using a trio of constitutive relationships from the dual-scale framework

The explicit stress return algorithm is usually simple and useful for verifying other more complicated stress return algorithms over very small incremental driving variables. This algorithm is operated with the determination of the tangent stiffness based on the enforcement of traction continuity in incremental form. With all formulations of the dual-scale constitutive structure of the generic model, the local constitutive relationships that governs the behaviour for the inside and outside of a localisation band can be described as:

$$\dot{\sigma}_{ij}^o = D_{ijkl}^o \dot{\epsilon}_{kl}^o = D_{ijkl}^o \left[\dot{\epsilon}_{kl} - \frac{f}{h} (\dot{u}_k n_l)^s \right] \quad (5.1)$$

$$\dot{\sigma}_{ij}^i = D_{ijkl}^i \dot{\epsilon}_{kl}^i = D_{ijkl}^i \left[\dot{\epsilon}_{kl} + \frac{1-f}{h} (\dot{u}_k n_l)^s \right] \quad (5.2)$$

where D_{ijkl}^o and D_{ijkl}^i are the tangent stiffness tensors for the zone outside and inside, respectively. As discussed in the previous section, these distinct governing relationships are connected through the internal equilibrium condition for traction, Eq. (3.49), and the kinematic compatibility conditions, Eqs. (3.43) and (3.44), to form the homogenised stress in the macroscopic description, Eq. (3.48).

As demonstrated, instead of using a single stress-strain relationship like traditional constitutive models, the proposed enriched framework operates with three relationships at two different length scales. While the macroscopic scale exhibits the behaviour of the entire sample, the mesoscopic scale possesses responses of the localisation band which consists of the material behaviour inside of the localised zone and those outside. In this study, by implementing the breakage mechanics model within the dual-scale framework, the local length scale is capable of capturing the evolution of microstructural mechanisms for these inside-outside zones.

Although the stress update for the two constitutive relationships at the mesoscale can be straightforwardly obtained with the conventional stress-return algorithms for plasticity-based models, the macroscopic stress cannot be obtained with a similar treatment. For this purpose, the generic constitutive relations for the inside-outside, Eqs. (5.1) and (5.2), are substituted into the traction equilibrium Eq. (3.49):

$$\left\{ D_{ijkl}^o \left[\dot{\epsilon}_{kl} - \frac{f}{h} (\dot{u}_k n_l)^s \right] \right\} n_j = \left\{ D_{ijkl}^i \left[\dot{\epsilon}_{kl} + \frac{1-f}{h} (\dot{u}_k n_l)^s \right] \right\} n_j \quad (5.3)$$

Given $\dot{\epsilon}_{kl}$ is the input for driving the constitutive model, Eq. (5.3) can be rearranged in terms of the velocity jump:

$$\dot{u}_k = h \underbrace{\left[f(D_{ijkl}^o n_l n_j) + (1-f)(D_{ijkl}^i n_l n_j) \right]}_{C_{ik}}^{-1} (D_{ijmn}^o - D_{ijmn}^i) \dot{\epsilon}_{mn} n_j \quad (5.4)$$

in which, C_{ik} serves as the localisation or acoustic tensor linking both diffuse and localised stages of deformation under constitutive scale. Furthermore, C_{ik} is the factor that enables the post-localisation analysis without disregarding the physical meaning by explicitly taking into account the relative length scale of the localisation band and the corresponding behaviour from the inside-outside zone.

Substituting the extended form velocity jump $\dot{u}_k$ from Eq. (5.4) to the mesoscale constitutive relations, Eqs. (5.1) and (5.2), and then entering it into the rate combination form in macroscale, Eq. (3.48), we obtain the macro stress-strain constitutive relation:

$$\dot{\sigma}_{ij} = \underbrace{\{fD_{ijkl}^i + (1-f)D_{ijkl}^o - f(1-f)C_{pm}^{-1}(D_{pqkl}^o - D_{pqkl}^i)n_q n_n(D_{ijmn}^o - D_{ijmn}^i)\}}_{D_{ijkl}^m} \dot{\epsilon}_k \quad (5.5)$$

Here, D_{ijkl}^m refers to the macroscopic tangent stiffness of which the first part is the upper bound in the stress return operation indicating the volume-averaged stress form; the second part is the “correction” stress for this upper bound that represents the enhancement for dealing with the non-homogeneous deformation. The term $(D_{ijkl}^o - D_{ijkl}^i)$ indicates the difference in incremental response. This whole formulation for localisation analysis will revert to a homogenous response when $D_{ijkl}^o = D_{ijkl}^i$ or when $f = 1$.

The formulation of the enriched constitutive framework covering two separate length scales has been demonstrated with a system of three constitutive relationships, Eqs. (5.1), (5.2) and (5.5), together with their connection. Accordingly, this framework allows modelling the response inside and outside of the localisation band with any constitutive model in conjunction with the macroscopic behaviour as their combining consequence.

The explicit algorithm starts with calculating the velocity jump by following Eq. (5.4). The localisation tensor, C_{ik} , and the tangent stiffness difference $(D_{ijmn}^o - D_{ijmn}^i)$ are determined from the state of the previous converged step. The obtained velocity jump is then substituted into Eqs. (3.43) and (3.44) to compute the inside and outside strain increments. Afterwards, by using the newly obtained strain increments, the corresponding inside-outside stress is computed within the stress return algorithm for the breakage model as mentioned in Section 3.2.2.

A common issue of explicit stress driving algorithms, in solving differential equations through the tangent stiffness, is the accumulated error. Because the enforcement of traction continuity is formulated in incremental forms, the error accumulates after each stress update leading to unreliable accuracy of the solutions. Therefore, an enhancement for the explicit stress return algorithm is introduced for more accurate stress computation using the total form of traction continuity. As numerical operation using the traction continuity, $t_k^i = t_k^o$, often produces a small residual:

$$r_i = (\sigma_{ij}^o - \sigma_{ij}^i)n_j \quad (5.6)$$

The first-order Taylor expansion based on the previous state of the residual results in:

$$r_i^{now} = r_i^{prev} + (\dot{\sigma}_{ij}^o - \dot{\sigma}_{ij}^i)n_j \quad (5.7)$$

Subsequently, the enhancement is applied on the displacement jump in incremental form as follows:

$$\dot{u}_k = hC_{ik}^{-1}[(D_{ijmn}^o - D_{ijmn}^i)\dot{\epsilon}_{mn}n_j + r_i^{prev}] \quad (5.8)$$

in which C_{ik} , D_{ijmn}^o and D_{ijmn}^i are obtained from the previous converged step.

Finally, the inside and outside strain increments, Eqs. (3.43) and (3.44), will be computed using the updated displacement jump above. The same procedure from the original explicit algorithm is applied with the macroscopic stress increment determined by Eq. (3.48).

5.1.2 The implicit stress return algorithm via an iterative process

In the stress update operation with finite strain increments, the first iteration using the explicit stress return algorithm often fails to satisfy the internal equilibrium condition that links the inside-outside stress. Therefore a residual traction vector, r_i , is introduced:

$$r_i = (\sigma_{ij}^o - \sigma_{ij}^i) n_j \quad (5.9)$$

Given a state associated with the residual traction r_i^{old} , the Taylor first-order expansion about this point will produce:

$$r_i^{\text{new}} = r_i^{\text{old}} + (\dot{\sigma}_{ij}^o - \dot{\sigma}_{ij}^i) n_j \quad (5.10)$$

Substituting the incremental stress-strain relationships, Eqs. (5.1) and (5.2), and the links between strain increments, Eqs. (3.43) and (3.44), into the above expression, providing that the macro strain increment $\dot{\varepsilon}_{kl}$ has been employed from the first iteration, we obtain:

$$r_i^{\text{new}} = r_i^{\text{old}} - D_{ijkl}^o \frac{f}{h} (\dot{u}_k n_l)^s n_j - D_{ijkl}^i \frac{1-f}{h} (\dot{u}_k n_l)^s n_j \quad (5.11)$$

By enforcing the condition $r_i^{\text{new}} = 0$ while solving the Eq. (5.11) for the incremental displacement jump $\dot{u}_k$ at the current iteration, one obtains:

$$\dot{u}_k = C_{ik}^{-1} r_i^{\text{old}} \quad (5.12)$$

in which C_{ik} was defined in Eq. (5.4). After obtaining the velocity jump $\dot{u}_k$, the iterative strain increments $\dot{\varepsilon}_{kl}^i$ and $\dot{\varepsilon}_{kl}^o$ at the second iteration will be:

$$\dot{\varepsilon}_{kl}^o = -\frac{f}{h} (\dot{u}_k n_l)^s \quad (5.13)$$

$$\dot{\varepsilon}_{kl}^i = \frac{1-f}{h} (\dot{u}_k n_l)^s \quad (5.14)$$

Subsequently, the stress increments $\dot{\sigma}_{ij}^o$ and $\dot{\sigma}_{ij}^i$ are updated along with the tangent stiffness and internal variables for the material in the corresponding zone. The iteration will be performed until reaching the converged solution, where the residual r_i becomes less than the tolerance (which, in this study, is set to 10^{-4}). The convergence criterion is determined as:

$$\text{error} = \frac{\|r_i^{\text{old}}\|}{\|\sigma_{ij} n_j\|} \leq \text{Tolerance} \quad (5.15)$$

Figure 5.1a-c demonstrates the performance of the explicit stress driving algorithm and the implicit stress return algorithm under a triaxial loading condition with a confining pressure, $p_c = 250 \text{ MPa}$, using the parameter-set of Bentheim sandstone. The thickness of the localisation band is fixed at $f = 0.3$ while the dimensions of the specimen are described in Figure 5.4. The implicit algorithm is performed with axial strain increments at $\Delta \varepsilon_a = 10^{-4}$ and 10^{-5} in two events that are the transition from softening to hardening ($\varepsilon_a = 2\%$) and the

hardening phase ($\varepsilon_a = 4\%$). In parallel, the explicit algorithm is conducted with reducing incremental strain considering $\Delta\varepsilon_a = 10^{-4}$; 10^{-5} ; 10^{-6} and 10^{-7} .

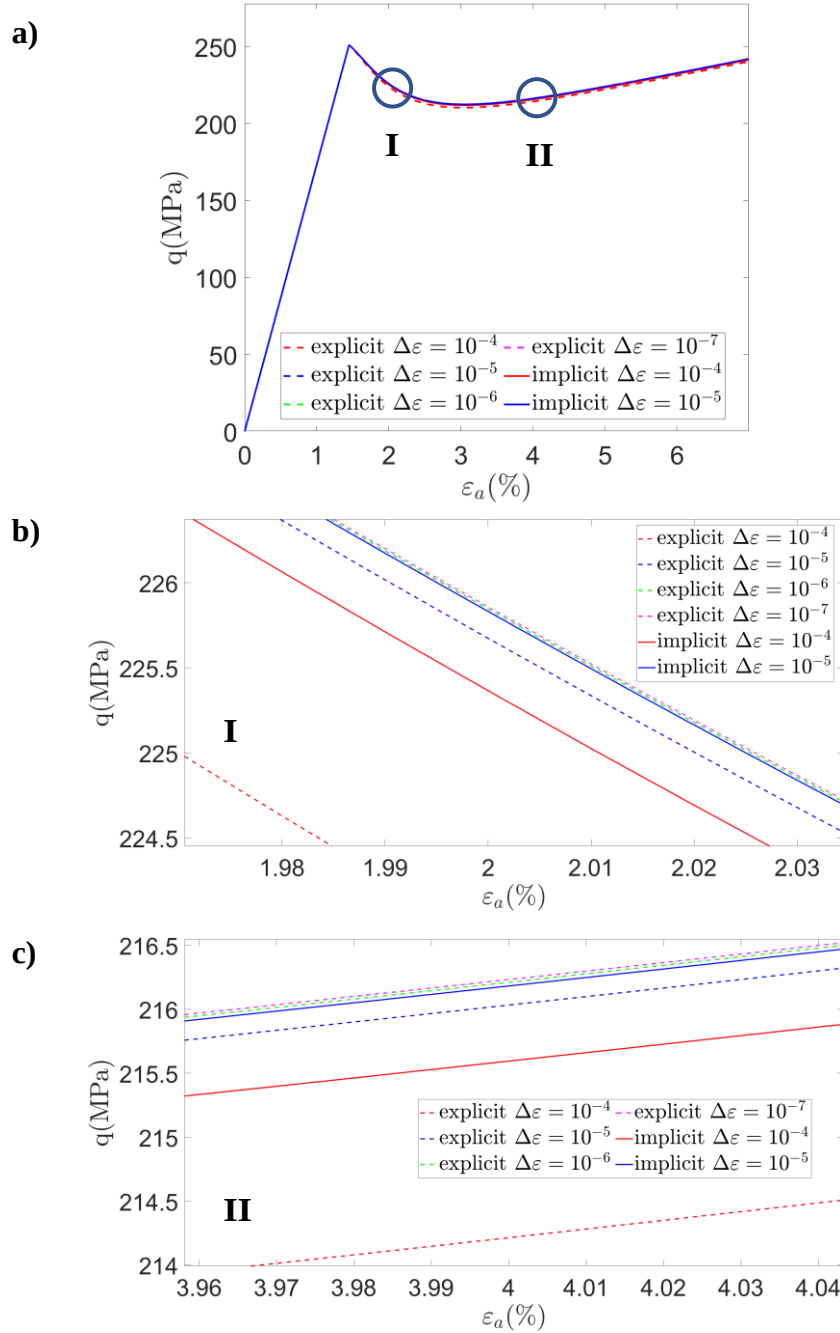


Figure 5.1. a) Comparison between the implicit and explicit stress-return algorithm by reducing the controlling strain increment where smaller increments lead to a more converging result. The performance is focused on two events that are: b) point I - the transition from softening to hardening ($\varepsilon_a = 2\%$); and c) point II - the hardening phase ($\varepsilon_a = 4\%$).

The implicit algorithm can maintain the traction error of an order of 10^{-17} which is the machine accuracy with double precision. We can see that the solutions obtained from the explicit algorithm with reducing strain increments from 10^{-4} to 10^{-7} converge to the implicit solution while a strain refinement in the implicit algorithm itself also reduces the relative error. It is

obvious that the implicit algorithm is more efficient as it does not require extra small strain steps to reach convergence. Besides, the error in the explicit algorithm does not accumulate after being employed with the enhancement using the residual from the previous state, r_i^{prev} , which shows the advantage of enforcing traction continuity in total form instead of its incremental form.

In Figure 5.2, the performance of the implicit algorithm is demonstrated at two events: softening-hardening transition ($\varepsilon_a = 2\%$) and during hardening phase ($\varepsilon_a = 4\%$). At the transition point, the return operation achieves the task in a more challenging condition which requires more iteration steps to solve larger errors. In general, the implicit algorithm has shown its effectiveness in reducing error through the iterative scheme which maintains the traction equilibrium in every single step.

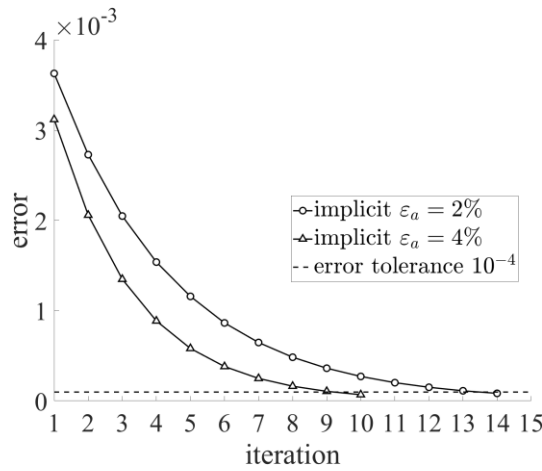


Figure 5.2. Error reduction of the implicit stress-return in a single strain step $\varepsilon_a = 2\%$ and $\varepsilon_a = 4\%$ showing an iterative scheme under $\Delta\varepsilon_a = 10^{-4}$ until a pre-set tolerance is met where the residual norm is sufficiently small ($error = 10^{-4}$).

5.1.3 Parameters calibration for the breakage model implemented in the dual-scale framework

As seen previously in the discussion on the formation of compaction bands under laboratory observations in Chapter 2, the episodic occurrence of compaction bands can be described by the activation and deactivation of a subparallel set of discrete bands during loading. The previous approach by Nguyen et al. (2017) enables the constitutive model to capture this swapping effect through a nested structure which allows inelastic behaviour in the zone outside of the first localisation band, thus, forming other localisation bands in this region. However, this nested structure would be resource consuming compared to the single-band approach while the necessity of whether this episodic detail at the constitutive level should be brought into the field-scale simulation still remains a question. Instead, the approach of a single diffuse band is employed of which thickness covers the zone of multiple discrete bands (Figure 5.3). Within the scope of this research, focus first directed to the case where elastic unloading is enforced on the behaviour on the outside of the localisation band while the inside is inelastic. Besides, the configuration case of inelastic behaviour on the outside, but not activating a second band in

this zone, will also be demonstrated and compared with the former configuration. Future work will approach the evolving thickness of the diffuse band so that it can cover newly formed discrete compaction bands as the pressure loading proceeds.

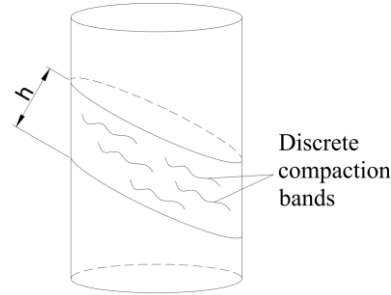


Figure 5.3. RVE embedded with a single band of which thickness covers the zone of multiple discrete localisation bands.

The enrichment involves both sizes h and H associated with the localisation band and the volume containing it, these sizes need to be determined, as they are parts of the dual-scale constitutive structure. While h is a material property measuring the width of the localisation band, H , varies with the specimen size in experiments or the size of the integration points in numerical analyses. In this study, the additional parameter H of the enriched breakage model is determined from the cylindrical sample (Figure 5.4) (Vajdova et al., 2004). The effective size H is computed from the specimen volume, the planar surface area and the orientation angle of the localisation band. The surface area S and the localisation angle γ vary between different sets of confining pressures p_c . Since the volume fraction $f = \frac{h}{H}$, indicating the thickness of localisation band in this study, is assumed to be fixed and the focus is on the behaviour in high-pressure regimes, it is acknowledged that although H varies with the loading condition (due to different orientations of the compaction bands), one can continue to use the same value of H for all cases ($H = 38.1\text{mm}$ is the result of confining pressure ranging from around 250 to 300 MPa).

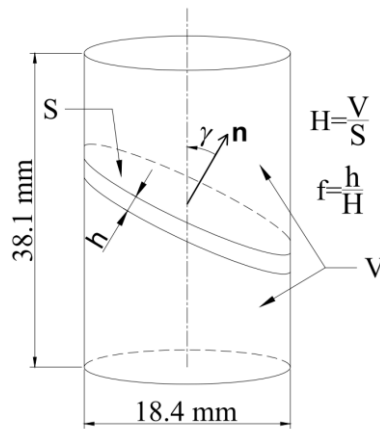


Figure 5.4. A finite thickness h localisation band embedded in a volume element with volume V , surface area S and size H .

The mechanical properties and parameters used for the double-scale breakage model are determined and calibrated based on various sources using the same sandstone from the Bentheim outcrop (Baud et al., 2004; Vajdova et al., 2004; Louis et al., 2005; Baud et al., 2006). The stress-strain response in the elastic portion is calibrated to obtain the elastic moduli (K and G). The critical breakage energy threshold is obtained from the crushing pressure, p_c , from the isotropic compression via the formulation $E_c = \frac{\vartheta p_c^2}{2K}$. The slope M of the critical state line is the ratio of the ultimate shear stress and ultimate volumetric stress $M = q_u/p_u$ from any conventional triaxial tests. The breakage-plastic coupling angle, ω , is obtained from the inelastic slope of stress-strain behaviour. The calibrated parameters of Bentheim sandstone were previously listed in Table 1. Since all parameters of the breakage model described can be determined under isotropic loading conditions, with the use of the experimental initial yield envelope, and are not subject to any conditions related to the localised mode of failure, they can be used straightforwardly in the dual-scale framework.

For the grading index, ϑ , representing the distance between the initial and ultimate grain size distribution, the procedure for obtaining ϑ will be presented in detail, given it is also important for the calculation of permeability due to grain crushing. The complex nature of atomization and dispersion produces a distribution of grain sizes. A graphical description of the grain size distribution is obtained by dividing the range of sizes into suitable intervals and producing a characteristic distribution or histogram. The ordinate can represent any size characteristic of the grains, e.g., number, volume, mass; which is of specific interest for the characterization of pharmaceutical aerosols. Normalizing the ordinate by the total mass of grains, M , yields the relative mass distribution. The probability distribution is obtained by dividing the relative mass by the grain size interval, ΔD_i (Dunbar and Hickey, 2000):

$$p_{m,i} = \frac{m_i}{M} \frac{1}{\Delta D_i} \quad (5.16)$$

$$F_{m,i} = \int_0^{D_i} p(D)_m dD \quad (5.17)$$

where $p_{m,i}$ is the probability density of the i^{th} interval (with units of μm^{-1}); $F_{m,i}$ is the cumulative percentage of mass for grains with diameters less than D_i . A smooth curve can be drawn through the data at the size interval mid-points to obtain the probability distribution curve. The probability that a selected mass of grains will be less or greater than a particular size can be calculated from the area under the curve. Integration of the probability distribution yields the cumulative mass distribution.

As suggested by Einav (2007a), it is useful to simplify the definition and view the breakage as a scalar variable that linearly weighs the relative proximity of the current grain size distribution (gsd) from the initial and ultimate gsd's as defined in Eq. (3.1). Einav (2007a) showed that the ultimate gsd may be given by the following Turcotte fractal distribution which has the limits of $D_m \rightarrow 0$ of the following distributions:

$$p_u(D) = (3 - \alpha) \frac{D^{2-\alpha}}{D_M^{3-\alpha} - D_m^{3-\alpha}} \quad (5.18)$$

$$F_u(D) = \frac{D^{3-\alpha} - D_m^{3-\alpha}}{D_M^{3-\alpha} - D_m^{3-\alpha}} \quad (5.19)$$

where α is the fractal dimension, ranging typically between 2.5–2.8, and D_M is the maximum grain size; and D_m is the minimum possible grain size. This seemingly minor additional dimension proves critical when the permeability reduction is analysed in the next section.

For the purpose of a parametric study, consider the initial and ultimate cumulative distributions given in Figure 5.5. The ultimate distribution is based on the fractal dimension Eq. (5.18). The criticality index property can be approximated by using Eq. (3.2).

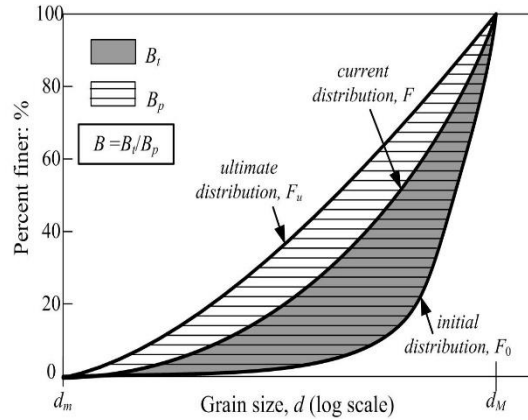


Figure 5.5. Breakage measurement and evolution law with the initial, F_0 , and ultimate, F_u , cumulative grain size distribution (Einav, 2007a,b).

The experimental observation of the gsd was obtained from a different research group (Louis et al., 2005) who also conducted Scanning Electron Microscope (SEM) observations on sandstones from the outcrop in Bentheim, Germany.

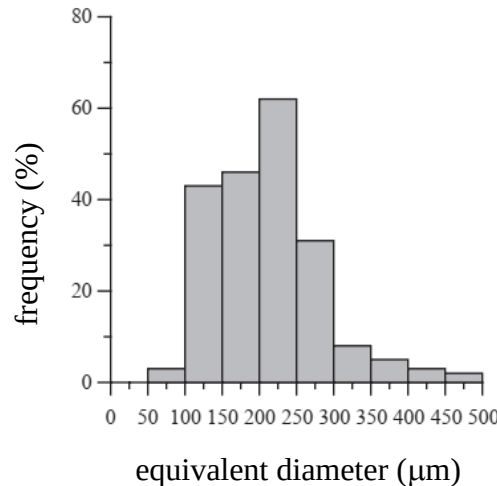


Figure 5.6. Scanning Electron Microscope (SEM) observation on the grain size distribution for Bentheim sandstone (Louis et al., 2005).

The gsd data set of the Bentheim sandstone is treated as the undamaged grain size characteristics, thus it can be considered as the initial gsd for the present analysis. In order to obtain the value of ϑ , the function describing the initial gsd curve is required for calculating its second-order moment. The gsd data set in Figure 5.6 is fitted by the normal distribution technique. Due to the lack of a fully comprehensive data set on the gsd, the given experiment chart (Louis et al., 2005) only provided the probability of grain size in a range, so this is treated as discrete random variables, although the gsd's nature should be continuous. The initial gsd probability density function, $p(D)$, following the normal distribution f along with the R-square/Adjusted R-square error (Akossou and Palm, 2013), have the following form:

$$f = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{D-\mu}{\sigma}\right)^2} \quad (5.20)$$

$$R^2 = 1 - \frac{\sum(x - \bar{x})^2}{\sum(x' - \bar{x})^2} \leq 1 \quad (5.21)$$

$$R_{adjusted}^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - q - 1} \quad (5.22)$$

where μ is the mean value and σ is the standard deviation; x is the sample data; $\bar{x}$ is the mean sample value; x' is the approximation value; N is the total sample size ($N = 9$); and q is the number of predictors ($q = 1$).

These two variables are calibrated until a good fit is obtained with an acceptable R-square/Adjusted R-square value. Figure 5.7 exhibits the fitted curve for the experimental gsd data of the Bentheim sandstone. The mean grain size and the standard deviations are $\mu = 210 \mu m$ and $\sigma = 65$ respectively, which are associated with the error R-square = 0.996 and the adjusted R-Square of 0.995. The cumulative distribution curve is obtained using Eqs. (5.17) and (5.20). The experimental cumulative density curve, Figure 5.7b, of the initial gsd is obtained by following the statistical technique of grain size fitting by Sehmel (1968).

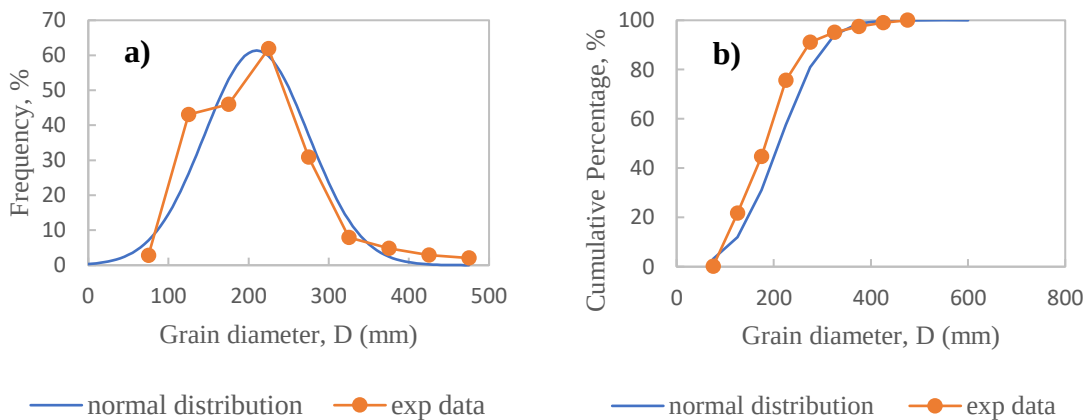


Figure 5.7. Curve fitting results for the initial distribution state of Bentheim sandstone a) grain size distribution; b) cumulative distribution.

When varying the theoretical ultimate and initial gsd, the distance between these two curves is described by ϑ . The closer the curves are, the smaller ϑ is, and vice versa. On the other hand,

the theoretical ultimate gsd and the experimental gsd should also describe the distance with ϑ . Das et al. (2011) used β for a "narrow initial gsd" based on observation (Schutjens et al., 1995) and α is 2.7 within the assumed fractal range of 2.5-2.8 (Sammis et al., 1987) for porous rock, resulting in $\vartheta = 0.85$, which is purely based on a theoretical formula. However, in order to obtain a suitable position of the ultimate gsd curve as compared to the position of the initial gsd obtained from the experiment by Louis et al., (2005), the fractal power, α , should be at around 4-6, which is incorrect for the fractal limit ($\alpha \leq 3$) and the recommended range 2.5 - 2.8 for rock (Sammis et al., 1987). Therefore, we cannot straightforwardly calculate the data set of cumulative distribution $F(D)$ with the fractal function. Instead, this study only adopts the fractal function to approximate the data set of the ultimate gsd, $p_u(D)$, with $\alpha = 4.5$. Then, the normal distribution is applied to this data set to obtain the curve-fitted function of $p_u(D)$, following by integral calculation in Eq. (5.17) to obtain the data set of $F_u(D)$. Finally, Eq. (3.5) is used for the determination of the second order moment for the determination of ϑ . The final result for the cumulative initial and ultimate gsd curves is demonstrated in Figure 5.8. Once the curve-fitted gsd function is obtained, it can be implemented in Eqs. (3.2) and (3.5) to obtain the grading index ϑ .

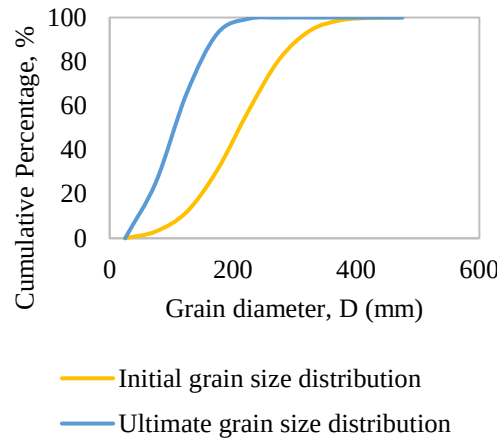


Figure 5.8. Spatial evolution of Bentheim sandstone limited by the initial gsd curve obtained by curve-fitting the experimental data (Louis et al., 2005) and ultimate gsd curves extracted from the approximation of fractal law (Sammis et al., 1987).

From the above initial and ultimate gsd results, it is straightforward to obtain the grading index $\vartheta = 0.72$. This is compared with the approach solely based on fractal theory, where $\vartheta = 0.85$ was used by Das et al. (2011) and then later by Collins-Craft et al. (2020) in a breakage model. As can be seen in Figure 5.9a, the volumetric response between the two ϑ values do not differ much and both are close to the experimental curves. However, the variation is well observed in the shear behaviour (Figure 5.9b) where $\vartheta = 0.72$ yields a more hardening behaviour, thus, it is better at fitting the response at high confining pressure ($p_c = 300 \text{ MPa}$). This can be well explained by the definition of ϑ where it measures the crushable capability of the material. A smaller ϑ value indicates that the material is less likely to be crushed. Under high confining pressure, the porous rock structure is reduced and compacted, thus, higher stress for triaxial

shearing is required. Therefore, in order to describe the sharp hardening slope of the behaviour under high confining pressure, ϑ should be sufficiently reduced.

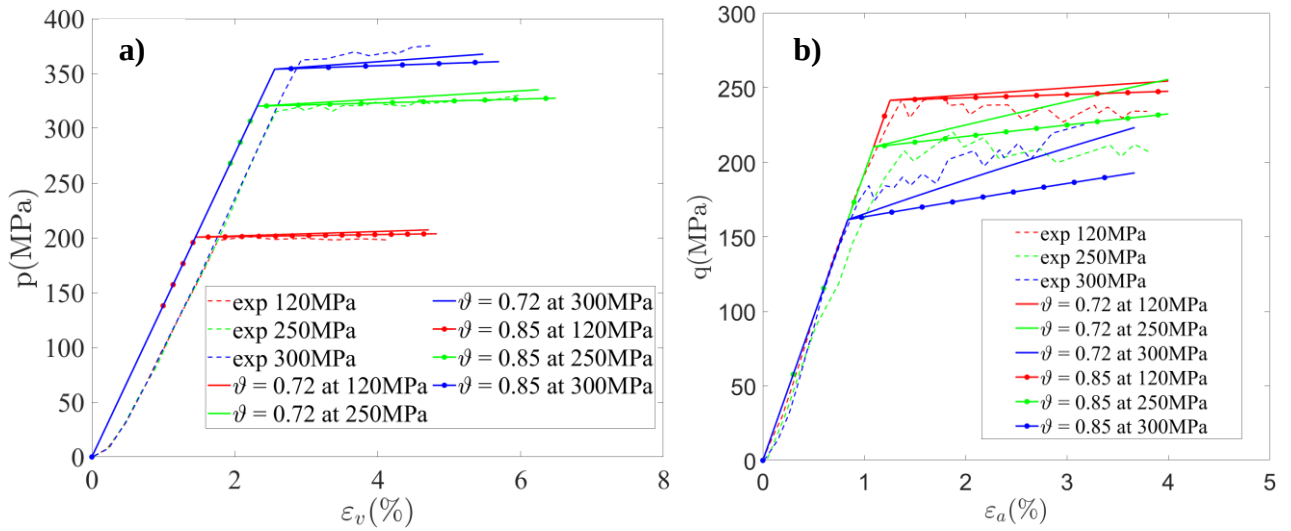


Figure 5.9. A comparison on the mechanical response, regarding a) volumetric; and b) shear behaviour, between the method using experimental data of the grain size distribution ($\vartheta = 0.72$) and the method based on fractal theory ($\vartheta = 0.85$) under different levels of triaxial confinement with the same parameter set used by Das et al. (2011). Experiment data are obtained from Baud et al. (2004) and Wong and Baud (2012).

5.1.4 Thickness of compaction localisation and breakage evolution

Instead of controlling the softening and hardening by a parameter in another traditional model, the dual-scale framework can describe that by incorporating a more physical parameter $f = \frac{h}{H}$ as the ratio between the thickness of the band and the volume element containing it. A parametric study is performed on the volume fraction f to understand its effect on the inelastic-elastic response when compaction localisation occurs by plotting the macroscopic shear response against axial strain at the three confining levels of 120, 250 and 300 MPa. Theoretically, f is an input related to the thickness h of the localisation band and can be defined by the measurement of the localised failure geometry in deformed porous rocks.

In Figure 5.10, the degree of breakage corresponding to the zone inside and outside of the compaction band is demonstrated at increasing axial strain steps under different confining pressures. These results are obtained from the breakage model in the dual-scale framework with the volume fraction $f = 0.3$. This illustration provides the concept of how the model describes the degree of grain crushing through the variable B and the width of the compaction localisation zone through the length scale-related h . The experimental results show that the total size of the compaction zone in the specimen increases during loading. In the proposed approach, only a single localisation band is considered embedded in a volume element, which is equivalent to lumping all inelastic effects into a band with size h . Given the experimental data in Figure 5.10, the expansion of this lumping phenomenon corresponds to the variations of the size h and volume fraction $f = h/H$ of the localisation zone in a specimen. Therefore, an evolution law

for f is in principle needed to fully capture the behaviour of Bentheim sandstone in the post-localisation stage. However, this feature is not considered yet in the current enriched framework and the value of the volume fraction is assumed to be a constant and is determined from the transmission optical micrograph (dark area), as the percentage of crushed grains over normal grains.

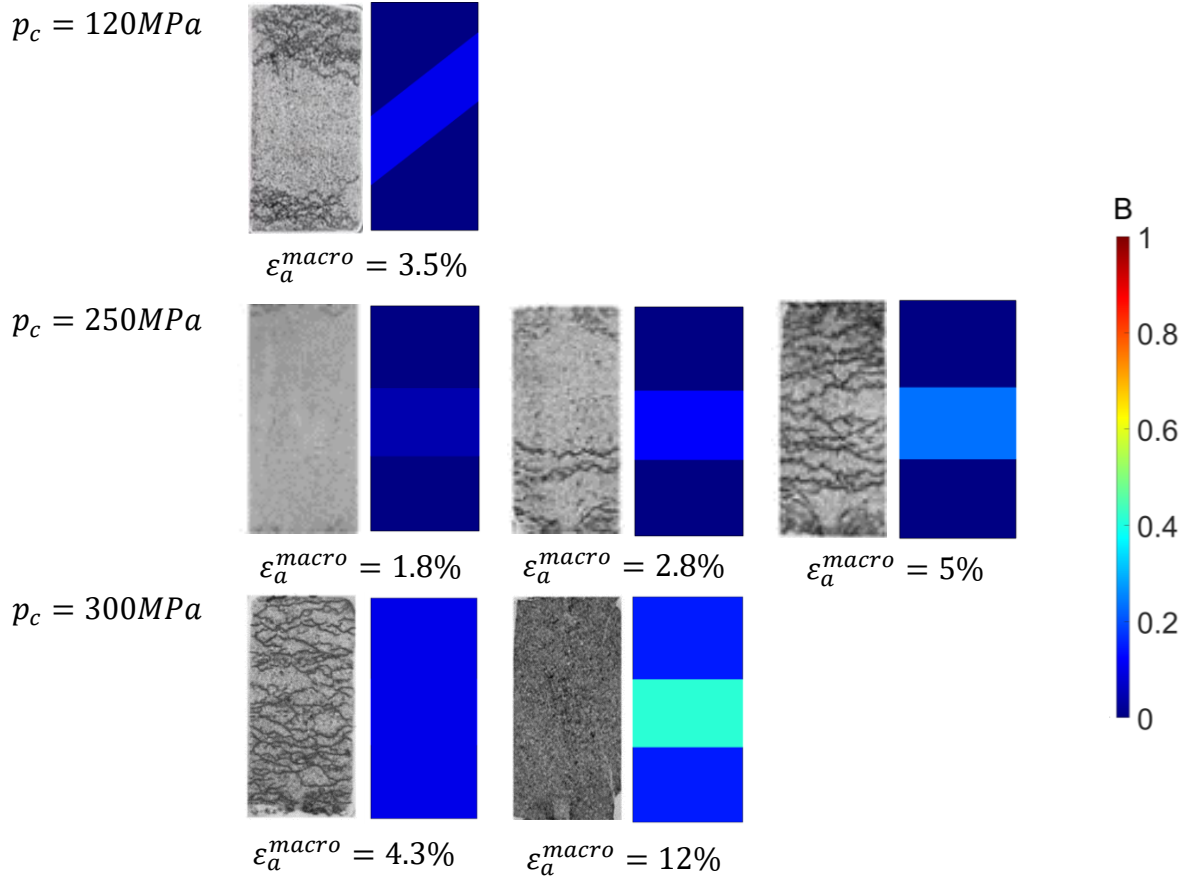


Figure 5.10. The evolution of compaction bands on the axial cross-section of the sample at the end of the triaxial loading test. The dark area indicates comminution of grain crushing (Wong et al., 2001; Vajdova et al., 2004).

The present parametric study demonstrates that the input values of f enable the overall behaviour of the model to capture the stress drop oscillation in the experimental response. The smaller f gets, the thinner the band is, leading to less dissipated energy and a softening macro behaviour is expected. On the other hand, larger values of f provide less intense softening, but the transition from softening to hardening would require more strain increments as well as the hardening progress. For all cases shown in Figure 5.11, $f = 0.1$ always exhibits the steepest softening slope at the initiation of localisation and the most immense surge in the hardening phase. For the case of 120 MPa and 250 MPa , $f = 0.3$ is a good match for the inelastic slope as well, as the stress drop level is appropriately represented (Figure 5.11a,b). However, for $p_c = 300 \text{ MPa}$, the behaviour does not exhibit localisation until it reaches an axial strain ϵ_a of about 5% (Figure 5.11c). It can be explained that this hardening jump is due to the effect of high confining pressure leading to crushed grain fragments to move and fill into the void of

pore collapse, causing the material to harden. Consequently, the numerical model detects the formation of a compaction band followed by a hardening response. Furthermore, the thickness of localisation zone h defines how the inelastic dissipation takes place through its associating volume fraction f with the host RVE size H .

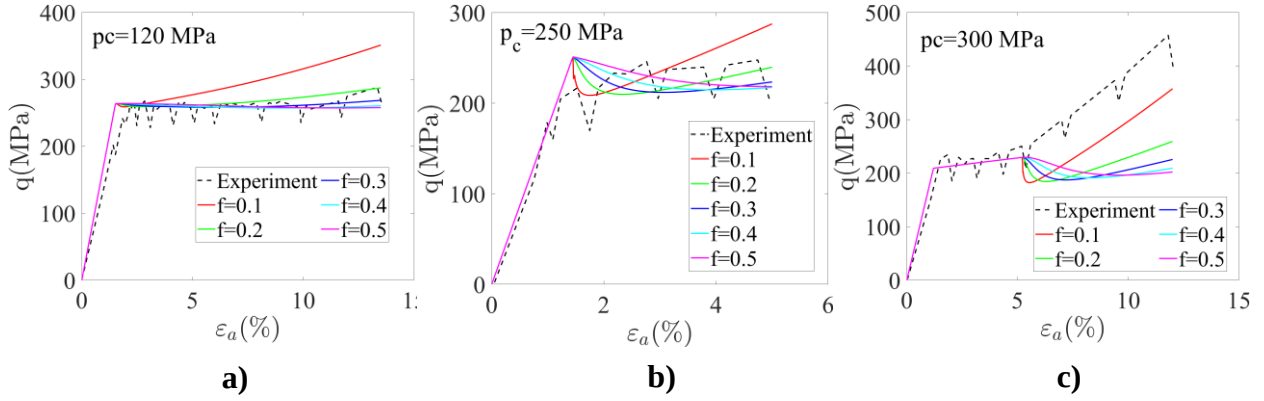


Figure 5.11. The effect of volume fraction f on the macroscopic behaviour compared with experimental data (Vajdova et al., 2004) under confining pressure at: a) 120 MPa; b) 250 MPa; and c) 300 MPa.

Nevertheless, the upward slope of hardening in the case of experimental response under 300 MPa confinement should not be calibrated with the volume fraction f . This is because the hardening behaviour should be initially dealt with by the capability of controlling the pore collapse effect by the breakage model using the breakage-coupling angle ω . It should be emphasised that when implementing the dual-scale framework, that takes into account the effects of strain localisation, it is aimed to capture the underlying physics of localised deformation without requiring adding more phenomenological or curve fitting parameters. In this sense, and also based on the above results, the improvement of the breakage model to better capture the effect of pore collapse, which leads to hardening behaviour, will require linking the evolution of f and the parameter ω controlling pore collapse affects. As discussed in Section 4.4, the underlying breakage model should be well connected to the mechanism of pore collapse before assessing the effect of band thickness f in the dual-scale framework. With the capability of the original breakage model by Einav (2007a,b), allows one to capture the compacted behaviour to a denser structure due to pore collapse. In future research, an enhancement on the evolution of the plastic-breakage coupling angle, ω , will better capture the steep hardening slope due to pore collapse in post-localisation for very high confining pressure. In such a case, the coupling angle, ω , is a function in terms of the internal variables from the breakage model which can be either the breakage variable, B , or the plastic strain increment, $\dot{\varepsilon}_{kl}^p$.

In summary, the stress drop is associated with the onset of localisation, which shows a steep slope at this point which increases when f gets smaller. For the case of increasing f , this means the thickness of the compaction band expands, indicating more discrete bands are forming. This could be a reason why the macroscopic response exhibits the stress drop effect, because as more discrete bands forms throughout the volume, the weaker points the RVE has and hence pore

collapse is taking place, leading to a denser state and strengthening effects. It should be noted that when f reaches its maximum value of 1, the dual-scale framework approaches homogenous behaviour. This agrees with the compaction failure observed in experiments where the material is fully crushed and the compaction band has taken over the whole volume.

5.2 Dual-scale enhancements for hydraulic response

5.2.1 Tracking the permeability via the evolving grain size

Permeability reduction due to grain crushing may have adverse effects in various engineering applications. The tortuosity of the fluid flow within granular materials constantly changes if the gsd evolves; this factor affects the permeability irrespective of whether the nominal porosity changes or not. Therefore, the connection between the gsd and the permeability is important, specifically in undrained conditions where the porosity effect on the permeability is eliminated. In particular, there has been a growing interest in the use of fractals to predict hydraulic properties from gsd (Rieu and Sposito, 1991; Tyler and Wheatcraft, 1992).

Characterization of number–size relations of fragments by a probabilistic approach, and its applications for estimating permeability, was recently made in relation to sand production in porous rocks (e.g., Karacan & Halleck, 2003.) A complimentary study links this important connection between the gsd and permeability further to the mechanics of stresses and strains. Papamichos et al. (1993) followed such a mechanistic approach but referred to the permeability reduction to a single size fraction of D_{10} (grain size for which 10% of the grains by mass is finer), and made use of the Hazen formula (i.e., permeability is proportional to D_{10} squared). Since the present work enables one to predict the entire gsd as it evolves, the permeability reduction issue is revisited in the expanding perforation problem by referring to the mean harmonic grain size D_H , rather than D_{10} , which has both theoretical and empirical advantages (Matyka et al., 2008).

Given the breakage variable from the breakage constitutive model, the harmonic mean grain size, D_H , is adopted following the work of Nguyen and Einav (2009):

$$\frac{1}{D_H} = \int_{D_m}^{D_M} p(D) \frac{dD}{D} = (1 - B) \frac{1}{D_{H_0}} + B \frac{1}{D_{H_u}} \quad (5.23)$$

where the initial and ultimate harmonic mean grain sizes (i.e., the distributions that correspond to the breakage of zero or unity) are defined by:

$$\frac{1}{D_{H_0}} = \int_{D_m}^{D_M} \frac{p_0(D)}{D} dD \quad (5.24)$$

$$\frac{1}{D_{H_u}} = \int_{D_m}^{D_M} \frac{p_u(D)}{D} dD \quad (5.25)$$

The permeability is defined in the Kozeny-Carman relationship derived from the porosity based on a simple capillary model for a porous medium:

$$K = c_0 \frac{\phi^3}{T^2 S^2} \quad (5.26)$$

where ϕ is the porosity of the porous medium; c_0 is a dimensionless Kozeny constant determined from the channel geometry (Bear, 1972); $S = 6/D_H$ is the specific surface area of a spherical grain in term of the harmonic grain size, which is different from the surface area of the localisation band as previously defined; and T is the hydraulic tortuosity which describes the streamlines of the porous medium by a dimensionless parameter. The ad hoc function of tortuosity T with respect to porosity ϕ is chosen in the review by Matyka et al. (2008):

$$T = \phi^{-\alpha} \quad (5.27)$$

where α is a fitting parameter that may vary between different pressures. In this study, α is the result of calibration to fit the experimental elastic slope of the permeability drop, which is described later in Section 5.3.4. Because the tortuosity for each specimen is unique despite being composed of the same material, and Eq. (5.27) is likely empirical-based, α should be adjusted for every single case and hence a universal parameter cannot be obtained. For this reason, after calibrating the elastic slope of permeability reduction, $\alpha = 5$ was chosen for specimens loaded under 250 MPa and 300 MPa confining pressures, while 120 MPa is set with $\alpha = 15$.

The permeability reduction R_K can now be obtained with respect to the initial permeability K_0 as:

$$R_K = \frac{K}{K_0} = \frac{(\phi/\phi_0)^3}{(T/T_0)^2} \left(\frac{D_H}{D_{H_0}} \right)^2 \quad (5.28)$$

5.2.2 Permeability evolution in the dual-scale framework

The relationship between the behaviour of flow and strain localisation may be summarised as a complex conduit system that neither suppresses nor enhances the hydraulic communication (Fossen et al., 2007). Accordingly, a low-porosity compaction band has been known for acting as a barrier that obstructs the flow of the fluid, while a dilation band leads to fluid pathways that facilitate the flow. Torabi et al. (2015) noted that such characteristics of the flow pattern may be governed by the variation of permeability, thickness or orientation along with a single band. The fluid's behaviour was described to move into fractures that have higher permeability than the outside zone, where the velocities across the interface rose rapidly and abruptly. On the other hand, in the opposite case where the permeability inside is lower, the flow tended to avoid the fracture. These findings led to the conclusion that the Darcy velocity on two sides of the fracture not identical. On this account, the term “geological barrier” was used by Martin et al. (2005) to specify the flow-interrupting effect of fractures which, implicitly, proved that two layers divided by that barrier could be under different pressures. In contrast, Borja and Alarcón (1995) implied that flow behaves the same inside and outside of the fractures, where the effective stress is mathematically consistent even at finite strain. However, it was just a

qualitative statement that had poorly supported numerical evidence, as their report vaguely involved the fluid-solid coupling behaviour in their theory and experiment.

In this research, the permeability on the inside and outside of the localisation band is assumed to be homogeneous. Similar to the mechanical descriptions, the permeability on the inside and outside of the material is assumed to be homogeneous. The isotropic permeability tensors $\mathbf{K}_i$ and $\mathbf{K}_o$ can be expressed as

$$\mathbf{K}_i = \begin{pmatrix} K_i & 0 \\ 0 & K_i \end{pmatrix} \text{ and } \mathbf{K}_o = \begin{pmatrix} K_o & 0 \\ 0 & K_o \end{pmatrix} \quad (5.29)$$

Deriving from the mass conservation applied on the whole RVE embedded with a localisation band (Nguyen et al., 2014)

$$\frac{\partial(\phi\rho)}{\partial t} = -\nabla \cdot [\rho(\mathbf{v}^f - \mathbf{v}^s)] \quad (5.30)$$

Where $\mathbf{v}^f$ is the fluid velocity, $\mathbf{v}^s$ is the solid velocity, ρ is the specific density of the fluid and ϕ is the porosity of the solid. Neglecting the gravitation force, the flow relative velocity $\mathbf{v}$ based on Darcy law is defined as

$$\mathbf{v} = \mathbf{v}^f - \mathbf{v}^s = -\frac{\mathbf{K}}{\mu} \nabla p \quad (5.31)$$

Where μ is the fluid viscosity; ∇p is the pressure gradient; $\mathbf{K}$ is the macroscopic permeability of the volume element which, in the dual-scale framework, is the combining result of both permeability inside, $\mathbf{K}_i$, and outside, $\mathbf{K}_o$, of the band linking through the volume fraction ratio. Eq. (5.31) can be expressed in matrix form as

$$\begin{pmatrix} v_n \\ v_s \end{pmatrix} = -\frac{1}{\mu} \begin{pmatrix} K_n & 0 \\ 0 & K_s \end{pmatrix} \begin{pmatrix} \nabla p_n \\ \nabla p_s \end{pmatrix} \quad (5.32)$$

Eq. (5.32) describes the permeability tensor in the local n-s coordinate system where the flow through the volume element is treated as two independent 1D problems for the normal n and the tangent s directions (Figure 5.12a). Within this context, the Darcy velocity can now be decomposed into two components v_n and v_s . Regarding the normal direction of the band, where $\mathcal{H}$ is the total hydraulic head and $\partial\mathcal{H}/\partial n$ is the hydraulic gradient across the whole volume element, the normal component of flow velocity can be written as

$$v_n = -\frac{K_n}{\mu} \frac{\mathcal{H}_1 - \mathcal{H}_2}{H} \quad (5.33)$$

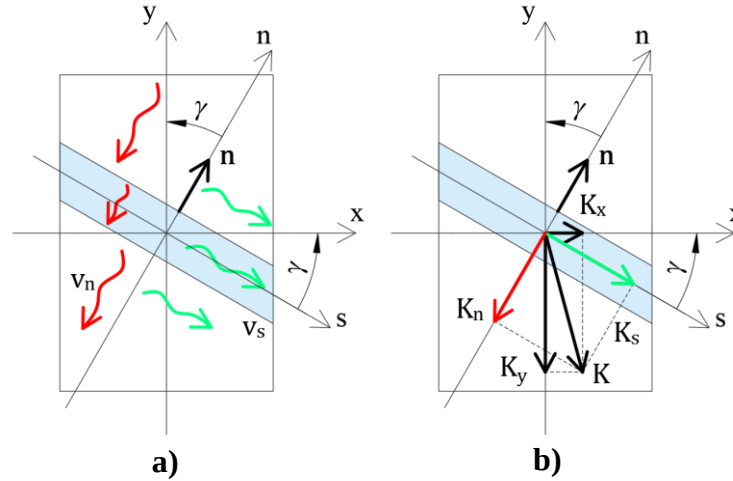


Figure 5.12. An RVE embedded with a localisation band of which n is the normal vector. The hydraulic components of the flow through the RVE are expressed in the global x - y coordinates and the local n - s coordinates rotated by angle γ . (a) The flow velocities are decomposed as normal velocity, v_n , and tangent velocity, v_s ; (b) The macro permeability, K , is decomposed into the local and global components, K_n - K_s and K_x - K_y , respectively.

Similarly, the fluid velocity in the region inside and outside of the band can also be written as

$$v_{o1} = -\frac{K_o}{\mu} \frac{\mathcal{H}_1 - \mathcal{H}_{i1}}{\alpha(H-h)}; \quad v_{o2} = -\frac{K_o}{\mu} \frac{\mathcal{H}_{i2} - \mathcal{H}_2}{\beta(H-h)}; \quad v_i = -\frac{K_i}{\mu} \frac{\mathcal{H}_{i1} - \mathcal{H}_{i2}}{h} \quad (5.34)$$

where $\alpha + \beta = 1$

The hydraulic gradient $\partial \mathcal{H} / \partial n$ is assumed constant throughout the volume element embedded with a localisation band. Thus, the continuity of the hydraulic head and hydraulic flux (Darcy velocity) at the interface between the localisation band and the outside region is enforced, which leads to $v_i = v_{o1} = v_{o2}$. Based on Eq. (5.31), and taking into account the case of the compaction band, the permeability inside reduces, while the hydraulic pressure increases and vice versa for the zone outside. Thus, it is safe to assume an equivalent velocity between these zones. It should be noted that, as seen in Figure 5.13, the continuity across the interfaces of the localisation band is not necessary for the tangent flow problem, given that the hydraulic gradient $\partial H / \partial s$ is similar on both regions. From Eq. (5.34) we obtain

$$\mathcal{H}_1 = \mathcal{H}_{i1} + \frac{K_i}{K_o} \frac{\alpha(H-h)}{h} (\mathcal{H}_{i1} - \mathcal{H}_{i2}) \quad (5.35)$$

$$\mathcal{H}_2 = \mathcal{H}_{i2} - \frac{K_i}{K_o} \frac{\beta(H-h)}{h} (\mathcal{H}_{i1} - \mathcal{H}_{i2}) \quad (5.36)$$

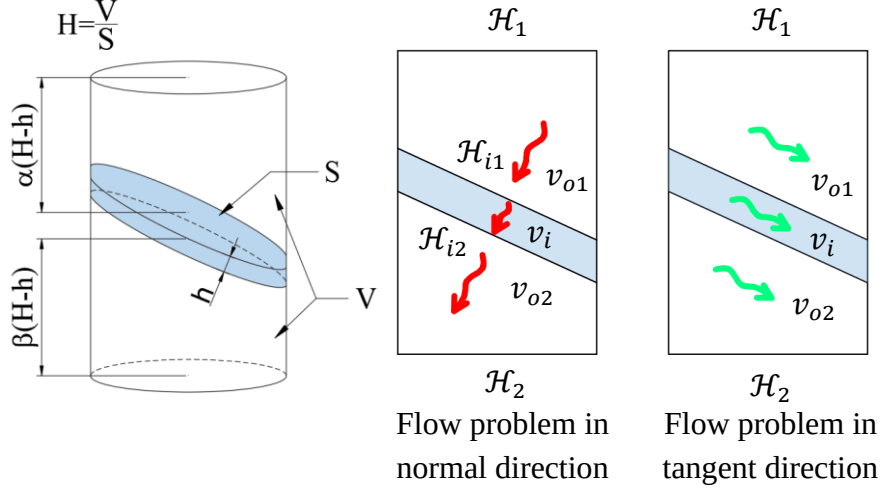


Figure 5.13. Decomposition of flow into the local n-s system. The flow from gradient head $\mathcal{H}_1$ to $\mathcal{H}_2$ through the RVE is divided with a localisation band. The Darcy velocity inside, v_i , and outside, v_o , is assumed to be continuous on the interface of the band.

Using the volume fraction $f = h/H$, Eqs. (5.35) and (5.36) become

$$\mathcal{H}_1 - \mathcal{H}_2 = \left[1 + \frac{K_i}{K_o} \frac{(H-h)}{h} \right] (\mathcal{H}_{i1} - \mathcal{H}_{i2}) = \frac{fK_o + (1-f)K_i}{fK_o} (\mathcal{H}_{i1} - \mathcal{H}_{i2}) \quad (5.37)$$

Since we assume the fluid velocity is uniform across the surface of the band, the normal permeability can then be determined from the condition $v_n = v_i$,

$$-\frac{K_n}{\mu} \frac{\mathcal{H}_1 - \mathcal{H}_2}{H} = -\frac{K_i}{\mu} \frac{\mathcal{H}_{i1} - \mathcal{H}_{i2}}{h} \quad (5.38)$$

Substituting Eq. (5.37) into Eq. (5.38), the normal permeability is obtained by

$$K_n = \frac{K_i K_o}{fK_o + (1-f)K_i} \quad (5.39)$$

Following the same procedure in the tangent direction with constant $\partial H / \partial s$, we obtain the tangent permeability

$$K_s = fK_i + (1-f)K_o \quad (5.40)$$

In order to express $\mathbf{K}$ in the global Cartesian x-y coordinate system, a rotation matrix $\mathbf{R} = \begin{pmatrix} -\sin \gamma & \cos \gamma \\ \cos \gamma & \sin \gamma \end{pmatrix}$ is required (Figure 5.12b). Multiplying Eq. (5.32) with $\mathbf{R}$ and its transpose matrix $\mathbf{R}^T$ ($\mathbf{R}\mathbf{R}^T = \mathbf{I}$), we obtain

$$\begin{pmatrix} v_x \\ v_y \end{pmatrix} = -\frac{1}{\mu} \begin{pmatrix} K_x & K_{xy} \\ K_{yx} & K_y \end{pmatrix} \begin{pmatrix} \nabla p_x \\ \nabla p_y \end{pmatrix} \quad (5.41)$$

$$\text{Where } \begin{pmatrix} K_x & K_{xy} \\ K_{yx} & K_y \end{pmatrix} = \mathbf{R} \begin{pmatrix} K_n & 0 \\ 0 & K_s \end{pmatrix} \mathbf{R}^T = \begin{pmatrix} K_n \sin^2 \gamma + K_s \cos^2 \gamma & (K_s - K_n) \sin \gamma \cos \gamma \\ (K_s - K_n) \cos \gamma \sin \gamma & K_n \cos^2 \gamma + K_s \sin^2 \gamma \end{pmatrix}$$

5.3 Permeability evolution analysis associating with the post-localisation behaviour in porous sandstone

In this section, the mechanical and hydraulic experimental results of highly porous Bentheim sandstone under triaxial compression tests will be used for the demonstration of the performance of the dual-scale breakage model in capturing the material behaviour in the localised mode of failure. Herein, the permeability evolution is addressed by tracking the mechanical response from micro- to macroscale via the bridge at the meso level. The key focus in this analysis is the coupled permeability-mechanical behaviour at different confining pressures, based on the description and observation from experimental resources, where:

- High (250 MPa) and very high (300 MPa) confining pressures exhibit inelastic response for the zone inside of compaction localisation band and the outside bulk as well. This configuration associates with the formation of pure compaction as (sub)parallel tabular arrays and the evolving thickness of the cumulative localised compaction zone.
- The intermediate confining pressure (120 MPa) possesses an inelastic behaviour for the material inside of the localised zone, while elastic or negligible inelastic response for the zone outside was observed. This indicates a mixed-mode of shear-enhanced compaction bands forming an inclined tabular plane with respect to the bedding surface.

Therefore, two configurations will be employed along with the analysis being demonstrated in a parallel structure in which one sub-section will describe the coupled mechanical-permeability evolution with the configuration. The computational technique for each configuration is straightforward where the “elastic outside” mode will use the breakage secant stiffness to produce the outside stress increments; whereas the “inelastic outside” mode utilises the yield-checking procedure and semi-implicit stress-return algorithm mentioned previously in Section 3.2.2.

For comparison with the experimental macroscopic measurements, permeability is plotted against the increment of macroscopic hydrostatic pressure, p , and macroscopic axial strain, ε_a^{macro} . It should be noted that the present analysis focuses on the mechanisms behind the permeability evolution rather than curve-fitting the experimental data. In particular, the macro-meso mechanical response affects the permeability of the zone inside and outside of the compaction band is investigated, as well as their combined effect on the macroscopic permeability. Account is also made of the four components of the permeability including the vertical (K_y) and horizontal (K_x) macro permeabilities; the inside (K_{in}) and outside (K_{out}) meso permeabilities, as all have been discussed above in Section 5.2.2. The reason for requiring inside-outside permeability is that there has been no experimental method that can measure the permeability inside this localisation band, but only the approximation of global permeability. The dual-scale framework in constitutive modelling provides us with a more comprehensive understanding of permeability evolution from the access to the inside of the localisation band, which shows a much different response compared to the global one. On the other hand, the

direction of macro permeability concerning the orientation of the band can be significantly different as some experimental works have demonstrated (mentioned in Section 2.3). Furthermore, a separate computation of K_x and K_y could be derived from the experimental technique, where permeability is measured for hydraulic flow in the either the axial or lateral directions. In this study, the experimental data by Vajdova et al. (2004) was obtained from permeability measurement in the axial direction, thus, the vertical numerical component of macro permeability will be examined.

5.3.1 Enforcing elastic behaviour for the zone outside of the compaction band

The stress path in $p - q$ triaxial space for the macro, inside and outside behaviour is illustrated in the correspondence with the initial breakage yield surface (Figure 5.14). It shows that the macroscopic behaviour is always linear with a slope $\frac{\Delta q}{\Delta p} = \frac{1}{3}$ under triaxial condition, while the responses inside and outside the localisation band can be observed once bifurcation occurs. The slope of this stress path also confirms the mixed stress-strain control algorithm is successful in mimicking triaxial loading conditions. In the case of confining pressure at 250 MPa , the outside behaviour unloads elastically by going down below the initial yield surface at first, while the inside is under inelastic loading which travels backward with respect to the $p - \text{axis}$ indicating softening. One can also notice that the bifurcation point of the 300 MPa case does not occur at the initial yield surface. In the current development, the breakage model could not provide reasonable results for low confining pressure, thus, one can see the macro stress path for cases below 100 MPa does not follow the slope $\frac{\Delta q}{\Delta p} = \frac{1}{3}$.

In general, inelastic responses inside and outside the localisation band evolves with their own governing responses during the early stage of the deformation, and gradually merge together when the whole volume element is compacting. This convergence indicates the formation of a localisation band. Because only a single band is allowed to form inside the volume, they only converge once and then deviate infinitely. The $p - q$ stress path shows that the occurrence of compaction localisation is responsible for the stress drop in the macro response at the bifurcation point. The episodic stress drop is the result of interaction between the responses inside and outside the band.

The stress-strain relationship is demonstrated with the capability of describing the experimental response in both volumetric and shear behaviour by employing the breakage model implemented in the dual-scale framework. The loading-reloading response taking place in the inelastic region is clear where multiple stress drops are observed (Figure 5.15). After the steep softening, the hardening process at the macro scale can be observed in all cases. This may be explained by the continuous loading of the compaction condition on the whole volume after grain crushing and pore collapse has resulted in a more compacted microstructure.

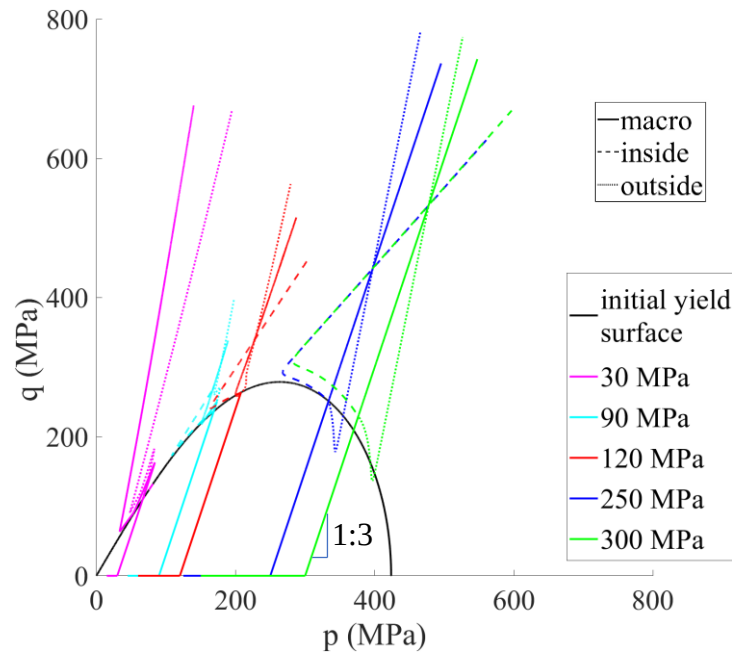


Figure 5.14. Stress path for the macro, inside and outside behaviour on the initial breakage yield surface for different confining pressures in the configuration of elastic outside.

The difference in macroscopic behaviour between the two configurations can also be examined by investigating the combining effect of the outside and inside behaviour. Clearly, the major difference lies in the response of the outside zone. In the case where linear-elasticity is enforced, initially after the bifurcation point, the outside curve develops unloading and then loading with the elastic slope, while volumetric softening takes place on the inside of the localisation band, resulting in the macro response exhibit softening (Figure 5.15 a, c and e). A similar phenomenon for the outside occurs in the shear response except that the deviatoric stress inside is hardening, leading to macro hardening behaviour. The mechanism behind this is straightforwardly explained as the macro behaviour is the combining effect of the inside and outside regions linked by the traction continuity condition. While outside unloading and reloading elastically are causing hardening, the deformation stage of the inside will drive the macro curve. However, because the experiment is under compression, the model will always end up hardening once the material is fully crushed and compacted.

The breakage evolution (Figure 5.16) demonstrates the correspondence between the stress response and the micro-mechanism which is also emphasising the capability of the breakage model. The breakage evolution curves for the inside and outside zones start to deviate right at the bifurcation, which indicates that the instability of behaviour has led to two separate zones with different degrees of grain crushing. Because the breakage variable is only associated with the inelastic response, forcing the zone outside to be elastic, has caused the breakage evolution curves to stay constant at zero for the case 120 MPa and 250 MPa as localisation is detected at the onset of yielding. For the case of the pure compaction band under very high confining pressure (300 MPa), there is a delay of bifurcation where it does not appear and the breakage evolves homogeneously over the entire sample until bifurcation. From here, the zone outside holds the breakage level of the last homogenous state and stays constant as loading continues

in an elastic manner. This does not match with observation in the experiment, where the zone outside exhibits another compaction band and keeps propagating over the undamaged zone outside of the existing localised zone. Hence, the need for allowing inelastic evolution for the outside zone is necessary.

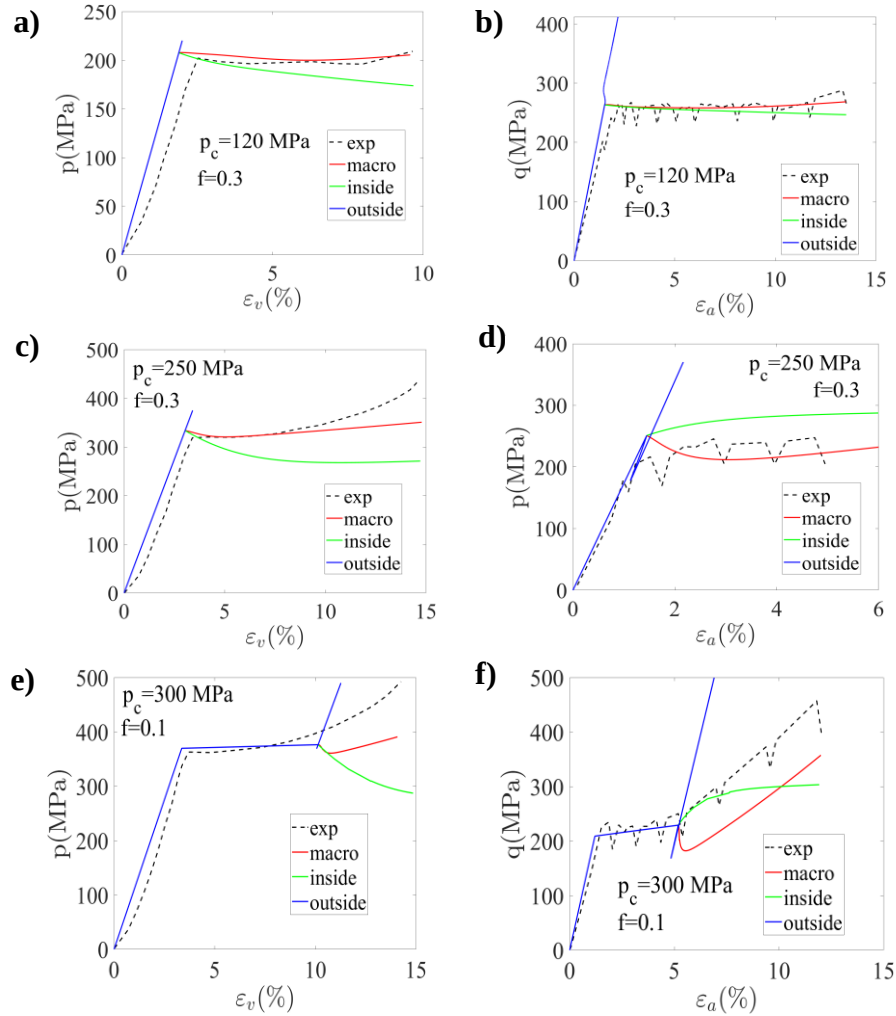


Figure 5.15. Volumetric and shear behaviour with the configuration of forcing the zone outside of localisation band to be linear elastic compared with the experiment data are taken from Vajdova et al. (2004) and Baud et al. (2006). The macro, inside and outside behaviour are plotted against their local volumetric strain ε_v and axial strain ε_a ; (a), (c), (e) demonstrate $p - \varepsilon_v$ at 120 MPa, 250 MPa and 300 MPa, respectively; (b), (d), (f) demonstrate $q - \varepsilon_a$ at 120 MPa, 250 MPa and 300 MPa, respectively.

The link between porosity and mechanical quantities is captured through the volumetric behaviour from the experiments (Figure 5.17). The initial porosity from the experiment was taken in between 22% to 23% by the ratio of the dry and water-saturated mass. Following this, the porosity change was determined from the initial bulk volume and the pore volume change. Hence, it is reasonable to consider the volumetric strain in the constitutive model to be equivalent to the porosity change in the experiment. The elastic slope of the numerical model and yield points share good agreement with the experimental curve indicating that the assumption of equivalent porosity-volumetric strain, as well as the calibrated parameters from

the mechanical analysis section, are correct. In the post-localisation region, especially for the case of confining pressure at 300 MPa, the macroscopic porosity drop of the dual-scale framework could not be well validated as the experimental data were not sufficiently measured. However, the large deviation observed in this case can be explained by the initiation of localisation behaviour in the numerical model, which intense softening is expected before the transition to hardening, while this softening effect is missed in the experimental curve.

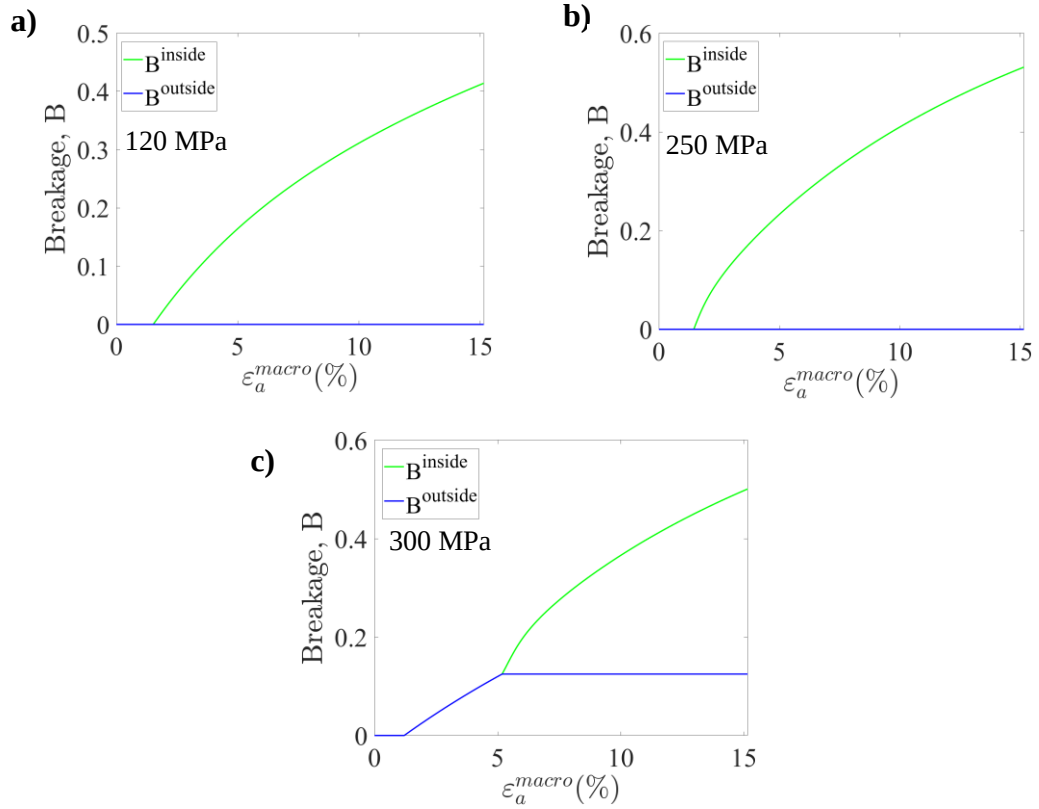


Figure 5.16. Breakage evolution of the zone inside and outside (elastic) of the compaction localisation band under different confining pressures: (a) 120 MPa; (b) 250 MPa; and (c) 300 MPa.

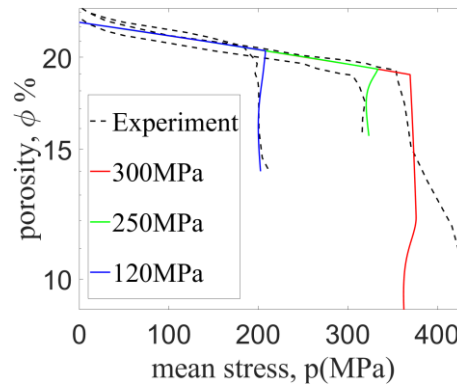


Figure 5.17. Porosity change in undrained triaxial test (Vajdova et al., 2004) under different confining pressures where the behaviour outside of the band is forced to be elastic.

In comparison with the permeability measurement (Vajodava et al., 2004), the model's permeability prediction exploits the stress-strain and breakage variable, B , from the inside and outside of the zone of compaction band calculated from the breakage model implemented in the dual-scale framework with the elastic enforcement of linear-elasticity for the outside zone. In general, the results of the permeability evolution from the breakage model match well with the experimental data in terms of the macro vertical permeability (K_y) given the experimental condition that fluid is forced to flow from upstream to downstream in the experiment.

Overall, regarding any value of confining pressure, the permeability inside of the localised compaction zone always exhibits the largest permeability drop compared to the other regions (Figure 5.18). With respect to volumetric behaviour, all four components show permeability reduction, of which values are relatively close to each other. Besides, the permeability in shear behaviour of the zone inside exhibits a significant decrease of around 20 orders of magnitude compared to the macroscopic experimental data. This is well explained by the compacted nature of the localisation band after the pore collapse process increases the density inside this region, thus, the material here will block the communication of the flow in both the normal and tangent directions.

In Figure 5.18a-b, the RVE under 120 MPa possesses an inclined shear-enhanced compaction band with angle $\gamma = 37.2^\circ$. The permeability inside of this band, K_{in} , has the largest permeability drop compared to the other three components, which implies that the band is strongly blocking the fluid flow, as expected from the pore collapse inside the compaction band. However, there is a major difference in vertical permeability, K_y , between the case of the pure compaction band under high confinement and the shear-enhanced compaction band under lower confining pressure. By comparing Figure 5.18b, d and f, the vertical permeability, K_y , in the 120 MPa case is similar to K_x and K_{out} , where slight permeability decrease is observed. Whereas in the case of 250 MPa and 300 MPa, the vertical permeability is significantly reduced, together with the inside permeability, K_{in} . This is because, in the case of the shear-enhanced compaction band, the band has allowed the fluid to flow down along the inclined direction, while the band itself is not compacted enough to completely block the flow. On the other hand, the pure compaction bands under high confinement possess a very dense micro structure in addition to the horizontal orientation, leading to a sharp permeability for the vertical component, K_y .

From the in-depth evolution of both the mechanical response and the permeability covering the local inside-outside details and their combined effect on the macro behaviour, the correspondence between the coupled mechanical-permeability behaviour is illustrated by plotting both the shear stress q and the macro vertical permeability, K_y , against axial strain, ε_a (Figure 5.19). In general, the permeability reduction starts immediately at the time when the material is put under pressure. In all cases, the decrease in permeability is insignificant, with a slow rate in the elastic loading regime. This downward trend continues even at the bifurcation point and the softening phase after the first compaction band appears. This indicates that the early existence of the localisation band does not cause much influence on the behaviour of

permeability, as the characteristics of compaction localisation have not developed completely, where the breakage level is just around 20% as indicated in Figure 5.16.

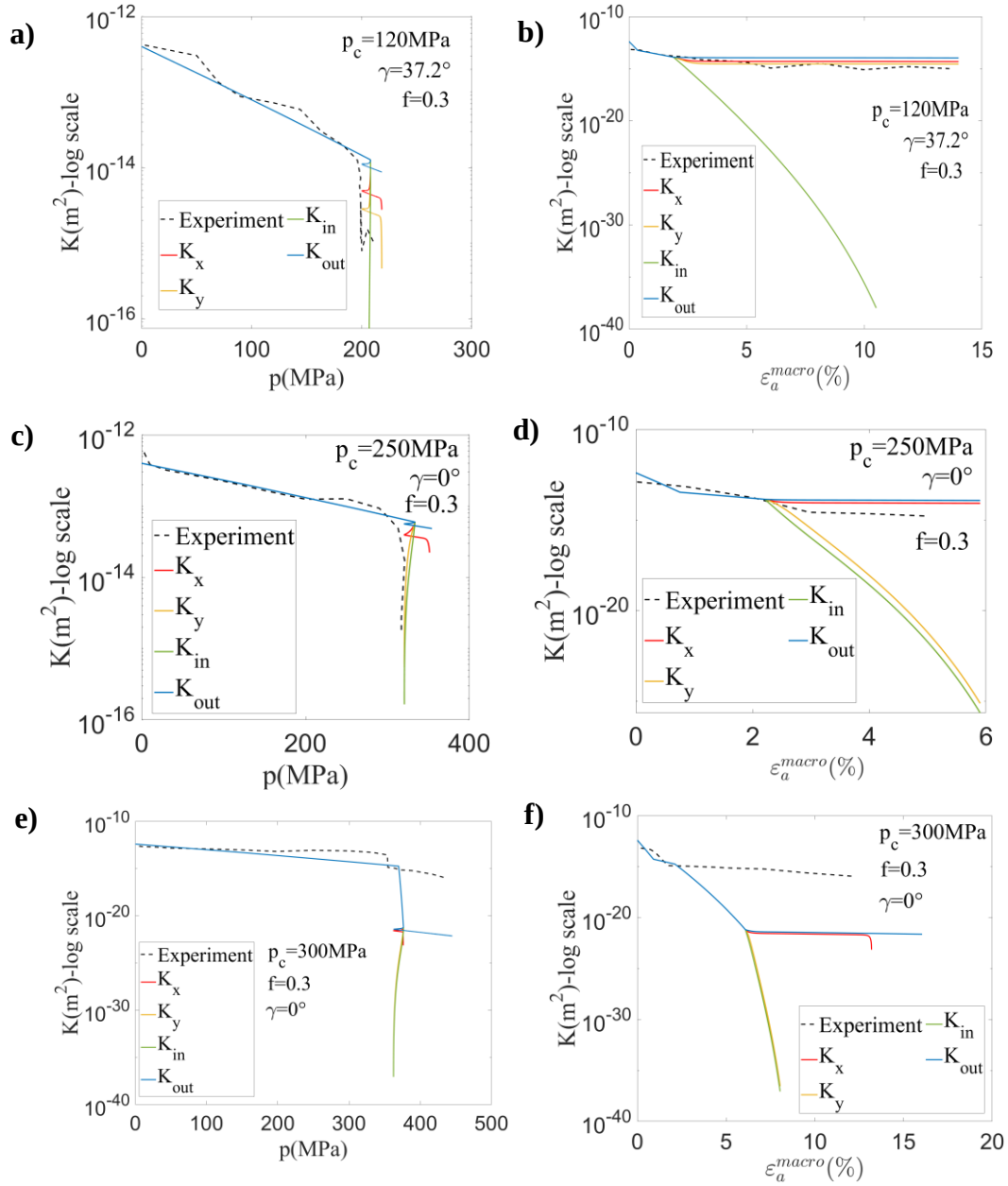


Figure 5.18. Permeability evolution of a volume element embedded with a single compaction band representing porous sandstone under fluid flowing from upstream to downstream. The zone outside of the localisation band is forced to be linear elastic. The experimental data are obtained from Vajdova et al. (2004). The permeability is plotted against volumetric change and the macro axial change under different confining pressures where (a), (c), (e) demonstrate $p - K$ at 120 MPa, 250 MPa and 300 MPa, respectively; (b), (d), (f) demonstrate $\varepsilon_a^{macro} - K$ at 120 MPa, 250 MPa and 300 MPa, respectively.

However, once the compaction band behaviour turns from softening to hardening, the abrupt permeability drop occurs, in which, the phenomenon can be clearly observed, with pure compaction bands under high to very high confining pressures (Figure 5.19b, c). For instance,

when the axial strain, ε_a , reaches 9% under a 300 MPa confining pressure, the permeability plummets quickly in association with the hardening phase, showing an almost blockage of fluid communication. The degree of grain crushing via the breakage variable at this sharp permeability drop state is almost double the value in the softening phase when the localisation band begins to form.

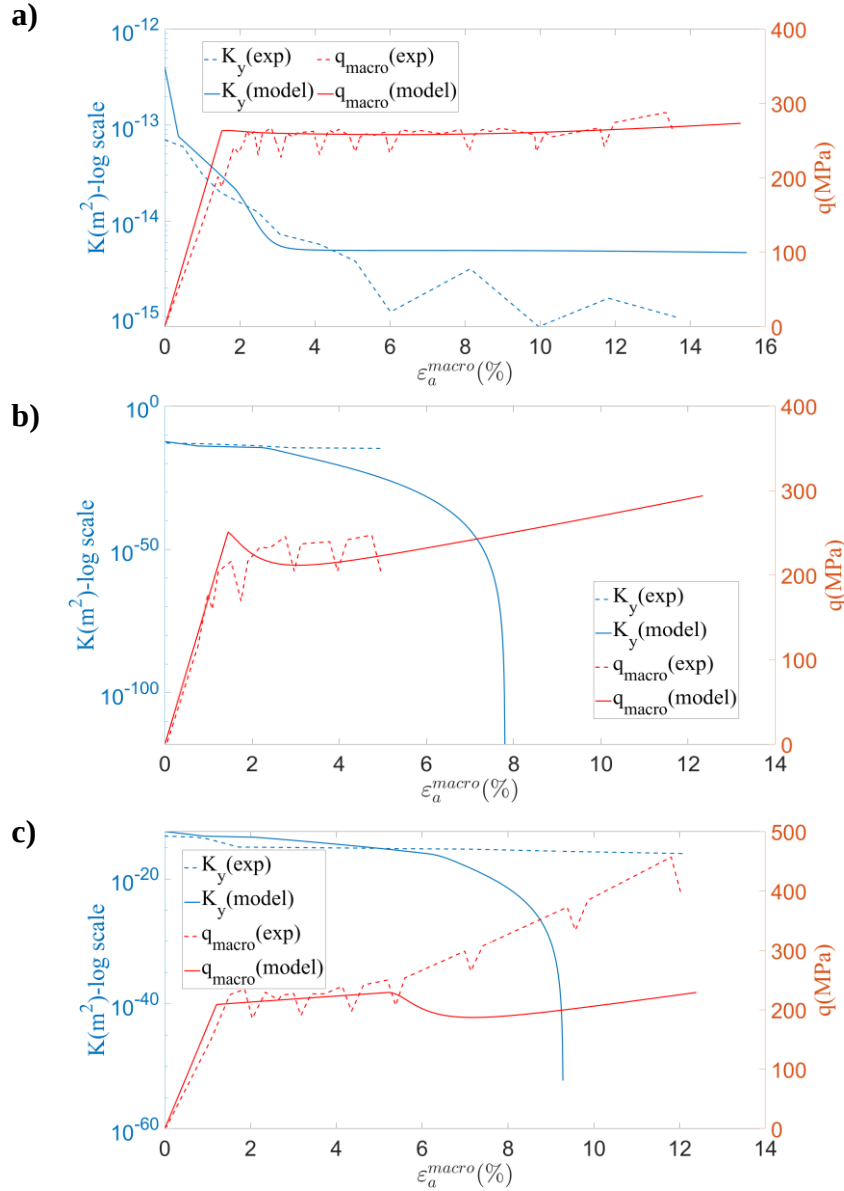


Figure 5.19. Comparison between permeability evolution and the mechanical response under axial strain. The degree of breakage and the size of breakage accumulation between the numerical model and experimental images are shown at some specific strain levels. The behaviour outside of the localisation band is forced to be elastic. The experimental data is obtained in Vajdova et al. (2004). The results are obtained with confining pressure at (a) 120 MPa; (b) 250 MPa; and (c) 300 MPa.

Nevertheless, the experimental curve does not exhibit a steep reduction of permeability like the present numerical prediction. This could be due to the inability of the model to capture dilation behaviour when confining pressures are not sufficiently high. This is an inherent issue of the

breakage model used in this study. In fact, failure of this porous rock involves two competing mechanisms: grain crushing & pore collapse, and dilation induced by sliding among grains. While dilation can enhance permeability, grain crushing and pore collapse lead to permeability reduction, and the competition of these mechanisms affects the hydraulic conductivity. The large permeability drop diminishes for the cases of lower confining pressure, where the shear-enhanced compaction band allows hydraulic conduction in the vertical direction, as hardening is not as intense as the two other cases, for the reasons given in the discussion for Figure 5.18a, b.

5.3.2 Allowing inelastic behaviour for the zone outside of the compaction band

In this section, the post-localisation analysis is performed in terms of two separate homogeneous responses for the zone inside and outside of the localisation, which can be either elastic or inelastic. Inelastic response occurring on the outside of the localisation band can be associated with localisation, and this behaviour can be linked to the progressive localisation with an episodic stress drop, which has been comprehensively described in Nguyen's previous works regarding the case with a single band (Nguyen et al., 2016b) or a nested structure with multiple bands (Nguyen et al., 2017). This section is coped with the scenario of inelastic allowance for the zone outside of a single band which represents a zone that covers multiple discrete bands as discussed in Section 5.1.4. Immediately after the bifurcation event, the zone outside is likely to unload elastically with softening macro behaviour being observed. As further strain increments occur, the computational operation will automatically decide either elastic or inelastic response via a stress-return procedure based on the current stress state and the tangent stiffness.

Since the performance of the dual-scale framework, and some fundamental mechanical characteristics of compaction localisation in porous sandstone, have been demonstrated in the previous section, this section will concentrate more on the permeability analysis under the configuration of inelastic allowance for both zones as well as its differences from the elastic enforcing technique. The key enhancement for this modification of the zone outside of the localisation band is that after elastic unloading, inelastic evolution takes place, which occurs after the inside response, instead of elastic reloading like in the other configuration. This kind of behaviour indicates the deactivation and activation of compaction localisation in terms of the first band, by which another compaction band occurs in the zone outside, as being confirmed by the progressive mechanism of localised failure observed in existing experimental results.

Figure 5.20 demonstrates the inelastic deactivation-activation behaviour via the breakage evolution and the stress path in triaxial space. It should be first noted that the current dual-scale breakage model fails to create separate responses for the inside and outside zone, of the shear-enhanced compaction band under low confining pressure, although bifurcation has been detected. This is related to the capability of this breakage model to capture softening behaviour under low confining pressures. Yet, these issues and related improvements are not within the scope of this study, which focus on the compacting behaviour at sufficiently high confining

pressures. The post-localisation analysis can still be conducted with a homogeneous response, and future work will address improvements to this bifurcation issue. As for the case of pure compaction bands under high and very high confining pressures, the separation of the inside and outside curves indicates a formation of a new compaction band, leading to deactivation of inelastic response inside and activating the inelastic on the outside. This trend can also be observed under breakage evolution where the value of B in one zone is increasing as the compaction band is developing while the other zone stays constant, and vice versa.

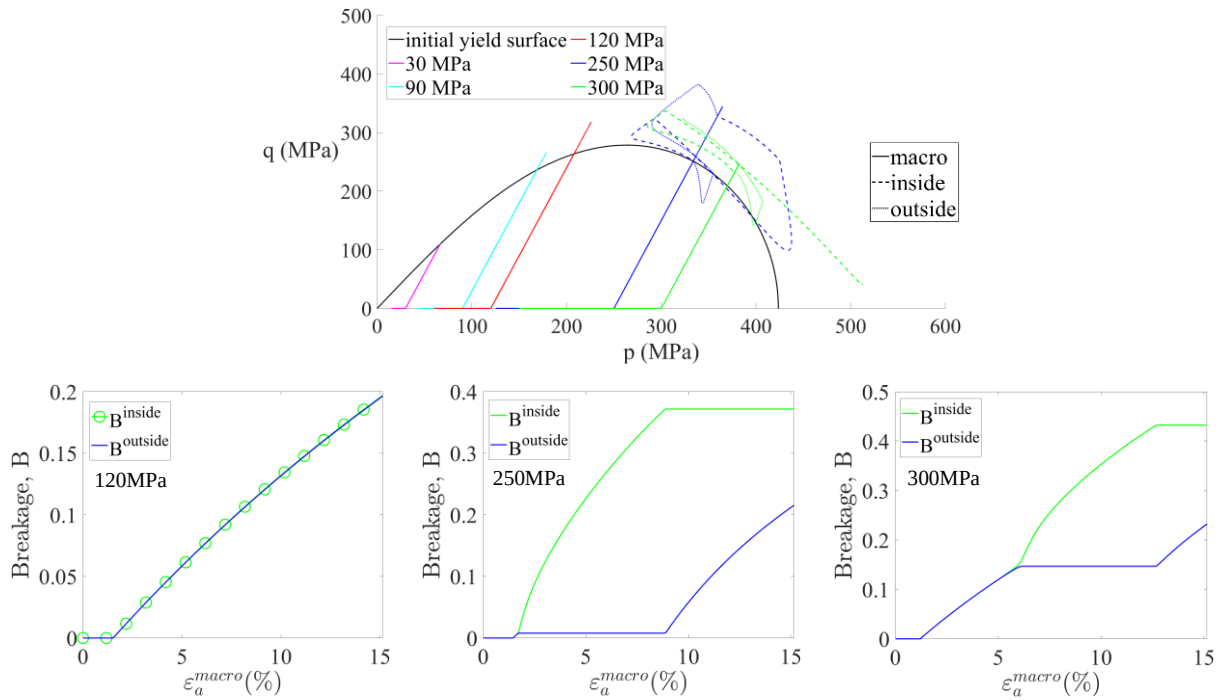


Figure 5.20. Stress path for the macro, inside and outside behaviour on the initial breakage yield surface for different confining pressures in the configuration of inelastic outside.

Regarding the demonstration of mechanical response with the inelastic configuration for both zones, there is an episodic stress drop at the macro scale which is the result of the inelastic activation-deactivation between the outside and the inside responses (Figure 5.21). Each time this stress drop occurs, we can associate it with the formation of a new compaction band. Because the current model only allows one occurrence of a single localisation band, there is only one stress drop in the stress-strain curve which can be clearly seen in Figure 5.21f. Inelastic loading occurs immediately when elastic unloading has been completed for zone outside of the band, together with the inelastic hardening for the zone inside, the macro RVE exerts softening behaviour as a consequential effect. When comparing the permeability evolution within the range of this softening response, an increasing drop that deviates off the gradual downward trend in the elastic loading regime can be clearly observed (Figure 5.22). The permeability drop, in this case, has a steeper slope than the one in the elastic unloading-reloading case. The drop may relate to the degree of breakage in the post-localisation phase where another compaction band occurs and the flow needs to penetrate through multiple bands. This has underscored the control effect of porosity and pressure level on permeability, more specifically, with the occurrence of compaction localisation. It is worth mentioning that the permeability evolution

also relies on the thickness of the localisation band which, according to the analysis in Section 5.1.4, the increasing size of band will lead to softening behaviour at the macroscopic scale which favours the process of grain crushing and pore collapse overall, leading to higher susceptibility to permeability reduction.

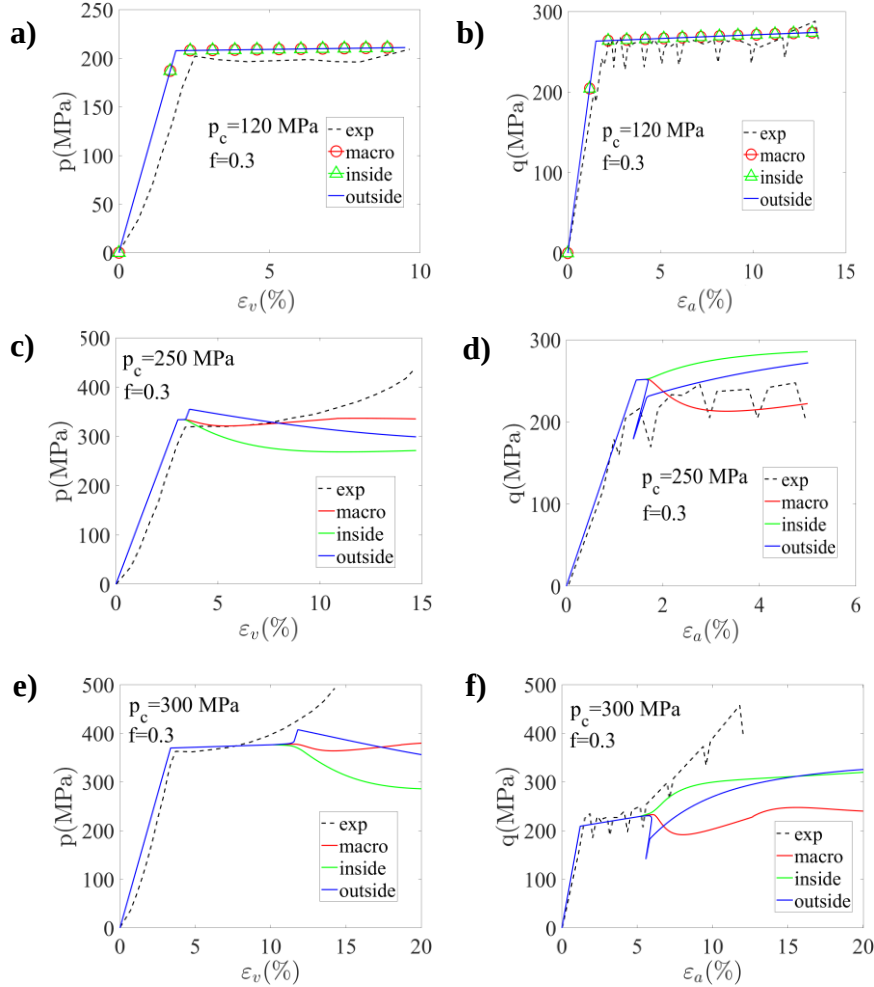


Figure 5.21. Volumetric and shear behaviour with the configuration of allowing the zone outside of localisation band to behave inelastically compared with the experiment data are taken from Vajdova et al. (2004) and Baud et al. (2006). The macro, inside and outside behaviour are plotted against their local volumetric strain ε_v and axial strain ε_a ; a) $p - \varepsilon_v$ at 120 MPa; b) $q - \varepsilon_a$.

As the loading continues, the hardening phase in the mechanical response curves starts to dominate. In association with this interaction, the macro permeability (vertical component, K_y) experiences an extreme reduction, which can be distinctly observed for the case of pure compaction bands. Within this context, the macro permeability drop is not so contradictory as compared to the configuration of elastic enforcement for the outside zone, because they both lead to a horizontal band that possesses severe grain crushing and pore collapse in a fully developed state with a steep hardening slope. In other words, no matter how the outside zone affects the permeability, the material inside of the localisation band still experiences a fully

compacted microstructure, which always results in a global blockage of the RVE in terms of vertical fluid conduction.

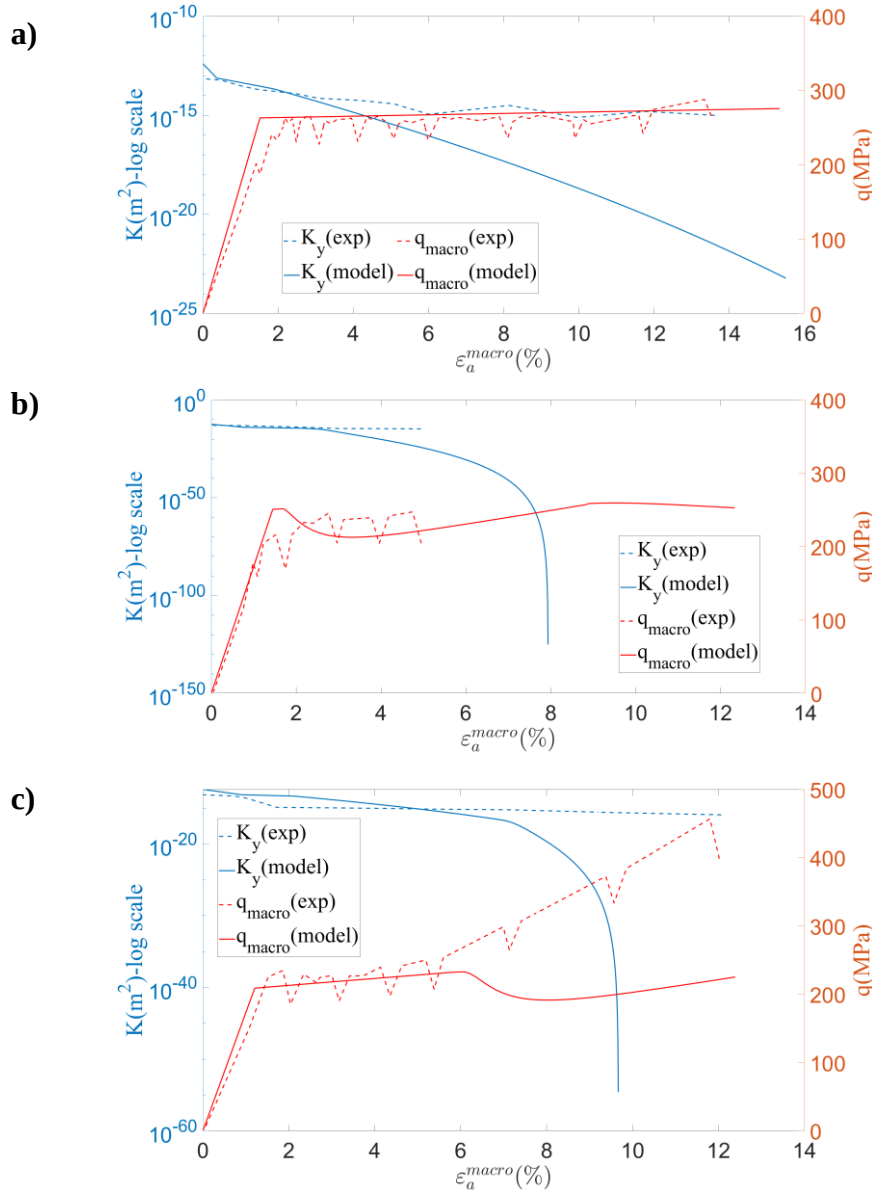


Figure 5.22. Comparison between permeability evolution and the mechanical response under axial strain. The degree of breakage and the size of breakage accumulation between the numerical model and experimental images are shown at some specific strain levels. The behaviour outside of the localisation band is allowed to be inelastic. The experimental data were obtained in Vajdova et al. (2004). The results are obtained with confining pressure at (a) 120 MPa; (b) 250 MPa; and (c) 300 MPa.

However, the same story does not repeat in the case of shear-enhanced compaction bands with an inclined orientation. By correlating the 120 MPa case in elastic enforcement mode (Figure 5.19) and inelastic allowance mode (Figure 5.22), we immediately notice that inelastic mechanical response for the zone outside has led to a sharper diminishment in permeability, though not as intense as in high confinement cases. An upsurge of grain crushing for the zone outside, as inelastic response is activated, can be linked to the increasing values of breakage

(Figure 5.20). This implies that by allowing inelastic behaviour outside of the first band, which may lead to the formation of another band and expand the localised compaction zone, the capability of hydraulic blockage of the material will increase disregarding the effect of the inclined orientation that may facilitate downstream flow. The result has underscored the control effect of porosity (Figure 5.23) and pressure level on permeability, more specifically, with the occurrence of compaction localisation. It is worth mentioning that the permeability evolution also relies on the thickness of the localisation band which, according to the analysis in Section 5.1.4, the increasing size of band will lead to softening behaviour at the macroscopic scale which favours the process of grain crushing and pore collapse in overall, leading to a higher susceptibility to permeability reduction.

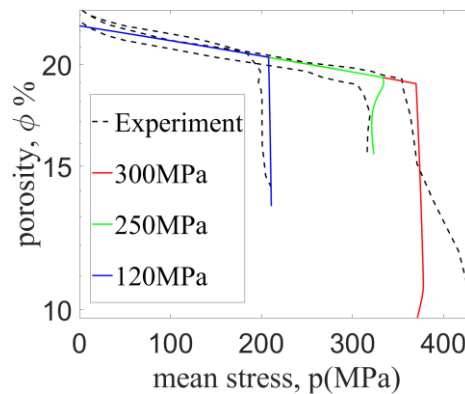


Figure 5.23. Porosity change in undrained triaxial test (Vajdova et al., 2004) under different confining pressures where the behaviour outside of the band is allowed to be inelastic.

The combining effect of the permeability inside and outside on the evolution of macro permeability does not differentiate much from the elastic enforcement mode (Figure 5.24). For any case of confining pressure, the permeability inside and the vertical macro component always share the same path which indicates the domination of the compaction band over the entire host volume with regards to the correspondence from the mechanical response and the hydraulic conductivity. Because the outside component is allowed to be inelastic, the permeability drop occurs more drastically which emphasises the role of capturing inelastic deformation associated with the micro-mechanisms on hydraulic conductivity. As mentioned above, the ultimate response provided by the model will always give an increasing hardening that leads to a fully compacted structure due to the impact of those happening at the mesoscale element.

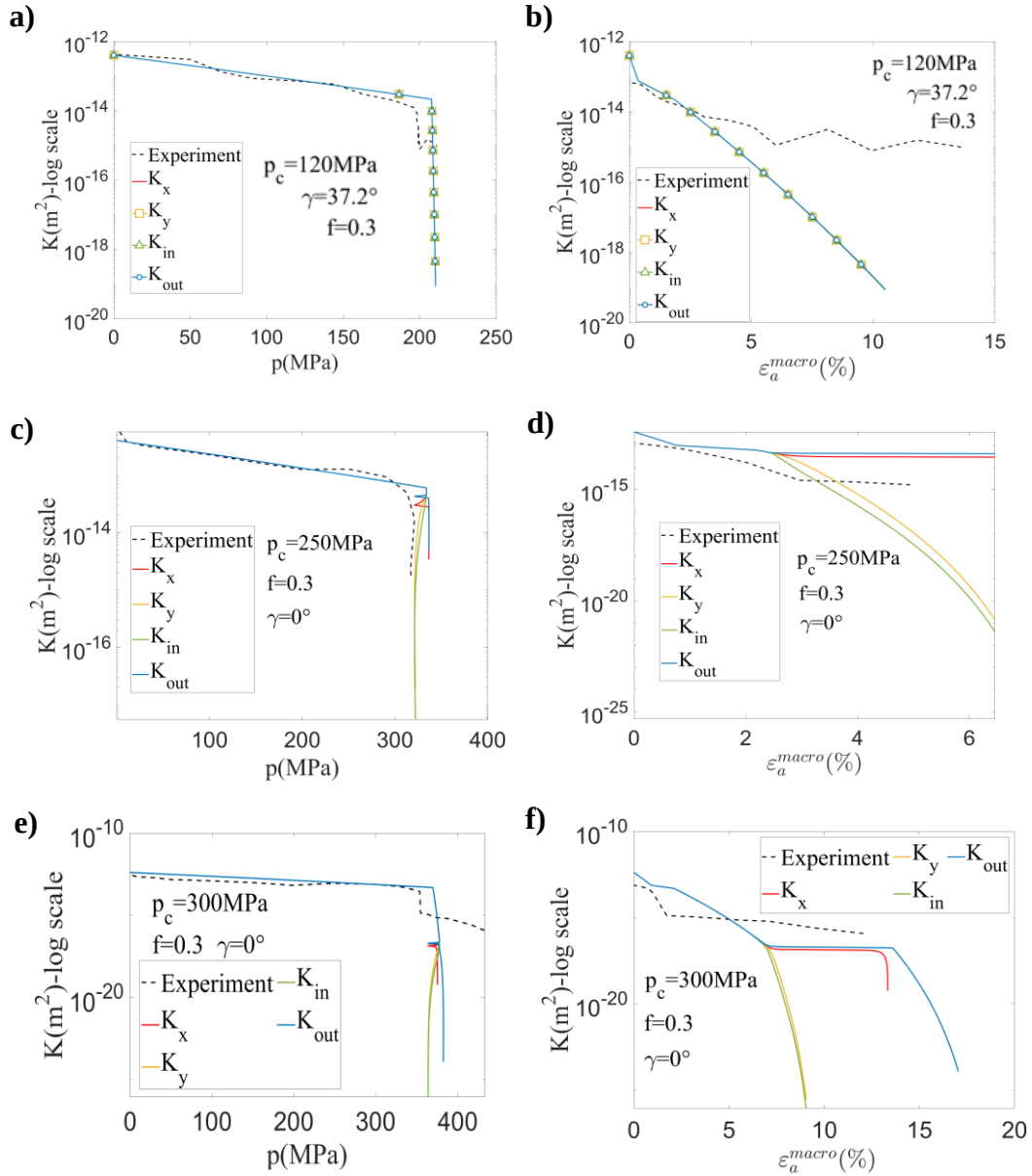


Figure 5.24. Permeability evolution of a volume element embedded with a single compaction band representing porous sandstone under fluid flowing from upstream to downstream. The zone outside of the localisation band is allowed to be inelastic. The experimental data are obtained from Vajdova et al. (2004). The permeability is plotted against volumetric change and the macro axial change under different confining pressures: a) $p - K_x, p_c = 120$ MPa; b) $\epsilon_a^{macro} - K, p_c = 120$ MPa; c) $p - K_x, p_c = 250$ MPa; d) $\epsilon_a^{macro} - K, p_c = 250$ MPa; e) $p - K_x, p_c = 300$ MPa; f) $\epsilon_a^{macro} - K, p_c = 300$ MPa.

Chapter 6

SUMMARY AND CONCLUSIONS

6.1 Summary

This thesis demonstrates a complete assembly of theoretical developments for numerical modelling in a consistent framework for describing the deformation of porous granular rocks in the case of compaction localisation. This is the first systematic study under a continuum mechanics framework that predicts the evolution of permeability by tracking the micro-mechanisms related to compaction localisation, as well as capturing the onset of localisation and the response in the post-localisation stage.

In summary, the effect of compaction localisation on the global behaviour of porous sandstones has been highlighted through the analysis of permeability using a constitutive framework that can link the micro-mechanism to the macro response via a mesoscale bridge. The intense permeability reduction provided by the proposed model in this research has drawn special attention to the necessity for the experimental technique to access the mechanisms inside a localisation band. The numerical investigation has demonstrated how important a correct mechanism of small details can influence the outcomes of the overall material behaviour. The development of a model based on breakage mechanics is required to describe correctly both pre, and post-localisation stages of behaviour. In particular, by implementing the internal variable B to enable tracking the grain size distribution, the grain crushing and pore collapse inside the zone of compaction localisation observed in experiments can be well captured on the macroscopic response. Whereas the proposed dual-scale enrichment with an intrinsic length scale h has dealt with the size-dependent problem from the constitutive level without further regularisation, which extends the capability to deal with compaction localisation in porous sandstones. In addition, the concept of an RVE embedded with a localisation band that has two distinct behaviour, for the zone inside of the band and the surrounding bulk can be extended in a multi-scale problem with effective computational cost and resources.

From the benefits of the dual-scale enriched breakage model, the permeability evolution has been inferred from the effect of mechanical response and the change in microstructure when compaction localisation appears inside the material. Based on the observation in existing experiments on permeability measurement, the numerical results from the dual-scale framework on the permeability inside and outside of compaction localisation have once again confirmed that homogenous assumption over the entire problem domain is invalid when dealing with localised problems. The analysis of permeability on different confining pressures in

triaxial conditions has verified the role of stress conditions on the material hydraulic conductivity in corresponding with different formations of compaction bands. The key features of permeability evolution under compaction localisation are listed below:

- The macroscopic permeability is heavily affected by the permeability inside of compaction bands. Due to intense grain crushing and pore collapse occurring inside a tabular horizontal zone, the downstream (vertical) permeability in triaxial tests is significantly influenced at the early stage of forming compaction localisation whereas the horizontal permeability will only be reduced during the late deformation stage.
- The reorganisation of crushed grains will trigger the reduction of porosity and permeability, which is indicated by the elastic loading and the softening response right after the bifurcation happens. However, intense permeability drop will only occur once the transition from softening to hardening of the first band is complete. In other words, the early stage of material hardening that is associated with the formation of the very first compaction band has already blocked the fluid communication. Further development of other compaction bands or the extension of the localised compaction zone will only intensify the blockage characteristics.
- As the first conclusion has already stated, the contribution of the permeability reduction of the zone outside of the band on the global hydraulic behaviour is insignificant. However, by studying different configurations for the outside zone, some factors affecting the permeability reduction have been noted. The inelastic response obtained from the breakage model is the key element that governs the breakage process and as a consequence, the reduction of permeability. Besides, the mode of localisation compaction, which is associated with different levels of confining pressures, governs the features of the band, such as its thickness and orientation.

6.2 Future improvements

Although valuable insights regarding the effects of localised compaction failure on permeability evolution in porous reservoir rocks have been provided from the proposed model, some limitations still need to be addressed to be improved in the future.

- Despite the modification on the bifurcation detection in a low-pressure regime, the current state of development for the breakage formulations is not capable yet to capture the response under shearing at low confining pressures during the post-localisation phase where dilatant behaviour is expected. Therefore the underlying breakage model should be improved to capture behaviour under a range of stress conditions, from tension to compression under a range of confining pressures. Although there have been derivatives of breakage models in the literature that can partly overcome inherent issues of the original breakage model, e.g. allowing dilation (Tengattini et al., 2016) or adding cohesion (Tengattini et al., 2014), these are related to specific features of the model.

Further enhancements to the framework of breakage mechanics, not individual or specific features of models derived from breakage mechanics theory, are needed.

- The progressive nature of localisation bands has not yet been well described by the current configuration of the dual-scale breakage model, as the thickness of the band is fixed with a constant value, while the model only allows the occurrence of one compaction band. However, this will need to be carefully considered as a nested structure of multiple bands is so complex that will cost more simulation time and computational resources. A reasonable approach could be the evolution of the thickness band that has been developed by Nguyen and Bui (2020). Nevertheless, an enhancement for the band thickness evolution, that takes into account the micro mechanism in porous rocks by exploiting the capability of the breakage model via the coupling angle ω , can be addressed. In such a case, the coupling angle, ω , is a function in terms of the internal variables from the breakage model which can be either the breakage variable, B , or the plastic strain increment ε_{kl}^p .
- The formulation and calibration of constitutive models for porous rocks under compaction would require the material behaviour obtained from experimental results. However, the current experimental technique can only measure the macro behaviour of the specimen, where the homogeneity assumption is sometimes applied. This may cause inaccuracy for computational work as this macro measurement is a mixed result between distinct responses from the zone inside and outside of the localisation band. A piece of evidence can be taken right from the analysis of this research where the experimental permeability data often matches with the outside permeability component, K_{out} , implying that the intense permeability drop for the zone inside K_{in} is missing. Therefore, in order to obtain a better set of parameters that can be used to validate the dual-scale framework result, it is critical to recalibrate and extract the macro data with respect to accessing the information inside of the localisation band based on the technique proposed by Le et al. (2021).
- The permeability analysis opens the first door into studying the hydraulic behaviour of porous media that takes into account the effects of compaction localisation. Further research work can dig deeper into the coupled hydraulic-mechanical analysis by addressing directly the quantities of flow that interacts with the structure inside of the localisation.

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