Analysis of underground excavations in argillaceous hard soils - weak rocks

by

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To my wife
“It is the science of calculation,—which becomes continually more necessary at each step of our progress, and which ultimately govern the whole of the applications of science to the arts of life.”

Charles Babbage (1791-1871)
Abstract

Stiff clayey materials, lying in the transition between hard soils and weak rocks, are being currently considered in several countries as possible host medium for deep geological disposal of high active and long-lived nuclear waste. This possibility has led to the construction of underground research laboratories (URL), excavated in these indurated clayey materials, to study their behaviour under real working conditions. Among the very different topics addressed in the URLs, the hydromechanical behaviour of the host rock is the one that most concerns the present research. In situ observations have revealed that excavation operations induce damage around the galleries, in the form of fracture networks, contained within a zone called excavation damaged zone (EDZ). The EDZ has been identified as one of the main aspects affecting the behaviour of the excavations.

In this context, the main objective of the present study is the numerical simulation of the hydromechanical behaviour of experimental excavations performed at the Meuse/Haute-Marne URL (France). For this purpose, a constitutive model has been developed to characterise the host formation. The modelling of these stiff argillaceous materials is a quite challenging task. They exhibit soil-like features like considerable plastic strains, rate-dependency, and creep, although they also show characteristics more typical of a rock such as significant softening and localised deformations. In addition, due to their sedimentary origin, they often exhibit anisotropy in properties like stiffness, strength, and permeability. Special attention has been paid to the reproduction of the EDZ and, therefore, to the objective simulation of localised deformations; a nonlocal approach has been employed for the regularisation of the continuum, avoiding the dependence on the employed mesh. The obtained results provide relevant insights into the hydromechanical behaviour of these stiff clayey materials, and they indicate the main aspects affecting the response of the underground excavations. In particular, the relevance of the EDZ has been demonstrated.

Keywords: anisotropic deconfinement; anisotropy; coupled hydromechanical analysis; elasto-plasticity; excavation damage zone; nonlocal plasticity; over-pressures; plane strain; stiff clays; strain localisation; time-dependent behaviour; tunnel excavation; visco-plasticity.
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Contents

List of Publications XV
List of Figures XIX
List of Tables XXVII
List of Symbols XXIX

1 Introduction 1
  1.1 Background .................................................. 1
  1.2 Objectives and methodology ................................. 3
  1.3 Thesis layout .................................................. 4

2 Geomechanics of shale repositories - Mechanical behaviour and modelling 7
  2.1 Introduction .................................................. 7
  2.2 Modelling framework ......................................... 9
    2.2.1 Plasticity theory ....................................... 12
  2.3 Yielding and degradation .................................... 13
    2.3.1 Response under compressive loading ................... 13
    2.3.2 Response under deviatoric loading .................... 15
    2.3.3 Yield surface ........................................... 17
    2.3.4 Degradation and softening ............................. 19
    2.3.5 Strain localisation .................................... 21
  2.4 Material anisotropy ........................................ 23
    2.4.1 Stiffness anisotropy ................................... 23
    2.4.2 Strength anisotropy .................................... 26
    2.4.3 Permeability anisotropy ................................ 29
  2.5 Time-dependent behaviour .................................. 29
    2.5.1 Viscoplasticity ......................................... 31
    2.5.2 Plasticity - creep partition ........................... 33
    2.5.3 Viscoplasticity - creep partition ...................... 34
  2.6 Conclusions .................................................. 34

3 A cross-anisotropic formulation for elasto-plastic models 35
  3.1 Introduction .................................................. 35
  3.2 Isotropic elasto-plastic model .............................. 37
  3.3 Cross-anisotropic formulation .............................. 38
List of Publications

This is an extensive list of all the work published, submitted or to be submitted, related to this PhD.

Peer reviewed journals


Book chapters


Conference proceedings

of an unsaturated seal structure. In 9th European conference on numerical methods in
geotechnical engineering, Porto.

and Application. In Ferrari, A. and Laloui, L., editors, Advances in Laboratory
Springer.

an unsaturated seal. In Second Pan American conference on unsaturated soils, pages
329 – 338, Dallas. ASCE.

with a nonlocal plasticity model. In Oñate, E., Owen, D. R. J., Peric, D., and
Chiumenti, M., editors, XIV International Conference on Computational Plasticity.
Fundamentals and Applications, pages 606–612, Barcelona. CIMNE.

an argillaceous rock: Formulation and application to an underground excavation case.
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Abstracts and Posters

Analysis of localized deformations around deep excavations in argillaceous rocks. In
7th International conference on clays in natural and engineered barriers for radioactive
waste confinement, pages 179–180, Davos (abstract).

a gallery sealing over the entire life of a deep repository. In 6th International Conference
on Coupled TGMC Processes in Geosystems, pages 120–121, Paris (abstract).

drift excavated in the Callovo-Oxfordian Argillite. In 8th Workshop of
CODE_BRIGHT, pages 2–6, Barcelona (abstract).

response of a gallery sealing over the entire life of a deep repository. In Clays in Natural
and Engineered Barriers for Radioactive Waste Confinement, pages 433 – 434, Brussels
(abstract and poster).
List of Figures

1.1 Conceptual model of the induced fracture networks at the MHM for drifts parallel to the (a) major and (b) minor horizontal stresses, (c) at Mont Terri, and (d) at HADES (modified from Armand et al., 2014; Blümling et al., 2007; Li et al., 2007). ......................................................... 2

1.2 Horizontal displacements of extensometer OHZ1501 (modified from Armand et al., 2014; Seyedi et al., 2017). ................................................................. 3

2.1 Degradation of a sample of argillaceous rock during cycles of relative humidity (Alonso and Alcoverro, 2004). .......................................................... 8

2.2 Variation of uniaxial compressive strength with content of calcium carbonate in Taylor and Austin chalk formation, Texas (Hsu and Nelson, 1993). .... 9

2.3 Schematic behaviour of rocks (Hoek and Bray, 1981). ............................ 10

2.4 Stress-strain response of two natural clay-based materials (Leroueil and Vaughan, 1990). ......................................................................................... 11

2.5 Typical limit envelope and critical state line for soils and soft rocks (Leroueil and Vaughan, 1990). .............................................................. 11

2.6 Compression of a structured and unstructured material (Leroueil and Vaughan, 1990). ......................................................................................... 14

2.7 One-dimensional compression behaviour of Boom clay (Horserman et al., 1987 referenced in B Burland, 1990). ................................................. 14

2.8 High-pressure oedometer test on Culebra shale (Banks et al., 1975 referenced in Gens, 2013). .............................................................. 14

2.9 Shear characteristics of stiff clayey materials (Skempton, 1964). .......... 15

2.10 Conceptual scheme for the strength of argillaceous hard soils and weak rocks (Jardine et al., 2004). .............................................................. 16

2.11 Stress-strain behaviour of Kimmeridge Bay Shale under triaxial loading (Nygård et al., 2006). .............................................................. 16

2.12 Peak failure strength envelope in Opalinus clay (Amann et al., 2012). ... 17

2.13 (a) Single yield function (Liu and Carter, 2002) and (b) combination of separate yield mechanisms (Galavi and Schweiger, 2009). ........ 17

2.14 Yield surface of natural Boom clay (Hong et al., 2016). ...................... 18

2.15 Mohr-Coulomb criterion (a) in the principal stress space and (b) in the deviatoric plane. .............................................................. 19

2.16 Hyperbolic approximation of the Mohr-Coulomb yield function (Abbo and Sloan, 1995). .............................................................. 19
2.17 A bounding plasticity model for structured clays (Rouainia and Muir wood, 2000). ................................................................. 20
2.18 Shale specimens after (a) unconfined compression and (b) triaxial compression test (Holt et al., 2015). ................................. 21
2.19 (a) Bar under tension, (b) stress-strain behaviour of the material, and (c) force-displacement response. ................................. 22
2.20 Perpendicular versus parallel Young’s modulus of various shales (modified from Sayers, 2013). ......................................... 23
2.21 Definition of elastic constants for the case of transverse isotropy (Wittke, 1990). ............................................................... 25
2.22 Strength variations (a) under triaxial loading of Tournemire shale (Niandou et al., 1997) and (b) under uniaxial loading of Boryeong shale (Cho et al., 2012). ............................................ 26
2.23 Strength predicted by the single weakness plane theory (Hoek, 1983). ................................................................. 27
2.24 Comparison between different anisotropic criteria and laboratory data from (a) Nova (1986b), (b) Gao et al. (2010), (c) Pietruszczak (2001) and (d) Mánica et al. (2016b). ........................................... 28
2.25 (a) Observed damaged zone in the analysed drift (Armand et al., 2014) and (b) contour plot of the cumulative plastic multiplier showing the obtained plastic zone configuration (Mánica et al., 2017c). ........................................ 29
2.26 Triaxial creep test on Haynesville shale (Sone and Zoback, 2014). ................................................................. 30
2.27 Influence of axial strain rate on (a) peak deviatoric stress and (b) axial strain at peak for undrained triaxial test Swan et al. (1989). ................................................................. 31
2.28 The overstress theory (Perzyna, 1966). ................................................................. 32
2.29 Simulation results of (a) triaxial creep tests and (b) of an underground excavation in Callovo-Oxfordian claystone from Mánica et al. (2017c). ........................................... 33

3.1 Cross-section damaged zone observed around a drift excavated under a quasi-isotropic stress state (Armand et al., 2014). ........................................... 36
3.2 (a) Global coordinate system and (b) local coordinate system. ................................................................. 38
3.3 Angles in the rotation matrix. ................................................................. 39
3.4 Effect of stress scaling when rotating the anisotropy direction: (a) effect of variation of the normal scaling factor, \( c_N \) and (b) effect of variation of the shear scaling factor, \( c_S \). ................................................................. 40
3.5 Effect of stress scaling on the yield surface plotted in principal stress space. ........................................... 40
3.6 Comparison of the cross-anisotropic criterion and triaxial test results from (a) Donath (1964), (b) Alliot and Boehler (1979) and (c) Fleming and Duncan (1990). ................................................................. 41
3.7 Finite-element spatial discretisation and boundary conditions of the numerical analysis. ................................................................. 43
3.8 Major principal stress directions close to the excavation. ................................................................. 44
3.9 Cumulative plastic multiplier and total displacements contour plots for the anisotropic model considering the isotropic plane horizontal: (a) cumulative plastic multiplier \( (c_N=1.4, c_S=1.0) \); (b) total displacements \( (c_N=1.4, c_S=1.0) \); (c) cumulative plastic multiplier \( (c_N=0.8, c_S=1.0) \) and (d) total displacements \( (c_N=0.8, c_S=1.0) \). ................................................................. 44

XX
3.10 Cumulative plastic multiplier and total displacements contour plots for the anisotropic model considering rotation of the isotropic plane ($c_N=1.4$, $c_S=1.0$): (a) cumulative plastic multiplier, isotropic plane rotated 30° to the horizontal; (b) total displacements, isotropic plane rotated 30° to the horizontal; (c) cumulative plastic multiplier, isotropic plane rotated 60° to the horizontal and (d) total displacements, isotropic plane rotated 60° to the horizontal.

4.1 Friction angle evolution in hardening and softening regimes.

4.2 (a) Global and (b) local coordinate systems.

4.3 Definition of the angles in the rotation matrix (Mánica et al., 2016b).

4.4 Stress-strain curves in triaxial tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.

4.5 Volume change in triaxial tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.

4.6 Creep tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.

4.7 Location of the GCS drift in a three-dimensional view of the MHM URL (Seyedi et al., 2017).

4.8 Extension of the damaged zone for drifts parallel to the major horizontal stress (Armand et al., 2014).

4.9 Horizontal and vertical convergences in drifts parallel to the major horizontal stress (Armand et al., 2013).

4.10 Variation of in situ measured hydraulic conductivity with distance to the drift wall (Armand et al., 2014). (a) Horizontal borehole, (b) vertical borehole.

4.11 Finite element mesh and boundary conditions.

4.12 Variation of boundary conditions on the excavation wall.

4.13 Location of measurement points used for comparison with simulation results.

4.14 Pore pressure evolution in measurement points of borehole OHZ1521. Observed (Seyedi et al., 2017) and computed values.

4.15 Pore pressure evolution in measurement points of borehole OHZ1522. Observed (Seyedi et al., 2017) and computed values.

4.16 Horizontal displacements at measurement points of borehole OHZ1501. Observed (Seyedi et al., 2017) and computed values.

4.17 Evolution of horizontal and vertical convergences. Observed (Seyedi et al., 2017) and computed values.

4.18 Contours of accumulated plastic multiplier at the end of the excavation.

4.19 Evolution of horizontal and vertical convergences. Observed (Seyedi et al., 2017) and computed values. No creep deformations considered.

5.1 Yield criterion in the (a) $p - J$ and (b) octahedral planes

5.2 Conceptual scheme for the strength of stiff plastic clays (Jardine et al., 2004)

5.3 Representation of weighting functions

5.4 Analysis domain and boundary conditions

5.5 Contours of shear strain from the set of analyses A

5.6 Load-displacement curves from the set of analyses A

5.7 Contours of shear strain from the 2D analyses of the set B
5.8 Load-displacement curves from the 2D analyses of the set B and from the 3D analysis (B04) ................................................................. 78

5.9 (a) Geometry, mesh, and boundary conditions from the 3D analysis of the set B (B04). (b) Computed shear strain contours ........................................... 78

5.10 Contours of shear strain from the set of analyses C .................................. 79

5.11 Load-displacement curves from the set of analyses C .................................. 80

5.12 Load-displacement curves from the set of analyses D ................................. 81

5.13 Load-displacement curves from the set of analyses E ................................. 81

5.14 Relationship between softening rate and $l_s$ in the set of analyses E ........... 82

5.15 Contours of shear strain from the set of analyses F ................................... 82

5.16 Evolution of $\epsilon''_s$ from analysis E03 ...................................................... 84

5.17 Theoretical and obtained shear band orientation from analysis E03 ............... 85

5.18 Theoretical and obtained shear band orientation from the set of analysis F .... 86

5.19 Contours of shear strain from the set of analysis G ..................................... 87

5.20 Theoretical and obtained shear band orientation from the set of analysis G ..... 87

5.21 Theoretical and obtained shear band orientation from analysis H01 .............. 88

5.22 Schematic diagram of the plane strain apparatus (Desrues and Viggiani, 2004) 89

5.23 Specimen MBLL16 after the test (Marello, 2004) ...................................... 89

5.24 Geometry, mesh, and boundary conditions for the simulation of the experiment. (b) Non-uniform distribution of the asymptotic cohesion. ............... 91

5.25 Experimental (Marello, 2004) and simulated axial load vs. global axial strain curves from a plane strain compression test on stiff Beaucaire marl .................. 91

5.26 Incremental field of shear strain from a plane strain compression test on stiff Beaucaire marl: (a) experimental (Marello, 2004) and (b,c) simulation results 92

6.1 Conceptual model of the induced fractures network around a drift parallel to the horizontal major stress (Armand et al., 2014) ................................. 96

6.2 Conceptual model of the induced fractures network around a drift parallel to the horizontal minor stress (Armand et al., 2014) ................................. 97

6.3 Location of measurement points used for comparison with the simulation. ....... 102

6.4 Geometry, boundary conditions and finite element mesh employed. ............. 104

6.5 Deconfinement curve for radial stresses on the tunnel wall. ......................... 105

6.6 Water retention curve employed and experimental data for the COx (Armand et al., 2017b) ................................................................. 108

6.7 Experimental (Andra, 2014a; Armand et al., 2017b) and simulated peak strengths as a function of confinement stress and strain rate. ......................... 108

6.8 Variation of cohesion (and tensile strength) with loading direction employed in the simulations. ................................................................. 110

6.9 Observed deviatoric creep strain rates in triaxial creep tests (Armand et al., 2017b) determination of the parameter $\gamma^c$. ........................................... 111

6.10 Obtained configuration of the EDZ in terms of shear strain contours for drifts parallel to the (a) major and (b) minor horizontal stresses ($t = 100$ days), compared to the observed extension of the EDZ (Armand et al., 2014) ........... 112

6.11 Obtained configuration of the EDZ in terms of shear strain contours for drifts parallel to the (a) major and (b) minor horizontal stresses ($t = 1400$ days) .... 113
6.12 Observed (Seyedi et al., 2017) and computed evolution of convergences for the GCS drift. ................................................................. 114
6.13 Computed evolution of convergences for a drift parallel to the minor horizontal stress. .............................................................. 115
6.14 Observed horizontal displacements of extensometer OHZ1501 (Seyedi et al., 2017) and simulation results. .......................... 115
6.15 Horizontal displacement contours. .............................................. 116
6.16 Observed pore water pressure evolution of borehole OHZ1521 (Seyedi et al., 2017) and simulation results. ......................... 117
6.17 Observed pore water pressure evolution of different boreholes (Seyedi et al., 2017) and simulation results. ......................... 117
6.18 Observed pore water pressure evolution of borehole OHZ1521 (Seyedi et al., 2017) and simulation results assuming a purely elastic constitutive behaviour. 119
6.19 Mechanism controlling water pressure increments in terms of a) shear strains, b) pore water pressures, c) incremental pore water pressures and d) incremental volumetric strains. .................................................. 120
6.20 Observed pore water pressure evolution of borehole OHZ1522 (Seyedi et al., 2017) and simulation results assuming a constant permeability. 121
6.21 Groundwater flux \( (t = 100 \text{ days}) \). .................................................. 122
6.22 Observed pore water pressure evolution of borehole OHZ1522 (Seyedi et al., 2017) and simulation results. ......................... 123
6.23 Different meshes employed to examine the mesh independence of the results. ................................................................. 124
6.24 Obtained shear strain contours for different meshes with and without nonlocal regularisation. .............................................. 125
6.25 Obtained convergences for different meshes with and without nonlocal regularisation. ......................................................... 125

7.1 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift and a drift parallel to the minor horizontal stress from the set of analyses A \( (t = 100 \text{ days}) \), compared to the observed extension of the EDZ (Armand et al., 2014). .................................................. 131
7.2 Different employed variations of cohesion (and tensile strength) with the loading direction for the set of analyses B. ................................. 132
7.3 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift and a drift parallel to the minor horizontal stress from the set of analyses B \( (t = 100 \text{ days}) \), compared to the observed extension of EDZ (Armand et al., 2014). .................................................. 133
7.4 Computed evolution of horizontal and vertical convergences from the set of analyses C, compared to base case and field measurements (Seyedi et al., 2017). 133
7.5 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses C, compared to base case and field measurements (Seyedi et al., 2017). .................................................. 134
7.6 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses D \( (t = 100 \text{ days}) \), compared to the observed extension of EDZ (Armand et al., 2014). .................................................. 135
7.7 Computed evolution of horizontal and vertical convergences from the set of analyses D, compared to base case and field measurements (Seyedi et al., 2017).

7.8 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses D, compared to base case and field measurements (Seyedi et al., 2017).

7.9 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses E ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).

7.10 Computed evolution of horizontal and vertical convergences from the set of analyses E, compared to base case and field measurements (Seyedi et al., 2017).

7.11 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses E, compared to base case and field measurements (Seyedi et al., 2017).

7.12 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the sets of analyses F and G ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).

7.13 Computed evolution of horizontal and vertical convergences from the sets of analyses F and G, compared to base case and field measurements (Seyedi et al., 2017).

7.14 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the sets of analyses F and G, compared to base case and field measurements (Seyedi et al., 2017).

7.15 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses H ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).

7.16 Computed evolution of horizontal and vertical convergences from the set of analyses H, compared to base case and field measurements (Seyedi et al., 2017).

7.17 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses H, compared to base case and field measurements (Seyedi et al., 2017).

7.18 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses I ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).

7.19 Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses I ($t = 1400$ days), compared to the observed extension of EDZ (Armand et al., 2014).

7.20 Computed evolution of horizontal and vertical convergences from the set of analyses I and J, compared to base case and field measurements (Seyedi et al., 2017).

7.21 Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses I and J, compared to base case and field measurements (Seyedi et al., 2017).

8.1 Flow chart of the script within $IDTask = 2$ .

8.2 Example of a cheat file for the activation of a UDFM .
A.1 Normalised undrained strength variation with the loading direction in soils with different OCRs (modified from Skempton and Hutchinson, 1969).

A.2 Identified types of undrained strength distributions in fine-grained soils.

A.3 Orientation of the isotropic plane for a) 3D and b) 2D problems.

A.4 Function Ω and its parameters.

A.5 Observed and computed undrained strength distributions.

A.6 Geometry and boundary conditions for the synthetic case.

A.7 Definition of the failure mechanism.

A.8 Variation of the stability number with slope inclination.

A.9 Failure mechanism obtained for different slope inclinations.

A.10 Direction of the major principal stress along the failure surface of the isotropic analysis for two slope inclinations.

A.11 Variation of the stability number with the direction of anisotropy.

A.12 Obtained failure mechanism for different directions of anisotropy.

A.13 Mean δ value along the failure surface for different directions of anisotropy.

A.14 Cross-section through the excavated trench at LASH terminal after failure (modified from Duncan, 2000).

A.15 Geometry and boundary conditions of the analysed underwater slope.

A.16 Undrained strength variation with depth for San Francisco bay mud at the LASH Terminal site (modified from Duncan, 2000).

A.17 Observed (Lade and Kirkgard, 2000) and computed normalised strength distribution.

A.18 Obtained failure mechanism and factor of safety for the a) isotropic and b) anisotropic analyses.
## List of Tables

3.1 Material parameters. ................................................................. 43

4.1 Reference properties of the COx claystone (modified from Gens, 2013). ...... 49
4.2 Evolution laws for the mobilised friction angle (see Fig. 4.1 for the location of
the strain zones). ............................................................................ 51
4.3 Constitutive law parameters used in the simulations. ............................... 57
4.4 Hydraulic parameters used in the drift excavation simulation. ................. 62

5.1 Parameters of base case analysis A01 ............................................ 74
5.2 Analyses performed ..................................................................... 75
5.3 Obtained shear band thickness from the set of analyses C ....................... 79
5.4 Reference properties of the Beaucaire marl (from Marello et al., 2004) ...... 88
5.5 Parameters of the simulation of the test on Beaucaire marl .................... 90

6.1 Parameters of base analysis A01 .................................................. 106

7.1 Analyses performed .................................................................... 129

A.1 Parameters of the adjusted strength distributions ............................... 205
List of Symbols

- **a**: rotation matrix for the stress tensor
- **a**$_{\text{hard}}$ constant that controls the curvature of the function in the hardening branch
- **a**$_{\text{soft}}$ constant that controls the curvature of the function in the softening branch
- **a**$^c$ parameter in the creep law
- **A**: parameter for the relative permeability
- **$\hat{A}$**: variable in $\Omega$
- **b**: vector of body forces
- **b**$_c$ softening rate for the cohesion and isotropic tensile strength
- **b**$_{\text{res}}$ softening rate for residual strength parameters
- **b**$_{\text{post}}$ softening rate for post-rupture strength parameters
- **b**$_{\phi}$ softening rate for the friction angle
- **b**$_{\omega}$ rate of reduction of $\omega$
- **B**: Biot’s coefficient
- **$\hat{B}$**: variable in $\Omega$
- **c**: cohesion
- **c**$_{ij}$ scaling factors
- **c**$_{\text{ini}}$ initial cohesion
- **c**$_{\text{mob}}$ mobilised cohesion
- **c**$_{\text{peak}}$ peak cohesion
- **c**$_N$ normal scaling factor
- **c**$_S$ shear scaling factor
- **c**$^*$ asymptotic cohesion
- **c**$^*_0$ asymptotic cohesion measured with $\sigma_1$ parallel to bedding
- **c**$^*_0$$_{\text{ini}}$ initial asymptotic cohesion measured with $\sigma_1$ parallel to bedding
- **c**$^*_0$$_{\text{post}}$ post-rupture asymptotic cohesion measured with $\sigma_1$ parallel to bedding
- **C**: elastic compliance
- **C**: unknown constant for error terms
- **$\hat{C}$**: variable in $\Omega$
- **C**$_{\alpha}$ index of secondary compression
- **D**$^e$ elastic stiffness matrix
- **$\hat{D}$**$^e$ elastic stiffness matrix for the actual orientation of the isotropic plane
- **D**$^{\text{ep}}$ elasto-plastic stiffness matrix
- **e**: void ratio
- **e**$_1$ exponential function in $\Omega$
- **e**$_2$ exponential function in $\Omega$
- **E**: estimates of the local truncation error
\( E \) Young’s modulus
\( E_1 \) Young’s modulus parallel to the isotropic plane
\( E_2 \) Young’s modulus perpendicular to the isotropic plane
\( E^\tau \) relative error

\( EPS \) machine specific upper bound on the relative error due to rounding in floating point arithmetic

\( f \) yield function
\( f_d \) deviatoric yield function
\( f_t \) tension yield function
\( f_v \) volumetric yield function
\( f_o \) reference normalisation stress
\( f_2 \) function defining the shape of \( f \) in the deviatoric plane
\( f^{rd} \) rate dependent yield function
\( f^w \) external supply of water

\( FOS \) factor of safety

\( g \) vector of gravity forces
\( g_p \) plastic potential
\( g_g \) gas phase

\( G_2 \) Shear modulus on planes perpendicular to the isotropic plane

\( h \) step size

\( H \) slope height

\( \hat{H} \) hardening modulus

\( H_R \) relative humidity

\( I \) identity matrix

\( j \) total mass flux

\( J \) Jacobian matrix

\( J \) square root of \( J_2 \)

\( J_2 \) second invariant of the deviatoric stress tensor

\( J^{ani} \) deviatoric stress invariant of the anisotropic stress tensor

\( k \) intrinsic permeability tensor

\( k_0 \) intrinsic permeability tensor of the intact rock

\( K \) hydraulic conductivity tensor

\( k \) error order of the approximation procedure

\( k_h \) horizontal intrinsic permeability

\( k_r \) relative permeability

\( k_v \) vertical intrinsic permeability

\( K_o \) lateral \textit{in situ} stress coefficient

\( l \) liquid phase

\( l_i \) variable in the transformation matrix

\( l_s \) length scale parameter

\( L \) total length

\( L_e \) weak element length

\( m \) material constant - Lemaitre’s creep

\( \hat{m} \) parameter controlling the dependence of \( p \) on the hardening law

\( \bar{m} \) elastic constant
$m_i$ variable in the transformation matrix
$M_w$ water molar mass
$n$ vector normal to the isotropic plane
$\hat{n}$ parameter in $\Omega$
$n_\varepsilon$ elastic constant
$n_i$ variable in the transformation matrix
$n^\theta$ parameter in van Eekelen function
$n$ material constant - Lemaitre’s creep
$N$ order of Perzyna’s formulation
$N_G$ number of Gauss points
$N_o$ stability number
$O$ big O notation
$p$ mean stress
$p'$ effective mean stress
$p_{atm}$ reference pressure equal to 100 kPa
$p_{res/dil}$ mean stress value from which $\hat{\omega}$ is equal to $\omega_{res}
$p_t$ isotropic tensile strength
$p_{t0}$ isotropic tensile strength measured with $\sigma_1$ parallel to bedding
$p_{t0\ ini}$ initial isotropic tensile strength measured with $\sigma_1$ parallel to bedding
$p_{t0\ post}$ post-rupture isotropic tensile strength measured with $\sigma_1$ parallel to bedding
$p_{ini}$ mean stress of the anisotropic stress tensor
$p_l$ liquid pressure
$P$ air entry value
$q$ fluid flux
$q$ deviatoric stress invariant
$Q$ acoustic or localisation tensor
$Q$ estimated size of the next sub-step
$r$ vector of residuals
$r_{post}$ post-rupture ratio
$R$ universal gas constant
$R_{cres}$ Undrained residual compressive strength
$s$ solid phase
$s$ deviatoric stress tensor
$s_u$ suction
$S_e$ equivalent degree of saturation
$S_i$ degree of saturation
$S_{ir}$ residual degree of saturation
$S_{ls}$ degree of saturation in saturated conditions
$S_u$ undrained strength
$S_u^*$ anisotropic undrained strength
$S_{u-f}$ undrained strength at failure
$t$ time
$T$ transformation matrix
$T$ normalised time
$T_e$ temperature

XXXI
TOL  tolerated relative error in the sub-stepping algorithm
  u  displacements
  $u_o$  displacement at peak
  $u_f$  displacement at failure
  $U$  unknown quantity
  v  major principal stress vector
  V  volume
  w  normalised weighting function
  $w_o$  weighting function
  x  vector of unknowns
  X  improved approximation of $U$
  $X$  Gauss points coordinates
  $\alpha$  angle in the transformation matrix
  $\alpha^\theta$  parameter in van Eekelen function
  $\beta$  angle in the transformation matrix
  $\beta^k$  evolution parameter for the intrinsic permeability
  $\beta^\theta$  parameter in van Eekelen function
  $\gamma$  column matrix of material parameters
  $\gamma^u$  unit weight
  $\gamma^c$  parameter in the creep law
  $\gamma^{vp}$  viscosity parameter - Lemaitre’s creep
  $\Gamma$  creep proportionality factor
  $\delta$  relative orientation between $n$ and the direction of $\sigma_1$
  $\delta_m$  parameter in $\Omega$
  $\delta_{\text{min}}$  value of $\delta$ where the minimum value of $\Omega$ occurs
  $\epsilon$  total strain tensor
  $\epsilon^e$  elastic strain tensor
  $\epsilon^c$  creep strain tensor
  $\epsilon^p$  plastic strain tensor
  $\epsilon^{ep}$  elastoplastic strain tensor
  $\epsilon^{vp}$  viscoplastic strain tensor
  $\tilde{\epsilon}$  column matrix of engineering total strain components
  $\tilde{\epsilon}^e$  column matrix of engineering elastic strain components
  $\tilde{\epsilon}^p$  column matrix of engineering plastic strain components
  $\epsilon_{\text{eq}}$  equivalent creep strain
  $\epsilon_{\text{eq}}^p$  equivalent plastic strain
  $\epsilon_{\text{eq}}^p$  stress dependent variable controlling hardening
  $\epsilon_{\text{eq}}^{vp}$  nonlocal equivalent plastic strain
  $\epsilon_{\text{eq}}^{\tau}$  state variable for the time-dependent response
  $\epsilon_f$  strain at failure
  $\epsilon_o$  strain at peak
  $\epsilon_s$  shear strain
  $\epsilon''$  global shear strain acceleration
  $\epsilon_{\text{thr}}$  value of $\epsilon_{\text{eq}}^p$ at which creep deformations are activated
  $\epsilon_1$  major principal strain

XXXII
\( \epsilon_3 \)  minor principal strain
\( \zeta \)  function controlling the dependence of the plastic potential with plastic strains
\( \eta \)  parameter for the change in the intrinsic permeability with damage
\( \eta_{p2} \)  viscosity parameter in Perzyna’s overstress
\( \theta \)  Lode’s angle
\( \theta^s \)  slope inclination
\( \theta_A \)  Arthur’s angle
\( \theta_C \)  Coulomb’s angle
\( \theta_R \)  Roscoe’s angle
\( \theta_{ani} \)  Lode’s angle of the anisotropic stress tensor
\( \Theta \)  measure of the relative orientation between loading and anisotropy directions
\( \kappa \)  coordinates of neighbouring Gauss points
\( \lambda \)  plastic multiplier
\( \lambda^p \)  cumulative value of the plastic multiplier
\( \lambda^r \)  parameter for the retention curve
\( \Lambda \)  parameter for the relative permeability
\( \mu \)  parameter in the over-nonlocal approach
\( \mu_w \)  dynamic viscosity
\( \nu \)  Poisson’s ratio
\( \nu_1 \)  Poisson’s ratio between the two strain components on the isotropic plane for loading parallel to the isotropic plane
\( \nu_2 \)  Poisson’s ratio between strain components on the isotropic plane and the component perpendicular thereto for loading perpendicular to the isotropic plane
\( \xi_1 \)  equivalent plastic strain at which the maximum strength is reached
\( \xi_2 \)  equivalent plastic strain at which softening begins
\( \xi_3 \)  equivalent plastic strain at which the residual state is reached
\( \rho \)  density
\( \sigma \)  stress tensor
\( \sigma' \)  effective stress tensor
\( \sigma_{ani} \)  anisotropic stress tensor
\( \sigma^r \)  stress tensor in the local coordinate system
\( \bar{\sigma} \)  column matrix of independent stress components
\( \bar{\sigma}_{ani} \)  column matrix of independent stress components of the anisotropic stress tensor
\( \sigma_h \)  minor horizontal stress
\( \sigma_H \)  major horizontal stress
\( \sigma_r \)  radial stress
\( \sigma_s \)  stress threshold - Lemaitre’s creep
\( \sigma_v \)  vertical stress
\( \sigma_y \)  yield stress
\( \sigma_1 \)  major principal stress
\( \sigma_2 \)  intermediate principal stress
\( \sigma_3 \)  minor principal stress
\( \Upsilon \)  coordinates of neighbouring Gauss points
\( \phi \)  friction angle
\( \phi_C \)  inclination of the plane of maximum stress ratio
\( \phi_{\text{ini}} \) initial friction angle
\( \phi_{\text{mob}} \) mobilised friction angle
\( \phi_{\text{peak}} \) peak friction angle
\( \phi_{\text{res}} \) residual friction angle
\( \phi^* \) asymptotic friction angle
\( \phi^*_{\text{ini}} \) initial asymptotic friction angle
\( \phi^*_{\text{peak}} \) peak asymptotic friction angle
\( \phi^*_{\text{res}} \) residual asymptotic friction angle
\( \Phi \) Perzyna’s overstress function
\( \varphi \) porosity
\( \mathbf{\chi} \) vector of state variables
\( \chi \) arbitrary state variable
\( \psi \) dilation angle
\( \psi^c \) parameter in the creep law
\( \omega \) non-associativity factor
\( \hat{\omega} \) stress-dependent non-associativity factor
\( \omega_{\text{res}} \) residual value of \( \hat{\omega} \)
\( \Omega \) function controlling the variation of strength with \( \delta \)
\( \Omega^c \) \( \Omega \) function for the cohesion and tensile strength
\( \Omega^\phi \) \( \Omega \) function for the friction angle
\( \Omega_m \) parameter in \( \Omega \)
\( \Omega_{90} \) parameter in \( \Omega \)
\( \langle \rangle \) Macaulay brackets
Chapter 1

Introduction

1.1 Background

Across the spectrum of geotechnical materials, ranging from normally consolidated soft soils to very hard igneous rocks, we can identify a transition zone where materials can be classified either as hard soils or weak rocks (Gens, 2013), and where the disciplines of soil and rock mechanics tend to overlap. Here, we can find sedimentary materials in which clay minerals are the main constituent. They exhibit soil-like features like considerable plastic strains, rate dependency, and creep. However, they also show characteristics more typical of a rock such as significant softening and localised deformations. In addition, due to their sedimentary origin, they often exhibit anisotropy in properties like the stiffness, strength, and permeability. These argillaceous formations are of particular interest in the context of nuclear waste management since they are being currently considered in several countries as possible host medium for deep geological disposal of high active and long-lived nuclear waste (Delage et al., 2010). In this regard, they show appealing characteristics like very low hydraulic conductivity, low molecular diffusion, and significant radionuclide retention capacity (Armand et al., 2017b), and they are now a prominent candidate along with other geological formations such as crystalline rocks and rock salt (Gens, 2004).

The possibility of using argillaceous formations to host nuclear waste repositories has motivated the construction of underground research facilities in these materials in order to study their behaviour under field conditions. Some of these laboratories are the Mont Terri rock laboratory, in Northwestern Switzerland, excavated in Opalinus clay (Bossart et al., 2017a); the HADES underground research facility, located in Mol, Belgium, excavated in Boom clay (Li et al., 2007); and the Meuse/Haute-Marne (MHM) underground research laboratory (URL), in Eastern France, excavated in the Callovo-Oxfordian argillite (Delay et al., 2007). A number of in situ experiments have been performed in them to assess the feasibility of these clayey materials as host formations. Among the very different topics covered by the experiments, we are particularly interested here in those dealing with the hydromechanical behaviour of the host material.

Experimental excavations have been performed at the underground laboratories, with much higher levels of instrumentation and control compared with conventional engineering works, to study the hydromechanical response of the host rock to excavation operations. Some salient examples are the CLIPEX project at HADES (Li et al., 2007), the ED-B mine-
by test at Mont Terri (Bossart et al., 2017b), and the GCS drift at the MHM URL (Armand et al., 2013). In spite of the differences between the formations, reflecting their various origins and geological histories, similar features can be identified in their behaviour (Gens, 2013). For instance, excavation operations induced damage around the galleries, in the form of fractures networks. In Fig. 1.1, conceptual models of the observed fracture networks around drifts at the three laboratories are depicted. They were derived combining a variety of techniques such as geological surveys, structural analysis of core samples, and overcoring of resin-filled fractures (Armand et al., 2014; Bossart et al., 2004). The zone containing the fracture network is usually known as the excavation damaged zone (EDZ), and significant changes in the flow and transport properties take place within it (Tsang et al., 2005).

Figure 1.1: Conceptual model of the induced fracture networks at the MHM for drifts parallel to the (a) major and (b) minor horizontal stresses, (c) at Mont Terri, and (d) at HADES (modified from Armand et al., 2014; Blümling et al., 2007; Li et al., 2007).

Particularly interesting are the excavations at the MHM URL. At the main level (-490 m), an anisotropic initial stress state has been estimated (Wileveau et al., 2007), with \( \sigma_v \approx \sigma_h \approx 12 \text{ MPa} \) and \( \sigma_H/\sigma_h \approx 1.3 \), where \( \sigma_v \) is the vertical stress and \( \sigma_H \) and \( \sigma_h \) are the major and minor horizontal stresses respectively. For drifts parallel to \( \sigma_h \), the EDZ extends further in the vertical direction (Fig. 1.1b) and measured vertical convergences are considerably larger than horizontal ones (Armand et al., 2013). In general terms, this behaviour can be easily explain using a simple isotropic elastoplastic constitutive description, and is mainly controlled by the initial stress anisotropy. On the other hand, in drifts parallel to \( \sigma_H \) a nearly isotropic stress state exists in the plane normal to the tunnel axis; however, the EDZ does not show radial symmetry, and it extends further in the horizontal direction (Fig. 1.1a), with larger horizontal convergences (Armand et al., 2013). In this case, the observed response cannot be explained without including material anisotropy.

The EDZ has been identified as one of the key issues affecting the behaviour of excavations. An example is shown in Fig. 1.2, where horizontal displacements from an extensometer near a drift parallel to \( \sigma_H \) are depicted. The extensometer was installed from an adjacent gallery in advance of the excavation (Seyedi et al., 2017). It is evident that deformations near
the drift are controlled by the fractures, and only those points inside of the EDZ experienced considerable displacements. The fractures also act as preferential pathways for water flow and, therefore, the observed hydraulic conductivity from *in situ* tests increases within the EDZ (Armand et al., 2014). In turn, this affects the evolution of pore water pressures, which are particularly sensitive to excavation operations (Gens, 2013).

![Figure 1.2: Horizontal displacements of extensometer OHZ1501 (modified from Armand et al., 2014; Seyedi et al., 2017).](image)

Along with the *in situ* experiments carried out at the MHM URL, a massive effort has been made to assess the hydromechanical behaviour of the COx through laboratory testing (Andra, 2005b). Some of the key features identified are: strength and stiffness anisotropy; a quasi-brittle behaviour, with a significant strength loss after the peak deviatoric stress; localised failures modes; loading-rate dependency; or considerable creep deformations with increasing deviatoric stresses.

Due to the complexity of the problem in hand, numerical methods, such as the finite element method, are the most appealing way (perhaps the only one) for trying to reproduce and explain the observed hydromechanical behaviour of the drifts at URL. The constitutive description of the claystone should include the most relevant behaviour features identified. However, the latter poses an important problem since the use of constitutive laws with softening to simulate localised deformations, in combination with numerical methods within the framework of continuum mechanics, derives in non-objective results showing a marked dependency with the employed mesh (de Borst et al., 1993). Different approaches exist to handle this issue, usually called regularisation techniques, that must be included for the successful simulation of the host formation.

### 1.2 Objectives and methodology

The general objective of this research is the numerical simulation of the hydromechanical behaviour of underground excavations in stiff clayey formations. The work was developed within the context of deep geological disposal of nuclear waste, particularly in relation with the activities carried out at the MHM URL. The experimental excavation GCS served as the
main case study of this research. This is a heavily instrumented drift parallel to $\sigma_H$, where measurements of convergences, ground displacements, pore water pressures, and the characterisation of fractures around the tunnel were available (Armand et al., 2014; Seyedi et al., 2017). Coupled hydromechanical finite element analyses were performed, aimed to reproduce field observations. In this regard, a constitutive model was developed including a number of features that are considered relevant for the satisfactory description of the behaviour of COx claystone. In addition, a nonlocal regularisation technique has been incorporated for the objective simulation of localised deformations. The obtained results are aimed to provide relevant insights into the behaviour of these stiff clayey formations, to indicate the main aspects affecting the response of the drifts, and to supply information to assist the design of the actual repositories.

1.3 Thesis layout

This thesis was prepared as a compendium of publications. It consists of six journal papers and a book chapter. Each publication corresponds to a chapter of the thesis (except chapters 8 and 9) and, therefore, they can be read independently. Because this, the reader should bear in mind that some repetition is unavoidable, especially in the introductory sections of the chapters. No attempt is made to infringe publisher’s copyright policies; each chapter was prepared based on the accepted (or submitted, or to be submitted) manuscript, of which the authors reserve the copyright for non-commercial purposes. Weblinks are provided to the version of record for the already published material. An effort was made to have a unique list of symbols throughout the document; therefore, some symbols might differ from the version of record. If the pdf version of the document is being used, please note that all references, sections, equations, figures, tables, and appendices are hyper-referenced to facilitate navigation through the document. If a link has been used, the reader can return to the previous position using Alt+Left in most of the softwares used to read pdf files. The way chapters were organised reflects the chronological progress of the research; this is further described in the following paragraphs.

Chapter 2 corresponds to a section of a book dealing with scientific and engineering aspects of shales. The chapter presents an overview of the modelling frameworks, within the theory of elastoplasticity, to simulate the mechanical behaviour of shale rocks. Nevertheless, the subjects addressed apply generally to stiff clayey materials. Consequently, it introduces the concepts employed later for the development of a constitutive model for the COx claystone.

In the context of the Transverse Action benchmark programme (Seyedi et al., 2017), a simulation of the GCS drift was performed. As briefly mentioned in section 1.1, material anisotropy is required to reproduce the observed behaviour of this kind of drifts; particularly, strength anisotropy is one of the major features that must be introduced in the constitutive description. Therefore, a cross-anisotropic extension for elastoplastic models was developed, and the resulting formulation is presented in chapter 3. It uses a non-uniform scaling of the stress tensor to modify indirectly the yield function and to account for strength anisotropy. This anisotropic extension was later applied to a constitutive model that includes relevant features of the COx behaviour, which was used in the benchmark simulations. The
description of the model and its application to the simulation of the GCS drift are presented in chapter 4. Nevertheless, localisation was not considered at this stage and, in the context of this thesis, it represents a first approximation of the problem in hand.

In chapter 5, the issue of simulating localisation objectively was considered. A plasticity model, intended for stiff clayey materials, was enhanced with a nonlocal regularisation; it represents a simplified version where features such as time dependency or anisotropy were not included. Through a number of plane strain analyses, the mesh independence of the formulation employed was verified. In addition, important aspects related to the numerical simulation of localised deformations were studied from the perspective of a boundary value problem.

In appendix A, a different approach to account for strength anisotropy was developed. Although the one presented in chapter 3 is quite versatile and straightforward to implement, the idea here is to control directly anisotropy through a dependence of the strength parameters on the loading direction. This work was derived from the supervision of a master’s thesis (Conesa, 2017), and is not part of the main body of the document because it was applied to the stability analysis of slopes. Nevertheless, the approach is later employed in chapters 6 and 7, and it is therefore relevant to this thesis.

In chapter 6, the formulation presented in chapter 5 was extended to account for all relevant behavioural features of the COx, including the anisotropic extension described in appendix A. A simulation of the GCS drift was performed, but in this case, dealing with the problem of localisation. Important insights are presented about the relevance of the EDZ in the short- and long-term behaviour of the excavation, in particular about the generation of over-pressures deep into the clay rock.

In chapter 7, a sensitivity study is presented to assess the influence of different parameters on the results of the GCS drift simulation given in chapter 6. Aspects studied include mechanical anisotropy, strength parameters, excavation size, hydraulic parameters and time dependency. Some of the main aspects of the COx hydromechanical behaviour affecting the response of the drift have been identified. Together with chapter 6, these works are the most relevant of this thesis, where the objectives set at the beginning of the research were fulfilled.

Chapter 8 deals with the implementation of the constitutive model employed in chapters 6 and 7. This chapter does not correspond to any published work, and it is only intended to present details of the implementation such as the stress integration algorithm, or the error-based sub-stepping scheme. A link to the compiled dynamic library, to be used directly in Plaxis, is provided. In addition, useful suggestions are given for those people interested in using the model.

Finally, in chapter 9 the general conclusions of the thesis are presented.
Chapter 2

Geomechanics of shale repositories
- Mechanical behaviour and modelling

Based on the submitted manuscript of the following book chapter:

Abstract

This chapter presents an overview of modelling frameworks available within the theory of elastoplasticity and able to capture main features of shale behaviour including: yield under compression, failure under deviatoric loading, strain-softening, degradation, anisotropy of elastic moduli, strength and permeability as well as creep and viscous response. For each aspect, a short illustration of material response is presented, followed by a brief presentation of the mathematical formulation used to capture it. When numerical simulations of real cases are available, the ability of the models to reproduce laboratory and field measurements is also presented.

2.1 Introduction

Shales are low porosity soft rocks with intermediate strength level between hard soils and rocks, although no precise limits have ever been uniformly defined. They are characterised by a significant fraction of clay-based materials that made them quite sensitive to water content changes. These types of materials are very widespread in nature; it has been estimated that they constitute as much as 50% of the global sedimentary rock mass (Pettijohn, 1975) and that they outcrop in about one-third of the emerged earth surface (Franklin, 1983).

A complete review of the geological origins of stiff sedimentary clays is given in the keynote paper by Chandler (2010). Diagenetic processes occurring after sedimentation generally include mineral precipitation and change in material structure under conditions of increased temperature and stress due often to the depth of burial or tectonic forces. These changes
cause recrystallisation of mineral grains components and result in a structure intruded by bonds whose strength bears no relationship to the sedimentary history of the clay, but reflects the combined effects of chemistry and stress imposed at the time of diagenesis (Chandler, 2010). The precipitated carbonate is the main source of bonds and plays a central role in the mechanical behaviour of shales.

As a consequence of the low level of porosity and the presence of bonds between minerals particles, several aspects of shale behaviour are similar to that of rocks, mainly controlled by micro-cracks development and coalescence, fracture propagation, and existing discontinuities. These materials fail in most of cases along localised paths that split the medium into several blocks of intact rock. On the other hand, shales are susceptible to suffer weathering and degradation as many argillaceous rocks, particularly in presence of water. During this process, the initial diagenetic structure is erased and the material transforms into an unbounded matrix provided with a mechanical response proper of soils. Fig. 2.1 presents the evolution of a marl sample submitted to cycles of relative humidity: from the simple observation of its aspect, it is possible to apprehend the huge degradation suffered after one cycle and the total transformation from a rock-like to a soft-like material after only four cycles. Such type of response typically appears when the material is exposed to sudden changes in environmental conditions like, for example, exposure to atmospheric conditions after excavation. A full modelling of their hydro-mechanical response should thus account for transitional phenomenological features between that of a rock and a soil.

![Intact Marl (w_i = 37, w_r = 18.7) After 1 wetting/drying cycle](image1)
![After 4 wetting/drying cycle](image2)
![After 5 wetting/drying cycle](image3)

Figure 2.1: Degradation of a sample of argillaceous rock during cycles of relative humidity (Alonso and Alcoverro, 2004).

The way in which shales integrate soil-like and rock-like types of response in their phenomenology can be reasonable expected to depend on the level of porosity and bonding, as in other carbonate materials. Fig. 2.2 shows, for example, the relationship established by Hsu and Nelson (1993) between uniaxial strength and carbonate content for Taylor and Austin chalk formations in Texas. Austing chalk immediately underlies Taylor formation, and both rocks represent a fairly continuous variation from very low to high %CaCO_3. The increase in strength with carbonate content, which is a good indicator of bonding level in unweathered shales, evidences the progressive transformation of the material from a hard soil to a rock.
Another example of this relationship is founded by Klinkenberg et al. (2009) and Kaufhold et al. (2013). They stated that the failure strength of the argillaceous formations Opalinus Clay and Callovo-Oxfordian increases with the carbonate content.

![Graph showing variation of uniaxial compressive strength with carbonate content in Taylor and Austin chalk formation, Texas (Hsu and Nelson, 1993).](image)

Figure 2.2: Variation of uniaxial compressive strength with content of calcium carbonate in Taylor and Austin chalk formation, Texas (Hsu and Nelson, 1993).

In consequence, the phenomenological description of shales responses should include challenging features from the point of view of modelling such as low porosity effects, significant bonding, marked anisotropy, stiffness decrease upon loading, brittle behaviour during shearing, crack opening during unloading, and mechanical degradation upon environmental actions. As exposed by Gens (2013), there have been in recent years a significant number of conferences and publications specially devoted to the behaviour of intermediate soil/rock materials and, in particular, to argillaceous materials to whose belong shale formations. Particularly, there exist several review papers arising from the 2007 Géotechnique Symposium, that provide updated information on engineering properties of stiff sedimentary clays. The description of these properties is not the objective of this chapter, devoted to the mathematical modelling of shale behaviour. The reader is thus referred to the previous literature for further insights into the phenomenological features on the bases of the modelling works addressed hereinafter.

### 2.2 Modelling framework

Because of the rock-soil transitional nature of shales responses, their modelling has been worked within theoretical frameworks existing for both brittle to ductile materials: fracture mechanics, damage elasticity and elastoplasticity.

Models developed on the basis of fracture theory focus on the definition of failure criteria for intact rock and joints as a function of rock type, joint orientation and roughness, and nature of filling material. Hoek and Bray (1981) presented a schematic picture of several shear failure envelopes for rocks, independently of the level of strength of the material (Fig. 2.3).

Elastic damage theory, initially developed for concrete, has been used to represent macro-
scopically the effect of micro-cracks development on the material stiffness (Hueckel and Maier, 1977; Kachanov, 1958; Mazars and Lemaitre, 1985). Examples of application are given by Chan et al. (1992) for salt rock; Shao et al. (1999) for granite; Renaud and Kondo (1997) for sandstone; Chiaielli (1999) and Zhu and Arson (2014) for argillite; Zhao et al. (2016) for brittle rocks. They have been progressively linked with the theory of fracture mechanics by recognising the localised nature of micro-cracks and the strong link between fracture propagation and crack coalescence. Particularly, Mazars and Pijaudier-Cabot (1996) propose a model for damage localisation into fracture, based on thermodynamic considerations. The assumed microstructural process underlying this type of approach may be favourably compared with recent tomography measurements performed by Viggiani et al. (2004) in stiff clay. They indicate extremely thin shear failure surface (around 1 µm), which seems to sustain that shear surfaces develop according to pre-discontinuity propagation-like rather than strain localisation mechanisms.

![Figure 2.3: Schematic behaviour of rocks (Hoek and Bray, 1981).](image)

The main alternative framework to fracture and damage mechanics relies on the theory of elastoplasticity used for soils. In that case, models aim at reproducing macroscopic phenomenological features of the soft rock, considered as a continuum. Similarity between stiff soils and soft rocks behaviours have been pointed out by Leroueil and Vaughan (1990). Fig. 2.4 shows for example a comparison between the stress-strain response of a soft natural sensitive clay with an undrained residual compressive strength $R_{cres}$ equal to 70 kPa and a high porosity oolitic limestone with $R_{cres} = 10$ MPa. Despite of the different levels of strength, both volumetric and deviatoric responses present very similar patterns, characterised by a transition from brittle to ductile behaviours as the level of confinement increases.

This type of response has motivated the application to soft rocks of the limit and critical state concepts, initially developed for soils. This framework introduces the effect of density on soil resistance by distinguishing the stress ratio at which plastic strain start (or yield locus) and the large strain shear failure. In between, the stress state evolves according to the changes in density experienced by the material. The large-strain shear failure is reached when volume changes finally vanish and material density attains a stationary value. Fig. 2.5 shows
typical loci in the stress space for the onset of plastic strain, also called limit envelope (Y-curve in the figure) and large-strain failure, also called critical state line (\(\phi'\) line destructured in the figure). The part of the limit envelope above the critical state line (CSL) provides the peak shear strength envelope of the soil, and is associated to the material dilatancy. The part below the CSL provides the yield points under compression at low deviatoric stress, and is associated to the material densification. In the extension of the framework to soft rocks conjectured by Nova (1986b) and further formalised by Gens and Nova (1993), the limit envelope depends moreover on a parameter expressing the effect of bonds. This parameter degrades with the plastic strain, which allows representing material softening under load. Application of this framework to soft rocks such as shales, tuff, calcarenite, marl or chalk can be found in Kavvadas and Amorosi (2000); Lagioia and Nova (1995); Nova and Castellanza (2001); Nova et al. (2003).

Figure 2.4: Stress-strain response of two natural clay-based materials (Leroueil and Vaughan, 1990).

Figure 2.5: Typical limit envelope and critical state line for soils and soft rocks (Leroueil and Vaughan, 1990).

The aim of this chapter is to not to address all the above mentioned frameworks but
to provide an overview of the different elastoplastic frameworks available to model the main behavioural features of shales including: yielding under compression, failure under deviatoric strain, strain-softening, degradation, anisotropy of elastic moduli, strength and permeability, and finally creep and viscous response. Before addressing these aspect, the theory of plasticity will be shortly introduced.

2.2.1 Plasticity theory

The conventional plasticity theory is based on the decomposition of strain into an elastic and plastic part. Under the assumption of small strain, the decomposition reads,

$$\bar{\epsilon} = \bar{\epsilon}^e + \bar{\epsilon}^p$$  \hspace{1cm} (2.1)

where $\bar{\epsilon}$ is the column matrix of engineering strain components, $\bar{\epsilon}^e$ and $\bar{\epsilon}^p$ are the elastic and plastic strain components. Elastic strains are the ones responsible for changes in stresses according to the elastic law,

$$\bar{\sigma} = D^e \bar{\epsilon}^e$$  \hspace{1cm} (2.2)

where $\bar{\sigma}$ is the column matrix of independent stress components, and $D^e$ is the elastic stiffness matrix.

The yield condition provides the zone where the stress state can move (sometimes called admissible or permissible zone),

$$f(\bar{\sigma}, \chi) \leq 0$$  \hspace{1cm} (2.3)

where $f$ is the yield function. Once reached the yield surface, plastic strains develop along the direction determined by the flow rule of the material,

$$d\bar{\epsilon}^p = d\lambda \frac{\partial g(\bar{\sigma}, \chi)}{\partial \bar{\sigma}}$$  \hspace{1cm} (2.4)

where $\lambda$ is the plastic multiplier, and $g$ is the plastic potential function describing the direction of the plastic flow. The yield surface can generally evolve when plastic strains develop. The evolution is given by the hardening law of the material,

$$d\chi = \frac{\partial \chi}{\partial \bar{\epsilon}^p} d\bar{\epsilon}^p$$  \hspace{1cm} (2.5)

where $\chi$ is a vector of parameters defining the size of the yield surface, and depending on the history of the soil (they are alternative called internal, hardening or history variables).

The formulation of the elastoplastic stiffness matrix is derived from the loading/unloading conditions, which sets that the stress state must stay on the yield surface during an elastoplastic increment,

$$d\lambda \geq 0, \quad f \leq 0, \quad d\lambda f = 0$$  \hspace{1cm} (2.6)

The yield function defines a surface in the stress space bounding the elastic domain. For $f < 0$ the response is elastic, for $f = 0$ the response is plastic, and $f > 0$ represents an impossible situation. The loading/unloading conditions (Eq. 2.6), in terms of the so-called Kuhn-Tucker complementary conditions, imply that plastic loading can only occur for states on the yield surface ($f = 0$). During plastic flow the yield function must remain equal to
zero, so its rate of change must also be equal to zero, leading to the so-called consistency condition,

$$df = 0$$  \hspace{1cm} (2.7)

From the latter assumption it is possible to derive an expression relating the stress and strain increments,

$$d\bar{\sigma} = \left( D^e \frac{\partial g}{\partial \bar{\sigma}} \frac{\partial f^T}{\partial \bar{\sigma}} - \frac{\partial f^T}{\partial \bar{\sigma}} D^e \frac{\partial g}{\partial \bar{\sigma}} + \hat{H} \right) d\bar{\varepsilon}$$  \hspace{1cm} (2.8)

where the expression in parenthesis is known as the elastoplastic constitutive matrix, and $\hat{H}$ is the so-called hardening modulus, defined as,

$$\hat{H} = -\frac{1}{d\lambda} \frac{\partial f^T}{\partial \chi} d\chi$$  \hspace{1cm} (2.9)

The hardening modulus plays a crucial role in the elastoplastic response of the material, since it is related to the slope of the stress-strain curve in the plastic regime. Particularly, depending on whether it is positive or negative, the material will exhibit a hardening or softening response.

2.3 Yielding and degradation

2.3.1 Response under compressive loading

From a general point of view, the mechanical behaviour of natural argillaceous geomaterials, including shale rocks, results from the combination of the different effects of sedimentation, gravitational compaction, uplift/unloading and cementation/bonding (Gens, 2013). These complex interactions give rise to structured materials, whose behaviour significantly differ from those of the soils originally deposited. Particularly, these materials are able to carry loads at densities lower than the ones of the original soil. As such, under isotropic or uniaxial compression, it is likely found that materials can bear a mean or vertical stress on the right side of the compression line of the original soil (Fig. 2.6). In this case, during further loading, soil structure starts to degrade and the material response progressively tends to that of the fully destructured. As illustrated in Fig. 2.6, this feature traduces into a gradual convergence of the compression line of the bonded material towards the compression line of the destructured soil. An example of such behaviour is shown in Fig. 2.7, where results of one-dimensional compression test on a sample of Boom clay are depicted. The intrinsic compression line (ICL) corresponds to the reconstituted material, whereas the sedimentation compression line (SCL) is obtained as the best-fit regression line of the field $e - \log(\sigma'_v)$ relationship for several argillaceous materials (see Burland, 1990 for more details). We can observe that the yield point lies beyond the ICL, and also beyond the in situ vertical stress. However, when loaded after yielding, the compression curve tends to converge to the ICL as the load is increased.

The degradation of the structure due to compression can also be identified from the slope of the swelling line after loading beyond the yield point. A remarkable example can
be observed in Fig. 2.8, which shows experimental results obtained during a high-pressure oedometer test on Culebra shale from the Panama Canal. Degradation takes place during compression (line with black symbols). Afterwards, the material is unloaded (line with white symbols) and experiences a huge swelling, that ends at a void ratio higher than the initial one.

Figure 2.6: Compression of a structured and unstructured material (Leroueil and Vaughan, 1990).

Figure 2.7: One-dimensional compression behaviour of Boom clay (Horseman et al., 1987 referenced in Burland, 1990).

Figure 2.8: High-pressure oedometer test on Culebra shale (Banks et al., 1975 referenced in Gens, 2013).
2.3.2 Response under deviatoric loading

In general, argillaceous hard soils and weak rocks fail in a quasi-brittle manner under deviatoric loading. Ductile behaviour can also be observed if samples are tested at very high effective confining stresses (e.g. Ohtsuki et al., 1981) but, in conventional geotechnical engineering situations, brittle failure predominates. One of the first descriptions of this kind of behaviour was put forward by Skempton (1964) on the basis of slow drained tests performed in the direct shear box apparatus on a stiff clayey material (Fig. 2.9). He identified a first stage, characterised by an increase of resistance up to a maximum value, denoted the peak strength. After this point, a process of strain softening starts to develop. It consists in a decrease of strength until the reach of a limit state, where the strength no longer decreases during further application of displacements. This lowest-bound constant strength is known as the residual strength, and had been early identified by Tiedemann (1937) and Hvorslev (1937) using the ring shear apparatus. As shown in Fig. 2.9, the cohesion intercept vanishes and the friction angle slightly decreases as the strength envelope moves from peak to residual values. Depending on the materials, the decrease of the friction angle may vary from 1° or 2° up to 10°. It is worth noting that water content increases during the process, evidencing the tendency of the material to dilate during shearing.

These phenomenological features were later used to distinguish between two different stages in the softening process (Fig. 2.10). The first stage occurs just after the peak, and is characterised by a high rate of strength loss associated with the degradation and breakage of interparticle bonds (Burland, 1990; Simpson, 1979). The second stage is subsequent to the first one, and is characterised with a gentler strength reduction until the residual value, generally attributed to a gradual realignment of clay particles along the failure plane (Gens, 2013). The strength between both stages is often known as fully softened strength (Mesri and Shahien, 2003; Skempton, 1970) or post-rupture strength (Burland, 1990).

Shale rocks are not an exception regarding this type of behaviour. As an example, Fig. 2.11 shows typical stress-strain curves of shales under triaxial loading presented by Nygård et al. (2006). The peak, fully softened, and residual strengths can be clearly identified in curves M2 and M3. It seems moreover that strain reachable in triaxial tests are not large enough to reach the residual strength for high confining pressures (M4 and M5), while post-
peak curve could not be experimentally followed at low confining pressures (curve M1), probably because the large dilatancy experienced by the sample at this level of stress leads to the loss of control of the test.

![Diagram]

Figure 2.10: Conceptual scheme for the strength of argillaceous hard soils and weak rocks (Jardine et al., 2004).

![Diagram]

Figure 2.11: Stress-strain behaviour of Kimmeridge Bay Shale under triaxial loading (Nygård et al., 2006).

Regarding the shape of the strength envelopes, the one associated with the residual strength is usually described through the linear Mohr-Coulomb criterion, characterised by a friction angle and null cohesion (e.g. Alonso and Gens, 2006). Nevertheless, the peak and post-rupture strength envelopes may show some curvature. For example, Fig. 2.12 shows the peak strength envelope of an Opalinus clay from Amann et al. (2012). It can be observed that, for confinement stresses in excess of 1.0 MPa, the strength envelope can be fitted by Mohr-Coulomb linear criterion, with a relatively high cohesion intercept. However, for lower confinements, the strength envelope shows a notorious curvature. It suggest that the cohesion estimated under high normal stress with a linear criterion over-estimates material true cohesion and tensile strength.
2.3.3 Yield surface

In the context of plasticity theory, the yield function (Eq. 2.3) defines the boundary between pure elastic and elastoplastic response in the stress space. The elastoplastic response includes essentially two main types of irreversible mechanisms, one related to the collapse of inter-particle pores under compressive loading, and the second to failure under deviatoric load or tension. In terms of modelling, two possibilities emerge: 1) to consider a single yield function that indistinctively defines the onset of plastic response due to both mechanism (Fig. 2.13a), or 2) to assign separate yield functions to each mechanism (Fig. 2.13b).

The first type of model is well illustrated by the modified Cam Clay (MCC) elastoplastic law (Roscoe and Burland, 1968), sometimes used to model structured argillaceous materials (Baudet and Stallebrass, 2004; Kavvadas and Amorosi, 2000; Liu and Carter, 2002; Rouainia and Muir wood, 2000). The model is characterised by an elliptical yield function in the $p - q$ plane (Fig. 2.13a) that intersects the mean effective axis at the value of the isotropic pre-consolidation pressure, and whose shape is controlled by the CSL. This original shape was developed essentially for soft deposits and soils reconstituted in the laboratory, and can significantly differ from yield surfaces identified for argillaceous natural deposits. Other single function have been alternatively proposed on the basis of MCC concept (McDowell and Hau, 2004; Yu, 1998), that presented a better agreement with experimental data obtained
in natural materials. An example is depicted in Fig. 2.14, where the yield surfaces from the MCC and from McDowell and Hau (2004) are compared with experimental results of Boom clay.

![Figure 2.14: Yield surface of natural Boom clay (Hong et al., 2016).]

The second type of model is based on the well-established theory of non-smooth multisurface plasticity (Simo and Hughes, 1998), and allows assigning different yield surface to volumetric, shear, and sometimes tensile plastic mechanism. For example, Galavi and Schweiger (2009) proposed a model for structured clayey materials based on the multilaminate framework. Three independent yield functions were employed (Fig. 2.13b), each one related to plastic processes under deviatoric ($f_d$), compressive ($f_c$), and tension ($f_t$) loading respectively. However, depending on the problem under consideration, not all the surfaces are necessarily activated, and it is possible to disregard some of them in specific applications. For example, in the case of deep underground excavations in stiff argillaceous materials, high increases in the mean stress are not likely to occur, but import deviatoric and tensile stresses are expected. In this case, the yield surface for compressive loading (e.g. $f_c$ in Fig. 2.13b) can be omitted.

A first approximation of the yield function for argillaceous natural materials under deviatoric loading is the Mohr-Coulomb criterion (e.g. Galavi and Schweiger, 2009; Mánica et al., 2017c), which draws a cone in the principal stress space with a hexagonal cross-section in the deviatoric plane (Fig. 2.15). This type of criterion possesses corners and an apex where gradients are not defined, which requires specific numerical implementation. A possibility is to smooth the corners, following e.g. Sloan and Booker (1986) procedure. In any case, as previously mentioned, this criterion tends to over-estimate the strength for low confinement pressures. A possible remedy is to consider an additional tension cut-off criterion that bounds the elastic zone at low stresses (e.g. Galavi and Schweiger, 2009; Mollon et al., 2011).

Another alternative is to work with yield criteria having non-linear shapes in the Mohr plane. Among this kind, a salient example is that of Hoek and Brown (1980), which has been widely employed to characterise the strength characteristics of brittle rocks (Hoek and Brown, 1997; Ramamurthy, 2001). As already shown in Fig. 2.12, this criterion can adequately reproduce the observed curvature of the strength envelopes of argillaceous rocks,
and predicts reasonable tensile strengths. Corners and an apex are also present, which can also be smoothed (Wan, 1992). Another possibility is to employ a hyperbolic approximation of the Mohr-Coulomb criterion (e.g. Abbo and Sloan, 1995). The criterion is asymptotic to the Mohr-Coulomb envelope for high stress (Fig. 2.16), which allows keeping the friction angle and the cohesion as model parameters, and provides the criterion with strong physical meaning. At low stress, the criterion departs from the Mohr-Coulomb envelope, and intercept the horizontal axis at the value of the tensile strength, considered as an independent parameter. The curvature of the yield function at low confinement can thus be controlled by the cohesion and the tensile strength.

![Figure 2.15: Mohr-Coulomb criterion (a) in the principal stress space and (b) in the deviatoric plane.](image)

**Figure 2.15:** Mohr-Coulomb criterion (a) in the principal stress space and (b) in the deviatoric plane.

![Figure 2.16: Hyperbolic approximation of the Mohr-Coulomb yield function (Abbo and Sloan, 1995).](image)

**Figure 2.16:** Hyperbolic approximation of the Mohr-Coulomb yield function (Abbo and Sloan, 1995).

In the case of compressive loading, elliptical functions has also been employed to independently characterise this yielding mechanism, although sometimes shifted to the left, with the centre of the ellipse coinciding with the stress origin in the \( p - q \) plane (e.g. Galavi and Schweiger, 2009; Schanz et al., 1999]). Parabolic functions has also been proposed to bound the permitted stress space for compressive loading (Resende and Martin, 1985).

### 2.3.4 Degradation and softening

From a general point of view, degradation and softening are often linked to the loss of material structuration. A simple conceptual approach to model structured geomaterials consists in
considering a yield surface that depends both on material density and structuration through a *bonding parameter* (Gens and Nova, 1993). This surface is larger than the yield surface of the destructured material, which open the possibility for the stress state to be outside the admissible destructured stress zone. When the stress state reaches the structured yield envelope, plastic strains develop, causing degradation and breakage of interparticle bonds, and a decrease of the bonding parameter. During this process, the yield surface shrinks towards the destructured envelope, while the latter shrinks or expands depending on the changes in the material density. The mechanism controlling yield changes is formally known as *strain hardening* (without making distinction if the surface is shrinking, expanding, or moving in the stress space), and it is included in the plastic theory through the dependency of the yield function with $\chi$ (Eq. 2.3), and through the dependency of $\chi$ with the plastic strains (Eq. 2.5). This straightforward approach has given rise to several constitutive models with varying degrees of complexity, and accounting for quite a number of significant features of structured geomaterials.

A relatively simple example is the MCC model enriched by several parameters describing the effects of structure (Li and Dafalias, 2002). More complex models have been alternatively developed by Kavvadas and Amorosi (2000), Rouainia and Muir wood (2000), Gajo and Muir Wood (2001), and Baudet and Stallebrass (2004) within the framework of bounding plasticity, pioneered by Dafalias and Popov (1977). As an example, Fig. 2.17 presents the yield surfaces considered in Rouainia & Muir Wood’s model. It consists of a small yield surface, usually called *bubble*, bounding the elastic region in the $p – q$ diagram. According to a kinematic hardening rule, this surface can move within a larger *bounding* surface, which contains information about the current magnitude of structuration. As plastic strains accumulate, this latter surface tends to collapse towards a third surface, representing the yield of the destructured material and generally controlled by a volumetric softening rule. This kind of models allows to naturally take into account the effect of structuration for both compressive and deviatoric stress paths.

![Figure 2.17: A bounding plasticity model for structured clays (Rouainia and Muir wood, 2000).](image)

Another alternative is to link the evolution of the destructuration process to the evolution of the strength parameters, as suggested by the conceptual scheme previously described in Fig. 2.9. In this type of framework, compressive and deviatoric yield mechanism have been usually accounted separately (Galavi and Schweiger, 2009). Some models also keep only the deviatoric part, if yielding by compressive loading is not expected (Mánica et al., 2017c;
According to this approach, degradation and breakage of interparticle bonds are directly related to the loss of cohesion and tensile strength of the material.

### 2.3.5 Strain localisation

Another key control aspect of softening and shear failure of shales is the process of strain localisation and fracture propagation. As already mentioned, shale rocks fail in a quasi-brittle manner under deviatoric loading after reaching the peak strength. The resulting strain field is generally not homogeneous and deformations tend to localise into thin zones of intense shearing, in the form of shear bands or fractures (Fig. 2.18). This phenomenon is known as strain localisation and challenges the validity of numerical models obtained using a constitutive law developed under the framework of continuum mechanics.

![Figure 2.18: Shale specimens after (a) unconfined compression and (b) triaxial compression test (Holt et al., 2015).](image)

When a boundary value problem (BVP) is solved using a constitutive model that accounts for softening behaviour, it is likely to obtained under certain conditions thin zones of localised plastic deformations. If no adequate techniques are used, the obtained results are not objective and will show a strong dependency on the mesh employed to discretise the problem. This pathology can be easily explained by considering the case of a one-dimensional bar under tension (Fig. 2.19a). The material obeys a linear elastic stress-strain relationship until the yield stress \( \sigma_y \), followed by linear softening behaviour up to zero (Fig. 2.19b). \( \epsilon_f \) is the strain value at which the strength is totally lost, \( \epsilon_o = \sigma_y/\sigma \) is the strain value at peak strength, and \( \sigma \) is the Young’s modulus. The bar is discretised in \( n \) elements of constant size, and we assumed that one of them is provided with a default that makes the yield stress slightly lower than in the other elements. If the bar is loaded, the response will be elastic and uniform in all the bar until the displacement reaches the value \( u_o = L\epsilon_o \) (Fig. 2.19c).
From this point, the element with slightly lower strength will soften following the stress-strain curve of Fig. 2.19b. During this process, due to equilibrium restrictions (the stress must be constant in the bar), all the other elements will unload elastically, since they had not reached the yield point. When the total failure is reached, the stress in the bar is null and all the adjacent elements have recover the deformation attained at the moment of bar yield. The total displacement computed at the extremity of the bar will be then governed only by the strain in the weak element \( u_f = L_e \epsilon_f \) (\( L_e \) is the length of the weak element). As a consequence, the total displacement depends on bar discretisation. By increasing the number of elements the displacements will decrease (Fig. 2.19c) and tend to zero for the case of a weak element of length zero. From a mathematical point of view, this pathology is related with the so-called loss of ellipticity of the governing differential equations, making the BVP ill-posed.

\[
\begin{align*}
\text{Figure 2.19: (a) Bar under tension, (b) stress-strain behaviour of the material, and (c) force-displacement response.}
\end{align*}
\]

Different methods exist to prevent such pathological response while conserving the framework of continuum mechanics, usually known as regularisation techniques. They return the objectivity to the BVP and avoid the dependency on the employed mesh. Among these techniques, we can highlight,

- The use of micropolar continuum (Cosserat and Cosserat, 1909).
- Adaptive mesh techniques (Deb, 1996; Ortiz and Quigley, 1991; Zienkiewicz and Huang, 1995).
- Viscoplastic models (Loret and Prevost, 1990; Oka et al., 1995; Prevost and Loret, 1990).
- The weak discontinuity approach (Ortiz et al., 1987).
- The strong discontinuity approach (Armero and Garikipati, 1996; Oliver, 1996a,b; Oliver et al., 2002; Regueiro and Borja, 2001).
- Strain gradient models (Aifantis, 1992; Mühlhaus and Alfantis, 1991).
- Nonlocal models (Bažant and Jirásek, 2002; Bažant and Pijaudier-Cabot, 1988; Jirásek, 1998).

All regularisation techniques have in common to incorporate a length scale to the material behaviour, which controls the size of the localised zone and avoids the dependency of the employed mesh. They must be employed to simulate strain localisation processes in shale rocks.
2.4 Material anisotropy

It has long been recognised that geomaterials may exhibit anisotropic behaviour (Donath, 1964; Ladd and Varallyay, 1965; McLamore and Gray, 1967), whose origin has been related to different sources such as deposition processes (Oda and Nakayama, 1989), tectonic processes (Amadei, 1996), loading history (Li and Yu, 2009) and fabric (Anandarajah, 2000), among others. Anisotropy can be generally observed in properties such as stiffness, strength or permeability. In shale rocks, it is essentially related to the process of sedimentation and compaction, which results in an oriented structure controlled by bedding planes and fissility. As a consequence, two main directions of anisotropy (parallel and orthogonal to the bedding plane) are generally identified and modelled in the framework of transverse isotropy (or cross-anisotropy). The degree of anisotropy has been been often related to the compaction process, due to both porosity reduction and smectite-to-illite transformation with diagenesis (Vernik and Liu, 1997), although micro-cracks and kerogen content may also play a role (Carcione, 2000; Vernik and Liu, 1997).

2.4.1 Stiffness anisotropy

Stiffness anisotropy in shale rocks has been usually assessed indirectly through its seismic velocity anisotropy (Vernik and Liu, 1997). Anisotropy can be inferred from field seismic measurements by considering the non-hyperbolic moveout of wave reflection (Alkhalifah, 1997), or in laboratory through multi- (Hornby, 1998) or single-core methods (Wang, 2002a,b). Direct stiffness measurements have also been reported (Niandou et al., 1997; Valès et al., 2004). In general, measurements indicate a marked tendency for higher stiffness (or wave velocities) in the direction parallel to the bedding planes than perpendicular thereto. In Fig. 2.20, Sayers (2013) collected data of various shales from the literature where the relationship between the Young’s moduli perpendicular and parallel to bedding is shown, and where the mentioned tendency is clearly identified.

Figure 2.20: Perpendicular versus parallel Young’s modulus of various shales (modified from Sayers, 2013).
In the most general case, stiffness anisotropy is incorporated in the elastoplastic framework by means of the generalised Hooke’s law. It expresses the elastic stiffness matrix (Eq. 2.2) as a function of 21 parameters. However, for many common situations, it is sufficient to consider that shale rocks exhibit transverse isotropy, which reduces the number of elastic constants to five. The stiffness matrix of transverse isotropic linear elastic materials can be found in the literature (e.g. Graham and Houlsby, 1983; Lings, 2001; Lings et al., 2000; Love, 1927; Pickering, 1970; Raymond, 1970; Wittke, 1990). It can be for instance written as,

$$D^e = \begin{bmatrix}
E_1 \frac{1 - \bar{n} \nu_2^2}{(1 + \nu_1) \bar{m}} & E_1 \frac{\nu_1 + \bar{n} \nu_2^2}{(1 + \nu_1) \bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\
E_1 \frac{\nu_1 + \bar{n} \nu_2^2}{(1 + \nu_1) \bar{m}} & E_1 \frac{1 - \bar{n} \nu_2^2}{(1 + \nu_1) \bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\
E_1 \frac{\nu_2}{\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & E_2 \frac{1 - \nu_1}{\bar{m}} & 0 & 0 & 0 \\
0 & 0 & 0 & E_1 & 0 & 0 \\
0 & 0 & 0 & 0 & 2(1 + \nu_1) & G_2 \\
0 & 0 & 0 & 0 & 0 & G_2
\end{bmatrix}$$

(2.10)

where $\bar{n} = E_1/E_2$, $\bar{m} = 1 - \nu_1 - 2\bar{n} \nu_2^2$ and $E_1$ $E_2$ $\nu_1$ $\nu_2$ $G_2$ are the five independent elastic constants defined in Fig. 2.21. The inverse relationship provides the elastic compliance $C$, that relates the strain vector to the stress vector. It is expressed as,

$$C = \begin{bmatrix}
1 & -\frac{\nu_1}{E_1} & -\frac{\nu_2}{E_2} & 0 & 0 & 0 \\
-\frac{\nu_1}{E_1} & \frac{1}{E_1} & \frac{\nu_2}{E_2} & 0 & 0 & 0 \\
-\frac{\nu_2}{E_2} & -\frac{\nu_2}{E_2} & \frac{1}{E_2} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{2(1 + \nu_1)}{E_1} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_2} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{G_2}
\end{bmatrix}$$

(2.11)

Love (1927), Pickering (1970) and Raymond (1970), among others, derived relationships and thermodynamic constrains between the different parameters. A comprehensive overview of these works can be found in Lings (2001). $E_1$, $E_2$, $\nu_1$ and $\nu_2$ were found to be strongly related and $G_2$ to be almost independent. Pickering (1970) showed that the requirement to have positive strain energy is equivalent to impose that $E_1$, $E_2$ and $G_2$ are all $\geq 0$, which leads to,

$$-1 \leq \nu_1 \leq 1$$

(2.12)

and

$$\frac{E_2}{E_1} (1 - \nu_1) - 2\nu_2^2 \geq 0$$

(2.13)
Raymond (1970) also found an upper bound for $G_2$ modulus,

$$G_2 \leq \frac{E_2}{\nu_2(1 + \nu_1) + \sqrt{(1 - \nu_2^2)(1 - \bar{n}\nu_2^2)}}$$  \hspace{1cm} (2.14)

This inequality was derived from the analytical solution for the stress-state below a point load (Barden, 1963), noting that the strain energy had to be positive and that all stresses had real values.

Figure 2.21: Definition of elastic constants for the case of transverse isotropy (Wittke, 1990).

In situations with non-horizontal bedding planes (e.g., due to tectonic processes), the global coordinate system does not coincide with the orientation of the material. In this case, the stiffness matrix has to be mapped to the global system according to the equation,

$${\tilde{D}}^e = T^T D^e T$$  \hspace{1cm} (2.15)

where $T$ is a transformation matrix, whose coefficients will depend on how the transformation is described. An example of $T$ can be found in Wittke (1990).
2.4.2 Strength anisotropy

Data on the strength anisotropy of shale rocks are scarce, although this issue is currently gaining increasing attention, especially in relation with hydraulic fracturing issues. Anisotropy is usually assessed by conventional methods for strength determination (e.g. uniaxial compression or triaxial compression test) on samples trimmed with different bedding orientations (Cho et al., 2012; Niandou et al., 1997; Valès et al., 2004). Fig. 2.22 shows typical strength distributions in shale rocks, where the minimum strength is generally obtained for intermediate orientations between the loading and the bedding planes.

Anisotropic failure criteria have been in parallel developed and implemented in comprehensive constitutive models. One of the first anisotropic criterion was proposed by Hill (1948) for sheet metals. In the case of geomaterials, an early example is provided by Jaeger (1960), who introduced the single weakness plane theory, later applied by Hoek (1983). The theory assumes that failure occurs along a weakness plane, but the predicted strength is bounded by the strength of the intact material, assumed isotropic (Fig. 2.23). The physical interpretation behind this concept relies on the fact that failure will not occur along the weakness plane but across it if the strength in the plane is higher than in the intact material. This approach is essentially considered for jointed rocks, where the concept of intact rock has a clear meaning. This is not the case for many shales, where the spacing between discontinuities may be of the order or even smaller than few millimetres (Potter et al., 1980), which makes difficult the estimation of the isotropic strength in-between discontinuities. Moreover, the strength distributions predicted by the weakness plane theory seems to not accommodate the observed behaviour in shales (e.g. Fig. 2.22), where the strength continuously varies through all bedding orientations and differs for bedding orientations at 0 and 90°.

According to than, it seems more appropriate to assume that failure does not necessarily follow the bedding planes, but can develop in the mass of a material provided with anisotropic bulk strength (including bedding). Following this idea, a straightforward approach, valid for both elastoplastic and damage constitutive laws, consists in considering an anisotropic yield (and/or failure and/or damage) surface (Eq. 2.3).
as,

\[ f = (\sigma, \chi, \Theta) \]  

(2.16)

where \( \Theta \) is a measure (scalar or tensorial variable/s) of the relative orientations between loading and anisotropy directions. A number of anisotropic (usually cross-anisotropic) criteria of this kind have been proposed in the literature to enhance isotropic models. For example, Nova (1986a) modified the isotropic CCM by including in the yield criterion a fourth-order tensor with cross-anisotropy strength parameters. Another example is given by Abelev and Lade (2004), who extended the isotropic Lade’s (1977) criterion by applying a rotation to the stresses in the triaxial plane. The applicability of the model is however limited because of the assumption of coaxiality between stress and anisotropy principal directions. Another way consists in formulating the failure criterion in terms of scalar orientation parameters, which provides a way to link the loading direction and the anisotropy direction (Pietruszczak and Mroz, 2000, 2001). This technique has been further used by Lade (2008) to propose a new cross-anisotropic extension of his initial failure criterion (Lade, 1977). Anisotropic failure criteria may also be formulated on the basis of the concept of the spatial mobilised plane (SMP) (Matsuoka, 1974), where the criterion is defined as a function of the angle between the SMP and the depositional plane (Yao and Kong, 2012). Another alternative is to describe the material anisotropy through the second order fabric tensor, and to represent the material anisotropic state by a scalar variable defined by joint invariants of the stress tensor and the fabric tensor (Gao and Zhao, 2012; Gao et al., 2010; Li and Dafalias, 2002). Anisotropy has also been included through the rotation of the yield surface in the stress space (usually for elliptical surfaces). This approach presents the advantage to easily capture the strain-induced evolution of anisotropy by introducing a rotational hardening mechanism (Gajo and Muir Wood, 2001; Wheeler et al., 2003; Whittle and Kavvadas, 1994). More recently, Mánica et al. (2016b) proposed a general cross-anisotropic extension for elastoplastic models, based on a non-uniform scaling of the stress tensor. The fictitious scaled stress are employed to modify the yield criterion to account for cross anisotropy. The main advantage of this approach lies in the fact that it can be easily incorporated into an already implemented isotropic model with only minor modifications.

![Figure 2.23: Strength predicted by the single weakness plane theory (Hoek, 1983).](image-url)
The different strategies to model anisotropic yield and failure criteria have been generally validated on laboratory data, and some examples are given in Fig. 2.24. Nevertheless, they have not always been implemented in software able to solve BVPs of real engineering situations. An example of such modelling can be found in relation with the experimental drifts in the Meuse/Haute-Marne (MHM) Underground Research Laboratory (URL), excavated in the Callovo-Oxfordian claystone formation (Armand et al., 2013). Detailed field monitoring has revealed that the excavation process induces damage in the surrounding rock and is associated with the development of extensional and shear fracture networks (Armand et al., 2014). In the case of drifts excavated parallel to the major horizontal stress, the in situ stresses in the plane orthogonal to the tunnel axis are reported as nearly isotropic. However, the damage zone extends significantly more in the horizontal than in the vertical direction (Fig. 2.25a). Larger horizontal converges are also observed, that suggest strong anisotropy characteristics of the rock mass. Mánica et al. (2017c) extended consequently an isotropic constitutive model to include strength cross-anisotropy in the simulation. The model was able to capture the main trends of behaviour, particularly its capability to reproduce asymmetrical plastic zone configurations (Fig. 2.25b) by considering the anisotropic characteristics of the rock mass, even in the presence of isotropic pre-excavation stress state.

![Figure 2.24](image-url)

Figure 2.24: Comparison between different anisotropic criteria and laboratory data from (a) Nova (1986b), (b) Gao et al. (2010), (c) Pietruszczak (2001) and (d) Mánica et al. (2016b).
2.4.3 Permeability anisotropy

The microstructural features of shale rocks may also result in anisotropy of permeability. In general, observations show that the permeability measured parallel to bedding is higher that the one measured perpendicular thereto (Bhandari et al., 2015; Kwon et al., 2004). This kind of anisotropy can be incorporated in the numerical formulation by considering that liquid (or gas) advective fluxes are governed by the generalised Darcy’s law,

$$ q_\alpha = -\frac{k_\alpha k_{\text{rel}}}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g_\alpha) \quad \alpha = l, g_p $$

(2.17)

where $q$ is the fluid flux, $k$ is the tensor of intrinsic permeability, $k_{\text{rel}}$ is the relative permeability of the fluid, $\mu_\alpha$ is the dynamic viscosity of the fluid, $p_\alpha$ is the pressure of the fluid, $\rho_\alpha$ is the density of the fluid, $g$ is the vector of gravity forces, and $l$ and $g_p$ refer to liquid and gas phases respectively.

Assuming that the direction parallel and perpendicular to bedding as principals directions, the tensor of intrinsic permeability reads,

$$ k = \begin{bmatrix} k_h & 0 & 0 \\ 0 & k_h & 0 \\ 0 & 0 & k_v \end{bmatrix} $$

(2.18)

where the $h$ and $v$ are the orientations parallel and orthogonal to the global coordinate system, respectively. In case of non-horizontal bedding planes, the tensor has to be mapped to the target coordinate by use of Eq. (2.15).

An example of this kind of formulations can be found in Olivella et al. (1994), which has been employed by Arnedo et al. (2013) to simulate gas flow through an anisotropic claystone.

2.5 Time-dependent behaviour

As many other geomaterials, shale rocks exhibit time-dependent phenomena, such as creep deformations (Sone and Zoback, 2014), stress relaxation (Olsson, 1980), and rate effects (Swan et al., 1989). Moreover, because of their low permeability these materials are suscept-
ible to experience excess pore fluid pressure under loading, whose further dissipation traduces into time-dependent changes in stress and strains. This process, often called consolidation, is however generally not considered as an intrinsic time-dependent phenomenon of the material. Whatever are the processes involved, the correct characterisation of the time-dependent behaviour of shale is a fundamental aspect for the long-term design of engineering works.

Creep deformations in shale rocks are generally studied by means of constant load test performed under uniaxial (Mishra and Verma, 2015), triaxial (Sone and Zoback, 2014) or laterally constrained (oedometer) (Powell et al., 2012) conditions, and involving single or multiple load steps. Fig. 2.26 depicts results from a multistep triaxial creep test carried out on Haynesville shale. They evidence a typical response, characterised by an initial instantaneous response upon loading, followed by a gentle accumulation of strains. The strain rate is high at the early stage of load application, and decreases then rapidly to null or very low values. The magnitude of the strain rate typically increases with the level of deviatoric stresses (Sone and Zoback, 2014). When the deviatoric stress is high enough, it is often reported that creep strain increases again after some time, and the sample reaches failure (Fabre and Pellet, 2006). It seems that shales present creep responses in agreement with the usual distinction between primary, secondary and tertiary stages (Mitchell, 1993). In addition to the effect of stress level, several authors have identified creep dependency on temperature (Eseme et al., 2007).

![Figure 2.26: Triaxial creep test on Haynesville shale (Sone and Zoback, 2014).](image-url)

Rate effects appears to be also an important phenomena in shale rocks. Fig. 2.27 shows results in undrained triaxial test conducted at different strain rates by Swan et al. (1989). The effect of strain rate on the deviatoric stress and axial strain at peak appears to be small up to a value close to 0.1min$^{-1}$, but increases rapidly for rates above this threshold. The authors reported that the change in rate effect is related to the switch from one deformation mechanism involving macroscopic failure plane formation at low rates, to another involving distributed shear micro-cracking at high rates.
Figure 2.27: Influence of axial strain rate on (a) peak deviatoric stress and (b) axial strain at peak for undrained triaxial test Swan et al. (1989).

Several models can be found in the literature to capture time-dependent characteristics of geomaterials. A comprehensive review can be found in Liingaard et al. (2004), who proposed the following classification,

- **Empirical models** are mainly obtained by fitting experimental results. The constitutive relationships are usually given by closed-form solutions or differential equations, and they are restricted to specific boundary and loading conditions.

- **Rheological models** describe uniaxial conditions. They are given in closed-form solutions or in a differential form, and are often used to obtain a conceptual understanding of time-dependent processes.

- **General stress-strain-time models** are three-dimensional models. They are often given in incremental form, and are not limited to the boundary conditions from which they were calibrated. This kind of models are readily adaptable to numerical implementation.

In the perspective of numerical modelling, the latter category is the one of greater interest. Some salient examples of this kind of constitutive models are described below.

### 2.5.1 Viscoplasticity

The viscoplasticity theory, also known as **Perzyna’s (1966) overstress theory**, has been frequently applied to reproduce time-dependent effects of geomaterials (Desai et al., 1995; Katona and Mulert, 1984; Malan, 1999; Yin et al., 2010). As in the classical theory of plasticity, an additive decomposition of strains is considered,

$$
\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^{vp}
$$

where $\dot{\varepsilon}$ is the total strain rate tensor, $\dot{\varepsilon}^e$ is the elastic strain rate tensor, and $\dot{\varepsilon}^{vp}$ is the viscoplastic strain rate tensor. The elastic component is assumed to obey the generalised
Hooke’s law and the viscoplastic component is computed through,

$$\dot{\epsilon}_{vp} = \frac{1}{\eta_{p\pi}} \langle \Phi(f) \rangle \frac{\partial g}{\partial \sigma}$$  \hspace{1cm} (2.20)

where $\eta_{p\pi}$ is the viscosity parameter, $\Phi$ is the overstress function that depends on the rate-independent yield function, and $\langle \rangle$ are the McCauley brackets such that,

$$\langle \Phi(f) \rangle = \begin{cases} 
\Phi(f) & \text{if } \Phi(f) \geq 0 \\
0 & \text{if } \Phi(f) < 0 
\end{cases}$$  \hspace{1cm} (2.21)

A widely-used expression for the overstress function is,

$$\Phi(f) = \left( \frac{f}{f_o} \right)^N$$  \hspace{1cm} (2.22)

where $f_o$ is a reference normalisation stress, and $N$ is a parameter that should satisfy $N \geq 1$ (Simo, 1989) and defines the order of the Perzyna’s viscoplasticity.

Unlike the plasticity theory, the overstress theory allows the stress state to lie above the rate-independent yield surface (Fig. 2.28). An expression for the rate-dependent yield function can be derived (Heeres et al., 2002),

$$f_{rd} = f - \left( \Phi^{-1} \eta_{p\pi} \dot{\lambda} \right)$$  \hspace{1cm} (2.23)

where $f_{rd}$ is the rate-dependent yield surface and the term in parenthesis represents the distance between both surfaces. The higher is the loading rate with respect to the viscosity parameter, the higher would be the distance. As a consequence, the overstress theory can naturally reproduce the strength increase observed in shale rocks due to the increase in the loading rate (Fig. 2.27).

This approach presents the advantage to readily extend rate-independent elastoplastic models to viscoplastic models, but suffers from its inability to capture long-term constant creep rate under constant load. In fact, as time advances and plastic strains accumulate, the

![Figure 2.28: The overstress theory (Perzyna, 1966).](image-url)
distance between viscoplastic and purely plastic yield surfaces vanishes, and the strain rate tends to a null value.

2.5.2 Plasticity - creep partition

Another type of constitutive relationship can be obtained considering two independent inelastic strain components,

\[ \dot{\varepsilon} = \dot{\varepsilon}^p + \dot{\varepsilon}^c \]  

(2.24)

where \( \dot{\varepsilon}^p \) is the standard rate-independent plastic strain increment and \( \dot{\varepsilon}^c \) represents an additional time-dependent strain increment, most of the time associated with creep.

This kind of models are commonly employed in metals to describe plasticity and creep phenomena simultaneously (Contesti and Cailletaud, 1989; Kawai and Ohashi, 1987; Murakami and Ohno, 1982; Pugh, 1983), and they are often referred as superposition models (Tirpitz and Schwesig, 1992). Although less exploited, this approach has also been applied for geomaterials (Borja and Kavazanjian, 1985; Mánica et al., 2017c; Souley et al., 2011). The main difference among models of this kind relies on the computation of \( \dot{\varepsilon}^c \). For instance, Borja and Kavazanjian (1985) compute it using the flow rule of the rate-independent plastic part of the model,

\[ \dot{\varepsilon}^c = \Gamma \frac{\partial f}{\partial \sigma} \]  

(2.25)

Nevertheless, \( \Gamma \) is not the usual plastic multiplier, but is another type of proportionality factor characterised using either the \( C_\alpha \) creep law or the Singh and Mitchell (1968) creep equation.

Another possibility is provided by Mánica et al. (2017c). In this case, \( \dot{\varepsilon}^c \) is computed from a modified form of the Lemaitre’s (1971) law. This model has been successfully employed to reproduce long-term triaxial creep test in an argillaceous rock (Fig. 2.29a), as well as the long-term behaviour of one of the drifts in the MHM URL (2.29b)). It worth noting that rate effects were not included in this formulation.

Figure 2.29: Simulation results of (a) triaxial creep tests and (b) of an underground excavation in Callovo-Oxfordian claystone from Mánica et al. (2017c).
2.5.3 Viscoplasticity - creep partition

Advantages of the over-stress theory and the plasticity-creep partitions can be combined by replacing the plastic strain in the strain partition,

$$\dot{\varepsilon} = \dot{\varepsilon}^p + \dot{\varepsilon}^c$$ (2.26)

where $\dot{\varepsilon}^p$ is the viscoplastic strain computed according to the Perzyna’s (1966) overstress theory, and $\dot{\varepsilon}^c$ is an independent strain component associated with creep mechanism. In this way, long-term creep and rate dependency and viscous effects can be simultaneously reproduced. An example of this combined approach can be found in Alonso et al. (2005), who used it to assess the long term behaviour of Beliche Dam. The combined model has been particularly applied to model the time-dependent response of rockfill shoulders, made of light compacted fractured schists and compacted greywacke.

2.6 Conclusions

The material presented in this chapter highlights that the theory of elastoplasticity encompasses presently extended mathematical formulations able to provide tools for modelling many aspects of the mechanical shale behaviour. One can particularly emphasise,

- The consideration of structuration parameters that degrade with plastic strain as a simple way to model strain-softening in structured geomaterials.
- The combination of anisotropic elasticity with yield surfaces whose parameters depend on the relative orientation between loading and anisotropic directions as a strategy to approach the complexity of anisotropic response of shales.
- The combination of creep and rate dependent yield surfaces as a tool to capture time-dependent responses.
- The consideration of anisotropic permeability tensor to further inquire into complex coupled hydro-mechanical responses of shales and soft argillaceous rocks.

Models able to integrate all these elements in a comprehensive manner are now in development, and it could be reasonably expected that they would provide at relatively short-term a consolidated framework to model shale as a continuum. These types of models present the advantage to be suitable for implementation in numerical codes, at the price of including strong non-linearities in the computations.

Other aspects of shale behaviour like degradation in presence of water, brittle failure, fissuration, fracture generation, and its effects on hydraulic properties would require coupling the pure mechanical elastoplastic framework with other continuum or discrete approaches, either at the macroscopic level or across several material scales. In this line, there are an increasing number of recent works based on coupled damage-elastoplastic frameworks (Le Pense et al., 2016; Zhu et al., 2016), multi-scale models (Xu et al., 2017; among others) or composite damage-elastoplastic models (Pinyol et al., 2007). When put in the perspective of works aiming at unifying damage and fracture mechanics (see introduction), the possibility of developing models covering the full rock-soil transitional behaviour of shale can be eventually contemplated at long-term.
Chapter 3

A cross-anisotropic formulation for elasto-plastic models

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Abstract

A cross-anisotropic formulation for elasto-plastic constitutive models based on a non-uniform scaling of the stress tensor is described. Taking advantage of the material symmetries characterising cross-anisotropy, only two scaling factors, one for the normal stress components and one for the shear stress components, are required. It is shown that the formulation can be easily introduced in already implemented models with minor modifications. The performance of this formulation is investigated by reproducing the strength variation of anisotropic rocks in triaxial tests. The numerical simulation of an unsupported excavation is also presented to show the effect of different scaling factors and bedding plane orientations.

3.1 Introduction

It has long been recognised that the behaviour of the geo-materials and their strength, in particular, depends on the loading direction (e.g. Ladd and Varallyay, 1965; McLamore and Gray, 1967). The origin of this anisotropy has been related to different sources such as deposition processes (Oda and Nakayama, 1989), tectonic processes (Amadei, 1996), loading history (Li and Yu, 2009) and fabric (Anandarajah, 2000). The effect of anisotropy in tunnelling works has been recently clearly demonstrated during the construction of drifts in the Meuse/Haute-Marne Underground Research Laboratory, that were excavated in the Callovo-Oxfordian claystone formation (Armand et al., 2013). Detailed field monitoring has revealed that the excavation process induces damage in the surrounding rock, and is associated with the appearance of extensional and shear fracture networks (Armand et al., 2014). In the case of drifts excavated parallel to the major horizontal stress, the *in-situ* stresses in the plane orthogonal to the tunnel axis are reported as nearly isotropic. However, the damaged zone extends significantly more in the horizontal than in the vertical direction.
(Fig. 3.1). Larger horizontal convergences are also observed that suggest strong anisotropy characteristics of the rock mass.

Figure 3.1: Cross-section damaged zone observed around a drift excavated under a quasi-isotropic stress state (Armand et al., 2014).

A number of anisotropic failure criteria have been developed; an early example is that of Hill (1948) for metals. For geomaterials, Nova (1986b) modified the Cam Clay isotropic model by including a fourth-order tensor in the yield criterion, the coefficients of which account for cross-anisotropic material strength. A different approach was proposed by Abelev and Lade (2004), for the cross-anisotropic extension of the isotropic Lade’s (1977) criterion, based on the rotation of stresses in the triaxial plane. Coaxiality was assumed between the direction of anisotropy and the stress axes; therefore, performance is limited to these conditions. Another way to consider anisotropy is by formulating the failure criterion in terms of scalar orientation parameters, that provide a way to link the loading direction with the anisotropy direction (Pietruszczak and Mroz, 2000, 2001). Following this approach, Lade (2008) proposed a different cross-anisotropic extension of his failure criterion (Lade, 1977). Anisotropic failure criteria may also be formulated based on the concept of spatial mobilised plane (SMP) (Matsuoka, 1974), where the criterion is defined as a function of the angle between the SMP and the depositional plane (Yao and Kong, 2012). Finally, another alternative is to describe the material anisotropy through a second-order tensor, the fabric tensor, and to represent the material anisotropic state with a scalar variable defined by joint invariants of the stress tensor and the fabric tensor (Li and Dafalias, 2002). Similar approaches have been employed by Gao et al. (2010) and Gao and Zhao (2012).

A different technique is presented here to incorporate anisotropy by way of a non-uniform scaling of the stress tensor. Stress tensor modification has also been proposed by Gajo and Muir Wood (2001) as a way to formulate hardening in an elegant and simple way; initial anisotropy is introduced through inclined bounding and yield surfaces. In the present paper, a non-uniform stress tensor scaling is used directly for the cross-anisotropic extension of an elasto-plastic constitutive model. This approach can be traced back to the Barlat (1991) anisotropic yield function for metals, where anisotropy was incorporated by transforming the deviatoric stress tensor through a series of factors controlling the anisotropic characteristics of the material.
A similar idea has been used here to incorporate inherent cross-anisotropy in any stress-based yield or strength criterion. The modified stress variables are only employed to change the yield and plastic potential functions; therefore, the elastic part is not affected. Elastic anisotropy can be incorporated independently, if desired, using a transverse anisotropic form of Hooke’s law. In some cases, it may be necessary to account for the evolution of anisotropy (Cudny and Vermeer, 2004; Dafalias, 1986; Nova, 1985; Wheeler et al., 2003). This can be achieved by varying the scaling factors in an appropriate manner. This issue, however, is not addressed in this paper.

Besides its simplicity, the main advantage of this approach lies in the fact that it can be easily incorporated into an already implemented isotropic constitutive model with only minor changes. To evaluate the performance of the formulation, results of triaxial tests carried out on specimens at different orientations have been matched using the proposed formulation. In addition, an unsupported deep underground excavation has been simulated to explore the capabilities of the cross-anisotropic model presented in a boundary value problem (BVP).

### 3.2 Isotropic elasto-plastic model

For completeness, the basic formulation of an isotropic elasto-plastic model is given here. Although the formulation can be equally applied to hardening plasticity models, a standard perfect plasticity model in the small strain range is used for simplicity. The conventional plasticity formulation can be expressed as follows:

- **elastic stress–strain relationship**
  \[
  \bar{\sigma} = D^e(\bar{\epsilon} - \bar{\epsilon}^p) \tag{3.1}
  \]

- **yield condition**
  \[
  f(\bar{\sigma}, \gamma) = 0 \tag{3.2}
  \]

- **flow rule**
  \[
  d\bar{\epsilon}^p = d\lambda \frac{\partial g}{\partial \bar{\sigma}} \tag{3.3}
  \]

- **and the loading/unloading conditions**
  \[
  d\lambda \geq 0, \quad f \leq 0, \quad d\lambda f = 0 \tag{3.4}
  \]

Here, \(\bar{\sigma}\) is the column matrix of independent stress components, \(D^e\) is the elastic stiffness matrix, \(\bar{\epsilon}\) is the column matrix of engineering total strain components, \(\bar{\epsilon}^p\) is the column matrix of engineering plastic strain components, \(f\) is the yield function, \(\gamma\) is a vector of material parameters, \(\lambda\) is the plastic multiplier and \(g\) is the plastic potential. For convenience, stress components can also be expressed in a second-order tensor format; in that format, the variable will not have the overbar (e.g. \(\sigma\)). In the following, the term stress always denotes effective stress.

Linearising the consistency condition \(df = 0\), the classical relationship relating stress and strain increments emerges,

\[
\begin{align*}
\dv{\bar{\sigma}} &= \left(D^e - \frac{D^e(\partial g/\partial \bar{\sigma})(\partial f/\partial \bar{\sigma})^T D^e}{(\partial f/\partial \bar{\sigma})^T D^e(\partial g/\partial \bar{\sigma})} \right)\dv{\bar{\epsilon}} = D^{ep}\dv{\bar{\epsilon}} \tag{3.5}
\end{align*}
\]
where $D^{\text{ep}}$ is the elasto-plastic constitutive matrix.

Isotropic elasto-plastic models are conveniently defined in terms of invariants and the following are often selected

$$p = \frac{1}{3}(\text{tr}\sigma) \quad (3.6)$$

$$J = \left(\frac{1}{2}\text{tr}s^2\right)^{1/2} \quad (3.7)$$

$$\theta = -\frac{1}{3}\sin^{-1}\left(\frac{3\sqrt{3}\det s}{2J^3}\right) \quad (3.8)$$

where $s$ is the deviatoric stress tensor, $s = \sigma - pI$. For instance, by using these variables, the Mohr–Coulomb yield criterion reads

$$f = \left(\cos\theta + \frac{1}{\sqrt{3}}\sin\theta\sin\phi\right)J - \sin\phi(p + cc\cot\phi) \quad (3.9)$$

where $\phi$ is the friction angle and $c$ is the cohesion. This expression results in a pyramid in the principal stress space, with a hexagonal cross-section in the deviatoric plane exhibiting a six-fold symmetry. This yield criterion is used subsequently in a perfect plastic model where it coincides with the failure criterion.

### 3.3 Cross-anisotropic formulation

As shown in Fig. 3.2a and 3.2b, axes $x$-$y$-$z$ represent the global coordinate system whereas axes 1–2–3 correspond to a local coordinate system aligned with the anisotropy axes. Stresses in the global coordinate system, $\sigma$, are transformed into the local system using the rotation matrix, $a$,

$$\sigma^i = a\sigma a^T \quad (3.10)$$

where $\sigma^i$ is the stress tensor in the local coordinate system. The rotation matrix is,

$$a = \begin{bmatrix} \cos\beta \cos\alpha & \sin\beta & -\cos\beta \sin\alpha \\ -\cos\alpha \sin\beta & \cos\beta & \sin\beta \sin\alpha \\ \sin\alpha & 0 & \sin\alpha \end{bmatrix} \quad (3.11)$$

where angles $\alpha$ and $\beta$ are indicated in Fig. 3.3.

![Figure 3.2: (a) Global coordinate system and (b) local coordinate system.](image)
The anisotropic stress tensor is obtained through the non-uniform scaling of the stress tensor oriented with the local coordinate system ($\sigma^r$),

$$
\sigma^{ani} = \begin{bmatrix}
    c_{11}\sigma_{11}^r & c_{12}\sigma_{12}^r & c_{13}\sigma_{13}^r \\
    c_{12}\sigma_{12}^r & c_{22}\sigma_{22}^r & c_{23}\sigma_{23}^r \\
    c_{13}\sigma_{13}^r & c_{23}\sigma_{23}^r & c_{33}\sigma_{33}^r
\end{bmatrix}
$$

(3.12)

where $c_{ij}$ are the scaling factors affecting each stress component. For an isotropic elastoplastic model defined in terms of stress invariants, the anisotropic formulation is obtained by simply replacing $pJ$ and $\theta$ in the failure criterion by $p^{ani}J^{ani}$ and $\theta^{ani}$, respectively, computed from the scaled stress tensor $\sigma^{ani}$.

Since cross-anisotropy is assumed in this paper, the scaling factors of the two normal stress components in the isotropic plane ($\sigma_{11}^r$ and $\sigma_{33}^r$) must be equal to obtain the same strength variation when rotating the anisotropy direction around $x$ or $z$ axes; therefore, $c_{11}$ must be equal to $c_{33}$. The same applies for the shear components $\sigma_{12}^r$ and $\sigma_{23}^r$, which leads to $c_{12} = c_{23}$. Moreover, it can be demonstrated that $c_{13}$ must be equal to 1.0, otherwise a variation of material behaviour would appear when a rotation around the anisotropy axis is applied. Finally, the following simplification is adopted using the fact that increasing $c_{22}$ produces an effect similar to reducing the other two normal stress scaling factors,

$$
c_{11} = \frac{1}{c_{22}}
$$

(3.13)

Therefore, only $c_{22}$ and $c_{12}$ are required to characterise the strength anisotropy of the material. In the following, they will be denoted as $c_N$ and $c_S$ to indicate that they are the normal and the shear scaling factors, respectively. Consequently, the scaled stress tensor takes the following form,

$$
\sigma^{ani} = \begin{bmatrix}
    \sigma_{11}^r & c_S\sigma_{12}^r & \sigma_{13}^r \\
    c_S\sigma_{12}^r & c_N\sigma_{22}^r & c_S\sigma_{23}^r \\
    \sigma_{13}^r & c_S\sigma_{23}^r & \frac{\sigma_{33}^r}{c_N}
\end{bmatrix}
$$

(3.14)

To examine the effect of stress scaling, the strength variation of a frictional material ($\phi = 30^\circ$) when rotated around the $z$ direction (i.e. $\alpha = 0$ and $\beta \neq 0$), is shown in Fig.
3.4.; the $y$ direction is the original anisotropy axis. In the left graph, $c_S$ is set equal to 1.0 and variations in $c_N$ are explored. In the right graph, $c_N$ is set equal to 1.0 and variations in $c_S$ are observed. It can be noted that $c_N$ controls the difference between the strengths of the material oriented orthogonal and parallel to the loading direction, whereas $c_S$ affects the strength for intermediate orientations.

Figure 3.4: Effect of stress scaling when rotating the anisotropy direction: (a) effect of variation of the normal scaling factor, $c_N$ and (b) effect of variation of the shear scaling factor, $c_S$.

The effect of the normal scaling factor on the yield surface can also be seen in principal stress space for the case in which global and local directions coincide, and the normal stress components are also principal values (Fig. 3.5). It can be observed that a reduction of the normal scaling factor causes an increase of strength for loading oriented along the anisotropy axis direction and vice-versa.

Figure 3.5: Effect of stress scaling on the yield surface plotted in principal stress space.

The strength response can be calibrated by selecting the scaling factors of the model that approximate the observed strength variation of the material. Some examples are shown.
in Fig. 3.6, where the presented formulation is used to fit the anisotropic response of three materials under triaxial loading. Fig. 3.6a shows results for a slate (Donath, 1964), Fig. 3.6b for a diatomite (Allirot and Boehler, 1979) and Fig. 3.6c for an Alaskan silt (Fleming and Duncan, 1990). In all three cases, a satisfactory match with the laboratory data is achieved.

When applying the resulting anisotropic model to BVPs, it is necessary to express the formulation within the global coordinate system. Applying the chain rule, the following
expressions for the gradients of the yield surface and the plastic potential are obtained,

\[ \frac{\partial f}{\partial \bar{\sigma}} = \left[ \left( \frac{\partial f}{\partial \bar{\sigma}^{ani}} \frac{\partial \bar{\sigma}}{\partial \bar{\sigma}^{ani}} + \frac{\partial f}{\partial J^{ani}} \frac{\partial J}{\partial \bar{\sigma}^{ani}} + \frac{\partial f}{\partial \theta^{ani}} \frac{\partial \theta}{\partial \bar{\sigma}^{ani}} \right)^{T} \right]^{T} \]  
\[ (3.15) \]

\[ \frac{\partial g}{\partial \bar{\sigma}} = \left[ \left( \frac{\partial g}{\partial \bar{\sigma}^{ani}} \frac{\partial \bar{\sigma}}{\partial \bar{\sigma}^{ani}} + \frac{\partial g}{\partial J^{ani}} \frac{\partial J}{\partial \bar{\sigma}^{ani}} + \frac{\partial g}{\partial \theta^{ani}} \frac{\partial \theta}{\partial \bar{\sigma}^{ani}} \right)^{T} \right]^{T} \]  
\[ (3.16) \]

where \( \bar{\sigma}^{ani} \) is the column matrix of independent components of the anisotropic stress tensor \( (\sigma^{ani}) \) and \( \frac{\partial \bar{\sigma}}{\partial \bar{\sigma}^{ani}} \) is a 6x6 Jacobian matrix containing the partial derivatives of the anisotropic stresses with respect to global stresses. The terms of \( \frac{\partial \bar{\sigma}^{ani}}{\partial \bar{\sigma}} \) are,

\[
\begin{bmatrix}
\cos^2 \beta \cos^2 \alpha & \sin^2 \beta & \cos^2 \beta \sin^2 \alpha & 2 \cos \beta \cos \alpha \sin \beta & 2 \cos^2 \beta \cos \alpha \sin \alpha & -2 \cos \beta \cos \alpha \sin \beta \\
-c_\beta \cos^2 \alpha \sin \beta & c_\beta \cos^2 \alpha & c_\beta \sin^2 \beta \sin^2 \alpha & -2 c_\beta \cos \beta \cos \alpha \sin \beta & 2 c_\beta \cos \beta \cos \alpha \sin \beta & -2 c_\beta \cos \beta \sin \beta \sin \alpha \\
\sin^2 \alpha & 0 & 0 & 2 \sin \beta \cos \alpha \sin \alpha & 2 \cos \beta \sin \alpha & 0 \\
-c_\beta \cos \beta \cos \alpha \sin \alpha & -c_\beta \cos \beta \cos \alpha \sin \alpha & -c_\beta \cos \beta \cos \alpha \sin \alpha & \cos \beta \cos^2 \alpha \cos \alpha & \cos \beta \sin \beta \sin \alpha & \cos \beta \sin \beta \sin \alpha \\
-c_\beta \cos \beta \sin \beta \sin \alpha & -c_\beta \cos \beta \sin \beta \sin \alpha & -c_\beta \cos \beta \sin \beta \sin \alpha & \cos \beta \sin^2 \alpha \cos \alpha & \cos \beta \sin \beta \sin \alpha & \cos \beta \sin \beta \sin \alpha \\
0 & c_\beta \cos \alpha \sin \beta \sin \alpha & -c_\beta \cos \alpha \sin \beta \sin \alpha & -c_\beta \cos \alpha \sin \beta \sin \alpha & \cos \beta \sin \beta \sin \alpha & \cos \beta \sin \beta \sin \alpha \\
\end{bmatrix}
\]

\[ (3.17) \]

If the model is formulated in terms of different invariants, Equations (3.15) and (3.16) should be modified accordingly; however, the definition of \( \frac{\partial \bar{\sigma}^{ani}}{\partial \bar{\sigma}} \) remains unchanged. It is also important to mention that the scaled stresses are only employed to evaluate the yield condition and the gradients of the yield function and plastic potential, used to define the plastic component of the model. Since the BVP is still solved in terms of unrotated and unscaled stresses, the anisotropy of the elastic behaviour of the model can be incorporated independently using a transverse anisotropic form of Hooke’s law.

### 3.4 Application to a BVP

Two-dimensional plain strain simulations of a circular unsupported deep underground excavation have been performed using the proposed cross-anisotropic model. The geometry of the problem and the spatial discretisation employed are depicted in Fig. 3.7, where the boundary conditions are also illustrated. An initial isotropic stress state is considered and the stress gradients due to gravity are neglected.

An elastic perfectly plastic constitutive model is used adopting the Mohr–Coulomb yield criterion of equation (3.9). Non-associativity is introduced in the definition of the flow rule through parameter \( \omega \),

\[ \frac{\partial f}{\partial \bar{\sigma}} = \left[ \left( \omega \frac{\partial f}{\partial \bar{\sigma}^{ani}} \frac{\partial \bar{\sigma}}{\partial \bar{\sigma}^{ani}} + \frac{\partial f}{\partial J^{ani}} \frac{\partial J}{\partial \bar{\sigma}^{ani}} + \frac{\partial f}{\partial \theta^{ani}} \frac{\partial \theta}{\partial \bar{\sigma}^{ani}} \right)^{T} \right]^{T} \]  
\[ (3.18) \]

The excavation process was simulated by reducing the tunnel boundary forces from the values corresponding to the initial \textit{in-situ} stresses to zero. Four analyses were performed adopting different scaling factors and different orientations of the anisotropy direction. The parameters used in these computations are listed in Table 3.1.
Table 3.1: Material parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>MPa</td>
<td>2000</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>Friction angle</td>
<td>$\phi$</td>
<td>$^\circ$</td>
<td>20</td>
</tr>
<tr>
<td>Cohesion</td>
<td>$c$</td>
<td>MPa</td>
<td>1.0</td>
</tr>
<tr>
<td>Non-associativity constant</td>
<td>$\omega$</td>
<td></td>
<td>0.7</td>
</tr>
<tr>
<td>Normal scaling factor</td>
<td>$c_N$</td>
<td></td>
<td>Variable</td>
</tr>
<tr>
<td>Shear scaling factor</td>
<td>$c_S$</td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>First rotation angle</td>
<td>$\alpha$</td>
<td>$^\circ$</td>
<td>0.0</td>
</tr>
<tr>
<td>Second rotation angle</td>
<td>$\beta$</td>
<td>$^\circ$</td>
<td>Variable</td>
</tr>
</tbody>
</table>

The extension and configuration of the plastic zone can be observed by plotting contours of the cumulative values of the plastic multiplier integrated over the complete simulation. Fig. 3.8 shows the directions of the major principal stresses close to the excavation wall before the appearance of plastic points. At a point close to the side-wall, the major principal stress is aligned with the vertical direction. If $\beta = 0^\circ$ and $\alpha = 0^\circ$, the major principal stress is perpendicular to the isotropic plane and therefore, an increase of the normal scaling factor will cause yielding at that point earlier. The results can be observed in Fig. 3.9a and 3.9b, where contours of cumulative plastic multiplier and total displacements are presented using a normal scaling factor of 1.4. In this case, the plastic zone extends more in the horizontal direction and it is associated with larger horizontal displacements. Fig. 3.9c and 3.9d represent the opposite situation, in which $c_N$ was reduced. As shown in Fig. 3.4, this causes an increase of the strength when loading is perpendicular to the isotropic plane or a reduction when loading is parallel. Therefore, yielding occurs earlier in points close to the top and bottom of the excavation, thus causing a plastic zone that extends more in the vertical direction.
CHAPTER 3

Major principal stress perpendicular to the isotropic plane
Major principal stress parallel to the isotropic plane
Horizontal isotropic plane for $\alpha = 0^\circ$ and $\beta = 0^\circ$

Figure 3.8: Major principal stress directions close to the excavation.

It is, of course, also possible to find situations where bedding planes are not horizontal (e.g. due to tectonic processes). Using the same formulation, the contour plots of the cumulative plastic multiplier and total displacements for two different orientations of the isotropic plane are shown in Fig. 3.10. The results are similar to those of Fig. 3.9, but they rotate, so that the larger size of the plastic zone and larger displacements remain parallel to the isotropic plane.

Figure 3.9: Cumulative plastic multiplier and total displacements contour plots for the anisotropic model considering the isotropic plane horizontal: (a) cumulative plastic multiplier ($c_N=1.4$, $c_S=1.0$); (b) total displacements ($c_N=1.4$, $c_S=1.0$); (c) cumulative plastic multiplier ($c_N=0.8$, $c_S=1.0$) and (d) total displacements ($c_N=0.8$, $c_S=1.0$).
3.5 Conclusions

In this paper, a simple formulation for the cross-anisotropic extension of an elasto-plastic constitutive model, based on a non-uniform scaling of the stress tensor, has been described. This concept can be applied to any stress-based yield/failure criterion, and its main advantage lies in the possibility of being incorporated to an already implemented isotropic constitutive model with only minor modifications.

The model has been able to match satisfactorily different published strength variations with loading orientation. An application to a BVP has demonstrated the ability of the formulation to obtain non-isotropic plastic zones and displacements in circular excavations with an isotropic initial stress state. Although only plane strain conditions have been examined, the formulation can be readily employed in a fully three-dimensional analysis, where the isotropic plane can have any orientation in the space. In addition to the two angles needed to define the orientation of the isotropic plane, only two scaling factors are required to define the cross-anisotropic characteristics of the material.
Chapter 4

A time-dependent anisotropic model for argillaceous rocks. Application to an underground excavation in Callovo-Oxfordian clayston

Based on the published manuscript of the following article:

Abstract

The paper presents a constitutive model for argillaceous rocks, developed within the framework of elastoplasticity, that includes a number of features that are relevant for a satisfactory description of their hydromechanical behaviour: anisotropy of strength and stiffness, behaviour nonlinearity and occurrence of plastic strains prior to peak strength, significant softening after peak, time-dependent creep deformations and permeability increase due to damage. Both saturated and unsaturated conditions are envisaged. The constitutive model is then applied to the simulation of triaxial and creep tests on Callovo-Oxfordian (COx) claystone. Although the main objective has been the simulation of the COx claystone behaviour, the model can be readily used for other argillaceous materials. The constitutive model developed is then applied, via a suitable coupled hydromechanical formulation, to the analysis of the excavation of a drift in the Meuse/Haute-Marne Underground Research Laboratory. The pattern of observed pore water pressures and displacements, as well as the shape and extent of the damaged zone, are generally satisfactorily reproduced. The relevance and importance of rock anisotropy and of the development of a damaged zone around the excavations are clearly demonstrated.
4.1 Introduction

Argillaceous rocks and stiff clay formations have great potential as possible geological host medium for radioactive waste. These materials have low permeability, significant retardation properties for radionuclide migration, no economic value (with the exception of gas or oil shales), and they often exhibit a significant capacity of hydraulic self-sealing of fractures (Gens, 2004, 2011). Therefore, a proper understanding and an appropriate modelling of their hydromechanical behaviour are of immediate interest. Although there are notable differences between different argillaceous formations (Gens, 2013; Jardine et al., 2015), reflecting their various origins and geological histories, there are also a number of common key features (e.g. time-dependent behaviour, anisotropy, some degree of softening, variation of permeability with damage) (Gens, 2013; Parry, 1972; Vitone et al., 2009; Wenk et al., 2008) that should be considered in any description of their behaviour.

There have already been quite a number of proposals of constitutive laws that incorporate one or more of those features listed above. From a macroscopic point of view models based on plasticity (Gens and Nova, 1993; Kavvadas and Amorosi, 2000; Liu and Carter, 2002; Nova et al., 2003; Rouainia and Muir wood, 2000; Souley et al., 2011; Suebsuk et al., 2010) or coupled damage-plasticity (Jia et al., 2010) have been widely employed. Also, combined micro- and macro-mechanical approaches have been recently applied via homogenisation techniques (Abou-Chakra Guéry et al., 2008; Huang et al., 2014). All of these models are capable of reproducing a post peak brittle behaviour and some of them also incorporate other features like time dependency (Huang et al., 2014; Souley et al., 2011).

The work presented in this paper has been developed in the context of the activities being carried out in the Meuse/Haute-Marne (MHM) Underground Research Laboratory (URL), located in Eastern France near the town of Bure, constructed and operated by the French national radioactive waste management agency (Andra). It consists of two shafts (an access shaft and a ventilation shaft) and a network of drifts, excavated at a depth of 490 m, in which several in situ experiments have been performed (Delay et al., 2007). The facility is excavated in Callovo-Oxfordian (COx) claystone, an argillaceous rock that has been intensively studied in recent years (Armand et al., 2017b); some reference properties are shown in Table 4.1. Laboratory studies have revealed, among others, the following features of behaviour:

- Anisotropy of strength and stiffness in the directions parallel and orthogonal to the bedding planes.
- Significant stress-strain nonlinearity and plastic strains prior to peak strength, with a yield limit identified at about 50% of the maximum deviatoric stress.
- A quasi-brittle behaviour at the in situ stress range, with a significant strength loss after the peak deviatoric stress.
- Creep deformations with increasing strain rates for higher deviatoric stresses.

In this paper, a constitutive model is described aimed to reproduce the main features of behaviour of the COx claystone as listed above. Specifically, it incorporates strength and stiffness anisotropy, nonlinear isotropic hardening to account for plastic deformations prior peak strength, softening behaviour after peak, a non-associated flow rule, time-dependent
deformations, and dependency of permeability on irreversible strains. Although the main objective has been the simulation of the behaviour of the COx claystone, the model can be readily applied to other argillaceous materials since they usually exhibit, as pointed out above, similar features of behaviour.

Table 4.1: Reference properties of the COx claystone (modified from Gens, 2013).

<table>
<thead>
<tr>
<th>Property</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry density (g/cm$^3$)</td>
<td>2.21 - 2.33</td>
</tr>
<tr>
<td>Porosity (%)</td>
<td>11 - 16</td>
</tr>
<tr>
<td>Water content (%)</td>
<td>&lt; 6.5</td>
</tr>
<tr>
<td>Liquid limit (%)</td>
<td>21 - 25</td>
</tr>
<tr>
<td>Plastic index (%)</td>
<td>11 - 19</td>
</tr>
<tr>
<td>Geological stage (millions years)</td>
<td>Callovo-Oxfordian 156-164</td>
</tr>
</tbody>
</table>

The constitutive law developed has then been applied to the simulation of an underground excavation in the MHM URL. The work has been developed in the context of the Transverse Action benchmark programme (Seyedi et al., 2017). Although all the calculations requested have been performed, for space reasons only the analysis corresponding to the hydromechanical modelling excavation of the GCS drift are reported here as it is the more fully instrumented case. Also, the GCS drift is aligned with the major horizontal principal stress resulting in a nearly isotropic stress state in the cross-section perpendicular to the axis of the opening. Thus, in this case, the effects of material anisotropy can be readily identified.

4.2 Hydromechanical constitutive model

Both saturated and unsaturated conditions have been considered in the development of the model. As shown later, consideration of unsaturated condition provides a more realistic setting for modelling laboratory tests. Also, potential desaturation of the rock during excavation can then be readily accommodated in the analysis, if necessary. To this end, a generalised effective stress expression has been adopted:

\[
\sigma' = \sigma + S_e s_u B I
\]  

(4.1)

where $\sigma'$ is the effective stress tensor, $\sigma$ is the total stress tensor, $S_e$ is the equivalent degree of saturation (defined below), $s_u$ is the suction, $B$ is the Biot’s coefficient and $I$ is the identity tensor. Naturally, for saturated conditions, Eq. (4.1) reduces to,

\[
\sigma' = \sigma - p_l B I
\]  

(4.2)

where liquid (water) pressure, $p_l$, is equated to $-s_u$.

From a number of experimental and in situ observations of COx claystone, two main deformation mechanisms can be identified: an instantaneous mechanism related to the immediate deformation due to changes in effective stress and a purely time-dependent response occurring under constant effective stress. Note that, the instantaneous response also includes the deformation caused by changes of effective stress associated with consolidation processes (i.e. hydromechanical coupling).
4.2.1 Instantaneous mechanism

The instantaneous response is described within the framework of elasto-plasticity because it provides a flexible platform to introduce the model features required to simulate the behaviour of argillaceous rock. Inside the yield surface, the response is assumed cross-anisotropic elastic, with a vertical symmetry axis. In this context, it is important to point out that when the term damage, is used in this paper, it refers to a state of the material and not to the concept associated with damage mechanics theory (e.g. Lemaitre, 1985).

At higher deviatoric stresses, plastic deformations develop. On reaching the yield surface, plastic strains accumulate, that are physically related to the development and growth of microcracks and they are modelled by hardening plasticity. Therefore, further loads can be sustained by the material until reaching the failure surface that represents the maximum strength of the material. From that point onwards, strength is gradually reduced to its residual value. This is related to the coalescence of microcracks into macrocracks and it is modelled through softening plasticity. The Mohr-Coulomb criterion is used for both yield and failure limits. In terms of stress invariants, this criterion is expressed by Eq. (4.3), which produces a cone in the principal stress space, with a hexagonal cross section in the deviatoric plane. Corners have been smoothed using Sloan and Booker (1986) procedure.

\[
f = \left( \cos \theta + \frac{1}{\sqrt{3}} \sin \theta \sin \phi \right) J - \sin \phi \left( c \cot \phi + p' \right) = 0 \quad (4.3)
\]

where \( \phi \) is the friction angle, \( c \) is the cohesion, and the remaining variables are stress invariants given by the following expressions,

\[
p' = \frac{1}{3} \left( \sigma'_{xx} + \sigma'_{yy} + \sigma'_{zz} \right) \quad (4.4a)
\]

\[
J = \left( \frac{1}{2} \text{tr} s^2 \right)^{1/2} \quad (4.4b)
\]

\[
\theta = -\frac{1}{3} \sin^{-1} \left( \frac{3 \sqrt{3} \det s}{2 J^3} \right) \quad (4.4c)
\]

where \( s \) is the deviatoric stress tensor \( s = \sigma' - p' I \).

The initial yield limit is denoted by using \( \phi_{ini} \) and \( c_{ini} \) in Eq. (4.3), which are material parameters. In the same way, the failure limit is obtained by replacing \( \phi \) and \( c \) by the peak values \( \phi_{peak} \) and \( c_{peak} \). Non-linear isotropic hardening is considered, driven by the evolution of the yield parameters. The equivalent plastic strain has been chosen as the state variable controlling this evolution, defined as,

\[
\epsilon_p^{eq} = \left( \frac{2}{3} \epsilon_p : \epsilon_p \right)^{1/2} \quad (4.5)
\]

where \( \epsilon_p \) is the plastic strain tensor.

The friction angle varies in a piecewise manner as shown in Fig. 4.1; the evolution laws corresponding to each zone are given in Table 4.2. Cohesion evolves in parallel with the
friction angle according to,

\[c_{\text{mob}} = c_{\text{peak}} \cot \phi_{\text{peak}} \tan \phi_{\text{mob}} \quad (4.6)\]

where \(c_{\text{mob}}\) is the mobilised cohesion, \(c_{\text{peak}}\) is the peak cohesion, and \(\phi_{\text{peak}}\) and \(\phi_{\text{mob}}\) are the peak and mobilised friction angles, respectively.

![Friction angle evolution in hardening and softening regimes.](image)

**Figure 4.1:** Friction angle evolution in hardening and softening regimes.

**Table 4.2:** Evolution laws for the mobilised friction angle (see Fig. 4.1 for the location of the strain zones).

<table>
<thead>
<tr>
<th>Zone</th>
<th>(\phi_{\text{mob}})</th>
<th>(\phi_{\text{ini}})</th>
<th>(\epsilon_{\text{eq}})</th>
<th>(\epsilon_{\text{eq}})</th>
<th>(\Delta \phi_{\text{hard}})</th>
<th>(\Delta \phi_{\text{soft}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\phi_{\text{mob}} = \phi_{\text{ini}} + \frac{\epsilon_{\text{eq}}}{a_{\text{hard}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{hard}}}})</td>
<td>(\phi_{\text{ini}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\Delta \phi_{\text{hard}} = \frac{\xi_{1}}{\phi_{\text{peak}} - \phi_{\text{ini}} - a_{\text{hard}}})</td>
<td>(\Delta \phi_{\text{soft}} = \frac{\xi_{3} - \xi_{2}}{\phi_{\text{peak}} - \phi_{\text{res}} - a_{\text{soft}}})</td>
</tr>
<tr>
<td>2</td>
<td>(\phi_{\text{mob}} = \phi_{\text{peak}})</td>
<td>(\phi_{\text{peak}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\Delta \phi_{\text{hard}} = \frac{\epsilon_{\text{eq}}}{a_{\text{hard}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{hard}}}})</td>
<td>(\Delta \phi_{\text{soft}} = \frac{\epsilon_{\text{eq}}}{a_{\text{soft}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{soft}}}})</td>
</tr>
<tr>
<td>3</td>
<td>(\phi_{\text{mob}} = \phi_{\text{peak}} - \frac{\epsilon_{\text{eq}} - \xi_{2}}{a_{\text{soft}} + \frac{\epsilon_{\text{eq}} - \xi_{2}}{\Delta \phi_{\text{soft}}}})</td>
<td>(\phi_{\text{peak}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\Delta \phi_{\text{hard}} = \frac{\xi_{3} - \xi_{2}}{a_{\text{hard}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{hard}}}})</td>
<td>(\Delta \phi_{\text{soft}} = \frac{\xi_{3} - \xi_{2}}{a_{\text{soft}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{soft}}}})</td>
</tr>
<tr>
<td>4</td>
<td>(\phi_{\text{mob}} = \phi_{\text{res}})</td>
<td>(\phi_{\text{res}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\epsilon_{\text{eq}})</td>
<td>(\Delta \phi_{\text{hard}} = \frac{\epsilon_{\text{eq}}}{a_{\text{hard}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{hard}}}})</td>
<td>(\Delta \phi_{\text{soft}} = \frac{\epsilon_{\text{eq}}}{a_{\text{soft}} + \frac{\epsilon_{\text{eq}}}{\Delta \phi_{\text{soft}}}})</td>
</tr>
</tbody>
</table>

\(\phi_{\text{mob}}\) = mobilised friction angle, \(\phi_{\text{res}}\) = residual friction angle, \(\xi_{1}\) = equivalent plastic strain at which the maximum strength is reached, \(\xi_{2}\) = equivalent plastic strain at which softening begins, \(\xi_{3}\) = equivalent plastic strain at which the residual strength is reached, \(a_{\text{hard}}\) = constant that controls the curvature of the function in the hardening branch, \(a_{\text{soft}}\) = constant that controls the curvature of the function in the softening branch.

It is well known that associated flow rules for geomaterials tend to overestimate volumetric strains during plastic flow. Therefore a non-associated flow rule is adopted in the model. Rather than deriving a specific function for the plastic potential, the flow rule is directly obtained from the yield/failure criterion in the following way,

\[\frac{\partial q}{\partial \sigma'} = \omega \frac{\partial f}{\partial \sigma'} \frac{\partial p'}{\partial \sigma'} + \frac{\partial f}{\partial J} \frac{\partial J}{\partial \sigma'} + \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial \sigma'} \quad (4.7)\]
where \( g \) is the plastic potential and \( \omega \) is a constant that controls the volumetric component of plastic deformations. With \( \omega = 1 \) an associated flow rule is recovered, while with \( \omega = 0 \) no volumetric plastic strains occur. An adequate value for geomaterials usually lies between these limits.

The model has been extended to consider cross-anisotropy through a non-uniform scaling of the stress tensor, as described in Mánica et al. (2016b). As Fig. 4.2 shows, the local coordinate system \( 1 - 2 - 3 \) corresponds to the principal axes of anisotropy with direction “2” oriented orthogonal to the isotropic plane. In a general case, the global coordinate system, \( x - y - z \), does not coincide with the local anisotropy one.

![Figure 4.2: (a) Global and (b) local coordinate systems.](image)

Transformation of the stress tensor from global to local coordinates is achieved via the usual rotation transformation,

\[
\sigma'^r = a \sigma' a^T
\]

where \( \sigma'^r \) is the stress tensor oriented with the local coordinate system and \( a \) is the rotation matrix,

\[
a = \begin{bmatrix}
\cos \beta \cos \alpha & \sin \beta & -\cos \beta \sin \alpha \\
-\cos \alpha \sin \beta & \cos \beta & \sin \beta \sin \alpha \\
\sin \alpha & 0 & \cos \alpha
\end{bmatrix}
\]

where \( \alpha \) and \( \beta \) are the angles indicated in Fig. 4.3.

![Figure 4.3: Definition of the angles in the rotation matrix (Mánica et al., 2016b).](image)
The cross-anisotropic extension of the model is obtained by replacing $p' J$ and $\theta$ in Eq. (4.3) by $p'_{ani} J_{ani}$ and $\theta_{ani}$ respectively. These variables are invariants with the same definition as shown in Eq. (4.4) but calculated from the anisotropic stress tensor $\sigma'^{ani}$. This tensor is obtained through the non-uniform scaling of the effective stress tensor oriented with the local coordinate system ($\sigma'^{r}$), as shown below,

$$
\sigma'^{ani} = \begin{bmatrix}
\sigma'^{r}_{11} & c_N \sigma'^{r}_{12} & \sigma'^{r}_{13} \\
\sigma'^{r}_{12} & c_N \sigma'^{r}_{22} & c_S \sigma'^{r}_{23} \\
\sigma'^{r}_{13} & c_S \sigma'^{r}_{23} & \sigma'^{r}_{33} / c_N \\
\end{bmatrix}
$$

(4.10)

where $c_N$ and $c_S$ are the normal and shear scaling factors respectively.

An appropriate selection of strength parameters and scaling factors allows a satisfactory matching of a specified strength variation with loading orientation. Details about the physical meaning of the anisotropy parameters, their effects, and of the derivation of the corresponding elastoplastic constitutive matrix are given in Mánica et al. (2016b)

### 4.2.2 Time-dependent mechanism

For the time-dependent response, an additional mechanism is considered characterised by a modified form of Lemaitre’s law. Assuming small strains, the total strain increment is decomposed as the sum of the two mechanisms,

$$
d\epsilon = d\epsilon^{ep} + d\epsilon^{vp} = d\epsilon^{ep} + dt(\dot{\epsilon}^{vp})
$$

(4.11)

where $d\epsilon$ is the total strain increment; $d\epsilon^{ep}$ is the elastoplastic strain increment, related to the instantaneous response; $d\epsilon^{vp}$ is the viscoplastic strain increment, related to the time-dependent response; $dt$ is the time increment; and $\dot{\epsilon}^{vp}$ is the viscoplastic strain rate tensor. This strain decomposition give rise to a class of constitutive relationship than can describe both, elastoplastic properties and viscous behaviour (Darve, 1990).

It is assumed that viscoplastic deformations are mainly caused by deviatoric stresses and the strain rates are given by,

$$
\dot{\epsilon}^{vp} = \frac{2}{3} \dot{\epsilon}^{vp} q \\
q = \left( \frac{3}{2} \mathbf{s} : \mathbf{s} \right)^{1/2}
$$

(4.12a)

$$
\dot{\epsilon}^{vp} = \gamma^{vp} (q - \sigma_s)^n (1 - \epsilon_{eq}^{vp})^m
$$

(4.12b)

(4.12c)

where $\gamma^{vp}$ is a viscosity parameter, $\sigma_s$ is a threshold from which viscoplastic strains are activated, $\langle \rangle$ are the Macaulay brackets, $n$ and $m$ are material constants, and $\epsilon_{eq}^{vp}$ is the state variable of the time dependent response given by,

$$
\epsilon_{eq}^{vp} = \int_0^t \left( \frac{2}{3} \dot{\epsilon}^{vp} : \dot{\epsilon}^{vp} \right)^{1/2} dt
$$

(4.13)
In this way, larger viscoplastic strain rates are obtained for higher deviatoric stresses, and those rate decrease as viscoplastic strains accumulate in time, as observed in laboratory tests. In the numerical implementation, an explicit scheme is employed, i.e. viscoplastic strains are computed from the stress state at the beginning of the step. These strains are subtracted from the total strain increment and the elastoplastic relationship is integrated only for $d\epsilon^p$ using now an implicit scheme. This procedure allows preserving the standard format of the elastoplastic constitutive matrix, and it is considered accurate enough if small time steps are used.

4.2.3 Unsaturation

In the case of unsaturation the retention curve linking suction and equivalent degree of saturation is given by the following modified van Genuchten (1980) expression,

$$S_e = \frac{S_l - S_{lr}}{S_{ls} - S_{lr}} = \left[1 + \left(\frac{S_u}{P}\right)^{\frac{1}{\lambda}}\right]^{-\lambda'}$$

(4.14)

where $S_l$ is the degree of saturation, $S_{lr}$ is the residual degree of saturation, $S_{ls}$ is the degree of saturation in saturated conditions (normally 1), and $P$ and $\lambda'$ are model parameters.

4.2.4 Hydraulic

Water flow is governed by Darcy’s law using a hydraulic conductivity, $K$, given by,

$$K = \frac{kk_r}{\mu_w}$$

(4.15)

where $k$ is the intrinsic permeability tensor, $k_r$ is the relative permeability, and $\mu_w$ is the water viscosity.

The relative permeability is considered a function of the effective degree of saturation, defined through a generalised power law,

$$k_r = AS_e^\Lambda$$

(4.16)

where $A$ and $\Lambda$ are material parameters.

In the context of argillaceous materials, it is necessary to take into account the large increase of permeability that occurs when the rock experiences damage. In order to reproduce this phenomenon, permeability cannot be constant but should evolve with damage growth. In the context of the current elastoplastic model, this feature is incorporated by including a dependency of the intrinsic permeability on the plastic multiplier. An exponential function has been adopted for this purpose:

$$k = k_0 e^{\eta \lambda_p}$$

(4.17)

where $k_0$ is the intrinsic permeability of the intact rock, $\eta$ is a constant that controls the rate of change, and $\lambda_p$ is the cumulative value of the plastic multiplier.
4.3 Simulation of COx claystone mechanical behaviour

The constitutive model above has been applied to the reproduction of triaxial and creep tests performed on COx claystone samples. Parameters derived from this exercise are later applied to the analysis of an underground excavation. In all cases (triaxial and creep tests), the major principal stress was orthogonal to the bedding planes of the sample. Due to deconfinement and sample preparation, the specimens became unsaturated with an associated suction that corresponds to a relative humidity of 90%. This resulted in an increase of the sample strength which had to be taken into account in the simulation of the tests in order to obtain consistent effective parameters.

The initial suction of the sample has been computed with the psychrometric equation:

\[ s_u = -\frac{RT_e}{M_w}\rho\ln(H_R) \]  (4.18)

where \( R \) is the universal gas constant, \( T_e \) is the temperature, \( M_w \) is the water molar mass, \( \rho \) is the density of the water, and \( H_R \) is the relative humidity. Assuming \( R = 8.314 \text{ J/mol/K} \), \( M_w = 0.018 \text{ kg/mol} \), \( \rho = 1000 \text{ kg/m}^3 \), and \( T_e = 20 \degree \text{C} \), a suction value of 14.26 MPa is obtained. It has been taken as the initial condition of the samples for the simulations.

Two triaxial tests under confinement pressures of 6 and 12 MPa respectively have been modelled. The tests were performed under displacement control with a constant strain rate of \( 10^{-6} \text{ s}^{-1} \) and conditions of null flux were applied to all boundaries. Fig. 4.4 shows the stress-strain curves obtained from the simulated triaxial tests together with the laboratory test results. Fig. 4.5 shows the results in terms of volumetric strains. From both figures a satisfactory agreement between the simulation results and the laboratory data can be noted. Table 4.3 summarises the parameters of the mechanical and hydraulic constitutive model employed. Both tests share the same parameters except for \( \xi_1, \xi_2 \) and \( \xi_3 \) that show a dependency with confinement pressure that has not been taken into account in the model.

![Figure 4.4: Stress-strain curves in triaxial tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.](image-url)
The simulated creep tests were also performed under triaxial loading conditions. In this case the controlled displacements were stopped once the desired deviatoric stress was reached, and, from then on, the stress state was kept constant for a specified period of time. Three test were performed at a confinement pressure of 12 MPa and with different ratios between applied and maximum deviatoric stresses (50%, 75% and 90%). Fig. 4.6 shows the results obtained in terms of time-dependent deformation. Somewhat larger differences compared with the results of the triaxial tests can be observed although the main trends of behaviour are adequately captured. The parameters related the time-dependent response are also given in Table 4.3.

![Figure 4.5: Volume change in triaxial tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.](image)

![Figure 4.6: Creep tests on COx claystone. Observations (Armand et al., 2017b) and constitutive model results.](image)
Table 4.3: Constitutive law parameters used in the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Input value</th>
<th>Parameter</th>
<th>Units</th>
<th>Input value</th>
</tr>
</thead>
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<tr>
<td><strong>Instantaneous mechanism</strong></td>
<td></td>
<td></td>
<td><strong>Instantaneous mechanism (cont.)</strong></td>
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</tr>
<tr>
<td>$E$</td>
<td>MPa</td>
<td>4000</td>
<td>$\xi_3$ (6 MPa)</td>
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<tr>
<td>$\nu$</td>
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<tr>
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<td></td>
<td></td>
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<td>$n$</td>
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<td>$Hydraulic$</td>
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<td>$\xi_1$ (6 MPa)</td>
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<td>$A$</td>
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<td>$\xi_1$ (12 MPa)</td>
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<td>MPa</td>
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<tr>
<td>$\xi_2$ (12 MPa)</td>
<td>-</td>
<td>0.0165</td>
<td>$\lambda'$</td>
<td>-</td>
<td>0.33</td>
</tr>
</tbody>
</table>

4.4 Theoretical formulation

To apply the constitutive model to a boundary value problem, it was incorporated into a general coupled hydromechanical formulation that is briefly described here. The formulation is a particular case of the general formulation presented in Olivella et al. (1994) for nonisothermal conditions. Only two phases are considered, solid ($s$) and liquid ($l$), corresponding to the two species mineral and water. In this case, the relevant balance equations are,

balance of solid,

$$\frac{\partial}{\partial t} \left[ \rho_s (1 - \varphi) \right] + \nabla \cdot (j_s) = 0 \quad (4.19)$$

balance of water mass,

$$\frac{\partial}{\partial t} \left( \rho_l S_l \varphi \right) + \nabla \cdot (j_l) = f^w \quad (4.20)$$

equilibrium,

$$\nabla \cdot \sigma + b = 0 \quad (4.21)$$

where $\rho$ is the density, $\varphi$ is the porosity, $j$ is the total mass flux, $S_l$ is the liquid degree of saturation, $f^w$ is an external supply of water, $\sigma$ is the stress tensor, $b$ is the vector of body forces.

Using the definition of material derivative,

$$\frac{D_s(\bullet)}{Dt} = \frac{\partial(\bullet)}{\partial t} + \frac{du}{dt} \cdot \nabla(\bullet) \quad (4.22)$$

Eq. (4.19) becomes,

$$\frac{D_s \varphi}{Dt} = \frac{1}{\rho_s} \left[ (1 - \varphi) \frac{D_s \rho_s}{Dt} \right] + (1 - \varphi) \nabla \cdot \frac{du}{dt} \quad (4.23)$$

where $u$ are displacements.

Now, the solid mass balance (Eq. 4.23) can be eliminated by introducing it into the water mass balance relationship (Eq. 4.20). Making use of the material derivative definition again,
the following equation results,
\[
\varphi \frac{D_s (\rho_l S_l)}{Dt} + \rho_l S_l \frac{D_s \varphi}{Dt} + (\rho_l S_l \varphi) \nabla \cdot \frac{du}{dt} + \nabla (j_l) = f^w
\] (4.24)

Any hydromechanical analysis involves the simultaneous solution of Eqs. (4.21) and (4.24) together with appropriate constitutive models and equilibrium restrictions. Displacements and pore water pressure are the main unknowns to be determined.

4.5 Application to an underground excavation in COx claystone

4.5.1 GCS drift excavation

The GCS drift was excavated at the -490 m level of the MHM URL in the location shown in Fig. 4.7. The drift alignment was parallel to the major horizontal principal stress. As a result, the state of stress perpendicular to the axis of the tunnel was practically isotropic with \(\sigma_v = 12.7\) and \(\sigma_h = 12.4\) MPa. The in situ pore water pressure at that level in zones not affected by excavations is 4.7 MPa. The drift section is circular with a 2.6 m radius and was excavated with a road header. The advances of the excavation were generally 1.2 m long and were supported by an 18 cm thick fibre reinforced shotcrete shell and a number of 3 m long bolts in the crown area. 12 yielding concrete props were also installed. In addition, 12 m long rock bolts were also used in the front face. More details of the GCS drift are given in Armand et al. (2014), while a complete description of the excavation work has been presented in Bonnet-Eymard et al. (2011a).

The excavation was monitored from instruments placed in boreholes drilled in advance from nearby openings. Displacements were measured by extensometers and inclinometers and pore water pressures by means of multipacker systems. In addition, convergences were
also measured just after a particular section had been reached by the excavation advance. A more detailed account of the instrumentation and the monitoring observations is given in Seyedi et al. (2017).

The damaged zone around the excavations has been the object of an intense site investigation (Armand et al., 2014). As Fig. 4.8 shows, the extent of the fractured zone is markedly larger in the horizontal direction compared to the vertical one in spite of the quasi-isotropic \textit{in situ} stress state, indicating plainly the role played by the anisotropy of the material. Anisotropy is also evident in the measured convergences in different sections (Fig. 4.9) with horizontal displacements significantly larger than vertical ones.

Another relevant observation for modelling concerns the permeability measured after excavation in boreholes drilled vertically and horizontally from the GCS drift (Armand et al., 2014). As Fig. 4.10 indicates, permeability increases sharply near the excavation and the extent of the zone of permeability increase is significantly larger in the horizontal direction, consistent with the observations of the damaged zone mentioned above.

![Figure 4.8: Extension of the damaged zone for drifts parallel to the major horizontal stress (Armand et al., 2014).](image)

![Figure 4.9: Horizontal and vertical convergences in drifts parallel to the major horizontal stress (Armand et al., 2013).](image)
Figure 4.10: Variation of in situ measured hydraulic conductivity with distance to the drift wall (Armand et al., 2014). (a) Horizontal borehole, (b) vertical borehole.

4.6 Main features of the numerical model

Many of the features of the analyses were specified in the “Action Transverse” benchmark (Seyedi et al., 2017) and correspond to a somewhat idealised simulation of the excavation process. They include the adoption of plane strain conditions and the assumption of no gravity effects. Plane strain models are not able to fully reproduce the actual stress history and tend to underestimate deformations. Nevertheless, the differences with respect to a fully threedimensional analysis tend to be small in the case of flexible supports with completion close to the face (Cantieni and Anagnostou, 2009). The mesh and main boundary conditions are illustrated in Fig. 4.11 where the quasi-isotropic initial stress state can be noted. The initial horizontal stress perpendicular to the analysed cross-section is 16.1 MPa. Advantage has been taken of the symmetry of the problem to analyse only a quarter of the domain. Excavation is simulated through the deconfinement curve specified in Seyedi et al. (2017) and shown in Fig. 4.12. Deconfinement ratio is defined as the ratio between the surface stress applied to the boundary and the value in equilibrium with the initial stress condition. A negative distance to front indicates that the excavation front has not yet reached the analysis section. It can be observed that the stresses on the drift boundary reduce to 0.3 MPa, assumed to correspond to the soft support provided by shotcrete, rock bolts and yielding props. Fig. 4.12 also shows the pore pressure applied to the boundary as a function of the nominal distance to the front. A Biot coefficient of 0.6 was adopted as specified in Seyedi et al. (2017).

The parameters used in the simulation are basically those obtained from the calibration of the constitutive model listed in Table 4.3. Regarding the values $\xi_1$, $\xi_2$ and $\xi_3$ that showed a dependency with the confinement pressure, the values for the triaxial test with $\sigma_3 = 6$ MPa have been employed, since this confinement pressure represents an intermediate value between the in situ conditions and the maximum deconfinement occurring in the tunnel wall.

Rock strength anisotropy was defined by adopting scaling factors $c_N = 1.33$ and $c_S = 1.0$, selected to obtain a reasonable configuration of the damaged zone. The stratification planes
in the COx formation are nearly horizontal; therefore the angles $\alpha$ and $\beta$ (Fig. 4.3) were set equal to zero. Regarding the elastic stiffness anisotropy, a ratio between the horizontal and vertical Young’s modulus of 1.3 was employed, consistent with the values obtained from measurements of wave velocities in cubic samples (Armand et al., 2013).

Figure 4.11: Finite element mesh and boundary conditions.

![Finite element mesh and boundary conditions](image)

In addition, it is necessary to specify the intrinsic permeability of the intact rock as well as the parameter controlling the variation of permeability with plastic multiplier, $\eta$ (Eq. 4.17), see Table 4.4. The selected intrinsic permeability corresponds to the values of hydraulic conductivity measured in situ far away from the excavation damaged zone.

Figure 4.12: Variation of boundary conditions on the excavation wall.

![Variation of boundary conditions on the excavation wall](image)
Table 4.4: Hydraulic parameters used in the drift excavation simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Input value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{0xx}$, $k_{0yy}$, $k_{0zz}$</td>
<td>m$^2$</td>
<td>$5 \times 10^{-2}$</td>
</tr>
<tr>
<td>B</td>
<td>-</td>
<td>0.6</td>
</tr>
<tr>
<td>$\eta$</td>
<td>-</td>
<td>300</td>
</tr>
</tbody>
</table>

4.7 Results of the analysis

The results from the numerical simulations are compared with field observations. Fig. 4.13 shows the location of the measurement points on the plane normal to the tunnel axis that have been used in the comparisons. They belong to three boreholes excavated from an adjacent drift (GAT); two devoted to the measurement of liquid pressure (OHZ1521, OHZ1522), and the other one to the measurement of rock displacements with an extensometer (OHZ1501). All of them were installed prior the excavation of the GCS drift. Also, a number of convergence sections installed along the drift during the excavation (OHZ170_24, OHZ170_36) are also considered.

Pore pressures are especially sensitive to the coupled hydromechanical rock behaviour. Fig. 4.14 shows the evolution of the liquid pressure at the measurement points of borehole OHZ1521, together with the results of the analysis. It should be noted that the simulation times have been slightly shifted from point to point to take into account the fact that the borehole is not perfectly orthogonal to the tunnel axis. An adequate match between the simulation results and the field data can be observed. Points PRE_02 and PRE_03 are quite close to the excavation and the liquid pressure drops very rapidly just after the front passes the corresponding cross section. Although this is partially explained by the decrease of the mean stress in this zone and the occurrence of dilatancy during plastic straining, the rate and the magnitude of this drop cannot be explained without considering the permeability increase due to the material damage. The model is also able to reproduce the liquid pressure increase in PRE_04 before the crossing of the excavation, although the observed maximum peak value was not quite reached. Even though the field data shows that this peak is maintained for
some time, in the model the liquid pressure begins to fall just after the front passes but it should be remembered that the three dimensional effects of tunnel excavation are modelled here in a quite approximate manner. At point PRE_05, model results and field data show a very similar behaviour, although the field data starts from a somewhat lower value of liquid pressure.

![Graph showing pore pressure evolution](image)

Figure 4.14: Pore pressure evolution in measurement points of borehole OHZ1521. Observed (Seyedi et al., 2017) and computed values.

Fig. 4.15 shows the evolution of the liquid pressure at the measurement points OHZ1522 corresponding to both field data and simulation results (again the fact that the borehole is not exactly normal to the drift axis has been taken into account in the comparison). Here a good agreement is observed for points PRE_01 and PRE_05, but some departures are observed in the other locations. Field measurements points PRE_02, PRE_03 and PRE_04 exhibit a rapid drop of the liquid pressure after the excavation front passes its correspondent section, suggesting a permeability increase in those locations. Both field observations and the numerical model indicate that those points are not damaged, so the permeability was assumed constant and equal to the undamaged value during the entire simulation. The cause of this drop in the measured pore pressures deserves further study.

The horizontal displacements recorded by the extensometer in borehole OHZ1501 are shown in Fig. 4.16, together with the result of the analysis. Again, the simulation times were shifted to match the time when the front was in the section of the measurement point. The extensometer is installed horizontally at the level of the axis of the drift, thus crossing the damaged zone at its maximum extent. The field data indicate that points DF0_02, DF0_03 and DF0_04 undergo relatively large displacements as they are within the damaged zone. In the simulation, points DF0_02 and DF0_03 show displacements of this order of magnitude and, in the case of DF0_02, with a very close quantitative agreement. Although point DF0_04 is within the plastic zone according to the simulation, computed displacements are smaller than the field observations; it seems that damage is underestimated at this location. The observed displacements at points further away than DF0_04 are quite small, both in the simulation and in the observations as expected for the undamaged zone of the rock.
Figure 4.15: Pore pressure evolution in measurement points of borehole OHZ1522. Observed (Seyedi et al., 2017) and computed values.

Figure 4.16: Horizontal displacements at measurement points of borehole OHZ1501. Observed (Seyedi et al., 2017) and computed values.

The computed and observed convergences are shown in Fig. 4.17. As convergence measurement points were installed just after the excavation front cleared the corresponding section, displacements that occur before the front reaches the analysis section were subtracted from the final results of the numerical model in order to achieve a proper comparison with field data. It can be observed that the computed horizontal convergences are quite close to the field observations and that they are, because of anisotropy, larger than the corresponding vertical ones. However, the degree of anisotropy observed in the convergence field data is underestimated by the model. It is also worth noting that the rate of development of displacements with time appears to be well reproduced, thus giving support to the adopted time-dependent model.
An estimate of the configuration of the damaged zone can be obtained by plotting contours of the cumulative plastic multiplier, as it is directly related to the magnitude of irreversible strains (Fig. 4.18). It can be seen that the configuration of the damaged zone is similar to that observed in situ, extending more in the horizontal direction (Fig. 4.8). As the initial stress state is nearly isotropic, the use of an isotropic model would have resulted in an axisymmetric damage zone configuration; only an anisotropic model can account for the pattern of field observations.

Finally, the same analysis has been performed without considering creep deformations. Fig. 4.19 shows the convergences obtained. When compared to Fig. 4.17, it can be observed that creep has a very small influence during the excavation stage; almost the same deformations are obtained. From this point on, the observed time dependency in Fig. 4.19 is caused by consolidation only, but these deformations are quite small compared to the field measurements, demonstrating the importance of incorporating creep in the modelling of this type of materials.
Figure 4.19: Evolution of horizontal and vertical convergences. Observed (Seyedi et al., 2017) and computed values. No creep deformations considered.

4.8 Conclusions

This paper presents a constitutive model for argillaceous rocks, developed within the framework of elastoplasticity, that includes a number of features that are relevant for a satisfactory description of their hydromechanical behaviour: anisotropy of strength and stiffness, behaviour nonlinearity and occurrence of plastic strains prior to peak strength, significant softening after peak, time-dependent creep deformations, and permeability increase due to damage. Both saturated and unsaturated conditions are envisaged. The constitutive model has been successfully used in the simulation of triaxial and creep tests on COx claystone.

The constitutive model has then been applied, via a suitable coupled hydromechanical formulation, to the analysis of the excavation of a drift in the MHM URL at a depth of 490 m. The pattern of observed pore water pressure and displacements, as well as the shape of the damaged zone, are generally satisfactorily reproduced, although a number of departures of the calculations from field measurements have also been noted. Some of them may be related to the fact that an essentially 3D tunnel excavation problem has been simulated by a 2D analysis.

It has been shown that it is essential to incorporate material anisotropy if the field observations are to be adequately represented. Field observations also show the paramount importance of the development of the excavation damaged zone on the behaviour of the rock mass close to the drift. In the analyses presented, damage has been simulated in an approximate manner via a continuum approach, whereas localisation and fractures are key characteristics of the damaged zone. Although the pattern of results has been largely recovered by the analyses performed, this continuum assumption can be considered the main limitation of the approach used in the calculations. Formulation and constitutive model are currently under development to simulate explicitly localisation and fracture phenomena in order to achieve a more realistic description of the damaged zone.
Chapter 5

Nonlocal plasticity modelling of strain localisation in stiff clays

Based on the published manuscript of the following article:

Abstract

The paper addresses the numerical simulation of strain localisation in stiff clays that exhibit softening behaviour. An elastoplastic constitutive model developed to incorporate key features of stiff clay behaviour is described first. A non-local formulation is then introduced for the regularisation of the analysis of localisation. A series of analyses were conducted to explore relevant aspects of the numerical simulation of localisation. A 3D analysis was also performed to assess the suitability of the approach presented for 3D applications. Finally, application to the simulation of a laboratory test on Beaucaire marl results in an excellent reproduction of experimental observations.

5.1 Introduction

Stiff clays usually show a quasi-brittle behaviour under deviatoric loading unless they are subjected to high confining stresses (Gens, 2013). They commonly exhibit strain softening, which means that, after reaching a maximum, strength decreases as displacements increase until reaching a residual state where the strength no longer decreases even when subject to large displacements (Hvorslev, 1937; Lupini et al., 1981; Skempton, 1964). The resulting strain field is generally non-homogeneous and deformations tend to localise into thin zones of intense shearing in the form of fractures or slip surfaces (Georgiannou and Burland, 2006; Lenoir et al., 2007). This phenomenon is known as strain localisation. The numerical simulation of this phenomenon under the framework of continuum mechanics involves a number of difficulties, since it is well-established that standard formulations tend to deliver non-objective results due to the loss of ellipticity of the governing equation at the onset of localisation (Hill, 1962; Mandel, 1966; Thomas, 1961). Particularly, in the simulation of boundary value problems (BVP), this non-objectivity traduces into a strong dependency on the employed mesh (de Borst et al., 1993). Vanishing energy dissipation and localisation into a zone of vanishing volume are obtained as the size of elements is reduced (Bažant...
and Pijaudier-Cabot, 1988), which is not physically reasonable. Indeed, the actual width of the localised zone in geomaterials seems to be related with their microstructure (Desrues and Viggiani, 2004), providing the material with an internal length scale, missing in the standard continuum formulations. The introduction of an internal length scale can prevent the usual pathologies arising when modelling problems involving localised deformations, and different enriched continuum theories have been proposed to introduce such a scale parameter. Following Bažant and Jirásek (2002), they can be broadly classified into continua with microstructure (e.g. Cosserat and Cosserat, 1909; Eringen, 1966), continua incorporating gradients of strain (gradient theories) (e.g. Mindlin, 1965), and nonlocal models of the integral type (e.g. Eringen, 1981; Pijaudier-Cabot and Bažant, 1987). Other techniques such adaptive mesh refinement (Ortiz and Quigley, 1991; Zienkiewicz and Huang, 1995) or viscoplasticity (Loret and Prevost, 1990; Prevost and Loret, 1990) have also been employed as localisation limiters. All the above-mentioned approaches, sometimes known as regularisation techniques, incorporate in some way a length scale to the material behaviour, which tends to control the size of the localised region and prevents the pathological dependency with the employed mesh.

In this paper, the nonlocal integral type approach was applied to a plasticity model, intended for the objective simulation of localised plastic deformations in stiff clays. It incorporates the special weighting function proposed by Galavi and Schweiger (2010), which has shown lower mesh dependency compared with the usual Gaussian function (Summersgill et al., 2017a). The model is employed in a series of two-dimensional (2D) plane strain analyses, to explore relevant aspects of the numerical simulation of localisation, such as the thickness of the shear band, its orientation, and the onset of localisation in BVPs. A 3D analysis was also performed, in order to assess the suitability of the approach presented for 3D applications. Finally, a real biaxial experiment on Beaucaire marl (Marello, 2004) has been simulated, and the results were compared not only with global measurements but with the entire strain field, observed experimentally using the false relief stereophotogrammetry technique (FRS) (Desrues and Viggiani, 2004).

5.2 Model formulation

The model described herein represents an enhanced version of the one presented in Mánica et al. (2017c), for stiff clayey materials. The main enhancement is the ability to simulate objectively the localisation phenomenon by the introduction of the nonlocal approach, which is the main focus of this work. In addition, a different yield function and evolution laws were employed, more consistent with the observed behaviour of stiff clays. However, only a partial version is presented here where some additional behaviour features of stiff clays such as stiffness and strength anisotropy or creep deformations were not included. The incorporation of these features within the present approach will be addressed in a subsequent paper.

5.2.1 Local constitutive model

An elastoplastic model is adopted as the basic constitutive law for analysis. Inside the yield surface the response is assumed linear elastic and characterised by Hooke’s law. The yield criterion is defined by a hyperbolic approximation of the Mohr-Coulomb envelope (Gens
et al., 1990) expressed as,

\[ f = \sqrt{\frac{J_2}{f_2(\theta)}} + (c^* + p_t \tan \phi^*)^2 - (c^* + p \tan \phi^*) \]  

(5.1)

where \( c^* \) is the asymptotic cohesion, \( \phi^* \) is the asymptotic friction angle, \( p_t \) is the isotropic tensile strength, \( p \) is mean stress, \( J_2 \) is the second invariant of the deviatoric stress tensor \( \mathbf{s} = \mathbf{\sigma} - p \mathbf{I} \), and \( \theta \) is Lode’s angle. At high mean stresses, Eq. (5.1) converges to the classical Mohr-Coulomb envelope, and the terms asymptotic cohesion and friction angle refers to this condition. However, at low mean stresses the envelope is curved, with an isotropic tensile strength directly indicated by \( p_t \). This allows us to consider the low tensile strength usually exhibited by stiff clays, generally overestimated by linear criteria. The shape in the octahedral plane is defined by \( f_2(\theta) \), where the following generalised function was employed (van Eekelen, 1980),

\[ f_2(\theta) = \alpha^\theta (1 + \beta^\theta \sin 3\theta)^n^\theta \]  

(5.2)

where \( \alpha^\theta \), \( \beta^\theta \) and \( n^\theta \) are parameters providing a family of surfaces. This can be simplified to a one-parameter function by assuming \( n^\theta = -0.229 \) and \( \beta^\theta = 0.85\sqrt{\alpha^\theta} \), as proposed by van Eekelen (1980). Fig. 5.1 shows the adopted yield function in the \( p - J \) and octahedral planes, compared to the classical Mohr-Coulomb criterion. An important limitation is that yielding cannot occur under isotropic compression, a characteristic generally observed in stiff clays (e.g. Burland, 1990). One possibility is to bound the permitted stress space for compressive loading with an additional yielding mechanism, within the framework of multi-surface plasticity (e.g. Simo et al., 1988). However, in the present work, only plastic processes under deviatoric loading are of interest and, therefore, yielding under isotropic compression was not included in the model.

Isotropic non-linear hardening/softening was considered to reproduce the strength evolution under loading generally observed in stiff clays, which is illustrated in Fig. 5.2 (Jardine et al., 2004). It assumes that the observed initial cohesion is mainly due to the effect of interparticle bonds. At reaching the peak, the breakage of these bonds takes place and the strength decreases very rapidly up to a value designated by Burland (1990) as post-rupture strength, at which most of the cohesion has been lost. Afterwards, a more gentle reduction takes place until reaching the residual strength at very large displacements. The remaining
cohesion (if any) is completely lost, and the friction angle has reduced considerably. This reduction is generally attributed to a gradual realignment of clay particles on the sliding surface (Gens, 2013). Experimental investigations supporting this conceptual scheme can be found for instance in Calabresi and Manfredini (1973) and Jardine et al. (2004). Following this conceptual framework, the evolution laws for the strength parameters are defined in this way,

\[
\tan \phi^* = \begin{cases} 
\tan \phi^*_{ini} + \frac{\varepsilon^P_{eq}}{\phi_{hard} + \frac{\varepsilon^P_{eq}}{\Delta}}, & (\varepsilon^P_{eq} \leq \xi_2) \\
\tan \phi^*_{peak} - \left( \tan \phi^*_{peak} - \tan \phi^*_{res} \right) \left[ 1 - e^{-b_c(\varepsilon^P_{eq} - \xi_2)} \right], & (\varepsilon^P_{eq} > \xi_2)
\end{cases}
\]

where \(\varepsilon^P_{eq}\) is a scalar state variable defined as,

\[
\varepsilon^P_{eq} = \left( \varepsilon^P : \varepsilon^P \right)^{1/2}
\]

and \(\varepsilon^P\) is the plastic strain tensor. The initial position of the yield envelope is given by \(\phi^*_{ini}\), \(c^*_ini\) and \(p^t_{ini}\). It is assumed that plastic deformations before peak strength can occur, so after reaching the yield limit hardening takes place, related to the mobilisation of the apparent friction angle from \(\phi^*_{ini}\) to \(\phi^*_{peak}\) according to a hyperbolic function of the equivalent strain. During this hardening phase, the apparent cohesion and tensile strength are assumed to remain constant. The peak strength is reached at \(\xi_2\), i.e. the value of the state variable separating the hardening and softening regimens. Thereafter softening occurs, characterised by an exponential decay function. It has been considered that the rate of softening is not the same for all the strength parameters. A high softening rate is assumed for the apparent cohesion and the tensile strength \(\left(b_c\right)\), related to the degradation and breakage of interparticle bonds. On the other hand, a smaller softening rate is assumed for the apparent friction angle \(\left(b_\phi\right)\), attributed to a gradual realignment of clay particles that takes the material towards the residual strength. In the residual state, only \(\phi^*_{res}\) remains, which in fact becomes a true friction angle, since the apparent cohesion and tensile strength have completely disappeared, and a linear criteria (in the \(p - J\) plane) is recovered.

As for the development of plastic strains, a non-associated flow rule is adopted. Rather than deriving a specific function for the plastic potential, the flow rule is directly obtained from the yield criterion in the following way,

\[
\frac{\partial g}{\partial \sigma} = \omega \frac{\partial f}{\partial p} \frac{\partial p}{\partial \sigma} + \frac{\partial f}{\partial J_2} \frac{\partial J_2}{\partial \sigma} + \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial \sigma}
\]
where $g$ is the plastic potential and $\omega$ is a constant that controls the volumetric component of plastic deformations. With $\omega = 1$ an associated flow rule is recovered, while with $\omega = 0$ no volumetric plastic strains occur. An adequate value for geomaterials should lie between those limits.

![Figure 5.2: Conceptual scheme for the strength of stiff plastic clays (Jardine et al., 2004)](image)

### 5.2.2 Nonlocal approach

The use of nonlocal models can be traced back to the beginning of the 20th century, although its application as a regularisation technique for numerical simulations did not occur until the 1980s; see Bažant and Jirásek (2002) for a comprehensive review. In a general sense, a nonlocal constitutive model is one where the behaviour at a material point (or at a Gauss point in a finite element simulation) depends not only on its state but also on the state of neighbouring points. This is accomplished by replacing a given variable by its nonlocal counterpart. If $f(X)$ is some local field within a body of volume $V$, the nonlocal field can be expressed as,

$$\bar{f}(X) = \int_V w(X, \kappa) f(\kappa) \, d\kappa$$

where $w(X, \kappa)$ is a weighting function controlling the importance of neighbouring points as a function of its position ($\kappa$), relative to the position of the actual point under consideration ($X$). Typically, only the distance between them is considered, thus $w(X, \kappa) = w_0(||X - \kappa||)$. A Gaussian function has been usually employed (e.g. Bažant and Lin, 1988), defined as,

$$w_0 = \frac{1}{l_s \sqrt{\pi}} e^{-\left(\frac{||X - \kappa||}{l_s}\right)^2}$$

where the highest influence occurs at the actual point, and reduces by increasing the distance (Fig. 5.3). The parameter $l_s$ controls the width of the bell-shaped curve, implicitly introducing a length scale to the continuum formulation. Close to the boundaries, averaging should be performed only on the part of the domain that lies within the body. In addition, averaging should not modify a uniform field. Therefore, the weighting function is usually defined in the following normalised form,

$$w(X, \kappa) = \frac{w_0 (||X - \kappa||)}{\int_V w_0 (||X - \Upsilon||) \, d\Upsilon}$$

Different nonlocal models are obtained depending on which variable (or variables) is considered nonlocal. For instance, in the case of nonlocal plasticity formulations, different
alternatives have been studied, such as elastic strains (Eringen, 1981), total strains (Eringen, 1983), plastic strains or the plastic multiplier (Bažant and Lin, 1988), or the state variable controlling softening (Planas et al., 1993). However, under certain circumstances, these formulations may show undesirable effects such as stress locking, vanishing energy dissipation, or localisation into a zone of vanishing volume (Bažant and Jirásek, 2002). An improved formulation, often called over-nonlocal, was proposed by Brinkgreve (1994) where the averaged softening variable is obtained through a linear combination of the local and nonlocal variables,

\[
\bar{\chi}(X) = (1 - \mu) \chi(X) + \mu \int_V w(X, \kappa) \chi(\kappa) d\kappa
\] (5.11)

where \(\chi\) is an arbitrary state variable controlling softening, and \(\mu\) is a new parameter controlling the relative proportion of the local and nonlocal variables. With \(\mu = 0\) the classical local model is recovered, while with \(\mu = 1\) the standard nonlocal formulation, described by Eq. (5.8) is obtained. Although intuition would suggest that an appropriate value should lie between those limits, Brinkgreve (1994) showed that the best results are obtained with \(\mu > 1\). The consequence is that the highest influence is removed from the actual point under consideration and displaced to some distance from it and, in an extreme case, the influence of the actual point can become negative in sign. This approach prevents the localisation of deformations into a zone of vanishing volume. However, the actual size of the localised region will be a combination of \(l_s\) and \(\mu\) and, therefore, their selection may be somewhat arbitrary.

Following this idea, Galavi and Schweiger (2010) proposed the alternative weighting function depicted in Fig. 5.3, and defined by,

\[
w_0 = \frac{|X - \kappa|}{l_s} \exp \left( - \frac{|X - \kappa|}{\tilde{l}_s} \right)^2
\] (5.12)

The influence of the actual point is removed and the maximum weight is located at a distance equal to 0.707\(l_s\). This function has a similar effect as the over-nonlocal approach, but no additional parameter is required and the size of the localised region is related only to \(l_s\). Summersgill et al. (2017a) recently compared this latter approach with the standard nonlocal formulation (i.e. Eq. 5.8 with a Gaussian weighting function) and with the over-
nonlocal approach (Brinkgreve, 1994), and concluded that the best results are obtained with the weighting function proposed by Galavi and Schweiger (2010).

In the present research, we applied the approach given by Galavi and Schweiger (2010) to the regularisation of the local model described in section 5.2.1. As shown later, and in accordance with the results from Summersgill et al. (2017a), this approach showed excellent results in terms of consistency and mesh independence. For the implementation of the stress point algorithm, Eq. (5.8) and (5.10) were replaced by the following discrete versions,

\[
\bar{\epsilon}_{eq}^p_k = \sum_{l=1}^{NG} w_{kl} \epsilon_{eq}^l
\]  
\[
w_{kl} = \frac{w_0 (||X_k - X_l||)}{\sum_{m=1}^{NG} w_0 (||X_k - X_m||)}
\]  

where \(\bar{\epsilon}_{eq}^p\) is the nonlocal state variable and \(NG\) is the total number of Gauss points in the simulation. However, as pointed out by Galavi and Schweiger (2010), the effect of neighbouring points at distances greater than 2\(l_s\) is quite small (<1.83%), and iteration throughout all Gauss points can be quite inefficient for large BVP. Therefore, only neighbouring points inside an interaction radius of 2\(l_s\) have been considered for averaging. Since the local model was originally implemented implicitly using the backward Euler method, its nonlocal extension implies that the stress integration cannot be performed in each Gauss point independently, since the resulting state variable in one point will depend (directly or indirectly) on all points regardless of whether they are inside or outside the interaction radius. To overcome this issue, but keeping the algorithm simple and efficient, the iterative technique proposed by Rolshoven (2003) was employed here. The stress integration is performed in each Gauss point independently by assuming that the state variables for all other points are frozen within the current global iteration. Since the actual integration point does not have any influence, nonlocal state variables of all Gauss points can be computed and stored together at the beginning of each global iteration. Furthermore, since Eq. (5.14) depends only on the relative position of points, it is only computed and stored once at the beginning of the simulation. The nonlocal state variable is computed only for points in the softening regime. In the hardening regime, before the state variable reaches the value of \(\xi_2\), the model is local.

The developed stress point algorithm incorporates a sub-stepping scheme with error control, based on Richardson’s (1911) extrapolation, which results in a robust implementation. This algorithm was incorporated as a user defined soil model in the finite element code Plaxis (Brinkgreve et al., 2017), which was used for the simulations described below.

5.3 Numerical strain localisation analyses

A number of 2D numerical analyses were performed to assess the performance of the developed constitutive model and the non-local formulation in the simulation of localised deformation patterns. They correspond to a drained biaxial plane strain test under displacement control. The analyses do not represent any particular experiment, and the conditions and parameters used in each simulation were simply chosen to evaluate the key aspects of
the employed nonlocal approach. Fig. 5.4 shows the size of the analysis domain and the two types of boundary conditions used. In the first type (Fig. 5.4a), fixed horizontal displacements were applied at the top and bottom boundaries to develop a non-homogeneous stress/strain field and favour the onset of localisation. In the second type (5.4b), frictionless boundaries are considered with free horizontal displacements at both ends, except for the central node of the bottom boundary in order to avoid an undetermined system. A prescribed downward vertical displacement of 5.0 mm was applied to the top boundary. Table 5.1 shows the parameters for the base case, while a summary of all performed analyses is presented in Table 5.2. Table 5.2 also shows the parameters and/or boundary conditions that have been changed in each analysis with respect to the base case. The following features of the localisation analyses are now examined: mesh independence, shear band thickness and softening scaling, effect of boundary conditions and imperfections, onset of localisation and shear band orientation.

![Figure 5.4: Analysis domain and boundary conditions](image)

Table 5.1: Parameters of base case analysis A01

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>kPa</td>
<td>20000</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
<td>-</td>
<td>0.2</td>
</tr>
<tr>
<td>Initial asymptotic friction angle</td>
<td>$\phi_{\text{ini}}^*$</td>
<td>°</td>
<td>10</td>
</tr>
<tr>
<td>Peak asymptotic friction angle</td>
<td>$\phi_{\text{peak}}^*$</td>
<td>°</td>
<td>20</td>
</tr>
<tr>
<td>Residual friction angle</td>
<td>$\phi_{\text{res}}^*$</td>
<td>°</td>
<td>15</td>
</tr>
<tr>
<td>Asymptotic cohesion</td>
<td>$c_{\text{ini}}^*$</td>
<td>kPa</td>
<td>200</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>$p_{t \text{ ini}}$</td>
<td>kPa</td>
<td>0</td>
</tr>
<tr>
<td>Equivalent strain at peak strength</td>
<td>$\xi_2$</td>
<td>-</td>
<td>0.01</td>
</tr>
<tr>
<td>Constant in hardening law</td>
<td>$a_{\phi}$</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>Rate of reduction of friction angle</td>
<td>$b_{\phi}$</td>
<td>-</td>
<td>2</td>
</tr>
<tr>
<td>Rate of reduction of cohesion</td>
<td>$b_c$</td>
<td>-</td>
<td>10</td>
</tr>
<tr>
<td>Non-associative constant</td>
<td>$\omega$</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Length scale parameter</td>
<td>$l_s$</td>
<td>cm</td>
<td>n/a</td>
</tr>
</tbody>
</table>
Table 5.2: Analyses performed

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Boundary conditions</th>
<th>No. elements</th>
<th>Variations with respect to A01</th>
</tr>
</thead>
<tbody>
<tr>
<td>A01</td>
<td>Rough</td>
<td>16</td>
<td>-</td>
</tr>
<tr>
<td>A02</td>
<td>Rough</td>
<td>63</td>
<td>-</td>
</tr>
<tr>
<td>A03</td>
<td>Rough</td>
<td>167</td>
<td>-</td>
</tr>
<tr>
<td>A04</td>
<td>Rough</td>
<td>343</td>
<td>-</td>
</tr>
<tr>
<td>A05</td>
<td>Rough</td>
<td>789</td>
<td>-</td>
</tr>
<tr>
<td>A06</td>
<td>Rough</td>
<td>1303</td>
<td>-</td>
</tr>
<tr>
<td>B01</td>
<td>Rough</td>
<td>343</td>
<td>( l_s = 1.0 \text{ cm} )</td>
</tr>
<tr>
<td>B02</td>
<td>Rough</td>
<td>789</td>
<td>( l_s = 1.0 \text{ cm} )</td>
</tr>
<tr>
<td>B03</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 1.0 \text{ cm} )</td>
</tr>
<tr>
<td>B04</td>
<td>Rough</td>
<td>4788</td>
<td>( l_s = 1.0 \text{ cm, 3D} )</td>
</tr>
<tr>
<td>C01</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.8 \text{ cm} )</td>
</tr>
<tr>
<td>C02</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.6 \text{ cm} )</td>
</tr>
<tr>
<td>C03</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm} )</td>
</tr>
<tr>
<td>D01</td>
<td>Rough</td>
<td>343</td>
<td>( b_c = 0 )</td>
</tr>
<tr>
<td>D02</td>
<td>Rough</td>
<td>789</td>
<td>( b_c = 0 )</td>
</tr>
<tr>
<td>D03</td>
<td>Rough</td>
<td>1303</td>
<td>( b_c = 0 )</td>
</tr>
<tr>
<td>E01</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.8 \text{ cm, } b_c = 8.6 )</td>
</tr>
<tr>
<td>E02</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.6 \text{ cm, } b_c = 7.0 )</td>
</tr>
<tr>
<td>E03</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2 )</td>
</tr>
<tr>
<td>F01</td>
<td>Smooth</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \text{ geometrical imperfection} )</td>
</tr>
<tr>
<td>F02</td>
<td>Smooth</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \text{ weak element} )</td>
</tr>
<tr>
<td>G01</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \omega = 0.8 )</td>
</tr>
<tr>
<td>G02</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \omega = 0.6 )</td>
</tr>
<tr>
<td>G03</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \omega = 0.4 )</td>
</tr>
<tr>
<td>G04</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \omega = 0.2 )</td>
</tr>
<tr>
<td>G05</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, \omega = 0.0 )</td>
</tr>
<tr>
<td>H01</td>
<td>Rough</td>
<td>1303</td>
<td>( l_s = 0.4 \text{ cm, } b_c = 5.2, b_\omega = 20 )</td>
</tr>
</tbody>
</table>

5.3.1 Mesh independence

As previously mentioned, analyses involving localised deformations exhibit a marked dependency with the finite element mesh employed. This pathology is demonstrated in the set of analyses A, where six different meshes with increasing number of elements were used. The first type of boundary conditions (Fig. 5.4a) was prescribed. The finite elements were 15-noded triangular with fourth-order interpolation and 12 integration points. In this set of analyses, the local version of the model was employed, i.e. without the nonlocal extension described in section 5.2.2. Fig. 5.5 shows contour plots of the computed shear strain, defined, in this plane strain condition, as,

\[
\epsilon_s = \frac{\epsilon_1 - \epsilon_3}{2}
\]  

(5.15)

where \( \epsilon_1 \) and \( \epsilon_3 \) are the major and minor principal strains. \( \epsilon_s \) is a very convenient way to observe the configuration of the localised deformation pattern. The employed meshes are also depicted in the figure. Because of the fixed horizontal displacements at the boundary, stresses concentrate in the four corners of the model, allowing the simultaneous formation of two X-shaped shear bands. However, in analyses A01 and A02 the large size of elements and its orientation interfere with the free propagation of shear bands, resulting in one of them developing more than the other one. In the remaining analyses, elements are small
enough to avoid this interference and, therefore, both bands are symmetrical to each other. In any case, the mesh dependency can be clearly recognised by the decreasing thickness of shear bands when increasing the number of elements (and therefore decreasing its size). After the onset of localisation, Gauss points outside the band unload elastically, and plastic processes concentrate within it. Therefore, a decreasing thickness of the band translates to a decreasing amount of dissipated energy. At the limit, with elements size tending to zero, the dissipation will also tend to zero, which is not physically reasonable. This decreasing dissipation is apparent in Fig. 5.6 that shows the vertical deviator load (per meter thickness) against the prescribed vertical displacement. A more brittle response is obtained when the number of elements is increased.

![Figure 5.5: Contours of shear strain from the set of analyses A](image)

In the B set of analyses, the nonlocal extension of the model was employed with an internal length scale of 1.0 cm. The nonlocal approach requires a minimum amount of Gauss points inside the interaction radius to compute the nonlocal variable. For the same kind of elements as the ones employed here, Galavi and Schweiger (2010) suggested that the following condition must be fulfilled,

\[ l_s \geq L_{el} \]  

(5.16)

where \( L_{el} \) is the maximum length of an element in the FE mesh. For this reason, meshes with 16, 63 and 167 elements were discarded for this set of analyses. Fig. 5.7 shows the obtained contour plots of shear strain. Unlike set A, the same localisation pattern and the same shear
band thickness were obtained in all analyses regardless the number of elements. Dissipated energy is now also mesh-independent and, therefore, a practically unique load-displacement curve was obtained in all three analyses (Fig. 5.8).

![Figure 5.6: Load-displacement curves from the set of analyses A](image)

Figure 5.6: Load-displacement curves from the set of analyses A

The plane strain cases analysed in this study offer a good opportunity to assess the non-local approach in a 3D simulation. A 2D plane strain analysis is, in fact, a representation of a 3D problem with infinite extent in the perpendicular direction. Therefore, a 3D simulation with a finite extent in this direction, but with appropriate boundary conditions representing the infinite extent, should give in principle the same results as the 2D model. This was verified by analysis B04, which is a 3D version of the other analyses of group B. Fig. 5.9a shows the model geometry and boundary conditions, which are analogous to those depicted in Fig. 5.4a, but with a thickness of three centimetres. The null displacements in the y direction at the front and back faces ensure plane strain condition. The employed mesh is also shown in the same figure. It comprises 4788 tetrahedral 10-noded finite elements with
second-order interpolation and four integration points. The condition given by Eq. (5.16) is also fulfilled here, but $L_{el}$ is interpreted as the larger edge of the tetrahedra. Fig. 5.9b shows the computed field of shear strain. By comparing it with Fig. 5.7, it can be noted that the same localisation pattern and the same width of the shear bands were obtained with the 3D model. The difference is that now the localised zone has an additional dimension, i.e. it is a 3D region where plastic deformations accumulate. The load-displacement curve of the 3D model is also depicted in Fig. 5.8. Notice that the results of the 3D analysis are also given in kN/m to allow direct comparison with the 2D analyses. The 3D model yielded almost exactly the same curve than the 2D models. These results provide confidence in the application of the employed approach for the simulation of 3D problems involving localised deformations.

Figure 5.8: Load-displacement curves from the 2D analyses of the set B and from the 3D analysis (B04)

Figure 5.9: (a) Geometry, mesh, and boundary conditions from the 3D analysis of the set B (B04). (b) Computed shear strain contours
5.3.2 Shear band thickness and softening scaling

The effect of $l_s$ was explored in the set C, where the case B03 was analysed for different values of $l_s$. Fig. 5.10 shows the computed contours of shear strain. As $l_s$ decreases, the interaction radius also decreases and, therefore, plastic deformations tend to localise in a narrower zone. Table 5.3 shows the shear band thickness from these analyses. The boundary of the shear zone is defined as the location where a sudden jump in the field of incremental displacements take place. The numerical shear band thickness is roughly equal to the length scale parameter, as already observed by Galavi and Schweiger (2010). Nevertheless, since the constitutive behaviour is the same in all analyses (the same local model, with the same parameters), a thinner shear band entails a lower energy dissipation and, therefore, a more brittle response (Fig. 5.11). Consequently, for a given load-displacement curve, there exists a relationship between the length scale parameter and the softening rate.

![Figure 5.10: Contours of shear strain from the set of analyses C](image)

Table 5.3: Obtained shear band thickness from the set of analyses C

<table>
<thead>
<tr>
<th>Analysis</th>
<th>$l_s$ [cm]</th>
<th>Shear band thickness [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>B01</td>
<td>1.00</td>
<td>0.95</td>
</tr>
<tr>
<td>C01</td>
<td>0.80</td>
<td>0.77</td>
</tr>
<tr>
<td>C02</td>
<td>0.60</td>
<td>0.58</td>
</tr>
<tr>
<td>C03</td>
<td>0.40</td>
<td>0.44</td>
</tr>
</tbody>
</table>

To properly apply the nonlocal approach in the simulation of a given material, $l_s$ should be chosen to obtain a shear band thickness similar than those observed experimentally. Then, the softening rate can be adjusted to match a given load-displacement curve. However, localisation processes in stiff clays tend to be more discrete, in the form of fractures or slip surfaces (Georgiannou and Burland, 2006; Lenoir et al., 2007), surrounded by a small zone of intense shearing of a few micrometres (Laurich et al., 2014). Since a number of Gauss points inside the interaction radius are required to compute the nonlocal variable, it appears unfeasible to apply the nonlocal approach for stiff clays as it would require an excessively refined mesh. However, this can be overcome by assuming that the effects of the actual
fracture and sheared zone can be merged into a numerical shear band of larger size. In this case, the mesh should be as refined as possible, but without exceeding available computational capacities. The length scale parameter should be chosen according to Eq. (5.16), which will result in the smallest allowable band thickness for a given mesh refinement. Then, the desired macroscopic material behaviour (e.g. a given load-displacement curve) can be reproduced by adjusting the softening rate of the model. Therefore, the post-localisation behaviour of the simulation will be the result of the combination of both, the length scale parameter and the softening rate. This technique is known as softening scaling, first suggested by Pietruszczak and Mroz (1981), and later applied by others (Brinkgreve, 1994; Galavi and Schweiger, 2010; Marcher, 2003; Schädlich, 2012), which allows us to merge the effects of the real fracture process zone into a larger numerical shear band in accordance with a reasonable amount of computational resources. This is of paramount importance when dealing with real engineering situations.

![Figure 5.11: Load-displacement curves from the set of analyses C](image)

In the constitutive model described here the total softening rate is defined by parameters $b_c$ and $b_\phi$, controlling the rate of reduction of cohesion (and tensile strength) and friction angle respectively. Thus, in principle, both parameters should be adjusted when defining the target softening rate. Nevertheless, as previously stated, the friction angle reduction in stiff clayey soils is generally slow, and requires large deformations. When dealing with small softening rates, the usual pathologies arising from the continuum simulation of strain localisation may become unimportant (Pietruszczak and Mroz, 1981). This is clearly demonstrated in Fig. 5.12, where different meshes were analysed using the local version of the model, but with $b_c$ set equal to zero, i.e. just considering a gentle reduction of the friction angle. Despite having used different sizes of elements, the response is not mesh-dependent, and a unique load-displacement curve was obtained from all analyses. Therefore, since the small rate of reduction of the friction angle does not result in mesh dependent results, the adjustment of the softening rate, for a given $l_s$, can be performed only through variation of $b_c$. 
Assuming, for example, that the load-displacement curve from the analysis B03 is the desired macroscopic behaviour, the analyses from set C were again performed (set E), but with a softening rate adjusted to retrieve the desired response. Fig. 5.13 shows how a unique load-displacement curve can be obtained from the different analyses by using in each of them an appropriate value of $b_c$. The relationship obtained between the softening rate and the length scale parameter is depicted in Fig. 5.14. Despite using an exponential softening law, the softening rate seems to scale linearly with $l_s$, as already suggested by others (Galavi and Schweiger, 2010; Marcher, 2003; Schädlich, 2012).

Figure 5.12: Load-displacement curves from the set of analyses D

Figure 5.13: Load-displacement curves from the set of analyses E
5.3.3 Effect of boundary conditions and imperfections

The overall behaviour of problems exhibiting localisation does not only depend on the constitutive behaviour, but boundary conditions have a profound influence on the obtained configuration of the localised deformation pattern. This is clearly shown by the analysis F01, where frictionless ends were used (Fig. 5.4b). Naturally, these conditions lead to a homogeneous stress/strain field, where localisation cannot take place. Therefore, a geometric imperfection was introduced to enforce localisation; the top boundary was shifted to the right 0.5 mm with respect to the bottom one. Upon loading, this imperfection causes a non-homogeneous stress/strain distribution, where plastic deformations first accumulate at the top-left and bottom-right corners. Therefore, unlike previous analyses where two X-shaped shear bands formed simultaneously, only a single shear band is generated across the sample, joining these two corners (Fig. 5.15a).
Another commonly employed method to induce the onset of localisation is to incorporate a weak element, from which the shear band can propagate. This was done in analysis F02 where the weak element was located at the top-right corner and had a cohesion of 100 kPa, i.e. half than the rest of elements. No geometrical imperfections are introduced in this analysis. A single shear band is also generated (Fig. 5.15b), but since it initiates in the top-right corner, it has the opposite orientation with respect to the analysis F01.

5.3.4 Onset of localisation

Strain localisation is a progressive process and the definition of an onset is difficult. Non-uniform strain fields can appear at very early stages of the deformation but experimental evidence suggests that the onset of a persistent shear band often occurs near the global peak strength or slightly before (Desrues and Viggiani, 2004). In the context of plasticity theory, the localised failure condition at the constitutive level has been related to the singularity of the so-called acoustic or localisation tensor (Hill, 1962; Ortiz, 1987; Rice, 1976), i.e. when the following condition is met,

$$\det(Q) = \det(n \cdot D^{ep} \cdot n) = 0$$ (5.17)

where $Q$ is the acoustic tensor, $D^{ep}$ is the tangent stiffness matrix and $n$ is the normal to the discontinuity surface. However, instability of a single Gauss point (or a number of them) does not necessarily imply a global instability of the BVP.

In the present study, the onset of localisation at a global level was objectively identified by the evolution of the second derivative of the shear strain with respect to time, averaged for all Gauss points,

$$\bar{\epsilon}''_s = \frac{1}{N_G} \sum_{i=1}^{N_G} \frac{d^2 \epsilon_s}{dt^2} i$$ (5.18)

where $t$ is the simulation time. It can be viewed as some sort of global shear strain acceleration. Fig. 5.16 shows the evolution of this variable during analysis E03. At the beginning the response is purely elastic, a linear relationship exists between the applied constant displacement rate and the shear strain rate and, therefore, $\bar{\epsilon}''$ is equal to zero. Due to the fixed horizontal displacements boundary condition, hardening is initially attained at Gauss points close to the corners of the model. As plastic hardening takes place, the rate of accumulation of shear strains slowly increases, as reflected in a gentle increase of $\bar{\epsilon}''$. Subsequently, softening is also initially attained at Gauss points close to the corners. From this point on, the increase of $\bar{\epsilon}''$ accelerates. Nevertheless, the remaining points, still in the hardening regime, contribute to the global stability of the model. When a sufficient number of Gauss points enter the softening regime (1909 in this case), plastic shear strains suddenly increase along what will be the shear bands, causing a jump in $\bar{\epsilon}''$. This point is taken here as the onset of localisation of the BVP (Fig. 5.16). From this point on, $\bar{\epsilon}''$ does not show a smooth evolution and exhibits oscillations during the rest of the simulation. It is interesting to notice that this instability point does not necessarily take place at the global peak strength, and in this case occurs slightly before it, as experimental evidence often indicates (Desrues and Viggiani, 2004).
A localisation analysis at a constitutive level was also performed in all Gauss points of the simulation E03 using the condition in Eq. (5.17). In Fig. 5.16, it can be appreciated that the first point where the localisation condition is satisfied coincides with the first point entering softening, and that Eq. (5.17) has been satisfied in 6.7% of the Gauss points when the global instability occurs. In between, the localisation condition is progressively satisfied in an increasing number of Gauss points. Therefore, the instability of a single point is not particularly relevant in the context of the BVP.

5.3.5 Shear band orientation

The orientation of shear bands in geomaterials (or at least in granular ones) has been historically bounded by two limits. The upper bound is given by Coulomb’s theory, in which shear band orientation coincides with the inclination of the plane where the maximum ratio of shear to normal stress occurs,

\[ \theta_C = 45^\circ + \frac{\phi_C}{2} \] (5.19)

where \( \theta_C \) is Coulomb’s angle and \( \phi_C \) is the friction angle defining the plane of maximum stress ratio. The lower bound is given by Roscoe’s (1970) criterion where the orientation is determined by the zero extension direction with respect to the axis of minimum principal strain rate, leading to,

\[ \theta_R = 45^\circ + \frac{\psi}{2} \] (5.20)

where \( \theta_R \) is Roscoe’s angle and \( \psi \) is the dilation angle. Most laboratory observations of shear banding fall within these limits (e.g. Alshibli and Sture, 2000; Arthur et al., 1977b; Desrues and Viggiani, 2004; Finno et al., 1997; Vermeer, 1990). Vermeer (1990) also suggested that a given material tends to one of them depending on the particle size; coarse sands tend towards Roscoe’s orientation, whereas fine sands tend to show Coulomb’s orientation. However, Desrues and Viggiani (2004) argued that the orientation of a shear band is not directly related to the particles size. They also pointed out that the orientation is not constant and may evolve throughout a test. An intermediate relationship between Coulomb’s and Roscoe’s solutions was also proposed by Arthur et al. (1977b) (Eq. 5.21) and later supported.
by Vardoulakis (1980) through a bifurcation analysis.

\[ \theta_A = 45^\circ + \frac{\phi_C + \psi}{4} \]  (5.21)

where \( \theta_A \) is Arthur’s angle.

In Fig. 5.17, the resulting shear band orientation from analysis E03 was compared to those obtained from Eq. (5.19) - (5.21). The angles \( \phi_C \) and \( \psi \) for the present plane strain condition were computed throughout the simulation at a Gauss point inside the shear band (its location is also shown in Fig. 5.17), according to:

\[ \phi_C = \arcsin \left( \frac{(\sigma_1/\sigma_3) - 1}{(\sigma_1/\sigma_3) + 1} \right) \]  (5.22)

\[ \psi = \arcsin \left( -\frac{(d\epsilon_1/d\epsilon_3) + 1}{(d\epsilon_1/d\epsilon_3) - 1} \right) \]  (5.23)

where \( \sigma_1 \) and \( \sigma_3 \) are the major and minor principal stresses and \( d\epsilon_1 \) and \( d\epsilon_3 \) are the major and minor principal strain increments. The vertical displacement at the peak of the global load-displacement curve is indicated in the figure, along with the value corresponding to the onset of localisation of the BVP. Coulomb’s and Arthur’s orientations seem to overestimate the obtained shear band inclination of 55\(^\circ\), which appears to coincide with Roscoe’s criterion computed at the onset of localisation.

![Figure 5.17: Theoretical and obtained shear band orientation from analysis E03](image)

In Fig. 5.18, Roscoe’s orientation was also compared with the shear bands from analyses of set F, where smooth boundary conditions were employed. Here, the geometrical imperfection and weak element in analyses F01 and F02, respectively used to favour the onset of localisation, did not produce large heterogeneities compared to models with rough boundaries. Fewer points have begun softening before the peak of the load-displacement curve, and their number is insufficient to produce the instability of the BVP. As a result, the onset of localisation coincides with the global peak strength in both analyses. Despite having used the same parameters than in E03, each analysis delivered a different shear band orientation. Nevertheless, both of them coincide with Roscoe’s orientation at the onset of localisation.
Since the amount of dilation at the onset of localisation seems to control the orientation of the shear band, a given BVP should yield a different orientation if the flow rule (Eq. 5.7) of the constitutive law is modified. The latter was demonstrated in the analyses of set G. They share the same characteristics with the analysis E03, but different values of \( \omega \) were employed, controlling the amount of plastic volumetric strains during loading. Fig. 5.19 shows the shear bands obtained in terms of shear strains contours. As \( \omega \) is reduced, a lower dilation angle operates at the onset of localisation, producing a gentler inclination of the shear bands. Fig. 5.20 compares the obtained inclinations to those computed from Eq. (5.20). Here the vertical displacements were normalised with the corresponding value at the onset of localisation. Again, the obtained orientations at the onset of localisation are consistent with Roscoe’s criterion.

The orientation of the numerical shear bands is not in fact constant throughout the simulations; a slight change has been observed in all analyses. For example, in analysis E03 the shear band orientation reduces by about 0.3° from the instant it is first identified, until the end of the simulation. Certainly, this change is small and does not alter the conclusions drawn before, but it suggests that once a persistent shear band has formed, its orientation may still evolve due to changes in the direction of plastic flow, that in this case occurs due to a small reduction of the friction angle during softening (see Eq. 5.1, 5.3 and 5.7). To verify this hypothesis, a severe modification in the flow rule was enforced in analysis H01, by considering that \( \omega \) is no longer constant but it evolves during the simulation according to,

\[
\omega = \begin{cases} 
1 & (\epsilon_{p_{eq}}^0 \leq \xi_2) \\
 e^{-b_{\omega} \epsilon_{p_{eq}}} & (\epsilon_{p_{eq}}^0 > \xi_2) 
\end{cases} 
\]  

where \( b_{\omega} \) is a parameter controlling the rate of reduction of \( \omega \) and takes a value equal to 20 in this analysis. Apart from this difference, analysis H01 share the same characteristics as analysis E03. Fig. 5.21 shows the evolution of the shear band orientation throughout the simulation compared to that derived from Eq. (5.20). The drastic change in the direction of plastic flow during the simulation is evidenced by a reduction over 23° in the dilation.
angle from its maximum value, which in turn leads to a reduction of 11.9° in the predicted shear band orientation. Unlike previous analyses, a noticeable reduction of the shear band inclination was identified here, of around three degrees. However, this reduction is much smaller than that predicted due to changes in the dilation angle. These results suggest that once a persistent shear band has formed it is difficult to modify its orientation, and it is only possible through important changes in the direction of plastic flow.

Figure 5.19: Contours of shear strain from the set of analysis G

Figure 5.20: Theoretical and obtained shear band orientation from the set of analysis G
5.4 Plane strain tests in Beaucaire marl

A real plane strain experiment on Beaucaire marl, reported by Marello (2004), was also simulated to demonstrate the capability of the developed constitutive model to simulate localised deformations in stiff clays. The Beaucaire marl is a sedimentary overconsolidated clayey material deposited during Pleistocene, lying in the transition zone between hard soils and weak rocks. Some reference properties are summarised in Table 5.4. In particular, attention is focused on test MBLL16 that is part of a large experimental program to investigate the phenomenon of shear banding in saturated stiff clayey soils (Marello, 2004; Marello et al., 2004; Viggiani and Desrues, 2004). Fig. 5.22 shows the dimensions of the sample and a diagram of the employed plane strain compression apparatus at the laboratory 3S of Grenoble. The glass plates allow taking photographs of the in-plane deformation of the sample throughout the experiment, from which the strain fields can be later determined. For the experiment considered (MBLL16), FRS was employed to derive the deformation fields. A detailed description of this technique and of the apparatus can be found in Desrues and Viggiani (2004).

Table 5.4: Reference properties of the Beaucaire marl (from Marello et al., 2004)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay content [%]</td>
<td>30</td>
</tr>
<tr>
<td>Calcium carbonate content [%]</td>
<td>up to 30</td>
</tr>
<tr>
<td>Water content [%]</td>
<td>23 - 25</td>
</tr>
<tr>
<td>Liquid limit [%]</td>
<td>40 - 45</td>
</tr>
<tr>
<td>Plastic index [%]</td>
<td>21 - 25</td>
</tr>
<tr>
<td>Vertical yield stress, (\sigma'_y) [kPa]</td>
<td>2000</td>
</tr>
<tr>
<td>Uniaxial compressive strength, UCS [kPa]</td>
<td>900</td>
</tr>
</tbody>
</table>

After backpressure saturation and swelling under the confinement pressure, an approximately isotropic initial stress condition of 313 kPa was attained in the specimen. Shearing was performed under displacement control, at a rate of 0.004 mm/min and under globally...
drained conditions. Fig. 5.23 shows a picture of the specimen after the test, where the localised nature of deformations can be readily identified. Two roughly symmetrical shear bands formed at the bottom of the sample, from a point where a weak spot is believed to exist. Details on the testing procedures and results are given in Marello (2004).

Figure 5.22: Schematic diagram of the plane strain apparatus (Desrues and Viggiani, 2004)

Figure 5.23: Specimen MBLL16 after the test (Marello, 2004)

Fig. 5.24a shows the geometry, mesh and boundary conditions of the 2D model used for the simulation of the experiment. As silicon grease was employed to lubricate surfaces in contact with the specimen, smooth boundaries were considered for the upper and lower ends. The node with fixed horizontal displacements, employed to prevent an undetermined
system, was placed in the upper boundary. Since the formation of the shear bands begins at the lower boundary (Fig. 5.23), the placement of the fixed node there would have interfered with their propagation. As the test was performed under globally drained conditions and with a low displacement rate, hydromechanical coupling was not considered here and only a mechanical simulation was performed.

The parameters adopted are listed in Table 5.5, and they define the stress-strain behaviour of the material. However, since the localised nature of deformations in the BVP is being considered, they cannot be directly obtained from the experimental results; they should be back-calculated from the simulation of the test by modelling the BVP as close as possible. The elastic parameters are the exception, and they were derived at the initial stages of the test. The strain field can be assumed approximately homogeneous at that point, and stresses and strains can be computed directly from global measurements. A first guess for the initial and peak strength parameters ($\phi^*_{ini}$, $\phi^*_{peak}$, $c^*_{ini}$, and $p^*_{ini}$) was also determined by assuming homogeneous deformations, and deriving the corresponding stress states in experiments performed with different confinement stresses (Marello, 2004). These values were later adjusted in the simulation of the BVP. As for the residual friction angle $\phi^*_{res}$, conventional triaxial or biaxial experiments are generally insufficient to bring stiff clays to its full residual strength (Gens, 2013). However, the residual friction angle of a number of stiff clays lie in a relatively narrow range between $10^\circ$ and $16^\circ$ (Zhan, 2012). A value of $\phi^*_{res} = 15^\circ$ was assumed here for the Beaucaire marl. The length scale parameter $l_s$ was arbitrarily chosen equal to 3 mm, and the non-associative constant $\omega$ was selected to obtain the correct inclination of the fractures observed in the experiment. The remaining parameters $\xi_2$, $a_{hard}$, $b_\phi$, and $b_c$ were back-calculated with the simulation of the BVP to adjust the observed load-displacement curve. A random variation ($\pm 5\%$) of the apparent cohesion was also introduced to generate a non-uniform deformation field and facilitate the formation and propagation of the shear bands (Fig. 5.24b). In addition, a single weak element with null asymptotic cohesion was included, the location is depicted in Fig. 5.24b. This element represents a weak spot in the material, from which the shear bands propagate.

Table 5.5: Parameters of the simulation of the test on Beaucaire marl

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>kPa</td>
<td>36000</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
<td>-</td>
<td>0.37</td>
</tr>
<tr>
<td>Initial asymptotic friction angle</td>
<td>$\phi^*_{ini}$</td>
<td>$^\circ$</td>
<td>25</td>
</tr>
<tr>
<td>Peak asymptotic friction angle</td>
<td>$\phi^*_{peak}$</td>
<td>$^\circ$</td>
<td>29.4</td>
</tr>
<tr>
<td>Residual friction angle</td>
<td>$\phi^*_{res}$</td>
<td>$^\circ$</td>
<td>15</td>
</tr>
<tr>
<td>Asymptotic cohesion (mean value)</td>
<td>$c^*_{ini}$</td>
<td>kPa</td>
<td>35</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>$p^*_{ini}$</td>
<td>kPa</td>
<td>0</td>
</tr>
<tr>
<td>Equivalent strain at peak strength</td>
<td>$\xi_2$</td>
<td>-</td>
<td>0.009</td>
</tr>
<tr>
<td>Constant in hardening law</td>
<td>$a_{hard}$</td>
<td>-</td>
<td>0.005</td>
</tr>
<tr>
<td>Rate of reduction of friction angle</td>
<td>$b_\phi$</td>
<td>-</td>
<td>0.05</td>
</tr>
<tr>
<td>Rate of reduction of cohesion</td>
<td>$b_c$</td>
<td>-</td>
<td>15</td>
</tr>
<tr>
<td>Non-associative constant</td>
<td>$\omega$</td>
<td>-</td>
<td>0.8</td>
</tr>
<tr>
<td>Length scale parameter</td>
<td>$l_s$</td>
<td>cm</td>
<td>0.3</td>
</tr>
</tbody>
</table>
Fig. 5.24: Geometry, mesh, and boundary conditions for the simulation of the experiment. (b) Non-uniform distribution of the asymptotic cohesion.

Fig. 5.25: Experimental (Marello, 2004) and simulated axial load vs. global axial strain curves from a plane strain compression test on stiff Beaucaire marl.

Fig. 5.25 shows the deviator load vs. the global axial strain (i.e. computed from the vertical displacement of the loading platen and the initial height of the sample) derived from the experiment, together with the simulation results. A good agreement between both is clearly apparent. The open crosses designate the points where photographs were taken during the test to obtain the deformation fields. Fig. 5.26, shows the incremental shear strain field between points 5 and 6, where the persistent localisation pattern was clearly visible. The two persistent shear bands were well captured by the FRS technique (compare with Fig. 5.23). Fig. 5.26b and 5.26c shows the incremental shear strain field obtained from the simulation in the same interval. In Fig. 5.26b results are presented in the same format than Marello (2004) to allow direct comparison between them. Note that the scale is also the
same. The simulation satisfactorily captured the localised deformation pattern observed in the experiment. In addition, similar values of shear strain were obtained. The point where the shear bands initiate was determined by the location of the weak element. However, no assumptions were made regarding the orientation of the shear bands, which is the result of the constitutive behaviour. The thickness of the shear bands is also quite similar although both, the FRS and the simulation, overestimate the real width of the localised zone (see Fig. 5.23). The first one due to the coarseness of the grid where the displacement field was computed and the second one is the result of the chosen length scale parameter. Nevertheless, these larger numerical shear bands represent adequately the real deformation process and, therefore, a good agreement with the global response was obtained.

Figure 5.26: Incremental field of shear strain from a plane strain compression test on stiff Beaucaire marl: (a) experimental (Marello, 2004) and (b,c) simulation results

5.5 Conclusions

A nonlocal approach was applied to an elastoplastic constitutive model for the objective simulation of localised deformations in stiff clays. A number of analyses were performed, from which the following conclusion can be drawn:

- The combination of the constitutive model with the nonlocal approach using the averaging function from Galavi and Schweiger (2010) provides excellent results preventing the usual pathologies arising from the continuum simulation of strain localisation. Shear band thickness and global load-displacement curves are independent of mesh refinement and element size.

- Softening scaling is required in the analysis of real problems because of the very small thickness of localised strains in stiff clayey materials. It has been found that, in spite of the nonlinearity of the behaviour modelled, the relationship between the length scale parameter and the softening rate seems to be linear.

- The overall behaviour of problems exhibiting localisation does not only depend on the constitutive behaviour, boundary conditions and the presence of imperfections have a significant influence on the computed configuration of the localised deformation pattern.
A criterion is proposed to identify objectively the onset of localisation in a BVP. It was observed that this onset occurs either at the global peak strength, or slightly before it. This is consistent with experimental evidence (Desrues and Viggiani, 2004).

The orientation of the numerical shear bands at the point identified as the onset of localisation seems to coincide with Roscoe’s criterion based on the orientation of the zero-extension line. It has also been observed that, once a persistent shear band has formed, it is difficult to modify its orientation. Modest orientation changes are only possible through drastic changes in the direction of plastic flow.

The formulation developed has proved to be readily transferable to 3D computations.

The satisfactory simulation of a real biaxial experiment provides additional confidence in the application of the presented approach for the simulation of localised deformation in stiff clays.
Chapter 6

Numerical simulation of an underground excavation using nonlocal regularisation. Part 1: formulation and base case

Based on a manuscript to be submitted.

Abstract

The paper addresses the numerical simulation of an underground excavation in the Callovo-Oxfordian argillaceous formation (COx), within the context of deep geological nuclear waste disposal. A constitutive model is described, including a number of features that are considered relevant for the satisfactory simulation of the COx. Particularly, the ability to simulate localised deformations objectively with the incorporation of a nonlocal regularisation. Important insights are presented about the relevance of the EDZ in the short- and long-term behaviour of the excavation and, in particular, with the generation of overpressures deep into the clay rock.

6.1 Introduction

Nowadays, there is a strong international consensus that deep geological disposal is the most appropriated solution for the management of high-activity and long-lived radioactive waste (NEA, 2008). As possible geological host medium, stiff clayey formations are an appealing alternative thanks to favourable properties such as its low hydraulic conductivity, low molecular diffusion, and significant radionuclide retention capacity (Armand et al., 2017b). In this context, the French national radioactive waste management agency (Andra) started in 2000 the construction of the Meuse/Haute-Marne (MHM) underground research laboratory (URL) at Bure, in the Callovo-Oxfordian argillaceous formation, in order to demonstrate the feasibility of this geological unit to host a nuclear waste repository (Andra, 2005a). The main level of the URL consists of a network of drifts excavated horizontally at a depth of 490 m, where several in situ experiments have been performed to assess the thermo-hydro-mechanical behaviour of the COx under real working conditions (Armand et al., 2017a; Delay
et al., 2007). These experiments have revealed that excavation operations induce damage and fracturing around the galleries (Armand et al., 2014), creating a zone known as the excavation damaged zone (EDZ), where significant changes in flow and transport properties take place (Tsang et al., 2005). The observed configuration of the EDZ depends on the orientation of the excavation with respect to the anisotropic in situ stress state. The drifts parallel to the major horizontal stress $\sigma_H$ have a nearly isotropic stress state in the plane normal to the tunnel axis. However, the EDZ extends further in the horizontal direction (Fig. 6.1), suggesting strong anisotropic characteristics of the rock mass. On the other hand, drifts parallel to the minor horizontal stress $\sigma_h$ exhibit an EDZ extending further in the vertical direction (Fig. 6.2).

![Diagram of induced fractures network around a drift](image)

Figure 6.1: Conceptual model of the induced fractures network around a drift parallel to the horizontal major stress (Armand et al., 2014).

The EDZ is identified as one of the key issues affecting the long-term behaviour of the tunnel near-field (Blümling et al., 2007). Major efforts have been made to simulate these experimental excavations (Seyedi and Gens, 2017), and to gain insights into the design of the actual repository. However, the localised nature of deformations occurring in the EDZ, as a result of the quasi-brittle behaviour of the COx, poses an important problem. Standard for-
nulations based on continuum mechanics, in combination with strain softening constitutive laws, tend to deliver non-objective results in the form of a strong dependency with the employed mesh (de Borst et al., 1993). Different approaches have been so far applied for the simulation of excavations dealing with localised deformations in the context of nuclear waste disposal. Perhaps, the most extended technique used is the local second gradient model (Pardoen and Collin, 2017; Pardoen et al., 2015; Salehnia et al., 2015; van den Eijnden et al., 2017), although other approaches such as the extended rigid block spring method (Yao et al., 2017) and the combined finite-discrete element method (Lisjak et al., 2014) have also been applied.

![Figure 6.2: Conceptual model of the induced fractures network around a drift parallel to the horizontal minor stress (Armand et al., 2014).](image)

The present paper presents a detailed simulation of the GCS drift at the MHM URL. In fact, in the context of the Transverse Action benchmark programme (Seyedi et al., 2017), the authors had performed a previous simulation of this drift. However, localised deformations were not treated in that research, which is the main focus of the present work. The constitutive model employed incorporates a number of features that are considered relevant for the satisfactory simulation of the COx claystone. Particularly, the ability to simulate localised deformations objectively with the incorporation of a nonlocal regularisation. By dealing with the localisation problem, new insights are presented about the relevance of the EDZ in the short- and long-term behaviour of the excavation, in particular with the generation of overpressures deep into the clay rock. In a second paper, a sensitivity study is presented where the influence of different parameters on the excavation response is addressed (Mánica et al., 2018c).

### 6.2 Constitutive model

The constitutive model employed represents an enhanced version with respect to that used in previous works (Mánica et al., 2017c, 2018a). At the uppermost level, it can be considered as a superposition model (Tirpitz and Schwesig, 1992) in which a small strain increment is decomposed as,

\[
d\epsilon = d\epsilon^e + \epsilon^{yp} + \epsilon^c
\]  

(6.1)
where $\epsilon$, $\epsilon^e$, $\epsilon^{vp}$, and $\epsilon^c$ are respectively the total, elastic, visco-plastic and creep strain tensors. The first two terms are described under the framework of elasto-visco-plasticity, particularly by the over-stress theory of Perzyna (1966), and an additional creep mechanism is considered. The main components of the local model are presented in section 6.2.1 assuming classical rate-independent elasto-plasticity, while extension to visco-plasticity and the additional creep mechanism are described in section 6.2.2. A brief description of the employed nonlocal regularisation for the simulation of localised deformations is given in section 6.2.3, and components of the hydraulic model are described in section 6.2.4. The resulting algorithm was implemented as a user-defined soil model in the finite element code Plaxis, which was used for the fully coupled hydro-mechanical simulations described below. Details about the hydro-mechanical formulation in Plaxis can be found elsewhere (Brinkgreve et al., 2017).

### 6.2.1 Rate-independent plasticity

Inside the failure surface the response is assumed linear elastic, characterised by a transverse isotropic (cross-anisotropic) form of the Hooke’s law (Wittke, 1990). The yield envelope is defined by a hyperbolic approximation of the Mohr-Coulomb criterion (Gens et al., 1990),

$$f = \sqrt{\frac{J_2}{f_2(\theta)}} + (c^* + p_t \tan \phi^*)^2 - (c^* + p' \tan \phi^*)$$  \hfill (6.2)

where $c^*$ is the asymptotic cohesion, $\phi^*$ is the asymptotic friction angle, $p_t$ is the isotropic tensile strength, $p'$ is the effective mean stress, $J_2$ is the second invariant of the deviatoric stress tensor $s$, $\theta$ is the Lode’s angle, and $f_2(\theta)$ defines the shape of the yield surface in the octahedral plane. For $f_2(\theta)$, the following generalised function was employed (van Eekelen, 1980),

$$f_2(\theta) = \alpha^\theta \left(1 + \beta^\theta \sin 3\theta\right)^n$$  \hfill (6.3)

Strength anisotropy is included by assuming that $c^*$ and $p_t$ depend on the relative orientation between bedding and principal effective stresses; the frictional component is considered isotropic. For instance, the asymptotic cohesion is defined as,

$$c^* = \Omega(\delta)c_0^*$$  \hfill (6.4)

where $c_0^*$ is the asymptotic cohesion measured with the major principal stress normal to bedding, $\delta$ is the angle between the normal to bedding and the major principal stress, and $\Omega(\delta)$ is a given function defining the variation of cohesion with $\delta$. The same variation applies for $p_t$. The function proposed in Conesa et al. (2018) is used here for $\Omega(\delta)$, defined as,

$$\Omega = \frac{\hat{A}e^{(\delta_m-\delta)m} + \hat{B}}{1 + e^{(\delta_m-\delta)m} + \hat{C}}$$  \hfill (6.5)

where

$$\hat{A} = \frac{2(e_1 + 1)(e_2 + 1)(e_1 - e_2 + \Omega_90 + e_1e_2 + e_1\Omega_90 - e_2\Omega_90 - 2e_1\Omega_m + 2e_2\Omega_m - e_1e_2\Omega_90 - 1)}{(e_1 - e_2)(e_1 - 1)(e_2 - 1)}$$  \hfill (6.6)
\[
\dot{B} = \frac{\Omega_{90} - \frac{\dot{A}e_1}{(e_1+1)^2} + \frac{\dot{A}e_2}{(e_2+1)^2} - 1}{\frac{1}{e_1+1} - \frac{1}{e_2+1}}
\]

(6.7)

\[
\dot{C} = 1 - \frac{\dot{A}e_2}{(e_2+1)^2} - \frac{\dot{B}}{e_2+1}
\]

(6.8)

\[
e_1 = e^{(\delta_m-90)\hat{n}}
\]

(6.9)

\[
e_2 = e^{\hat{n}\delta_m}
\]

(6.10)

and \(\Omega_{90}, \Omega_m, \delta_m\) and \(\hat{n}\) are material parameters (see Conesa et al., 2018, for further details).

After reaching the failure surface, non-linear softening is considered, driven by the evolution of the strength parameters. An exponential law is employed, but distinction is made between the post-rupture and residual strengths (Burland, 1990),

\[
\tan \phi^* = \tan \phi_{ini}^* - (\tan \phi_{ini}^* - \tan \phi_{res}^*) \left[ 1 - e^{-b_{res}(\varepsilon_{eq}^p - \xi_2)} \right]
\]

(6.11)

\[
\varepsilon_0^* = (\varepsilon_0^*_{ini} - \varepsilon_0^*_{post}) e^{-b_{post}(\varepsilon_{eq}^p - \xi_2)} + \varepsilon_0^*_{post} e^{-b_{res}(\varepsilon_{eq}^p - \xi_2)}
\]

(6.12)

\[
p_0 = (p_0^*_{ini} - p_0^*_{post}) e^{-b_{post}(\varepsilon_{eq}^p - \xi_2)} + p_0^*_{post} e^{-b_{res}(\varepsilon_{eq}^p - \xi_2)}
\]

(6.13)

where \(b_{post}\) and \(b_{res}\) are the softening rates related to the post-rupture and residual strengths respectively, \(\varepsilon_{eq}^p\) is a state variable controlling the evolution of the mobilised strength as a function of plastic deformations, defined as,

\[
\varepsilon_{eq}^p = (\varepsilon^p : \varepsilon^p)^{1/2}
\]

(6.14)

A post-rupture ratio is defined so that the post-rupture parameters are a function of the initial ones,

\[
r_{post} = \frac{\varepsilon_0^*_{post}}{\varepsilon_0^*_{ini}} = \frac{p_0^*_{post}}{p_0^*_{ini}}
\]

(6.15)

In the residual state, cohesion and tensile strengths have completely disappeared, and only the residual frictional component remains (Gens, 2013).

A non-associated flow rule is adopted for the development of plastic deformations. Rather than deriving a specific function for the plastic potential, the flow rule is directly obtained from the yield criterion in the following way,

\[
\frac{\partial g}{\partial \sigma'} = \omega \frac{\partial f}{\partial p'} \frac{\partial p'}{\partial \sigma'} + \frac{\partial f}{\partial J_2} \frac{\partial J_2}{\partial \sigma'} + \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial \sigma'}
\]

(6.16)

where \(g\) is the plastic potential, \(\sigma'\) is the effective stress tensor, and \(\omega\) is a constant controlling the volumetric component of plastic deformations. With \(\omega = 1\) an associated flow rule is recovered, while with \(\omega = 0\) no volumetric plastic strains occur. An adequate value for geomaterials should lie between those limits.
6.2.2 Visco-plasticity and creep deformations

Following Perzyna (1966), extension to visco-plasticity is obtained by defining the visco-plastic strain increment as,

$$d\varepsilon_{vp} = \left\langle \frac{\Phi(f)}{\eta_{pz}} \frac{\partial g}{\partial \sigma'} \right\rangle$$  \hspace{1cm} (6.17)

where $\eta_{pz}$ is a viscosity parameter and $\Phi$ is the over-stress function expressed as,

$$\Phi(f) = \left( \frac{f}{p_{atm}} \right)^N$$  \hspace{1cm} (6.18)

where $p_{atm}$ is a normalising stress, set here to 100 kPa, and $N$ is a parameter that should satisfy $N \geq 1$ (Simo, 1989), and defines the order of the Perzyna’s formulation.

As for the creep component, strain increments are computed as,

$$d\varepsilon_c = \dot{\varepsilon}_c dt$$  \hspace{1cm} (6.19)

where $t$ is the time and $\dot{\varepsilon}_c$ is the creep strain rate tensor, defined as,

$$\dot{\varepsilon}_c = \begin{cases} 
0 & (\varepsilon_{eq}^p \leq \varepsilon_{thr}) \\
\dot{\varepsilon}_c = \gamma_c e^{(-\alpha_c^v \varepsilon_{eq})} (s + \psi_c p I) & (\varepsilon_{eq}^p \leq \varepsilon_{thr})
\end{cases}$$  \hspace{1cm} (6.20)

where $\gamma_c$, $\alpha_c$ and $\psi_c$ are material parameters, $\varepsilon_{eq}^p$ is the state variable for the creep component (Eq. 6.21), and $\varepsilon_{thr}$ is a threshold defining the level of plastic deformations at which creep deformations are activated.

$$\varepsilon_{eq}^c = (\varepsilon^c : \varepsilon^c)^{1/2}$$  \hspace{1cm} (6.21)

Creep strains are coupled with the visco-plastic component, and can mobilise the strength. The latter is achieved by defining the plastic strain tensor $\varepsilon^p$, used in Eq. (6.14), as the sum of the visco-plastic and creep strains $\varepsilon^p = \varepsilon^{vp} + \varepsilon^c$. This allows the occurrence, under certain circumstances, of creep failure.

6.2.3 Nonlocal regularisation

The model employed is capable to simulate objectively localised deformations using a nonlocal regularisation. Here, the local state variable $\varepsilon_{eq}^p$ is replaced by its nonlocal counterpart,

$$\varepsilon_{eq}^{vp} = \int_V w(X, \kappa) \varepsilon_{eq}^p \kappa d\kappa$$  \hspace{1cm} (6.22)

where $V$ stands for volume and $w$ is a weighting function controlling the importance of neighbouring points as a function of its position ($\kappa$), relative to the position of the actual point under consideration ($X$). The weighting function is usually defined in the following normalised form,

$$w(X, \kappa) = \frac{w_0(||X - \kappa||)}{\int_V w_0(||X - Y||) dY}$$  \hspace{1cm} (6.23)
where \( w_0 \) is characterised here by the expression proposed by Galavi and Schweiger (2010),

\[
w_0 = \frac{||X - \kappa||}{l_s} e^{-((||X - \kappa||/l_s)^2)}
\]  

(6.24)

where \( l_s \) is a parameter introducing an internal length scale to the material behaviour. Compared to the widely employed Gaussian function (e.g. Bažant and Lin, 1988), the use of Eq. (6.24) has shown improved results in terms of consistency and mesh independence (Summersgill et al., 2017a). Details about the implementation of the employed nonlocal approach and its ability to simulate localised deformations in stiff clays has been given elsewhere (Mánica et al., 2018a).

### 6.2.4 Hydraulic

The constitutive law described is defined in terms of effective stresses, accounting for the influence of the pore water pressure. A generalised expression has been adopted here for the definition of the effective stress tensor,

\[
\sigma' = \sigma + S_e s_u B I
\]  

(6.25)

where \( \sigma \) is the total stress tensor, \( S_e \) is the effective degree of saturation, \( s_u \) is the suction, \( B \) is Biot’s coefficient and \( I \) is the identity tensor. For saturated conditions, Eq. (6.25) reduces to,

\[
\sigma' = \sigma - p_l B I
\]  

(6.26)

where the pore water pressure \( p_l \) is equated to \(-s_u\).

In case of unsaturation the retention curve, linking suction and the effective degree of saturation, is given by the following modified van Genuchten (1980) expression,

\[
S_e = \frac{S_i - S_{ir}}{S_{ls} - S_{ir}} = \left[ 1 + \left( \frac{s_u}{P} \right)^{\frac{1}{\lambda'}} \right]^{-\lambda'}
\]  

(6.27)

where \( S_i \) is the degree of saturation, \( S_{ir} \) is the residual degree of saturation, \( S_{ls} \) is the degree of saturation in saturated conditions (normally 1), and \( P \) and \( \lambda' \) are model parameters.

Water flow is governed by Darcy’s law using a hydraulic conductivity given by,

\[
K = \frac{k k_r}{\mu_w}
\]  

(6.28)

where \( k \) is the intrinsic permeability tensor, \( k_r \) is the relative permeability, and \( \mu_w \) is the water viscosity. The relative permeability is considered a function of the effective degree of saturation, where the expression from van Genuchten (1980) has been employed,

\[
k_r = S_e^{1/2} \left[ 1 - \left( 1 - S_e^{1/\lambda'} \right)^{\lambda'} \right]^2
\]  

(6.29)

As for the intrinsic permeability, it is assumed that it evolves with deformation in order
to account for the observed permeability increase due to damage in the COx (e.g. Armand et al., 2014). The expression from Pardoen et al. (2016) was used here, which is inspired on the classical cubic law (Witherspoon et al., 1980),

\[ k = k_0 \left[ 1 + \beta^k (\epsilon^p_{eq})^3 \right] \] (6.30)

where \( \beta^k \) is an evolution parameter.

6.3 Simulation of the GCS drift

6.3.1 The GCS drift

The constitutive model described above was applied to the simulation of the drift GCS, excavated at the main level of the MHM URL (-490 m). Fig. 4.7 shows the location of the drift in a three-dimensional view of the URL. The \textit{in situ} stress state was determined by Wileveau et al. (2007). At the main URL level, an anisotropic state is found with \( \sigma_H \approx 16 \text{MPa} \) and \( \sigma_v \approx \sigma_h \approx 12 \text{MPa} \), where \( \sigma_v \) is the vertical stress. The initial pore water pressure (i.e. unaffected by excavation works) at this level is estimated to be around 4.7 MPa (Armand et al., 2014, 2013). The GCS drift is oriented N155°E, parallel to \( \sigma_H \), and, therefore, a nearly isotropic stress state exists in the plane normal to the excavation axis. As mentioned before, this corresponds to excavations where the EDZ extends further in the horizontal direction (Fig. 6.1) and where horizontal convergences are larger than vertical ones (Armand et al., 2013; Seyedi et al., 2017).

The drift was excavated using a road header with advances of about 1.2 m long (three passes \( \approx 40 \text{ cm each} \)) at an approximate rate of 2.5 m per week (Bonnet-Eymard et al., 2011b). A flexible support system was adopted to allow the deformation of the rock (Bonnet-Eymard et al., 2011b) and, hence, to study the hydro-mechanical response of the COx to excavation operations. It comprises an 18 cm thick fiber reinforced shotcrete shell, interrupted by 12 yielding wedges, and a crown of 3 m-long 12 HA25 radial bolts every meter.

![Image: Location of measurement points used for comparison with the simulation.](image_url)
(Armand et al., 2013). A comprehensive description of the excavation works can be found in Bonnet-Eymard et al. (2011a,b). Monitoring of displacements and pore water pressures were performed from boreholes drilled from nearby tunnels and from the actual drift behind the excavation front. In the former case, observations included the ground response in advance of the excavation. Convergences were also monitored in a number of measurement sections. A detailed account of the instrumentation at the GCS is given in Seyedi et al. (2017). Fig. 6.3 shows the field measurement points that are used for comparison with the numerical simulation. They correspond to the horizontal extensometer OHZ1501 and the two pressure measurement boreholes OHZ1521 and OHZ1522. Numerical results are also compared with the vertical and horizontal convergences recorded at different sections.

6.3.2 Main features of the finite element model

Several characteristics of the FE simulation presented here correspond to the Action Transverse benchmark (Seyedi et al., 2017) and, consequently, to the previous simulation of the GCS drift carried out by the authors (Mánica et al., 2017c). Improvements with respect to this previous work concern mainly the constitutive description of the COx and, particularly, the objective simulation of localised plastic deformations (Mánica et al., 2018a). The two main simplifying assumptions in the present analysis are the adoption of plane strain conditions and neglecting the gravity gradient. Regarding the first one, underground excavations are intrinsically a three-dimensional (3D) problem. Nevertheless, in the presence of localised plastic deformations, a fine discretisation of the domain is generally required and, therefore, 3D simulations tend to exceed conventional computational capacities. In those situations, 2D plane strain analyses are, for the moment, the main alternative to incorporate localisation in the simulation of geotechnical problems such as the stability of slopes (Summersgill et al., 2017b) or underground excavations (Pardoen et al., 2015). Furthermore, in the case of flexible supports with completion close to the face (as in the GCS drift), the difference between 2D (plane strain) and 3D analyses tend to be small (Cantieni and Anagnostou, 2009). Concerning the gravity assumption, it has been shown that the stress magnitudes at the Bure site do not vary linearly with depth and that the vertical variations are controlled by the rheological characteristics of the various formations (Cornet and Röckel, 2012). Therefore, neglecting the gravity gradient is, in fact, a reasonable assumption. In addition, it allows us to preserve two axes of symmetry and to model only a quarter of the gallery.

Fig. 6.4 shows the geometry of the problem, the boundary conditions, and the FE mesh employed in the analysis. The mesh comprises 20028 6-noded triangular finite elements with second-order interpolation. It is highly refined around the excavation, where localised plastic deformations are expected to occur. The criterion given by Galavi and Schweiger (2010) was fulfilled in this zone; it requires that,

$$l_s \geq L_{el}$$  \hspace{1cm} (6.31)

where $L_{el}$ is the maximum length of an element. As shown later, all plastic processes take place in this zone. The remaining elements stay elastic the entire simulation and, therefore, such a high refinement is not required. A uniform initial stress state and pore water pressure distribution was considered in the model. The actual magnitudes correspond to those suggested in the benchmark specifications (Seyedi et al., 2017). The nearly isotropic stress state
on the plane of analysis can be noted in Fig. 6.4. For comparison, a hypothetical excavation oriented parallel to \( \sigma_h \) was also analysed, i.e. with an anisotropic stress state on the plane of analysis. As previously mentioned, this corresponds to excavations in the URL where the EDZ extends further in the vertical direction (Fig. 6.2) and where vertical convergences are larger than horizontal ones (Armand et al., 2013; Seyedi et al., 2017).

![Figure 6.4: Geometry, boundary conditions and finite element mesh employed.](image)

In the tunnel wall, the corresponding radial stresses were applied to ensure initial equilibrium. Then, this stresses were gradually reduced to simulate the excavation as a function of the position of the front. The deconfinement curve in Fig. 6.5 was adopted (Unlu and Gercek, 2003). In that figure, and throughout the paper, time equal to zero corresponds to the excavation front at the analysis section. The flexible support system, previously described, was not explicitly considered in the simulation. Nevertheless, field measurements at the GCS drift indicate that this type of support applies to the ground a mean radial stress of about
Therefore, the deconfinement ratio is not reduced to zero, but to the value corresponding to the observed confinement applied by the support. Regarding the hydraulic boundary conditions, null fluxes were prescribed at the excavation wall while the front face lies behind the analysis section. Thereafter, zero water pressure is prescribed at this boundary. Actually, a complex interaction takes place between the COx, the shotcrete support, and the circulating air in the gallery, resulting in water transfer and potential desaturation of the claystone. Efforts for a more comprehensive simulation of this kind of boundary condition can be found for instance in Pardoen et al. (2016). In the present analysis, the simulation of the unsaturated zone in the COx is not a main objective and, therefore, the zero liquid pressure boundary condition is considered sufficient. In addition, ventilation experiments at the Mont Terri (Mayor et al., 2007) and MHM (Armand et al., 2016) URLs revealed that the effect of dry air circulation is limited, and the unsaturated zone only extends a few tens of centimetres into the claystone.

![Figure 6.5: Deconfinement curve for radial stresses on the tunnel wall.](image)

### 6.3.3 Model parameters for the COx claystone

A summary of the employed parameters is given in Table 6.1.

#### Elastic parameters

For the Young’s modulus $E_2$ and Poisson’s ratio $\nu_2$, the commonly reported values of 4000 and 0.3 were respectively used (Armand et al., 2014, 2013). The anisotropy ratio between $E_1$ and $E_2$ is found to vary between 1.2 and 2.0 (Armand et al., 2013); the former value has been employed in this research. As it will be shown later, this ratio is closely related with the observed over-pressures in the COx due to excavation operations. Regarding $\nu_1$ and $G_2$, experimental evidence is scarce and more research is needed to fully characterise the transverse-isotropic elastic constants of the COx. In similar materials, such as the Opalinus clay, $\nu_1$ is somewhat smaller than $\nu_2$ (Gens et al., 2007). A value of 0.25 was adopted here for $\nu_1$. In the case of the independent shear modulus $G_2$, the theoretical upper bound from Kiehl (1980) was used, derived from a plane strain analysis of the expansion of a cylindrical cavity (Eq. 6.32).
Table 6.1: Parameters of base analysis A01.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic</strong></td>
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<td></td>
</tr>
<tr>
<td>Young’s modulus parallel to the isotropic plane</td>
<td>$E_1$</td>
<td>MPa</td>
<td>8000</td>
</tr>
<tr>
<td>Young’s modulus perpendicular to the isotropic plane</td>
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<td>MPa</td>
<td>4000</td>
</tr>
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<td>Poisson’s ratio between the two strain components on the</td>
<td>$\nu_1$</td>
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</tr>
<tr>
<td>isotropic plane for loading parallel to the isotropic plane</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio between strain components on the isotropic</td>
<td>$\nu_2$</td>
<td>-</td>
<td>0.3</td>
</tr>
<tr>
<td>plane and the component perpendicular thereto for loading</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>perpendicular to the isotropic plane</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Shear modulus on the planes perpendicular to the isotropic</td>
<td>$G_2$</td>
<td>MPa</td>
<td>2010</td>
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<tr>
<td><strong>Peak, post-rupture, and residual strength</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Peak asymptotic friction angle</td>
<td>$\phi^*_{\text{peak}}$</td>
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<td>20</td>
</tr>
<tr>
<td>Residual friction angle</td>
<td>$\phi^*_{\text{res}}$</td>
<td>$^\circ$</td>
<td>16</td>
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<td>Asymptotic cohesion</td>
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<td>MPa</td>
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<td>Isotropic tensile strength</td>
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<tr>
<td>Post-rupture softening rate</td>
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</tr>
<tr>
<td>Residual softening rate</td>
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<td><strong>Plastic potential</strong></td>
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<td>Non-associativity constant</td>
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<tr>
<td><strong>Visco-plasticity</strong></td>
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</tr>
<tr>
<td>Order of Perzyna’s formulation</td>
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<td>-</td>
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<tr>
<td>Viscosity parameter</td>
<td>$\eta_{\text{ps}}$</td>
<td>MPa-day</td>
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<td><strong>Strength anisotropy</strong></td>
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<td>Parameter for the variation of cohesion with the loading</td>
<td>$\Omega_{90}$</td>
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<tr>
<td>Parameter for the variation of cohesion with the loading</td>
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<td>direction</td>
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<td></td>
</tr>
<tr>
<td><strong>Creep</strong></td>
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<td>Parameter in the creep law</td>
<td>$\gamma^c$</td>
<td>MPa$^{-1}$day$^{-1}$</td>
<td>7.4E-7</td>
</tr>
<tr>
<td>Parameter in the creep law</td>
<td>$\psi^c$</td>
<td>-</td>
<td>0.3</td>
</tr>
<tr>
<td>Parameter in the creep law</td>
<td>$a^c$</td>
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<tr>
<td>Threshold for creep activation</td>
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<td>-</td>
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<td><strong>Hydraulic</strong></td>
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<td></td>
</tr>
<tr>
<td>Intact horizontal intrinsic permeability</td>
<td>$k_{0xx}$</td>
<td>m$^2$</td>
<td>5E-20</td>
</tr>
<tr>
<td>Permeability anisotropy ratio</td>
<td>$k_{0xx}/k_{0yy}$</td>
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<td>2</td>
</tr>
<tr>
<td>Parameter for the increase of permeability with damage</td>
<td>$\beta^k$</td>
<td>-</td>
<td>4E7</td>
</tr>
<tr>
<td>Parameter in the retention curve</td>
<td>$\chi^r$</td>
<td>-</td>
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</tr>
<tr>
<td>Parameter in the retention curve</td>
<td>$P$</td>
<td>MPa</td>
<td>17.6</td>
</tr>
<tr>
<td>Biot’s coefficient</td>
<td>$B$</td>
<td>-</td>
<td>0.6</td>
</tr>
<tr>
<td><strong>Nonlocal approach</strong></td>
<td></td>
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<tr>
<td>Length scale parameter</td>
<td>$l_s$</td>
<td>m</td>
<td>0.15</td>
</tr>
</tbody>
</table>
\[ G_2 \leq \frac{E_2}{2 \left[ \nu_2 (1 + \nu_1) + \sqrt{(E_2/E_1 - \nu_1^2)} \left( 1 - \nu_1^2 \right) \right]} \] (6.32)

**Peak, post-rupture, and residual strength**

Due to the viscous effects brought about by the overs-stress formulation (Eq. 6.17 and 6.18), the peak strength obtained from the constitutive model depends on the loading rate. In fact, this behaviour is observed in the COx, and the strength seems to increase for higher loading rates (Andra, 2014a). Therefore, peak strength parameters were calibrated together with the viscosity parameter \( \eta_{pz} \). A first-order over-stress function was adopted \((N = 1)\). A set of triaxial tests with different confinement stresses and loading rates (Andra, 2014a; Armand et al., 2017b) were simulated to back-calculate the peak strength and viscosity parameters. In the experiments, the samples were equilibrated to a 90% relative humidity \((H_R)\) environment to guarantee uniform conditions between different samples (Armand et al., 2017b). However, this preconditioning may have resulted in an increased strength due to the related suction, which must be accounted so as not to overestimate the effective strength parameters. The initial suction imposed, related to a 90% \( H_R \), was estimated using Kelvin’s equation,

\[ s_u = -\frac{RT_e}{M_w} \rho_l \ln(H_R) \] (6.33)

where \( R \) is the universal gas constant, \( T_e \) is the temperature, \( M_w \) is the water molar mass, and \( \rho_l \) is the density of the water. Assuming \( R = 8.314 \text{ J/mol/K} \), \( M_w = 0.018 \text{ kg/mol} \), \( \rho_l = 1000 \text{ kg/m}^3 \) and \( T_e = 20^\circ C \) \((293.15^\circ K)\), a suction of 14.26 MPa was determined. This value was considered as the initial condition of the samples for the simulation, and as a boundary condition for the top and bottom ends. The parameters for the retention curve and relative permeability models employed (Eq. 6.27 and 6.29) are also given in Table 6.1. The retention curve is depicted in Fig. 6.6 representing a mean curve of a number of experimental studies to characterise the water retention behaviour of the COx (Armand et al., 2017b). The intact saturated intrinsic permeability in the horizontal direction was assumed equal to 5.0E-20, a commonly reported value for the COx (Armand et al., 2017b, 2014, 2013), and the ratio between horizontal and vertical permeabilities equal to 2. Regarding Biot’s coefficient, a value of 0.6 was adopted, which is a frequently employed value in numerical simulations of the COx (Jia et al., 2010; Pardoen et al., 2015; Seyedi et al., 2017). Fig. 6.7 shows the obtained values of peak strength along with the experimental data. A reasonable agreement can be noticed. It is important to mention that all parameters involved in the simulation of the tests were also employed in the analyses of the drifts, except for the initial unsaturation. An initial saturated condition was assumed in that case, as observed in the URL.

From a comprehensive literature review on stiff clayey materials, Zhan (2012) showed that at the post-rupture strength the cohesion is generally not completely lost. He found mean values of \( r_{post} = c_{post}/c_{peak} \) between 0.3 and 0.5, this ratio becoming larger with increasing clay activity. A value of 0.3 was employed here for the COx, which shows a rather low clay activity (around 0.29). Zhan (2012) also confirmed that at the residual state, the remaining cohesion is completely lost and only a frictional strength remains. The values of the residual friction angle of a number of stiff clays lie in a relatively narrow range between 10° and
16°, with a slight tendency to decrease with increasing clay activity (Zhan 2012). Here, the residual friction angle was assumed equal to 16°.

![Figure 6.6: Water retention curve employed and experimental data for the COx (Armand et al., 2017b).](image)

![Figure 6.7: Experimental (Andra, 2014a; Armand et al., 2017b) and simulated peak strengths as a function of confinement stress and strain rate.](image)

As shown in Mánica et al. (2018a), the softening rate is closely related to the length scale parameter of the nonlocal regularisation $l_s$. In the model described in section 6.2.1, explicit distinction is made between post-rupture and residual strengths (Eq. 6.12 and 6.13), and different softening rates are considered for each one of them. The rate associated with the residual strength is generally assumed small, since very large displacements are required to reach this stage (Gens, 2013). In the case of small softening rates, Mánica et al. (2018a) showed that mesh dependency issues are negligible, and the scaling of the softening rate according to $l_s$ is not required. On the other hand, the drop form peak strength to post-rupture strength is very fast, and the softening rate must be scaled according to the selected...
$l_s$, which in turn is related to the size of the finite elements (Eq. 6.31). For $b_{res}$, a value of 2 was considered adequate (Mánica et al., 2018a). In the case of $b_{post}$, a calibration was performed with the drift simulation, and a value of 160 was found reasonable according to the employed $l_s$ of 15 cm. This value was also found to be of the same order of magnitude than the one obtained extrapolating the linear relationship between the softening rate and the length scale parameter given in Mánica et al. (2018a).

**Strength anisotropy**

Although experimental evidence regarding strength anisotropy of the COx is scarce, it is fairly accepted that the minimum strength is found when the specimen is oriented at an intermediate orientation with respect to the major principal stress ($\delta$), around 45° to 60° (Armand et al., 2017b). However, there is still no consensus about the difference in the strength when the major principal stress is oriented parallel and perpendicular to bedding. In the late 1960s, Skempton and Hutchinson (1969) presented experimental evidence suggesting the progressive evolution of anisotropy in clayey soils with over-consolidation ratio. They noted that for normally- or lightly over-consolidated clays the undrained strength is highest when loading is perpendicular to bedding ($\delta = 90^\circ$). The strength monotonically decrease with orientation or there is minimum value at an intermediate angle, but with a strength just slightly lower than for loading parallel to bedding. On the other hand, in over-consolidated materials the behaviour is similar for low values of $\delta$, but then the strength rises rapidly so that the value for $\delta = 90^\circ$ can be higher than for $\delta = 0^\circ$. Both types of behaviours described have been more recently verified using the hollow cylinder apparatus (e.g. Nishimura et al., 2007; Zdravkovic and Jardine, 2000). Experimental results in indurated shale rocks also show a similar trend as the one suggested by Skempton and Hutchinson (1969) for over-consolidated clays, with a minimum compressive strength at an intermediate orientation, but with the highest strength for loading parallel to bedding (Cho et al., 2012; McLamore and Gray, 1967). The same behaviour was also reported in an extensive testing programme on Opalinus clay (Naumann et al., 2007), although contrasting results have also been presented by Faverio et al. (2018), where there is no considerable difference between the strengths for $\delta = 0^\circ$ and $\delta = 90^\circ$. In addition, recent results on the strength anisotropy of the COx also show a maximum strength occurring for loading parallel to bedding and with a minimum strength for an orientation around 45° (Bésuelle et al., 2017). Finally, Mánica et al. (2016b) demonstrated that in underground excavations with an initial isotropic stress state, a higher strength for $\delta = 90^\circ$ is required to obtain a plastic zone extending further in the horizontal than in the vertical directions (for horizontal bedding), as it occurs with the EDZ at the GCS drift (Armand et al., 2014).

The actual variation of cohesion (and tensile strength) with the loading direction employed in this research is depicted in Fig. 6.8, corresponding to the type described in Skempton and Hutchinson (1969) for over-consolidated clays. As shown later, this distribution resulted in a remarkable reproduction of the EDZ configuration for both types of drifts, parallel and perpendicular to the major horizontal stress. In addition, a sensitivity study is also presented in the companion paper (Mánica et al., 2018c), where different types of cohesion variations were explored, and the best results were obtained with the one variation shown in Fig. 6.8.
Time-dependent behaviour

Time-dependent behaviour in the employed constitutive model results from Perzyna’s (1966) visco-plasticity (Eq. 6.17 and 6.18) and the additional creep mechanism (Eq. 6.19 and 6.20) (consolidation due to hydro-mechanical coupling also results in time-dependent behaviour, but this is naturally accounted for by the formulation of the constitutive model in terms of effective stress). However, after any loading phase (where loading does not result in an unsustainable stress state) the over-stress will eventually fade away and only creep deformations will remain in time. Therefore, the creep strain rate parameter $\gamma^c$ was selected by considering the time-dependent deformations of the COx where the effects of the loading phase appear negligible. For instance, Fig. 6.9 shows the vertical and horizontal deviatoric strain rates against the corresponding deviatoric stress components of a number of creep tests carried out on COx samples (Armand et al., 2017b). They were performed under confinement stresses of 2 and 12 MPa and with different ratios of $q/q_{\text{max}}$ ($q = \sigma_1 - \sigma_3$). In such a graph, $\gamma^c$ is the slope of a line passing through the origin. It can be observed that a value of $\gamma^c = 7.4E-5$ MPa$^{-1}$ day$^{-1}$ fits well the experimental results. Volumetric creep strains are somewhat smaller than the deviatoric ones, and a value $\psi^c = 0.3$ was considered adequate. In addition, it is not expected that the initial strain rate will stay constant indefinitely. In the absence of creep failure, this rate will tend to decrease slowly in time according to a value of $a^c = 50$. To avoid excessive propagation of creep-induced yielding, a threshold $\epsilon_{\text{thr}} = 5E-3$ was employed for the activation of the creep deformations.

Permeability evolution

Finally, the parameter for the increase of permeability with damage $\beta^k$ was not selected based on any experimental evidence, and it was back-calculated from the drift simulation to obtain a reasonable behaviour of the observed pore pressure drop around the drift. Its importance to capture properly the observed behaviour will be demonstrated.
6.4 Simulation results: Excavation damaged zone and ground displacements

6.4.1 Excavation damaged zone

Contours of shear strains are an excellent means to observe the configuration of localised plastic deformations (Mánica et al., 2018a), and have been used to assess the extension of the EDZ. Under plane strain conditions, shear strains are defined as,

\[ \varepsilon_s = \frac{\varepsilon_1 - \varepsilon_3}{2} \]  

(6.34)

where \( \varepsilon_1 \) and \( \varepsilon_3 \) are the major and minor principal strains respectively.

Although only a quarter of the excavation was simulated (Fig. 6.4), contour plots are presented for the entire excavation by mirroring results for both symmetry axes. Fig. 6.10a shows the shear strain contours for the GCS drift at \( t = 100 \) days, when the position of the excavation front is far away and it no longer affects the behaviour of the drift. Shear bands extend from the tunnel wall in the horizontal direction up to 4.2 m into the claystone. In addition, a more diffuse zone of shear deformations can be identified very close to the excavation, between the shear bands. Comparing Fig. 6.1 and Fig. 6.10a, a remarkable similarity can be noticed between the observed and obtained configurations of the EDZ. However, in the observed EDZ (Fig. 6.1) a higher number of shear fractures can be identified. In the simulation, the thickness of shear bands is related to \( \ell_s \), and does not represent the actual width of the fracture processes (Mánica et al., 2018a). The observed extension of the EDZ is also added to Fig. 6.10a (dashed lines), which neatly matches the simulation. It has been verified that the obtained results are mesh independent (see Appendix).

Fig. 6.10b shows contours of shear strain for the drift oriented parallel to \( \sigma_h \). This simulation does not correspond to any particular excavation at the URL and has the same characteristics than the one for the GCS drift; only the stress state is different. A similar EDZ configuration as for the GCS drift is obtained, but in this case, shear bands extend in
the vertical direction as observed in the field for a drift excavated parallel to $\sigma_h$ (Fig. 6.2). The observed extension of the EDZ is also shown in Fig. 6.10b (dashed lines). Again, a satisfactory agreement with the simulation can be noted.

Figure 6.10: Obtained configuration of the EDZ in terms of shear strain contours for drifts parallel to the (a) major and (b) minor horizontal stresses ($t = 100$ days), compared to the observed extension of the EDZ (Armand et al., 2014).

Creep strains occur in Gauss points where the prescribed threshold has been reached (Eq. 6.20), i.e. when the material has experienced some level of damage. However, in terms of the BVP, creep deformations can also cause further stress re-distributions and, therefore, be responsible for the yielding of new points, resulting in the evolution of the EDZ. Fig.
6.11a and Fig. 6.11b show contours of shear strain for drifts parallel to the major and minor horizontal stresses respectively at $t = 1400$ days. In both cases, the growth of the shear bands can be readily observed although no new ones develop.

![Figure 6.11: Obtained configuration of the EDZ in terms of shear strain contours for drifts parallel to the (a) major and (b) minor horizontal stresses ($t = 1400$ days).](image)

6.4.2 Ground displacements

The observed and computed evolution of convergences for the GCS drift are plotted in Fig. 6.12. Here, deformations occurring before the installation of the measurement sections have been subtracted from the numerical results to allow a direct comparison with field
observations. The position of the front with respect to the measurement sections, at the moment of installation, ranged between 0.04 and 1.5 m (Andra, 2014b); an intermediate value of 1.0 m was employed in the simulation. A good agreement between the observed and computed convergences can be noted. In drifts oriented along the major horizontal principal stress, horizontal convergences are larger than the vertical ones, and the difference between the two has been satisfactorily captured by the simulation. Only a faster accumulation of displacements occur in the simulation compared with field measurements in the first 100 days. Convergences obtained for the drift parallel to the minor horizontal stress are shown in Fig. 6.13. As this simulation does not correspond to a particular excavation, no comparison is made with field observations. Nevertheless, vertical convergences are considerably larger than horizontal ones, corresponding to the main trend of behaviour of this drift orientation (Armand et al., 2013).

In Fig. 6.14, horizontal deformations from the extensometer OHZ1501 are compared with the simulation results. Since the extensometer was installed before the excavation of the GCS drift, from the adjacent tunnel GAT (Fig. 4.7), comparison with the simulation can be made directly. By observing the position of the measurement points with respect to the extension of the EDZ (Fig. 6.3), it is evident that only those points inside the EDZ experience considerable deformations (DFO, 02, 03 and 04). In DFO, 02, which is 61 cm away from the excavation wall, the agreement is quite good. However, field measurements at DFO, 03 show just slightly lower displacements than DFO, 02, while in the simulation displacements are quite smaller. The difference can be explained by reference to Fig. 6.15, which shows contours of horizontal displacements around the excavation. The areas enclosed by the shear bands (compare with Fig. 6.10a) tend to move together as a rigid block. DFO, 03 is just outside the moving block closest to the excavation wall and, therefore, displacements are considerably different than in DFO, 02. If for instance, we consider a point just 35 cm to the right from DFO, 03 (Simulation, 03b in Fig. 6.15), then much higher displacements are obtained, more consistent with field measurements (Fig. 6.14). In DFO, 04, the computed displacements are also somewhat smaller than field values. The remaining points (DFO, 05, 06 and 07)
lie outside the EDZ (Fig. 6.3) and displacements are small. Nevertheless, simulation results show somewhat larger values. In addition, around \( t = 45 \) days field measurements change direction and begin to move away from the drift. This behaviour was not well captured by the simulation and its cause deserves further study.

![Figure 6.13: Computed evolution of convergences for a drift parallel to the minor horizontal stress.](image)

Figure 6.13: Computed evolution of convergences for a drift parallel to the minor horizontal stress.

![Figure 6.14: Observed horizontal displacements of extensometer OHZ1501 (Seyedi et al., 2017) and simulation results.](image)

Figure 6.14: Observed horizontal displacements of extensometer OHZ1501 (Seyedi et al., 2017) and simulation results.

### 6.5 Simulation results: Pore pressures and water flow

#### 6.5.1 Pore water pressure response

A good understanding of the pore water pressure response due to excavation operations is also a major concern at the URL. As shown below, hydro-mechanical coupling, and particularly the configuration and extent of the EDZ, play a major role in the pore pressure response.
Fig. 6.16a shows the observed and computed evolution of pore water pressures in the borehole OHZ1521, which is oriented in the horizontal direction (Fig. 6.3), and was excavated from the GAT drift (Fig. 4.7). The same graph is shown in Fig. 6.16b, but with emphasis on the first days. Simulation results are in good agreement with field observations. Points PRE02 and PRE03 lie inside the EDZ very close to the excavation wall (1.1 and 1.9 m respectively). Water pressure raises at those locations as the front approaches the measurement points up to a value of about 6.5 MPa, i.e. 1.5 MPa above the initial value. Thereafter, pressure drops rapidly to almost zero as soon as the excavation front passes the corresponding measuring points. The simulation results show the same behaviour reaching almost exactly the same pressures. Only the maximum value and the pressure drop occurs a little later in the simulation. Null fluxes are prescribed at the wall while the excavation front lies behind the analysis section. However, in the actual drift drainage can occur in the out-of-plane direction and, therefore, could affect a given section before the front reaches it. Point PRE04 is 4.8 m away from the wall just outside the EDZ (Fig. 6.3). Nevertheless, at this location water pressure reached 7.5 MPa; the maximum value recorded in this borehole. Unlike points PRE02 and PRE03, the maximum occurs sometime after the front passes the measurement point. Subsequently, the pressure also drops rapidly to a value around 2.0 MPa. Afterwards, a more gentle reduction is observed reaching about 1.0 MPa at $t = 3$ years. Simulation results show a quite similar behaviour at this location, but with a somewhat smaller peak pressure. PRE05 is 9.9 m away from the wall and, still, an increase of about 1.0 MPa takes place. A similar increase is obtained in the analysis; however, field data starts from a lower initial pressure and, therefore, simulation results lie above it in the first 400 days. Thereafter, both seem to coincide.

Fig. 6.17 shows pore water pressures measured at different horizontal boreholes in the GCS drift as a function of the distance to the excavation wall. Overpressures have been measured as far as 17.5 m away from the wall. A remarkable agreement can be noticed with the simulation results (solid lines) except for the borehole OHZ1524, where somewhat higher pressures were recorded.
Figure 6.16: Observed pore water pressure evolution of borehole OHZ1521 (Seyedi et al., 2017) and simulation results.

Figure 6.17: Observed pore water pressure evolution of different boreholes (Seyedi et al., 2017) and simulation results.
6.5.2 Overpressure mechanism

From the results of this study, the mechanism underlying the overpressures observed deep into the claystone has been recognised. Guayacán-Carrillo et al. (2017) already pointed out the importance of the elastic anisotropy of the COx, particularly the ratio between $E_1$ and $E_2$. By increasing this ratio, higher pressures are obtained in the horizontal direction, while lower pressures are obtained in the vertical one (for drifts parallel to the major horizontal stress). This can be understood easily by assuming a circular tunnel under an isotropic stress state and plane strain conditions. During excavation, at the sidewalls, horizontal stresses decrease while vertical stresses increase. Therefore, the material tries to expand in the horizontal direction and compress in the vertical one. If the material is isotropic, both deformations have the same magnitude, and the ground deforms isochorically. However, if the material is anisotropic, with a higher stiffness in the horizontal direction (as it occurs in the COx), the expansive component is smaller than the compressive one resulting in a decrease of volume. In a saturated low permeable material, as the COx, this results in an increase of the pore water pressure. Exactly the opposite occurs at the crown, where pore pressures tend to decrease during excavation, since the material is trying to expand. This anisotropic deconfinement can occur even in isotropic materials if the initial stress state is anisotropic. In that case, the expansive and compressive deformation components will be different because of the different initial horizontal and vertical stresses, causing the tendency of the material to compress or expand depending on the orientation around the tunnel. However, despite the fact that this is actually the main mechanism controlling the generation of overpressures, it does not provide the full explanation of the observed behaviour. For instance, if the simulation of the GCS drift is performed assuming only an elastic behaviour of the COx, the results shown in Fig. 6.18 are obtained. Only the point closest to the wall (PRE\_02) shows a maximum value similar to field observations. In the remaining locations, significantly smaller values are obtained, especially in PRE\_04. In addition, the reduction of the pore pressure after the maximum is less pronounced, and higher values are obtained in time at all locations except for PRE\_05.

The full mechanism controlling the observed evolution of pore water pressures can however be understood using Fig. 6.19. In Fig. 6.19a and 6.19b, contours of shear strains and pore pressures are shown at three different times during excavation. Fig. 6.19c and 6.19d show contours of incremental pore pressures and volumetric strains corresponding to the last increment of the finite element solution. Attention is focused on the increases in water pressures and, therefore, only positive values are plotted in Fig. 6.19c and 6.19d (i.e. positive water pressures and compressive deformations). As excavation progresses, shear bands develop around the gallery, and higher water pressures can be noticed in the horizontal direction. However, unlike the elastic analysis, the zone with the highest pressure moves away from the gallery, as the shear bands grow. An evident correspondence between the incremental pore pressures and volumetric strains can be noticed, since it is the tendency of the COx to compress due to the anisotropic deconfinement that drives the increase of water pressures. However, the quasi-brittle response of the COx (softening) causes this anisotropic deconfinement to occur further away, outside the EDZ. In fact, pressure increases take place only at elastic points, just outside the plastic zone (Fig. 6.19c). In the plastic (softening) points dilation occurs, causing the decrease of water pressures. In addition, permeability...
increase in those locations (Eq. 6.30) propagating faster the pressure gradient produced by the zero pore pressure boundary condition at the wall and, therefore, further enhancing the pressure drop. Since these competing phenomena interact at the boundary of the EDZ, the rate at which pore pressure increases are generated will be relevant to the magnitude of the resulting overpressures. Therefore both softening and excavation rates will affect the pore pressure response.

Figure 6.18: Observed pore water pressure evolution of borehole OHZ1521 (Seyedi et al., 2017) and simulation results assuming a purely elastic constitutive behaviour.

6.5.3 Role of the evolution of permeability

To illustrate the relevance of the permeability evolution due to damage in the development of pore pressures, the analysis of the GCS drift has also been performed assuming a constant permeability. The resulting evolution of pore water pressures at the borehole OHZ1521 is shown in Fig. 6.20. The maximum pressures reached are similar to those of the previous case (Fig. 6.16). However, the pressure reduction after the maximum is underestimated by the simulation, and higher pressure values are obtained in all locations compared with field observations. The evolution of permeability appears therefore essential to capture properly the pore water pressure response.
Figure 6.19: Mechanism controlling water pressure increments in terms of a) shear strains, b) pore water pressures, c) incremental pore water pressures and d) incremental volumetric strains.
Since plastic deformations concentrate within the shear bands, permeability increases due to damage are also concentrated there. This results in preferential pathways for the water flux. For instance, Fig. 6.21 shows flux vectors for $t = 100$ days, where the localised nature of groundwater flux can be identified. Although the permeability increase is assumed isotropic (Eq. 6.30), the direction of the flux is parallel to the shear bands, towards the zone with the lower pressure. Nevertheless, experimental evidence suggests that the self-sealing capacity of the COx can restore to some degree the initial permeability of the intact rock (Liu et al., 2015; Zhang, 2011). This was not included in the simulation, and further research is needed to determine if these preferential pathways can persist in time, or if the initial permeability can be completely restored.

Figure 6.20: Observed pore water pressure evolution of borehole OHZ1522 (Seyedi et al., 2017) and simulation results assuming a constant permeability.

### 6.5.4 Pore pressures above the crown

In the zone above the tunnel crown, pressures decrease (Fig. 6.19b). However, the EDZ barely grows in this direction and the effect of the anisotropic deconfinement affects only a limited depth into the clay rock. In addition, permeability remains almost constant and the
pressure gradient due to the boundary condition at the wall takes longer to propagate. Fig. 6.22 shows the evolution of pore pressures at the borehole OHZ1522 (Fig. 6.3), compared with the simulation results. There is a slight increase of pore pressures as the excavation front approaches the measurement points, which was not captured by the analysis. In addition, the pressure drop is underestimated by the simulation, especially at PRE_02, PRE_03 and PRE_04. A possible explanation for this difference is that, under plane strain conditions, the out-of-plane deformation component is neglected. However, this strain component does exist in the field, and could enhance the pressure drop in this zone. A 3D simulation will be necessary to confirm this hypothesis.

![Figure 6.21: Groundwater flux (t = 100 days).](image)

### 6.6 Conclusions

This paper presents a detailed simulation of the GCS drift at the MHM URL. The constitutive model employed incorporates a number of features that are considered relevant for the satisfactory simulation of the behaviour of COx claystone. In particular, the ability to simulate localised deformations objectively with the incorporation of nonlocal regularisation is crucial.
The configuration and extent of the EDZ after excavation obtained from the simulation, in terms of shear strains, resembles remarkably the observed fracture network at the GCS drift. The same positive outcome was obtained from the analysis of a hypothetical drift parallel to the minor horizontal stress. Nevertheless, a fewer number of shear bands occur in the simulation, which may be related to their unrealistic thickness required for computational purposes. Due to creep deformations, the simulated EDZ evolved with time, and a limited growth of the existing shear bands was noticed in the long-term. To the best authors’ knowledge, this has not yet been observed in the URL in drifts with a flexible support system, and it is of course not expected to occur in the case of a rigid support. In fact, the self-sealing capacity of the COx, that was not explicitly included in the simulation, might act as a competing phenomenon preventing the potential long-term growth of fractures. More laboratory research about the self-sealing capacity of the COx, as well as periodic surveys of the fractures around the drifts, are required in this respect. The survey will also be relevant for the computed localised water flux, to determine if the created preferential pathways can persist in time, or if the initial permeability of the claystone can be restored. The observed pattern of displacements was also satisfactorily reproduced. Convergence measurements at the GCS drift were well captured by the simulation, including the observed anisotropy between horizontal and vertical convergences. The importance of the EDZ configuration on the resulting deformation field was also demonstrated.

As for the pore water pressure response, field observations were also adequately captured. A full explanation for the complete mechanism behind the observed overpressures in the horizontal direction of the GCS drift was presented. Pore pressure increases are generated by what is called here *anisotropic deconfinement*, which depends on the anisotropic elastic properties and the initial anisotropic stress state, as previously pointed out by Guayacán-Carrillo et al. (2017). However, the quasi-brittle behaviour of the COx causes this anisotropic deconfinement to occur further away as the EDZ grows. Therefore, the configuration and extension of the EDZ are responsible for the overpressures occurring deep into the claystone, which cannot be reproduced without including softening in the constitutive description.
Nevertheless, the actual pore pressure distribution and its evolution will be the result of a complex interaction between different factors, including the initial permeability and its evolution with damage.

### 6.7 Appendix - Mesh independence

To verify the mesh independence of the obtained results, the analysis of the GCS drift was also performed using two additional meshes with 36582 and 59104 elements. They are compared in Fig. 6.23, together with the original one. Simulations were also performed for all meshes assuming the standard version of the constitutive model (i.e. without the nonlocal approach), in order to stress the importance of regularising the solution when using a constitutive law with softening within the framework of continuum mechanics.

Fig. 6.23: Different meshes employed to examine the mesh independence of the results.

Fig. 6.24 show contours of shear strains for $t = 100$ days with and without nonlocal regularisation respectively. When the nonlocal approach is employed, the same configuration of the EDZ and the same thickness of the shear bands are obtained regardless of the number (and consequently the size) of finite elements. On the other hand, with the standard constitutive model, the configuration of the EDZ varies for each case and the shear bands thickness reduces as the size of elements is reduced. In addition, convergence issues occurred early in the simulation with the standard model, and none of the analyses reached $t = 100$ days. Convergence difficulties increased with the number of elements of the mesh. Similar conclusions can be drawn from Fig. 6.25, where the evolution of horizontal convergences is plotted for the first 100 days. Using nonlocal regularisation practically a single curve is
obtained from all meshes. In the standard model, displacements are not unique, but they depend on the selected mesh.

Figure 6.24: Obtained shear strain contours for different meshes with and without nonlocal regularisation.

Figure 6.25: Obtained convergences for different meshes with and without nonlocal regularisation.
Chapter 7

Numerical simulation of an underground excavation using nonlocal regularisation. Part 2: sensitivity analysis

Based on a manuscript to be submitted.

Abstract

A sensitivity study is presented to evaluate the influence of different parameters on the simulation results of an underground excavation in an indurated claystone, given in a companion paper (Mánica et al., 2018b). Aspects studied include mechanical anisotropy, strength parameters, excavation size, hydraulic parameters, and time-dependency. Results reveal some of the main aspects affecting the hydro-mechanical behaviour of the excavation.

7.1 Introduction

The work presented here has been developed within the context of the activities carried out at the Meuse/Haute-Marne (MHM) Underground Research Laboratory (URL), located in Eastern France; a facility constructed to demonstrate the feasibility of the Callovo-Oxfordian argillaceous formation (COx) to host a nuclear waste repository (Andra, 2005a). A detailed simulation of the GCS drift, an experimental excavation aimed to assess the hydromechanical response of the COx to excavation operations (Seyedi et al., 2017), has been presented by the authors in a companion paper (Mánica et al., 2018b). The elasto-visco-plastic formulation employed, able to simulate localised deformations objectively with a nonlocal regularisation (Mánica et al., 2018a), has been described. The parameters used in this research were derived, to the extent possible, from experimental evidence. In situ observations have been reproduced satisfactorily, and relevant insights about the importance of the excavation damaged zone (EDZ) in the short- and long-term behaviour of the drift have been presented. However, significant variability has been reported regarding the mechanical and hydraulic properties of the COx claystone (e.g. Andra, 2005b; Armand et al., 2013; Belmokhtar et al.,
The observed dispersion can be attributed to different sources such as natural variability of the material, different sample conditions, different experimental procedures, or different tests interpretations, and introduces uncertainty into the results of performed numerical simulations.

In this paper, a sensitivity study is presented to evaluate the influence of different parameters on the results of the GCS drift simulation given in the companion paper (Mánica et al., 2018b). Aspects studied include mechanical anisotropy, strength parameters, excavation size, hydraulic parameters, and time-dependency. Only a brief description of the hydro-mechanical boundary value problem (BVP) solved is given herein. Details about the nonlocal elasto-visco-plastic formulation employed, the modelling approach, and the selection of parameters for the base case are given in the companion paper (Mánica et al., 2018b). Results from the sensitivity study reveal some of the main aspects of the COx hydro-mechanical behaviour affecting the response of the drift.

7.2 Main features of the finite element model

Two-dimensional (2D) plane strain finite element analyses have been performed to evaluate the response of the GCS drift. The geometry, mesh, and main boundary conditions are depicted in Fig. 6.4. Only a quarter of the excavation was simulated and, therefore, the gravity gradient was neglected. The initial stress state corresponds to that estimated at the main level of the URL for drifts parallel to the major horizontal stress $\sigma_H$ (Seyedi et al., 2017). To assess the influence of in situ stresses, additional analyses were also performed considering an initial stress state corresponding to drifts parallel to the minor horizontal stress $\sigma_h$ (Seyedi et al., 2017). A pore water pressure of 4.7 MPa, equal to the estimated value at the main level of the URL unaffected by excavation operations (Armand et al., 2014, 2013), was applied as initial condition for all the domain and as a boundary condition at the upper and right boundaries. Radial stresses were applied at the tunnel wall to ensure equilibrium. Then, these stresses were gradually reduced to simulate the excavation as a function of the front position, following a deconfinement curve derived from Unlu and Gercek (2003). Stresses were not brought to zero, but to a value corresponding to the observed confinement applied by the support system to the ground (Bonnet-Eymard et al., 2011b). Details and limitations of the adopted modelling approach are discussed in Mánica et al. (2018b).

The solution of the described BVP was performed using the finite element code Plaxis (Brinkgreve et al., 2017), through a fully coupled hydro-mechanical simulation. The constitutive model employed has been described in Mánica et al. (2018b), and was implemented in Plaxis as a user-defined soil model. The parameters used for the base case are given in Table 6.1. This analysis serves as a baseline, to which the results of the sensitivity study are compared.

7.3 Sensitivity analysis

A summary of the analyses performed is given in Table 7.1, where differences with respect to the base case (Table 6.1) are specified for each analysis. A monothetic approach was followed, where the studied parameters where varied one at a time. Strength anisotropy is an exception since four parameters are involved, although they correspond to a single strength distribution.
Due to the high computational cost involved, several analyses were simultaneously executed in the cloud of a commercial provider (Amazon, 2018). Cloud computing is becoming an attractive alternative for accessing to high-performance computational resources on demand, without the need of purchasing and maintaining hardware that rapidly becomes obsolete.

Table 7.1: Analyses performed

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Variation with respect to the base case</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mechanical anisotropy</strong></td>
<td></td>
</tr>
<tr>
<td>A01a</td>
<td>Mechanically isotropic, parallel to $\sigma_H$</td>
</tr>
<tr>
<td>A01b</td>
<td>Mechanically isotropic, parallel to $\sigma_h$</td>
</tr>
<tr>
<td>A02a</td>
<td>Strength anisotropy only, parallel to $\sigma_H$</td>
</tr>
<tr>
<td>A02b</td>
<td>Strength anisotropy only, parallel to $\sigma_h$</td>
</tr>
<tr>
<td>A03a</td>
<td>Stiffness anisotropy only, parallel to $\sigma_H$</td>
</tr>
<tr>
<td>A03b</td>
<td>Stiffness anisotropy only, parallel to $\sigma_h$</td>
</tr>
<tr>
<td>B01a</td>
<td>$\Omega_{90} = 1.15, \Omega_m = 0.806, \delta_m = 47.86^\circ, \hat{n} = 0.1, \parallel \sigma_H$</td>
</tr>
<tr>
<td>B01b</td>
<td>$\Omega_{90} = 1.15, \Omega_m = 0.806, \delta_m = 47.86^\circ, \hat{n} = 0.1, \parallel \sigma_h$</td>
</tr>
<tr>
<td>B02a</td>
<td>$\Omega_{90} = 1.00, \Omega_m = 0.800, \delta_m = 45.00^\circ, \hat{n} = 0.1, \parallel \sigma_H$</td>
</tr>
<tr>
<td>B02b</td>
<td>$\Omega_{90} = 1.00, \Omega_m = 0.800, \delta_m = 45.00^\circ, \hat{n} = 0.1, \parallel \sigma_h$</td>
</tr>
<tr>
<td>B03a</td>
<td>$\Omega_{90} = 0.90, \Omega_m = 0.805, \delta_m = 41.46^\circ, \hat{n} = 0.1, \parallel \sigma_H$</td>
</tr>
<tr>
<td>B03b</td>
<td>$\Omega_{90} = 0.90, \Omega_m = 0.805, \delta_m = 41.46^\circ, \hat{n} = 0.1, \parallel \sigma_h$</td>
</tr>
<tr>
<td>C01</td>
<td>$E_1/E_2 = 1.6, \parallel \sigma_H$</td>
</tr>
<tr>
<td>C02</td>
<td>$E_1/E_2 = 1.3, \parallel \sigma_H$</td>
</tr>
<tr>
<td><strong>Strength parameters</strong></td>
<td></td>
</tr>
<tr>
<td>D01</td>
<td>$c_0^{\text{ini}} = 2.0 \text{ MPa}, p_{10}^{\text{ini}} = 0.75 \text{ MPa}$</td>
</tr>
<tr>
<td>D02</td>
<td>$c_0^{\text{ini}} = 6.0 \text{ MPa}, p_{10}^{\text{ini}} = 2.25 \text{ MPa}$</td>
</tr>
<tr>
<td>D03</td>
<td>$\phi_0^{\text{ini}} = 16^\circ$</td>
</tr>
<tr>
<td>D04</td>
<td>$\phi_0^{\text{ini}} = 25^\circ$</td>
</tr>
<tr>
<td>D05</td>
<td>$\phi_{\text{res}} = 13^\circ$</td>
</tr>
<tr>
<td>D06</td>
<td>$\phi_{\text{res}} = 10^\circ$</td>
</tr>
<tr>
<td>D07</td>
<td>$r_{\text{post}} = 0.15$</td>
</tr>
<tr>
<td>D08</td>
<td>$r_{\text{post}} = 0.60$</td>
</tr>
<tr>
<td><strong>Excavation size</strong></td>
<td></td>
</tr>
<tr>
<td>E01</td>
<td>Excavation diameter = 8 m</td>
</tr>
<tr>
<td>E02</td>
<td>Excavation diameter = 11 m</td>
</tr>
<tr>
<td><strong>Hydraulic parameters</strong></td>
<td></td>
</tr>
<tr>
<td>F01</td>
<td>$k_{0xx} = 5.00\times10^{-19} \text{ m}^2$</td>
</tr>
<tr>
<td>F02</td>
<td>$k_{0xx} = 2.75\times10^{-20} \text{ m}^2$</td>
</tr>
<tr>
<td>F03</td>
<td>$k_{0xx} = 5.00\times10^{-21} \text{ m}^2$</td>
</tr>
<tr>
<td>G01</td>
<td>$k_{0xx}/k_{0yy} = 1.0$</td>
</tr>
<tr>
<td>G02</td>
<td>$k_{0xx}/k_{0yy} = 3.0$</td>
</tr>
<tr>
<td>G03</td>
<td>$k_{0xx}/k_{0yy} = 4.0$</td>
</tr>
<tr>
<td>H01</td>
<td>$B = 0.7$</td>
</tr>
<tr>
<td>H02</td>
<td>$B = 0.8$</td>
</tr>
<tr>
<td>H03</td>
<td>$B = 1.0$</td>
</tr>
<tr>
<td><strong>Time dependency</strong></td>
<td></td>
</tr>
<tr>
<td>I01</td>
<td>$\eta = 75 \text{ MPa-day}$</td>
</tr>
<tr>
<td>I02</td>
<td>$\eta = 300 \text{ MPa-day}$</td>
</tr>
<tr>
<td>I03</td>
<td>$\eta = 1000 \text{ MPa-day}$</td>
</tr>
<tr>
<td>J01</td>
<td>Without creep deformations</td>
</tr>
</tbody>
</table>
Results were evaluated in terms of the obtained EDZ configuration, the pore water pressure response, and the horizontal and vertical convergences. The simulated EDZ was assessed in terms of contours of shear strains (Mánica et al., 2018b), which for the assumed plane strain condition are defined as,

$$\epsilon_s = \frac{\epsilon_1 - \epsilon_3}{2}$$  \hspace{1cm} (7.1)

where $\epsilon_1$ and $\epsilon_3$ are respectively the major and minor principal strains. The contour plots are given for the entire excavation (by mirroring results for both symmetry axes) and for $t = 100$ days. At this time, the position of the excavation front is far enough and no longer affects the behaviour of the drift. The pore water pressure was studied at three locations corresponding to the measurement points PRE_02, PRE_04 and PRE_05 of the borehole OHZ1521 (see in Fig. 7.5 the location of measuring points with respect to the EDZ), which is oriented horizontally and was excavated from an adjacent drift in advance of the excavation (Seyedi et al., 2017). The three locations are particularly relevant since one is located inside the observed EDZ, one just outside, and the last one about 5.45 m away from the EDZ. In all the graphs presented here, $t = 0$ corresponds to the front at the analysis section.

7.3.1 Mechanical anisotropy

At the URL, drifts oriented parallel to $\sigma_h$ show an EDZ that extends further in the vertical direction (Armand et al., 2014), together with larger vertical than horizontal convergences (Armand et al., 2013). This behaviour is mainly due to the anisotropic stress state in the plane normal to the tunnel axis ($\sigma_H/\sigma_h \approx 1.3$), and can be explained even with a simple isotropic elasto-plastic constitutive model. On the other hand, drifts parallel to $\sigma_H$ have a nearly isotropic stress state in the plane normal to the tunnel axis ($\sigma_h/\sigma_v \approx 1$), and yet the EDZ does not show circular symmetry; it extends more in the horizontal direction than in the vertical direction (Armand et al., 2014). Also, horizontal convergences larger than the vertical ones are measured (Armand et al., 2013). These observations suggest strong anisotropic characteristics of the rock mass. Results from Mánica et al. (2018b) captured this behaviour adequately for both types of drifts (Fig. 6.10) by including mechanical anisotropy (stiffness and strength) in the constitutive description of the COx. The importance of this feature is examined in the present section.

In the set of analyses A, three cases have been studied: mechanically isotropic, only with strength anisotropy, and only with stiffness anisotropy. The obtained contours of shear strain are shown in Fig. 7.1 for both cases, parallel to the minor and major horizontal stresses. The observed extensions of the EDZ are also depicted in the figure. The analysis A01a did not result in a symmetric response. The symmetry may have been broken by the slight difference between the vertical and horizontal stresses (Fig. 6.4), or by the anisotropic permeability (Table 6.1). In fact, localisation cannot take place under a perfectly isotropic excavation. In any case, the resulting configuration differs greatly from the observed EDZ. On the other hand, the obtained contours of shear strain from analysis A02 resembles both, field observations and the base case (Fig. 6.10). The analysis A03a did not yield the observed EDZ configuration and, in fact, the results are quite similar to those from the mechanically isotropic analysis A01a. This suggests that stiffness anisotropy has only a minor influence on the resulting configuration of localised deformations, and that strength anisotropy is the controlling factor. Although differences exist between the three analyses for the drift parallel
to $\sigma_h$ (Fig. 7.1d, 7.1e and 7.1f), the observed trend was preserved with a damage zone extending more in the vertical direction. The latter implies that for drifts parallel to $\sigma_h$, the initial stress anisotropy dominates over the effect of strength anisotropy.

![Diagram of shear strain contours](image)

Figure 7.1: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift and a drift parallel to the minor horizontal stress from the set of analyses A ($t = 100$ days), compared to the observed extension of the EDZ (Armand et al., 2014).

As described in Mánica et al. (2018b), strength anisotropy was included by assuming that the cohesion and the isotropic tensile strength depend on the relative orientation between the major principal stress and the normal to bedding (angle $\delta$). The normalised strength distribution employed in the base case is shown in Fig. 7.2. The main characteristics are a minimum value for $\delta = 45^\circ$ and a value for $\delta = 90^\circ$ larger than for $\delta = 0^\circ$. Although it was not directly derived from experimental results, a strong justification for this distribution was presented in Mánica et al. (2018b). It is generally accepted that the minimum strength of the COx is found for an intermediate orientation of $\delta$, around $45^\circ$ and $60^\circ$ (Armand et al., 2017b). However, there is still no consensus about the difference in the strength when the major principal stress is oriented parallel and perpendicular to bedding. In this context, the set of analyses B studied the effect of different strength distributions on the obtained configuration of the EDZ. The minimum value at $\delta = 45^\circ$ is preserved in the three analyses, but different values for $\delta = 90^\circ$ were considered. The employed strength distributions and their corresponding parameters are shown in Fig. 7.2 and Table 7.1 respectively, and the obtained shear strain contours are depicted in Fig. 7.3. As in the set A, results for the drift parallel to $\sigma_h$ showed similar results, with an EDZ extending in the vertical direction. This confirms the dominant effect of the initial stress anisotropy. For B01, a strength distribution
similar to the base case was employed, but with \( \Omega_{90} = 1.15 \). The contours of shear strain in the analysis B01a are quite similar to the base case and, therefore, shows an excellent agreement with the observed EDZ. In analysis B02a, both strengths for \( \delta = 0^\circ \) and \( \delta = 90^\circ \) are assumed equal and, although the EDZ is indeed more developed horizontally than vertically, the shear bands do not extend as far as the field observations and the configuration of localised deformations does not resemble the observed fracture pattern (Armand et al., 2014). Similar conclusions can be drawn from B03a, where the strength for \( \delta = 90^\circ \) is lower than for \( \delta = 0^\circ \), but higher than for \( \delta = 45^\circ \). In fact, the results are quite similar to those from the analysis where strength anisotropy was not employed (Fig. 7.1c). These results suggest that, for the drifts with a nearly isotropic initial stress state in the plane normal to the tunnel axis, the strength when the principal stress is parallel to bedding must be higher than when the principal stress is normal to bedding to obtain a damage zone configuration resembling field observations. Similar conclusions were presented previously by Mánica et al. (2016b) using much simpler simulations.

In the set of analyses C, the effect of the ratio between the stiffness normal and perpendicular to bedding was explored. According to Armand et al. (2013), this ratio varies between 1.3 and 2 for the COx, the latter being used for the base case (Mánica et al., 2018b). Therefore, values of 1.6 and 1.3 were considered for analyses C01 and C02 respectively. In addition, the analysis A02a corresponds to a ratio of 1.0. In accordance with the results from the set A, there were no significant differences in the configuration of localised deformations with respect to the base case; therefore, contours of shear strains were not plotted here. However, this ratio does have a relevant effect on the magnitude of the computed convergences, as shown in Fig. 7.4. Horizontal and vertical convergences increased by decreasing this ratio, the effect being more important in the case of the horizontal ones. Since the value of \( E_2 \) was kept constant, larger convergences are an obvious result because the elastic stiffness is being reduced. However, the differences are larger compared to those obtained performing elastic analysis only; results from those elastic calculations are not presented here.
Figure 7.3: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift and a drift parallel to the minor horizontal stress from the set of analyses B \((t = 100 \text{ days})\), compared to the observed extension of EDZ (Armand et al., 2014).

Figure 7.4: Computed evolution of horizontal and vertical convergences from the set of analyses C, compared to base case and field measurements (Seyedi et al., 2017).

In the companion paper (Mánica et al., 2018b), the mechanism controlling the variation of pore water pressure \((\text{anisotropic deconfinement, AD})\) was described. In the case of the GCS drift, parallel to \(\sigma_H\), this AD can occur due to the anisotropic elastic properties of the COx. Therefore, by reducing the ratio \(E_1/E_2\) pore water pressure increases in the horizontal
direction are expected to be smaller. The water pressure response for different stiffness ratios is depicted in Fig. 7.5. For the observation point PRE_02 (Fig. 7.5a), the graph only shows until day 80 from the time the front reached the analysis section because relevant responses at this location occur before that time. As expected, reducing the elastic anisotropy ratio causes smaller values of the obtained maximum water pressure at all locations. Due to the nearly isotropic initial stress state, in the analysis A02a ($E_1/E_2 = 1.0$) no increases in pressure would be expected. In PRE_02, this is exactly what happens, and no significant increase take place before the pressure drop brought about by the gradient from the excavation wall and the permeability increase due to damage. However, in locations PRE_04 and PRE_05
pressure increases take place even in the analysis A02a. This occurs because the development of the EDZ causes stress re-distributions around itself. When points PRE_04 and PRE_05 experience the AD due to the softening occurring in the shear bands, the stress state is in fact no longer isotropic and, therefore, the AD occurs in this case due to some stress anisotropy. Consequently, in the base case, AD occurs because of both, stress and stiffness anisotropy.

### 7.3.2 Strength parameters

The set of analysis D addressed the impact of different strength parameters on the results of the GCS simulation. Particularly, the effects of the asymptotic initial cohesion, the asymptotic initial and residual friction angles, and the post-rupture ratio were evaluated (Table 7.1). The obtained contours of shear strain, convergences, and the pore water pressure response are given in Fig. 7.6, 7.7, and 7.8 respectively.

![Diagrams showing different strength parameters](image)

Figure 7.6: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses D \((t = 100 \text{ days})\), compared to the observed extension of EDZ (Armand et al., 2014).
In analyses D01 and D02, values for the asymptotic initial cohesion of 2 and 6 MPa and values for the isotropic tensile strength of 0.75 and 2.25 MPa, respectively, have been employed. The analysis D01 resulted in a damage zone configuration much larger than the actual observed EDZ. The same behaviour can be noticed in terms of convergences, where values about 4 times larger than the recorded ones were obtained (note that the right scale in Fig. 7.7 corresponds only to analysis D01). In fact, numerical convergences issues occurred around $t = 700$ days, and the analysis was not completed; this raises the question whether if the BVP can be stable with the strength parameters considered for this analysis. In terms of water pressures, the large damage zone and its related permeability increase, caused a very rapid dissipation at PRE_02 and PRE_04. At PRE_05, the highest pressures of the considered locations occurred. This point ended just outside the EDZ; therefore, it was less affected by the permeability increase enhancing pressure drops, but close enough where the effects of the AD are larger. In analysis D02, very little damage is observed in the shear strain contours, and convergences are quite smaller than field values, with a small difference between horizontal and vertical ones. Due to the small plastic deformations taking place, the maximum water pressures at PRE_04 was considerably lower than field observations. In PRE_02, the maximum pressure was adequately captured, since at this location the peak values are more related to the elastic response of the ground (Mánica et al., 2018b).

In analyses D03 and D04, values for the asymptotic initial friction angle of 16° and 25° were employed. In analysis D03, the configuration of the EDZ is not much affected compared to the base case, and only a larger size can be noticed. Nevertheless, convergences are about two times the field values. The pore pressure response is similar than in D01, but with a lower maximum pressure and a slower dissipation at PRE_05; here, the EDZ is farther from PRE_05 and, therefore, the AD and the permeability increase had a smaller effect at this location. Regarding the analysis D04, results are quite similar to the analysis D02, but with some larger horizontal convergences.
Figure 7.8: Computed pore water pressure evolution at three location of the borehole OHZ1521 from the set of analyses D, compared to base case and field measurements (Seyedi et al., 2017).

In analyses D05 and D06, values of the asymptotic residual friction angle of 13° and 10° were employed. Along with the value of 16° used for the base case, the considered range covers the residual friction angles observed in a number of argillaceous materials (Zhan, 2012). Nevertheless, results in terms of shear strains contours, convergences, and pore water pressures did not vary significantly with respect to the base case. According to the employed $b_{\text{res}}$ (Table 6.1), deformations larger to those occurring are required to reach the fully residual state and, therefore, the residual friction angle did not have a considerable impact on the simulations results.
Finally, analyses D07 and D08 assessed the effect of the post-rupture ratio $r_{\text{post}}$, i.e. the relative amount of cohesion and tensile strength that is not degraded according to the post-rupture softening rate $b_{\text{post}}$; values of 0.15 and 0.6 were employed respectively. The contours of shear strain of analysis D07 are similar than the base case, although the outer shear bands are more developed and managed to intersect each other. However, the obtained convergences are quite larger than the base case and field values. Regarding the pore pressure response, the most interesting result occurred at PRE$_{04}$; a maximum pressure of 8.5 MPa was reached at this location. Since it is the brittle behaviour of the COx that causes the AD deep into the claystone, a higher amount of cohesion (and tensile strength) being lost in the post-rupture state enhanced the AD and, therefore, higher pressures were obtained at the vicinity of the EDZ in the horizontal direction. On the other hand, the lower amount of strength being lost in analysis D08 is not enough to cause important plastic strains, and a defined pattern of localised deformations. Therefore, the response in terms of convergences and pore water pressure is similar to the analyses D02 and D04. Nevertheless, at later times horizontal convergences accelerated due to the fact that creep deformations can also mobilise the strength (Mánica et al., 2018b) and can, therefore, reduce the cohesion.

### 7.3.3 Excavation size

*In situ* observations at the URL suggest that there is no significant scale effect on the configuration and extent of the EDZ. For instance, full-size excavations ($\bar{D} \approx 5$ m), micro-tunnels ($\bar{D} \approx 0.7$ m), and boreholes ($\bar{D} \approx 0.05$ m) parallel to $\sigma_H$ exhibit the same fracture pattern with an extent that seems to scale approximately proportional to the excavation size (Armand et al., 2014). In this regard, the set of analyses E studied the effect of the excavation size on the simulation results. In order to maintain exactly the same parameters than the base case (Table 6.1), including the same length scale $l_s$, larger excavation sizes were considered. For smaller excavations, the thickness of the shear bands would be too large compared to the tunnel and, therefore, this could affect the resulting localisation pattern. Diameters of 8 and 11 m were considered for analyses E01 and E02 respectively.

The resulting contours of shear strains are shown in Fig. 7.9. The hypothetical extents of the damaged zone, according to the excavation diameter for the GCS drift (Armand et al., 2014), are also depicted in the figure. As observed in the field, the pattern of localised plastic deformations is quite similar to the base case (Fig. 6.10). However, a slight increase in size of the damage zone can be noticed with respect to the corresponding field observations, being more noticeable for larger excavation sizes. This moderate scale effect emerged also in the resulting convergences (Fig. 7.10); normalising the results with the tunnel diameter did not yield a single curve, and somewhat larger relative convergences are obtained as the excavation diameter is increased.

The evolution of water pressures is depicted in Fig. 7.11. To allow comparison with the base case, the location of the observation points was adjusted according to the excavation size. Therefore, the ratio between the distance of a given observation point and the tunnel axis and the excavation diameter is the same for all analyses. At the location PRE$_{02}$, there is no much difference in the observed response. Only slightly higher pressures were obtained in analyses E01 and E02 with respect to the base case. Nevertheless, significant differences can be identified in locations PRE$_{04}$ and PRE$_{05}$. By increasing the excavation
Figure 7.9: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses E \((t = 100 \text{ days})\), compared to the observed extension of EDZ (Armand et al., 2014).

size, higher pressures are obtained in the point just outside the EDZ (PRE\textsubscript{04}); in the analysis E02, a maximum pressure above 8.5 MPa was attained. In PRE\textsubscript{05}, the differences in the maximum values are smaller, although the rate of dissipation decreases considerably by increasing the size of the excavation. These results can be easily explained by the fact that in a larger excavation, the zone affected by the AD outside the EDZ, driving increases of water pressure, is also larger. Therefore, drainage distances increase with the excavation size, reducing dissipation. The resulting pressure at the vicinity of the EDZ in the horizontal direction is the result of a competition between pressure increases bring about by the AD and the dissipation due to the pressure gradient. Therefore, by decreasing dissipation, higher water pressures can be attained, especially where the effect of the AD is higher, as it occurs at PRE\textsubscript{04}. This phenomenon might explain the moderate scale effect observed in the obtained extent of the EDZ and convergences.

Figure 7.10: Computed evolution of horizontal and vertical convergences from the set of analyses E, compared to base case and field measurements (Seyedi et al., 2017).
To the authors’ best knowledge, the scale effect identified in the simulations has not been observed at the URL. Nevertheless, its existence cannot be dismissed and could be masked by the natural variation of field measurements.

Figure 7.11: Computed pore water pressure evolution at three locations of the borehole OHZ1521 from the set of analyses E, compared to base case and field measurements (Seyedi et al., 2017).

### 7.3.4 Hydraulic parameters

On the basis of a large amount of laboratory and *in situ* testing, the intrinsic permeability of the intact COx at the main level of the URL has been estimated in the range of 5E-21 and 5E-20 m² (Armand et al., 2017b), i.e. with a variability of an order of magnitude. In the base case, the value of 5E-20 m² was employed for the horizontal initial permeability (Table 6.1).
The set of analyses F explores the effect of different permeabilities within the reported range. In analyses F02 and F03, values of 2.75E-20 and 5E-21 m² respectively have been employed (Table 7.1) (the ratio $k_{0xx}/k_{0yy} = 2$ has been preserved). In addition, in analysis F01 a larger value of 5E-19 m² was used. The contours of shear strain are depicted in Fig. 7.12. In analysis F01, the extension of the damaged zone was reduced considerably with respect to the base case (Fig. 6.10). In F02 and F03, the EDZ is very similar to the base case, but with a slightly larger extension as the permeability is reduced. Consistent with the latter, convergences also increase when the permeability has been reduced (Fig. 7.13), although differences are only significant in the analysis F03, having the lowest permeability. In terms of water pressures (Fig. 7.14), the large permeability of F01 enhances dissipation and, therefore, peak pressure values are quite small in PRE02 and PRE04; at the three measurement locations, water pressures tend to steady state values much faster than field measurements. On the other hand, analyses F02 and F03 resulted in larger peak pressures and lower dissipation rates compared to the base case. Particularly important is the evolution of water pressures in the analysis F03 at PRE05, where the pressure has kept increasing throughout the simulation. This means that the tendency to increase water pressures, brought about by volumetric compressive creep deformations, is able to overcome dissipation and causes the continuous increase of pressure during the whole simulation. These results suggest that it is unlikely that the COXs has such a low permeability value since this behaviour has not been observed in the field.

Figure 7.12: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the sets of analyses F and G ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).
The horizontal permeability of the COx appears to be larger than the vertical one, and ratios between 1.75 and 5 have been reported in the literature (Armand et al., 2017b; Enssle et al., 2011). Nevertheless, uncertainties on the permeability measurements are large, and they do not allow to verify with certainty the existence of this anisotropy (Armand et al., 2017b). In this regard, the set of analyses G assessed the impact of different $k_{0xx}/k_{0yy}$ ratios on the simulation results. In analysis G01, an isotropic permeability was assumed, while in G02 and G03 ratios of 3 and 4 were employed respectively; the base case uses a ratio of 2.

The configuration and extent of the damaged zone in terms of shear strains (Fig. 7.12) is quite similar to the base case (Fig. 6.10) in analyses G01 and G02. Only in analysis G03, with a permeability ratio of 4, important differences can be noticed. The outer shear bands did not grow much and, therefore, the extension of the EDZ is smaller than the observed one. In terms of convergences (Fig. 7.13), there are no significant differences between analyses of the set G. The same occurs in terms of pore water pressures (Fig. 7.14); only at PRE_04, analysis G03 showed a slower dissipation which can be explained by the limited permeability increase near this location due to the smaller extent of the EDZ. In general, results showed that the anisotropy ratio has a small impact on the behaviour of the drift, at least for anisotropy ratios between 1 and 3.

Another parameter showing a particularly large dispersion is the Biot’s effective stress coefficient; values ranging from 0.32 to 0.95 has been reported (Escoffier, 2002). In addition, it seems that this coefficient is not isotropic, showing different values when measured parallel and perpendicular to bedding (Belmokhtar et al., 2016), and it is unlikely to be constant (Gens, 2013). In the base case analysis (Mánica et al., 2018b), a constant and isotropic coefficient of 0.6 was used, which is a frequently employed value in numerical simulations of the COx (Jia et al., 2010; Pardoen et al., 2015; Seyedi et al., 2017). In this context, the set of analyses H studied the effect of the Biot’s effective stress coefficient on the simulation results. As in the base case, an isotropic approach was followed, and the effect of the ratio between coefficients parallel and perpendicular to bedding was not studied here. In analyses H01, H02, and H03 values of 0.7, 0.8, and 1.0 were considered respectively. The calculated contours of shear strain are shown in Fig. 7.15. Localised deformations of the analysis H01
do not show significant differences with respect to the base case (Fig. 6.10). On the other hand, results from H02 and H03 resulted in a damage zone having a smaller extent in the horizontal direction, with the outer shear bands less developed. In terms of convergences (Fig. 7.16), they tend to reduce when Biot’s coefficient increases, although differences are relatively small. Regarding water pressures (Fig. 7.17), the differences at PRE_02 and PRE_05 are also quite small, with slightly higher pressures for higher B values. Only a significantly slower dissipation occurs at PRE_04 in analyses H02 and H03, which is related with the smaller extent of their EDZ; the zone with a strong increase of permeability due to damage is farther from PRE_04.
Figure 7.15: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses H (t = 100 days), compared to the observed extension of EDZ (Armand et al., 2014).

Figure 7.16: Computed evolution of horizontal and vertical convergences from the set of analyses H, compared to base case and field measurements (Seyedi et al., 2017).

7.3.5 Time dependency

The influence of the viscosity parameter, appearing in Perzyna’s (1966) visco-plasticity formulation, has been addressed in the set of analyses I. For the base case, a value of $\eta_{pz} = 150$ MPa-day was employed (Table 6.1). It was selected to account for the observed increase of strength, for increasing loading rates, in a particular set of experimental results (Andra, 2014a). However, laboratory data assessing the dependence of the loading rate on the COx behaviour is scarce, and even in the set of results employed for the base case significant dispersion is apparent. In general, increasing $\eta_{pz}$ causes a greater delay in the development of plastic deformations and higher apparent strengths for a given loading rate. The particular effect on the present BVP was studied in this set of analyses. Values of 75, 300 and 1000 MPa-day were employed for analyses I01, I02, and I03 respectively. The obtained contours of shear strain are shown in Fig. 7.18. In analysis I01, where $\eta_{pz}$ was reduced, the configuration of localised deformations is similar to the base case, although with the outer shear
bands more developed and a slightly more flattened damage zone. The opposite occurred in analyses I02 and I03, where $\eta_{pz}$ was increased. The outer shear bands were less developed and the damage zone extended slightly more vertically. Since increasing $\eta_{pz}$ causes a greater delay of plastic deformations, the obtained results were expected. Nevertheless, the configuration of localised deformation in the different analyses does not converge to a unique solution as plastic strains develop in time. This is shown in Fig. 7.19, where the contours of shear strain for $t = 1400$ days are depicted. The delaying of plastic deformations during excavation resulted in a different redistribution of stresses and, therefore, the analyses resulted in different configurations of the damage zone. In the analysis I02, the outer shear bands ended
up intersecting each other with time. On the other hand, in I03 this did not occur and little evolution of the damage zone can be noticed. In terms of convergences (Fig. 7.20), increasing $\eta_{pz}$ causes a more time-dependent response after excavation, although the magnitude does not follow a clear pattern, and lower convergences than the base case were obtained by both, increasing and decreasing $\eta_{pz}$. Nevertheless, differences between the analyses are relatively small. In terms of water pressures, the more significant differences take place at PRE_04. For lower $\eta_{pz}$ values, more damage occurred during excavation, resulting in higher peak pressures due to the AD. In addition, a faster dissipation occurred in the analysis I01 and in the base case, since the damage zone extends further in the horizontal direction bringing the increase of permeability closer to PRE_04. Nevertheless, as the outer shear bands in the analysis I02 ended up intersecting each other, the permeability increase accelerated dissipation around $t = 700$ days.

Figure 7.18: Obtained configuration of the EDZ in terms of shear strain contours for the GCS drift from the set of analyses I ($t = 100$ days), compared to the observed extension of EDZ (Armand et al., 2014).

Finally, the analysis J01 was performed without creep, in order to stress the importance of this deformation mechanism on the observed response. The obtained evolution of convergences is also depicted in Fig. 7.20. Before $t = 80$ days, convergences are almost identical to the base case, where visco-plasticity dominates the time-dependent behaviour.
However, from this time onwards, horizontal and vertical convergences tend to stabilise, and beyond $t = 120$ days convergence increases are negligible. Therefore, consolidation (caused by the hydromechanical coupling) has little effect on the evolution of convergences, and a creep deformation mechanism is required to reproduce the evolution of convergence with time observed in the field. Similar conclusions have already been presented by Mánica et al. (2017c).

Figure 7.20: Computed evolution of horizontal and vertical convergences from the set of analyses I and J, compared to base case and field measurements (Seyedi et al., 2017).

7.4 Conclusions

In this paper, a sensitivity study was conducted following a detailed simulation of the GCS drift presented in a companion paper (Mánica et al., 2018b). A number of analyses were performed, in which the effect of different parameters was studied. The following conclusions can be drawn from the results obtained:

- The initial stress state and the strength anisotropy are two of the main factors controlling the resulting localised deformation patterns. For drifts parallel to $\sigma_h$, where a considerable difference between the horizontal and vertical stresses occurs in the plane normal to the tunnel axis ($\sigma_H/\sigma_h \approx 1.3$), this initial stress anisotropy dominates on the resulting configuration of the damage zone. On the other hand, for drifts parallel to $\sigma_H$, where a nearly isotropic stress state exists in the plane normal to the tunnel axis ($\sigma_h/\sigma_v \approx 1$), strength anisotropy becomes a crucial factor on the resulting configuration of the EDZ.

- For drifts parallel to $\sigma_H$, it seems that the strength when the principal stress is parallel to bedding must be higher than the strength when the principal stress is perpendicular to bedding to obtain a damage zone configuration resembling field observations. The minimum strength can take place at an intermediate orientation, as it is observed in the laboratory.
- Stiffness anisotropy has a minor influence on the pattern of localised deformations. However, it does have a considerable effect on the magnitude of deformations and, more importantly, on the obtained maximum overpressures in the vicinity of the EDZ. These overpressures are the result of the anisotropic deconfinement, which is enhanced as the ratio $E_1/E_2$ increased.
Peak and post-rupture strength parameters have a major impact on the obtained response. The pattern of localisation, extending in the horizontal direction, is generally not altered. However, the extent of the EDZ and the magnitude of deformations are particularly sensitive to modest changes in the peak and port-rupture strength parameters.

In general, pore water pressures are strongly affected by the initial stress state, the stiffness anisotropy, the configuration and extent of the EDZ, the amount and rate of softening, and the initial permeability and its evolution.

By increasing the size of the excavation, the same pattern of localised deformations as the base case was obtained. Only a moderate scale effect was noticed, increasing the relative extent of the EDZ and the relative convergences as the excavation size was increased. This might be explained by the fact that drainage distances increase with the excavation size, reducing dissipation, and resulting in higher water pressures at the vicinity of the EDZ (in the horizontal direction).

Permeability values at the lower bound of the reported range (between 5E-21 and 5E-20 m²) resulted in unrealistic dissipation rates compared to field observations. These results suggest that a representative permeability value for the intact COx might be closer to the upper bound of the reported range of permeabilities.

Permeability anisotropy did not have a considerable impact for ratios $k_{0xx}/k_{0yy}$ between 1 and 3. Only when $k_{0xx}/k_{0yy} = 4$, the extent of the damage zone was reduced compared to the observed EDZ.

Although the effect of Biot’s coefficient was moderate, values between 0.8 and 1.0 had an impact on the configuration of the damage zone. An EDZ with a somewhat lesser extent was obtained for $B$ values in that range.

The viscosity parameter $\eta_{pz}$ in the Perzyna’s (1966) formulation affected the resulting configuration and extent of localised deformations, as well as their evolution in time. A less developed EDZ was obtained as $\eta_{pz}$ was increased, although the magnitude of deformations was similar in all analyses.

Finally, the importance of including a creep deformation mechanics to reproduce the time-dependent behaviour of the excavations has been demonstrated.
Chapter 8

Numerical implementation

This chapter deals with the implementation of the constitutive model employed to simulate the behaviour of stiff clayey materials. A brief summary of the model is first presented. Then, the stress integration algorithm and the error-based sub-stepping scheme are outlined. Finally, the implementation as a user-defined soil model in PLAXIS is described.

8.1 Constitutive model summary

In the articles presented in chapters 5, 6, and 7 the implemented constitutive model is partially described. Nevertheless, for coherence a brief summary is presented here, corresponding to the latest version of the model which is given in appendix D. This also gives the opportunity to describe some implemented features that were not employed in the mentioned chapters. Most of the symbols have already been defined and, therefore, definitions are not presented here for most cases; the reader is referred to the list of symbols for a missing definition.

At the uppermost level, the model can be considered as a superposition model (Tirpitz and Schwesig, 1992), in which a small strain increment is decomposed as,

\[ \text{d}\varepsilon = \text{d}\varepsilon^e + \text{d}\varepsilon^{vp} + \text{d}\varepsilon^c \] (8.1)

where \( \text{d}\varepsilon^e \), \( \text{d}\varepsilon^{vp} \), and \( \text{d}\varepsilon^c \) are respectively the elastic, visco-plastic, and creep strain increments. The first two terms are described under the framework of elasto-visco-plasticity, and an additional creep mechanism is considered. The main components of the local model are presented in sections 8.1.1 to 8.1.4 assuming rate-independent elasto-plasticity, while extension to visco-plasticity and the additional creep mechanism are described in sections 8.1.5 and 8.1.6 respectively. The nonlocal regularisation employed is given in section 8.1.7 and the permeability evolution model in section 8.1.8.

8.1.1 Elasticity

Inside the yield surface the response is assumed linear elastic, where the increment of stresses from a given increment of elastic strains is given by,

\[ \text{d}\sigma = D^e \text{d}\varepsilon^e \] (8.2)
Transverse isotropy (or cross-anisotropy) is assumed and, therefore, the stiffness matrix $D^e$ has the form given in Eq. (8.3) (Wittke, 1990), where the anisotropy direction (i.e. normal to the isotropic plane) is aligned with the $z$ axis.

$$
D^e = \begin{bmatrix}
E_1 \frac{1-\bar{n} \nu_1^2}{(1+\nu_1)\bar{m}} & E_1 \frac{\nu_1+\bar{n} \nu_2^2}{(1+\nu_1)\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\
E_1 \frac{\nu_1+\bar{n} \nu_2^2}{(1+\nu_1)\bar{m}} & E_1 \frac{\nu_1+\bar{n} \nu_2^2}{(1+\nu_1)\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\
\frac{E_1 \nu_2}{\bar{m}} & \frac{E_1 \nu_2}{\bar{m}} & E_2 \frac{1-\bar{m} \nu_1^2}{(1+\nu_1)\bar{m}} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{E_1}{2(1+\nu_1)} & 0 & 0 \\
0 & 0 & 0 & 0 & G_2 & 0 \\
0 & 0 & 0 & 0 & 0 & G_2
\end{bmatrix} \tag{8.3}
$$

where $\bar{n} = E_1/E_2$ and $\bar{m} = 1 - \nu_1 - 2\nu_2^2$. A graphical interpretation of the elastic constants $E_1$, $E_2$, $\nu_1$, $\nu_2$, and $G_2$ is given in Fig. 2.21. If the isotropic plane is not assumed horizontal (parallel to the $xy$-plane), the stiffness matrix can be mapped to a local system aligned with the anisotropy axes of the material in the following way,

$$
\hat{D}^e = T^TD^eT \tag{8.4}
$$

where $\hat{D}^e$ is the stiffness matrix for the actual orientation of the isotropic plane and $T$ is a transformation matrix which depends on how the orientation of the isotropic plane is defined. Here, a different definition from that of Wittke (1990) is considered, described by the two rotations depicted in Fig. A.3a, leading to the following transformation matrix,

$$
T = \begin{bmatrix}
l_1^2 & m_1^2 & n_1^2 & l_1m_1 & m_1n_1 & l_1n_1 \\
l_2^2 & m_2^2 & n_2^2 & l_2m_2 & m_2n_2 & l_2n_2 \\
l_3^2 & m_3^2 & n_3^2 & l_3m_3 & m_3n_3 & l_3n_3 \\
2l_1l_2 & 2m_1m_2 & 2n_1n_2 & l_1m_2 + l_2m_1 & m_1n_2 + m_2n_1 & l_1n_2 + l_2n_1 \\
2l_2l_3 & 2m_2m_3 & 2n_2n_3 & l_2m_3 + l_3m_2 & m_2n_3 + m_3n_2 & l_2n_3 + l_3n_2 \\
2l_1l_3 & 2m_1m_3 & 2n_1n_3 & l_3m_1 + l_1m_3 & m_3n_1 + m_1n_3 & l_3n_1 + l_1n_3
\end{bmatrix} \tag{8.5}
$$

where

$$
l_1 = \cos \alpha \quad m_1 = \sin \alpha \quad n_1 = 0 \\
l_2 = -\sin \alpha \cos \beta \quad m_2 = \cos \alpha \cos \beta \quad n_2 = \sin \beta \\
l_3 = \sin \alpha \sin \beta \quad m_3 = -\cos \alpha \sin \beta \quad n_3 = \cos \beta \tag{8.6}
$$

For two-dimensional problems contained in the $xy$-plane, where the direction $y$ stands for the depth, the simplest approach is to re-arrange the terms in Eq. (8.3) so that the anisotropy direction is aligned with the $y$ axis, and assume $\beta = 0^\circ$ in Eq. (8.6). In that case, only $\alpha$ is required to define the orientation of the isotropic plane, defining a rotation around the axis perpendicular to the analysis plane (see Fig. A.3b).

### 8.1.2 Yield function and flow rule

The yield criterion is defined by the following hyperbolic approximation of the Mohr-Coulomb envelope (Gens et al., 1990),

$$
f = -(c^* + p^* \tan \phi^*) + \sqrt{\frac{J_2}{J_2(\beta)} + (c^* + p^* \tan \phi^*)^2} \tag{8.7}
$$
where $f_2(\theta)$ is a function defining the shape in the deviatoric plane (van Eekelen, 1980) given by,

$$f_2(\theta) = \alpha \theta \left(1 + \beta^3 \sin 3\theta\right)^n$$

where $\beta = 0.85\sqrt{\alpha}$ and $n = -0.229$ were assumed (van Eekelen, 1980).

The flow rule is directly derived from the yield function as follow,

$$\frac{\partial g}{\partial \sigma} = \omega \frac{\partial f}{\partial p} \frac{\partial p}{\partial \sigma} + \frac{\partial f}{\partial J_2} \frac{\partial J_2}{\partial \sigma} + \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial \sigma}$$

where $\omega$ controls the amount of volumetric plastic deformations. It can be assumed constant or a function of the mean stress $p$ and of $\dot{\varepsilon}^p_{\text{eq}}$ (later defined). In the second case, $\omega$ is defined as,

$$\omega(p, \dot{\varepsilon}^p_{\text{eq}}) = \hat{\omega}(p) \zeta(\dot{\varepsilon}^p_{\text{eq}})$$

where

$$\hat{\omega}(p) = \begin{cases} 1 & (p + \frac{J}{\sqrt{3}} < 0) \\ \frac{1}{2} \left[ (1 + \omega_{\text{res}}) + (1 - \omega_{\text{res}}) \cos \left(\pi \frac{p + \frac{J}{\sqrt{3}}}{p_{\text{resdil}} + \frac{J}{\sqrt{3}}} \right) \right] & (0 \leq p + \frac{J}{\sqrt{3}} \leq p_{\text{resdil}} + \frac{J}{\sqrt{3}}) \\ \omega_{\text{res}} & (p > p_{\text{resdil}}) \end{cases}$$

and

$$\zeta(\dot{\varepsilon}^p_{\text{eq}}) = \begin{cases} 1 & (\dot{\varepsilon}^p_{\text{eq}} \leq \xi_2) \\ \frac{\tan \phi^* - \tan \phi_{\text{res}}^*}{\tan \phi_{\text{peak}} - \tan \phi_{\text{res}}^*} & (\dot{\varepsilon}^p_{\text{eq}} > \xi_2) \end{cases}$$

In the code $\omega$ is assumed constant, but the dependence with $p$ and $\dot{\varepsilon}^p_{\text{eq}}$ is included in the implementation through the commented lines 1038 to 1077 of the file main.for. If this is to be included, parameters $\omega_{\text{res}}$ and $p_{\text{resdil}}$ must be added to the model.

### 8.1.3 Strength anisotropy

The strength parameters are assumed a function of the angle $\delta$ between the normal to the isotropic plane and the direction of the major principal stress. For instance, in the case of apparent cohesion,

$$c^* = \Omega(\delta)c_0^*$$

where $\Omega$ is a given function and $c_0^*$ is the cohesion measured with the major principal stress normal to the isotropic plane. The angle $\delta$ is obtained as,

$$\delta = \cos^{-1} \frac{\mathbf{n} \cdot \mathbf{v}}{|\mathbf{n}| |\mathbf{v}|}$$

where $\mathbf{v}$ is the eigenvector of the major principal stress and $\mathbf{n}$ is a unit vector normal to the isotropic plane. According to the considered rotation (see Fig. A.3), $\mathbf{n}$ is given by,
\[
\mathbf{n} = \begin{cases}
\begin{bmatrix}
\sin \beta \sin \alpha \\
- \cos \alpha \sin \beta \\
\cos \beta 
\end{bmatrix} & \text{for 3D where } z \text{ stands for the depth} \\
\begin{bmatrix}
- \sin \alpha \\
\cos \alpha \\
0 
\end{bmatrix} & \text{for 2D where } y \text{ stands for the depth}
\end{cases}
\] (8.15)

The function \( \Omega \), defining the variation of the strength parameters with \( \delta \), is given by,
\[
\Omega = \frac{\hat{A}e^{(\delta_m - \delta)n}}{1 + e^{(\delta_m - \delta)n}} + \frac{\hat{B}}{1 + e^{(\delta_m - \delta)n}} + \hat{C}
\] (8.16)

where
\[
\hat{A} = \frac{2(e_1 + 1)(e_2 + 1)(e_1 - e_2 + \Omega_90 + e_1e_2 + e_1\Omega_90 - e_2\Omega_90 - 2e_1\Omega_m + 2e_2\Omega_m - e_1e_2\Omega_90 - 1)}{(e_1 - e_2)(e_1 - 1)(e_2 - 1)}
\] (8.17)
\[
\hat{B} = \frac{\Omega_90 - \frac{\hat{A}e_1}{(e_1 + 1)^2} + \frac{\hat{A}e_2}{(e_2 + 1)^2} - 1}{e_1 + 1 - e_2 + 1}
\] (8.18)
\[
\hat{C} = 1 - \frac{\hat{A}e_2}{(e_2 + 1)^2} - \frac{\hat{B}}{e_2 + 1}
\] (8.19)
\[
e_1 = e^{(\delta_m - 90)n}
\] (8.20)
\[
e_2 = e^{\delta_m n}
\] (8.21)

A graphical interpretation of \( \Omega_{90} \), \( \Omega_m \), \( \delta_m \), and \( \hat{n} \) is given in Fig. A.4. In the code, \( c^* \) and \( p_t \) are assumed to have the same strength distribution and \( \phi^* \) is assumed isotropic. Nevertheless, anisotropy in \( \phi^* \) is also included in the implementation through lines 984, 985, 1003, and 1004 of the file \textit{main.for}. If this is to be included, parameters \( \Omega_{90} \), \( \Omega_m \), \( \delta_m \), and \( \hat{n} \) for the variation of \( \phi^* \) with the loading direction have to be added to the model.

### 8.1.4 Hardening laws

Non-linear isotropic hardening is considered, driven by the evolution of the strength parameters. They vary in piecewise manner as follow,
\[
\tan \phi^* = \begin{cases}
\tan \phi_{\text{ini}}^* + \frac{\varepsilon_p^p}{\varepsilon_{\text{eq}}} & (\varepsilon_{\text{eq}} \leq \xi_2) \\
\tan \phi^*_{\text{peak}} - \tan \phi^*_{\text{ini}} - a_{\text{hard}} & (\varepsilon_{\text{eq}} > \xi_2)
\end{cases}
\] (8.22)
\[ c_0^* = \begin{cases} c_0^{ini} & (\epsilon_{eq} \leq \xi_2) \\ (c_0^{ini} - c_0^{post}) e^{-b_{post}(\epsilon_{eq}^{p} - \xi_2) + c_0^{post} e^{-b_{res}(\epsilon_{eq}^{p} - \xi_2)}} & (\epsilon_{eq} > \xi_2) \end{cases} \] (8.23)

\[ p_{t0} = \begin{cases} p_{t0}^{ini} & (\epsilon_{eq} \leq \xi_2) \\ (p_{t0}^{ini} - p_{t0}^{post}) e^{-b_{post}(\epsilon_{eq}^{p} - \xi_2) + p_{t0}^{post} e^{-b_{res}(\epsilon_{eq}^{p} - \xi_2)}} & (\epsilon_{eq} > \xi_2) \end{cases} \] (8.24)

where \( \epsilon_{eq}^{p} \) is a function of the state variable \( \epsilon_{eq}^{p} \) and the mean stress \( p \),

\[ \epsilon_{eq}^{p} = \begin{cases} \epsilon_{eq}^{p} + \left(\frac{\langle p \rangle}{p_{atm}}\right)^2 \hat{m}^2 & (\epsilon_{eq}^{p} \leq \xi_2) \\ \epsilon_{eq}^{p} - \xi_2 \left(\frac{\langle p \rangle}{p_{atm}}\right)^2 \hat{m}^2 & (\epsilon_{eq}^{p} > \xi_2) \end{cases} \] (8.25)

where \( p_{atm} \) is a reference pressure, here assumed equal to 100 kPa, \( \hat{m} \) is a parameter controlling the influence of \( p \) on the hardening evolution, and

\[ \epsilon_{eq}^{p} = (\epsilon^p : \epsilon^p)^{1/2} \] (8.26)

When \( \hat{m} = 0 \), the dependence with \( p \) disappears and the hardening laws (Eq. 8.22 to 8.24) become a function of the state variable \( \epsilon_{eq}^{p} \) only. However, when \( \hat{m} > 0 \), a higher value of \( \epsilon_{eq}^{p} \) is required to start softening, resulting in a more ductile behaviour by increasing \( p \). The actual state variable is \( \epsilon_{eq}^{p} \), and \( \epsilon_{eq}^{p} \) serves to include a dependence of the hardening laws on the mean stress. This implies that, when \( \hat{m} > 0 \), the strength parameters also depend on \( p \), and they contribute to the volumetric component of plastic deformations in the flow rule (Eq. 8.9). In that case, the flow rule is given by Eq. (C.26).

A post-rupture ratio is defined so that the post-rupture parameters are a function of the initial ones,

\[ r_{post} = \frac{c_0^{post}}{c_0^{ini}} = \frac{p_{t0}^{post}}{p_{t0}^{ini}} \] (8.27)

8.1.5 Perzyna’s overstress

The extension to visco-plasticity is obtained by defining the visco-plastic strain increment as,

\[ d\epsilon^{vp} = \langle \Phi(f) \rangle \frac{\partial g}{\partial \sigma} \] (8.28)

where the following expression for the over-stress function \( \Phi \) was employed,

\[ \Phi(f) = \left(\frac{f}{p_{atm}}\right)^N \] (8.29)
It is possible to derive an equation for the rate-dependent yield surface (Heeres et al., 2002),
\[ f_{\text{rd}} = f - \Phi^{-1}(\eta_{px} \dot{\lambda}) = 0 \] (8.30)
where the second term is referred as the *overstress*, defining how far can the stress state be from the rate-independent yield surface.

### 8.1.6 Creep deformations

For the creep component, strain increments are computed as,
\[ d\epsilon^c = \dot{\epsilon}^c dt \] (8.31)
where the creep strain rate tensor \( \dot{\epsilon}^c \) is defined as,
\[ \dot{\epsilon}^c = \begin{cases} 0 & (\epsilon^p_{\text{eq}} \leq \epsilon_{\text{thr}}) \\ \dot{\epsilon}^c = \gamma^c e^{-\alpha^c \epsilon^c_{\text{eq}}} (s + \psi^c p I) & (\epsilon^p_{\text{eq}} > \epsilon_{\text{thr}}) \end{cases} \] (8.32)
and
\[ \epsilon^c_{\text{eq}} = (\epsilon^c : \epsilon^c)^{1/2} \] (8.33)

According to (8.32), creep strains will not take place until the material has undergone some amount plastic deformations, i.e. when the material experience some damage. Another important characteristic is that creep strains are coupled with the visco-plastic component, and can mobilise the strength. The latter is achieved by defining the total plastic strain tensor \( \epsilon^p \), used in Eq. (8.26), as the sum of the visco-plastic and creep components,
\[ \epsilon^p = \epsilon^p_{\text{vp}} + \epsilon^c \] (8.34)

### 8.1.7 Nonlocal approach

If the flag for nonlocality is activated, then the state variable \( \epsilon^p_{\text{eq}} \) is replaced by its nonlocal counterpart \( \bar{\epsilon}^p_{\text{eq}} \), defined as
\[ \bar{\epsilon}^p_{\text{eq}} = \int_V w(X, \kappa) \epsilon^p_{\text{eq}}(\kappa) d\kappa \] (8.35)
where \( w \) is a normalised weighting function defined as
\[ w(X, \kappa) = \frac{w_0(||X - \kappa||)}{\int_V w_0(||X - Y||) dY} \] (8.36)
\[ w_0(||X - \kappa||) = \frac{||X - \kappa||}{l_s} e^{-||(X - \kappa)||/l_s} \] (8.37)

In the implementation, \( \epsilon^p_{\text{eq}} \) is only replaced by Eq. (8.35) once softening has started, and points only inside a radius of \( 2l_s \) are considered to compute the nonlocal state variable.
8.1.8 Permeability evolution

The intrinsic permeability is assumed to evolve with deformation. The expression from Pardoen et al. (2016) was used here, which is inspired on the classical cubic law (Witherspoon et al., 1980),

\[ k = k_0 \left[ 1 + \beta^k (\epsilon_{eq})^3 \right] \]  

(8.38)

where \( \beta^k \) is an evolution parameter.

8.2 Stress integration algorithm

A backward Euler method is assumed for the time discretisation and, therefore, the system of equations to be solved is given by,

\[ \sigma_{n+1} = \sigma_n + d\sigma_{n+1} \]  

(8.39)

\[ \chi_{n+1} = \chi_n + d\chi_{n+1} \]  

(8.40)

satisfying also the yield condition in the case of plastic loading,

\[ f^{rd} = 0 \]  

(8.41)

It is important to notice that is the rate-dependent yield surface (Eq. 8.30) which must be satisfied. \( \chi \) is the vector of state variables. From the assumed strain decomposition (Eq. 8.1), we defined the unknown increments of stress and state variables as

\[ d\sigma_{n+1} = D^e (d\epsilon_{n+1} - d\epsilon_{vp} - d\epsilon_{c}) \]  

(8.42)

\[ d\chi_{n+1} = \frac{\partial \chi}{\partial \epsilon_{vp}} d\epsilon_{vp} + \frac{\partial \chi}{\partial \epsilon_{c}} d\epsilon_{c} \]  

(8.43)

where

\[ d\epsilon_{vp} = \frac{\partial g}{\partial \sigma} |_{n+1} d\lambda_{n+1} \]  

(8.44)

\[ d\epsilon_{c} = \dot{\epsilon}_{c}^c d\lambda_{n+1} \]  

(8.45)

It is also important to notice that both, the visco-plastic and creep components, contribute to \( \chi \). Substituting Eq. (8.44) and (8.45) into Eq. (8.42) and (8.43), leads to the non-linear system of equation to be solved,

\[ r^\sigma_{n+1} = d\sigma_{n+1} - D^e \left( d\epsilon_{n+1} - \frac{\partial g}{\partial \sigma} |_{n+1} d\lambda_{n+1} - \dot{\epsilon}_{c}^c d\lambda_{n+1} \right) = 0 \]  

(8.46)

\[ r^\chi_{n+1} = d\chi_{n+1} - \frac{\partial \chi}{\partial \epsilon_{vp}} |_{n+1} \frac{\partial g}{\partial \sigma} |_{n+1} d\lambda_{n+1} - \frac{\partial \chi}{\partial \epsilon_{c}} |_{n+1} \dot{\epsilon}_{c}^c d\lambda_{n+1} = 0 \]  

(8.47)

\[ r^f_{n+1} = f_{n+1} - \Phi_{n+1}^{-1} \eta_{p2} \frac{d\lambda_{n+1}}{dt} = 0 \]  

(8.48)
with the unknowns \( d\lambda_{n+1} \), \( d\sigma_{n+1} \), and \( d\chi_{n+1} \) constrained by the Kuhn Tucker loading/unloading conditions (Eq. 3.4). For its solution, the Newton’s method is employed, where a set of non-linear equations \( \mathbf{r}(\mathbf{x}) = 0 \) is solved iteratively as,

\[
J^j \Delta \mathbf{x}^j = -\mathbf{r}(\mathbf{x}^j) \quad (8.49)
\]

\[
\mathbf{x}^{j+1} = \mathbf{x}^j + \Delta \mathbf{x}^j \quad (8.50)
\]

where \( j \) refers to the iteration number, \( \mathbf{x} \) is the vector of unknowns, and \( J \) is a Jacobian matrix containing the partial derivatives of the equations with respect to each unknown,

\[
J = \begin{bmatrix}
\frac{\partial r_1}{\partial x_1} & \cdots & \frac{\partial r_1}{\partial x_i} \\
\frac{\partial r_2}{\partial x_1} & \cdots & \frac{\partial r_2}{\partial x_i} \\
\vdots & \ddots & \vdots \\
\frac{\partial r_i}{\partial x_1} & \cdots & \frac{\partial r_i}{\partial x_i}
\end{bmatrix} \quad (8.51)
\]

Applying Newton’s method to Eq. (8.46) to (8.48) gives

\[
\begin{bmatrix}
\frac{\partial r^\sigma}{\partial \sigma} & \frac{\partial r^\sigma}{\partial \chi} & \frac{\partial r^\sigma}{\partial \lambda} \\
\frac{\partial r^\chi}{\partial \sigma} & \frac{\partial r^\chi}{\partial \chi} & \frac{\partial r^\chi}{\partial \lambda} \\
\frac{\partial r^f}{\partial \sigma} & \frac{\partial r^f}{\partial \chi} & \frac{\partial r^f}{\partial \lambda}
\end{bmatrix}^j \begin{bmatrix}
\Delta \sigma^j \\
\Delta \chi^j \\
\Delta \lambda^j
\end{bmatrix} = \begin{bmatrix}
-r^\sigma^j \\
r^{-\chi}^j \\
r^{-f}^j
\end{bmatrix} \quad (8.52)
\]

\[
d\sigma^{j+1} = d\sigma^j + \Delta \sigma^j \\
d\chi^{j+1} = d\chi^j + \Delta \chi^j \\
d\lambda^{j+1} = d\lambda^j + \Delta \lambda^j \quad (8.53)
\]

where,

\[
\frac{\partial r^\sigma}{\partial \sigma} = I + d\lambda \mathbf{D}_e \frac{\partial^2 g}{\partial \sigma^2} + dt \mathbf{D}_c \frac{\partial \dot{\epsilon}^c}{\partial \sigma} \quad (8.54)
\]

\[
\frac{\partial r^\sigma}{\partial \chi} = d\lambda \mathbf{D}_e \frac{\partial^2 g}{\partial \sigma \partial \chi} + dt \mathbf{D}_c \frac{\partial \dot{\epsilon}^c}{\partial \chi} \quad (8.55)
\]

\[
\frac{\partial r^\sigma}{\partial \lambda} = \mathbf{D}_e \frac{\partial g}{\partial \sigma} \quad (8.56)
\]

\[
\frac{\partial r^\chi}{\partial \sigma} = -d\lambda \frac{\partial \chi}{\partial \epsilon^{vp}} \frac{\partial^2 g}{\partial \sigma^2} - dt \frac{\partial \chi}{\partial \epsilon^c} \frac{\partial \dot{\epsilon}^c}{\partial \sigma} \quad (8.57)
\]

\[
\frac{\partial r^\chi}{\partial \chi} = I - d\lambda \frac{\partial \chi}{\partial \epsilon^{vp}} \frac{\partial^2 g}{\partial \sigma \partial \chi} - dt \frac{\partial \chi}{\partial \epsilon^c} \frac{\partial \dot{\epsilon}^c}{\partial \chi} \quad (8.58)
\]
\[
\frac{\partial r^\chi}{\partial \lambda} = - \frac{\partial \chi}{\partial \epsilon^{vp}} \frac{\partial g}{\partial \sigma}
\] (8.59)

\[
\frac{\partial r^f}{\partial \sigma} = \left[ \frac{N \eta_{pz} \, d\lambda}{dt \, p_{atm} (f/p_{atm})^{N+1} + 1} \right] \frac{\partial f}{\partial \sigma}
\] (8.60)

\[
\frac{\partial r^f}{\partial \chi} = \left[ \frac{N \eta_{pz} \, d\lambda}{dt \, p_{atm} (f/p_{atm})^{N+1} + 1} \right] \frac{\partial f}{\partial \chi}
\] (8.61)

\[
\frac{\partial r^f}{\partial \lambda} = - \eta_{pz} \frac{d\lambda}{dt (f/p_{atm})^N}
\] (8.62)

Derivatives involved in Eq. (8.54) to (8.62) are given in appendix C.

The two state variables of the model are \( \epsilon_{eq}^p \) and \( \epsilon_{eq}^c \). Both, visco-plastic \( (\epsilon_{eq}^{vp}) \) and creep strains \( (\epsilon_{eq}^c) \) contribute to the first one, but only creep strains contribute to the second one. Therefore, to ease implementation, all the components of the total plastic strain tensor (Eq. 8.34) are stored instead of \( \epsilon_{eq}^p \), leading to the following definition for the vector of state variables \( \chi \),

\[
\chi = \begin{bmatrix} \epsilon^p \\ \epsilon_{eq}^c \end{bmatrix}
\] (8.63)

This leads to a system (Eq. 8.52) with 14 equations and 14 unknowns.

### 8.3 Error-based sub-stepping scheme

To solve the established implicit system of equations using Newton’s method an initial guess of the unknowns \( (x^j) \) is required. In fact, convergence is only guaranteed if this initial guess is reasonably close to the solution. In computational plasticity, it is customary to use the elastic solution as the initial guess for Newton’s method. However, for highly non-linear problems this initial guess for a given step size may be too far and the method might diverge. In addition, the backward Euler is only a second-order method (for the local truncation error) and, therefore, situations can exist were convergence is possible, but the error will be too large.

Due to the above-mentioned issues, an error-based sub-stepping scheme was implemented in the stress integration algorithm. The general structure is based on the scheme from Sloan (1987). However, in Sloan (1987) two different methods of different order are employed to estimate a second order local truncation error, which serves as the basis for the step size estimation. Here, a second order local truncation error is estimated using only the backward Euler method. This is possible using a numerical technique known as Richardson’s (1911; 1927) extrapolation, which allow us to derive a higher order solution by solving the problem with two different steps sizes; the derivation is given in appendix B. For instance, by using the step sizes \( h \) and \( h/2 \), the second order local truncation error in \( U(h/2) \) for the backward Euler method reads,

\[
error(h/2) = \frac{U(h/2) - U(h)}{4 - 1} + O(h^3)
\] (8.64)

where \( U(h) \) and \( U(h/2) \) are approximations of \( U \) (the exact solution) using step sizes of \( h \).
and $h/2$ respectively. By dropping the higher order terms $O(h^3)$, we obtain our second order
local error estimation.

The actual sub-stepping scheme, for sub-step sizes $dT$ and $dT/2$, reads as follow,

1. Set $T = 0$
   
   \[dT = 1\]

   which are the normalised time of the step and the size of the current sub-increment respectively.

2. While $T < 1$, do points 3 to 11.

3. Set $\sigma_n^a = \sigma_n$
   
   $\sigma_n^b = \sigma_n$

   $\chi_n^a = \chi_n$

   $\chi_n^b = \chi_n$

   $de^a = de \cdot dT$

   $de^b = de \cdot dT/2$

   where the superscripts $a$ and $b$ relate with the sub-step sizes $dT$ and $dT/2$ respectively.

4. Calculate $\sigma_{n+1}^a(\sigma_n^a, \chi_n^a, de^a)$

   $\chi_{n+1}^a(\sigma_n^a, \chi_n^a, de^a)$

   If divergence occurs in Newton’s method, then $dT = dT/2$ and return to point 2.

5. Calculate $\sigma_{n+1}^b(\sigma_n^b, \chi_n^b, de^b)$

   $\chi_{n+1}^b(\sigma_n^b, \chi_n^b, de^b)$

   If divergence occurs, then $dT = dT/2$ and return to point 2.

6. Set $\sigma_n^b = \sigma_{n+1}^b$

   $\chi_n^b = \chi_{n+1}^b$

7. Calculate $\sigma_{n+1}^b(\sigma_n^b, \chi_n^b, de^b)$

   $\chi_{n+1}^b(\sigma_n^b, \chi_n^b, de^b)$

   This corresponds to the second half of the step using $dT/2$. If divergence occurs, then $dT = dT/2$ and return to point 2.

8. Calculate an estimate of the local truncation error as (Eq. 8.64),

   \[E = \frac{\sigma_{n+1}^b - \sigma_{n+1}^a}{3}\]

9. Determine the relative error for the sub-step as,

   \[E^r = \max \left\{EPS, \frac{\|E\|}{\|\sigma_{n+1}^a\|} \right\}\]

   where EPS is a machine specific constant that gives an upper bound on the relative error due to rounding in floating point arithmetic. It is considered enough to check for the error in stresses, but state variables can also be included in the error definition.

10. If $E^r > TOL$, then go to point 12. Else, this sub-step is accepted and variables are updated,

    \[T = T + dT\]

    \[\sigma_n = \sigma_{n+1}^b\]

    \[\chi_n = \chi_{n+1}^b\]
11. Estimate the size of the next sub-step as,

\[
Q = \min \left\{ 0.8 \left( \frac{TOL}{E^*} \right)^{1/2}, 2 \right\}
\]

\[
dT = QdT
\]

\[
dT = \min \{dT, 1 - T\}
\]

The factor 0.8 gives a conservative estimation helping to reduce the number of sub-steps that are likely to be rejected in the integration process, and the constrain in the relative size of 2 prevents an excessively large sub-step (Sloan, 1987).

12. If the sub-step failed, estimate an smaller one as,

\[
Q = \max \left\{ 0.8 \left( \frac{TOL}{E^*} \right)^{1/2}, 0.1 \right\}
\]

\[
dT = QdT
\]

and return to point 2. In the same way as for the successful sub-step, the relative size is constrained to prevent an excessively small sub-step (Sloan, 1987).

### 8.4 User-defined soil model - PLAXIS

The constitutive model described was implemented as a user-defined soil model (UDSM) in PLAXIS. In general terms, for the implementation the user provides information about the current stresses and state variables, and PLAXIS provides information about the previous ones and also the strain and time increments. This section is not intended to describe in detail the facility for UDSM; the reader is referred to the PLAXIS’ user manual for that (Brinkgreve et al., 2017). Here, only a brief description of the Fortran files contained in the generated dynamic-link library (DLL) are presented, which are given in appendix D.

#### 8.4.1 Files in the DLL

**File call.for**

This file contains the subroutine *User.mod*, which is called by the calculation program when a UDSM is being used in PLAXIS. The arguments in this subroutine define the communication between the calculation program and the UDSM. More than one model can be contained in the same DLL, and the selection is performed in this subroutine according to the argument *iMod*, taking its value directly from the input program according to the selected model in the parameter tabsheet. For the selected model, a given task is expected to be performed in each call, defined by the argument *IDTask*. These are,

- \( IDTask = 1 \) Initialise state variables
- \( IDTask = 2 \) Calculate constitutive stresses
- \( IDTask = 3 \) Create effective material stiffness matrix
- \( IDTask = 4 \) Return the number of state variables
- \( IDTask = 5 \) Return matrix attributes
\textit{IDTask} = 6 \quad \text{Create elastic material stiffness matrix}

Although they can be performed within \textit{User\_mod}, it is always a good practice to have a separate subroutine, especially when there is more than one model in the DLL. Here, the different tasks are performed in the subroutine \textit{const\_law}, contained in the file \textit{main\_for}.

**File \textit{main\_for}**

This file contains the subroutine \textit{const\_law}, where the tasks requested by the calculation program are performed. In addition, a number of subroutines, employed by \textit{const\_law}, are also contained in this file. They are,

- \textit{Stiff\_mat} \quad \text{Calculates the elastic stiffness matrix with transverse isotropy (line 513).}
- \textit{SPA} \quad \text{Stress point algorithm - Backward Euler method (line 633).}
- \textit{Jacobian} \quad \text{Calculates the Jacobian matrix for the Newton-Raphson method (line 780).}
- \textit{HMC} \quad \text{Hyperbolic Mohr-Coulomb - Verification of the yield condition and calculation of plastic parameters (line 906).}
- \textit{Mob\_strg} \quad \text{Mobilised strength parameters and derivatives of evolution laws (line 1221).}
- \textit{Creep\_st} \quad \text{Calculation of the creep strain rates and its derivatives (line 1437).}
- \textit{Stress\_inva} \quad \text{Calculation of stress invariants (line 1553).}
- \textit{Stress\_inva\_dev} \quad \text{Calculation of derivatives of stress invariants (line 1613).}
- \textit{Stress\_inva\_2dev} \quad \text{Calculation of second derivatives of stress invariants (line 1687).}
- \textit{Ludcmp} \quad \text{LU decomposition of a square matrix (Press et al., 1992) (line 1796).}
- \textit{Lubksb} \quad \text{Solves the set of } n \text{ linear equations } AX = B \text{ from the results of the LU decomposition (Press et al., 1992) (line 1863).}
- \textit{Fomega} \quad \text{Calculation of } \Omega \text{ that controls strength anisotropy (line 1901).}
- \textit{Fomega\_dev} \quad \text{First derivative of } \Omega \text{ with respect to stresses (central difference) (line 1948).}
- \textit{Delta} \quad \text{Angle between the isotropic plane and the major principal stress (line 1994).}
- \textit{Eigen} \quad \text{Calculates eigenvalues and eigenvectors of a real symmetric matrix (Press et al., 1992) (line 2074).}
- \textit{Eigsrt} \quad \text{Sorts the eigenvalues into descending order (Press et al., 1992) (line 2177).}
- \textit{Nonlocal1} \quad \text{Creates information files for the nonlocal model at the beginning of a phase (line 2212).}
Nonlocal2 Calculates the nonlocal state variable at the beginning of a global iteration (line 2293).

The arguments passed between the calculation program and the UDSM, through User_mod, are described in lines 29 to 58 of main.for. Before any tasks are executed, a consistency check is performed (IDTask = 0) with respect to the parameters inputted from the parameter tabsheet and contained in the vector Props. If any inconsistency is found, the calculation is stopped and a messagebox appears with an explanation. The specific procedures executed for each IDTask are described below.

In IDTask = 1, state variables must be initialise. However, no specific initialisation procedure with respect to the initial stress state is required in the model. Nevertheless, const.law is called for IDTask = 1 at the beginning of a phase, and iterates through all Gauss points. Since coordinates are passed as arguments, these are written to a file (file1.txt) to be later used if the flag for the nonlocal approach has been activated. The initial value of $\epsilon_{eq}^P$ is also written in the file. Since a global index is assigned to each Gauss point while writing this information, the index for the first Gauss point of an element is written in file2.txt. PLAXIS does not use a global numbering for the Gauss points, and this file is used to obtain the global index from the element number and the local Gauss point number.

IDTask = 2 is the main task performed by the UDSM, corresponding to the integration of constitutive stresses. Given the initial stress and state variables and the increments of strain and time, the UDSM must return the new stresses and state variables according to the constitutive law (section 8.1). The general structure of the script executed within this task is depicted in Fig. 8.1, including the error-based sub-stepping scheme described in detail in section 8.3. The actual stress integration is performed by the subroutine SPA, where the implicit scheme described in section 8.2 was implemented. If the nonlocal approach has been activated, the required files are created at the beginning of a phase by the subroutine Nonlocal1, and the nonlocal variable is computed at the beginning of each global iteration by Nonlocal2. Including those mentioned for IDTask = 1, the files employed if the nonlocal approach has been activated are,

file1.txt Stores the coordinates and the initial local state variable $\epsilon_{eq}^P$ for all the Gauss points.

file2.txt Stores the global index of the first Gauss point of each element.

file3.txt Stores the number of Gauss points inside the interaction radius for each Gauss point.

file4.txt Stores the global indices of the Gauss points inside the interaction radius for each Gauss point.

file5.txt Stores the radial distances between the Gauss points inside the interaction radius for each Gauss point.

file6.txt Stores the local state variable $\epsilon_{eq}^P$ during calculation for each Gauss point.

file7.txt Stores the nonlocal state variable $\bar{\epsilon}_{eq}^P$ during calculation for each Gauss point.
Figure 8.1: Flow chart of the script within $IDTask = 2$
To speed-up I/O operations, the files are created using random access and binary format. They are stored in the temporary directory created by PLAXIS and, therefore, they are deleted once the calculation program stops.

In \textit{IDTask} = 3, the material stiffness matrix, used to derive the stiffness matrix employed in the global solution, must be supplied. If the quadratic convergence rate of the global Newton-Raphson method is desired, then the consistent material tangent matrix has to be computed and passed during this task (Simo and Taylor, 1985). On the other hand, an elastic stiffness matrix might result in a more robust iterative procedure (Brinkgreve et al., 2017). The second alternative was preferred here for the implementation and, therefore, the subroutine \textit{Stiff\_mat} was employed to derive the effective material stiffness matrix. Since in \textit{IDTask} = 6 the elastic material stiffness matrix is requested, this two task (3 and 6) are performed with the same piece of code.

In \textit{IDTask} = 4, the number of state variables is passed. Seven state variables were defined in section 8.2, corresponding to the six plastic strain components $\epsilon^p$ and the creep state variable $\epsilon^c_{eq}$. However, $\epsilon^p_{eq}$ is computed and stored also as a state variable, so that it is available in the output program. Therefore, the total number of state variables is eight.

In \textit{IDTask} = 5, attributes of the material stiffness matrix are passed in order to properly update this matrix during calculation. Those attributes define if the matrix is non-symmetric, stress dependent, if it is the consistent tangent, or if it is time-dependent. Since the elastic stiffness matrix is being employed as the material stiffness matrix, all these attributes are false and, therefore, zeros are passed for all of them. In addition, since \textit{IDTask} = 5 is called once at the beginning of a phase, the files \textit{file1.txt} and \textit{file2.txt}, used in \textit{IDTask} = 1, are created here. Finally, a procedure was also implemented here to allow considering a particular spatial distribution of the cohesion and isotropic tensile strength. A text file named \textit{file9.txt}, containing a list of strength factors for each Gauss point, must be supplied. The information of this file is rewritten to \textit{file10.txt} using random access and binary format, which is used by the subroutine \textit{Mob\_strg} to derived the desired cohesion and tensile strength. The use of this feature is further explained in section 8.4.2.

\textbf{File \textit{perm\_for}}

This file contains the subroutine \textit{perm}, where the permeability evolution model, described in section 8.1.8, was implemented. The possibility to modify the permeability during calculations, according to a state variable of the mechanical law, is possible due to the new facility of PLAXIS for user-defined flux models (UDFM); it gives the possibility to use custom groundwater and thermal flow laws. Because this feature is still in a validation stage, it has not being included in the input program yet. The activation has to be done via a so-called \textit{cheat file}, placed in the PLAXIS 2D project folder. This section is not intended to describe in detail the facility for UDFM, and the reader is advised to contact PLAXIS for further information. Only the specific cheat file employed for the analyses presented in chapters 6 and 7 is presented in Fig. 8.2.

The file name is fixed, and only the last character must be modified to indicate on which phase this file needs to be applied. In this case, the letter \textit{a} indicates that it must be applied to all phases. The file is a list of JSON structures, one per model and material set. Here,
a single structure was employed, and the items contained define the material set number to
which the UDFM is applied, the name of the DLL containing the UDFM, the name of the
UDFM, the function to be replaced, and the parameters of the UDFM.

```
data.udfm.rsa

[{
  "material": 1,
  "file": "ahw_Manica2018_64.dll",
  "model": "perm",
  "replace": "saturated_permeability",
  "parameters": [4.0e7]}
]
```

Figure 8.2: Example of a cheat file for the activation of a UDFM

**File param.for**

This file contains a number of subroutines allowing the interaction between the PLAXIS
user-interface and the user-defined models. For instance, they allow the input of parameters
of the UDSM directly from the parameter tabsheet. The structure of those subroutines was
directly taken from the examples at PLAXIS website; they were only modified accordingly
to the particular model implemented. These subroutines are,

- **GetModelCount** Return the maximum model number in this DLL.
- **GetmodelName** Return the name of the different models.
- **GetParamCount** Return the number of parameters of the different models.
- **GetParamName** Return the parameters name of the different models.
- **GetParamUnit** Return the units of the different parameters of the different models.
- **GetParamAndUnit** Return the parameters name and units of the different models.
- **GetStateVarCount** Return the number of state variables of the different models.
- **GetStateVarName** Return the name of the different state variables of the different models.
- **GetStateVarUnit** Return the units of the different state variables of the different models.
- **GetStateVarNameAndUnit** Return the name and unit of the different state variables of the different models.
File `okmsg.for`

Finally, this file contains the subroutine `Ok_messagebox`, which displays a message-box with an OK button. The message to be displayed is passed as an argument to this subroutine. Its structure was also taken from the examples at PLAXIS website.

8.4.2 Using the Argillaceous Hard Soils - Weak Rocks (AHW) model

The files described in the previous section have to be compiled to a 64-bits dynamic-link library using a Fortran compiler. The last two characters of the DLL’s name must be “64” so that PLAXIS can recognize the file. The DLL must be placed in the UDSM folder of PLAXIS, which is generally located in the following path: “C:\ProgramFiles\Plaxis\PLAXIS2D\udsm”. For those readers interested in directly using the model, an already generated DLL can be downloaded from the following website: https://1drv.ms/f/s!AvWYaNd33pAhqdoPSRqU5H7EGkscDw. It was generated using the Intel® Visual Fortran Composer XE 2013 SP1, and it has been tested in PLAXIS version 2017.01, running in a Windows 10 operating system.

In the following, the parameters of the AHW model are described. Since several features of the behavior of argillaceous hard soils - weak rocks were included, the model has as many as 40 parameters. Nevertheless, a modular approach was followed, and several of those features can be deactivated if desired.

Elastic parameters

01. $E_1$ Young’s modulus parallel to the isotropic plane
02. $\nu_1$ Poisson’s ratio between the two strain components on the isotropic plane for loading parallel to the isotropic plane
03. $E_2$ Young’s modulus perpendicular to the isotropic plane
04. $\nu_2$ Poisson’s ratio between strain components on the isotropic plane and the component perpendicular thereto for loading perpendicular to the isotropic plane
05. $G_2$ Shear modulus on the planes perpendicular to the isotropic plane

A graphical interpretation of the elastic parameters is given in Fig. 2.21. For transverse isotropic (or cross-anisotropic) elasticity, all five are required. However, if only isotropic elasticity is desired, then $E_1 = E$ and $\nu_1 = \nu$ and parameters 3 to 5 must be zero.

Anisotropy direction

06. $\alpha$ Angle for the orientation of the isotropic plane
07. $\beta$ Angle for the orientation of the isotropic plane

In 3D analyses, where the $z$ axis stands for the depth, the orientation of the isotropic plane can be described according to Fig. A.3a; in that case, parameter 40 must be zero. For 2D analyses, where the $y$ axis stands for the depth, parameter 7 must be zero, parameter 40 must be one, and the orientation of the isotropic plane should be done only with parameter
6 according to Fig. A.3b. This orientation of anisotropy applies to both, the elastic stiffness
anisotropy just described and the strength anisotropy later described.

**Strength parameters**

08. $\phi_{ini}^*$ Initial asymptotic friction angle

09. $\phi_{peak}^*$ Peak asymptotic friction angle

10. $\phi_{res}^*$ Residual asymptotic friction angle

11. $c_{0ini}^*$ Initial asymptotic cohesion for $\delta = 0$

12. $p_{0ini}$ Initial isotropic tensile strength for $\delta = 0$

13. $r_{post}$ Post-rupture ratio

14. $\alpha^\theta$ Parameter for the shape of the yield function in the octahedral plane

Parameters 8, 11, 12 and 14 define the initial yield surface (see Eq. 8.7 and 8.8). Following
van Eekelen (1980), $\beta^\theta = 0.85\sqrt{\alpha^\theta}$ and $n^\theta = -0.229$ are assumed in Eq. (8.8). Parameters 9,
11, 12 and 14 define the peak yield surface; note that cohesion and isotropic tensile strength
are assumed constant between initial and peak states (see Eq. 8.23 and 8.24). Parameter
13 define the relative amount of cohesion and tensile strength that is lost according to the
post-rupture softening rate $b_{post}$, so that $r_{post} = c_{0post}^*/c_{0ini}^* = p_{0post}^*/p_{0ini}^*$. It is assumed
that at the residual state all the cohesion and tensile strength have been lost and, therefore,
the residual envelope is defined by parameters 10 and 14.

**Plastic potential**

15. $\omega$ Non-associativity constant

Parameter 15 controls the amount of volumetric plastic deformations according to Eq. (8.9).
With $\omega = 1$ an associated flow rule is recovered, while for $\omega = 0$ no plastic volumetric strains
occur. The value of $\omega$ should lie within this range.

**Hardening/softening**

16. $\xi_2$ Value of $\epsilon_{eq}^p$ at which softening begins (for $p' = 0$ when $\dot{m} > 0$

17. $\dot{m}$ Parameter controlling the influence of $p'$ on the hardening evolution

18. $a_{hard}$ Parameter in the hyperbolic hardening law

19. $b_{post}$ Post-rupture softening rate

20. $b_{res}$ Residual softening rate

When parameter 17 is equal to zero, parameter 16 defines the value of $\epsilon_{eq}^p$ at which softening
begins (see Eq. 8.22). However, if $\dot{m} > 0$, then parameter 16 defines the value $\epsilon_{eq}^p$ at which
softening begins for $p' = 0$; for larger $p'$ values, softening will start at larger values of $\epsilon_{eq}^p$. 
(see Eq. 8.25). If hardening is not desired, then parameters 8 and 9 should be equal and parameters 16, 17, and 18 should be equal to zero.

Parameter 18 defines the softening rate for the part of the cohesion and tensile strength associated with the post-rupture state, according to an exponential decay function. Parameter 19 defines the softening rate for the remaining part of the cohesion and tensile strength and for the friction angle from $\phi^*_\text{peak}$ to $\phi^*_\text{res}$ (see Eq. 8.22, 8.23, and 8.24). If softening is not desired, then parameters 9 and 10 should be equal, parameters 19 and 20 should be zero, and parameter 13 equal to one.

**Strength anisotropy**

21. $\Omega_{90}$ Parameter in the function $\Omega$

22. $\Omega_m$ Parameter in the function $\Omega$

23. $\delta_m$ Parameter in the function $\Omega$

24. $\hat{n}$ Parameter in the function $\Omega$

Parameter 21 to 24 define the variation of cohesion and isotropic tensile strength with respect to the loading direction (see section 8.1.3). Parameter 21 defines the strength for $\delta = 90^\circ$, while the rest define the shape of the function for intermediate values of $\delta$. A graphical interpretation of the parameters is depicted in Fig. A.15. If strength anisotropy is not desired, then they should all be equal to zero.

**Perzyna’s (1966) visco-plasticity**

25. $N$ Order of Perzyna’s formulation (default = 1)

26. $\eta_{pz}$ Viscosity parameter (default = 1E-3)

Parameter 25 defines the exponent of the overstress function and 26 is a viscosity parameter (see Eq. 8.28 and 8.29). They should be chosen according to experimental evidence; for instance, to account for the increase of strength with increasing loading rates (see Fig. 6.7). If parameters 25 and 26 are equal to zero, by default they are assumed equal to one and 1.0E-3 respectively. This small viscosity helps to prevent numerical issues during stress integration (especially for high softening rates), but it should not affect the response. However, these values do not change by changing the units of a project, and depending on the loading rate and the duration of the phase, they might be too large. If rate-dependency is not desired, the user is advised to verify the response with different loading rates to ensure that the response is not affected by viscosity in the studied range. If that is the case, an $\eta_{pz}$ smaller than 1.0E-3 should be used.

**Creep deformations**

27. $\gamma^c$ Parameter in the creep law

28. $\psi^c$ Parameter in the creep law

29. $a^c$ Parameter in the creep law
30. $\epsilon_{\text{thr}}$ Threshold for creep activation

Parameters 27 to 29 define the creep strain rate according to Eq. (8.32). Parameter 30 defines the value of $\epsilon_{eq}^p$ at which the creep mechanism is activated. If creep deformations are not desired, then parameters 27 to 30 should be equal to zero.

Nonlocal approach

31. Nonlocal flag Activation flag for the nonlocal approach

32. $l_s$ Length scale parameter

With parameter 31 equal to zero, a local plasticity model is recovered. On the other hand, if parameter 31 is equal to one, the nonlocal approach is activated (see section 8.1.7). In the latter case, $l_s > 0$. In fact, it should be chosen according to the size of the mesh in the zones where localisation is expected. See chapter 5 for more details.

Weak element

33. Weak element? Number of an element with reduced strength

For problems involving localised deformations, sometimes it is useful to define an element with a reduced strength, so that localisation can start from this weak spot; this is done with parameter 33. It should indicate the number of the desired element (global PLAXIS numbering for elements). In the Gauss points within this element, all the strength parameters are reduced by 80%.

It is also possible to define a custom variation of cohesion and isotropic tensile strength. In that case, parameter 33 must be equal to -1. When the calculation of a phase starts, a message-box will appear asking for the file file9.txt. The file should be placed in the temporary folder created by PLAXIS during calculation, and then the user should press OK in the message-box. This file should contain a list of factors, one for each Gauss point where the AHW model is being used. The cohesion and tensile strength will be equal to those indicated in the parameter tabsheet times the corresponding factor in the file. The first line of the file must be the total number of gauss points using the AHW model. Then, the list of factors (a number from 0 to 1) for each Gauss point.

Control parameters

34. Ctrl - $p_{\text{atm}}$ Reference pressure

35. Ctrl - tol yield Tolerance in the yield criterion (default = 1E-8)

36. Ctrl - max NR iter Maximum number of Newton-Raphson iterations (default = 30)

37. Ctrl - num subinc Number of sub-increments in the error-based sub-stepping scheme (default = 3)

38. Ctrl - rel tol error Tolerated relative error (default = 1E-3)

39. Ctrl - rel min dt Minimum relative size of the step (default = 1E-50)
40. Ctrl - 2D? Flag for 2D analyses

Parameter 34 is a reference pressure that it is assumed equal to 100 kPa. However, if the units of the project are changed, the corresponding value should be entered here. Parameters 35 to 39 are control parameters of the implicit stress integration algorithm and the error-based sub-stepping scheme; in general, the default values should be sufficient and, therefore, they can be left equal to zero. Finally, parameter 40 should be equal to one for 2D simulations and zero otherwise. Nevertheless, this is only relevant if strength or/and stiffness anisotropy is being considered.

**Some important hints**

The AHW model is a time- and rate-dependent constitutive model and, therefore, arc-length control option should never be used together with it.

It is very important to always assign a time interval to all calculation phases; if this is not done, wrong results will be obtained.

The automatic step size procedure in PLAXIS will reduce the step size if important non-linear behaviour is encounter. Nevertheless, if the AHM model is used to simulate localised deformations, it is always recommended to control the max load fraction per step, to bound the maximum size of a step. In this way, too steep traditions in the step size are avoided.
Chapter 9

Conclusions

Since this thesis was prepared as a compendium of publications, conclusions for each of them have already been presented in the corresponding chapters. Only the essential insights extracted from each publication are presented here. If the pdf version of the document is being used, the reader can click on the header of each paragraph to go to the extended conclusions of the corresponding chapter.

Chapter 2

The theory of elastoplasticity encompasses currently extended mathematical formulations able to provide tools for modelling many aspects of the mechanical behaviour of argillaceous stiff materials. These extensions address features like strength degradation, regularisation techniques for the objective simulation of localised deformations, stiffness anisotropy, anisotropic and rate-dependent yield surfaces, or creep deformation mechanisms, to name the most relevant ones to the present research.

Chapter 3

The non-uniform scaling technique provides a simple way for the anisotropic extension of any stress-based yield/failure criterion. Although the scaled stress tensor lacks physical meaning, and it is only a mathematical tool to modify the yield criterion as a function of the loading direction. The main advantage of the approach lies in the fact that it can be easily incorporated into an already implemented isotropic model with only minor modifications.

Chapter 4

Through the introduction of a constitutive model including relevant features of the behaviour of stiff clayey materials, a coupled hydromechanical simulation of the GCS excavation at the MHM URL has been performed. The pattern of observed pore water pressure and displacements, as well as the shape of the damaged zone, are generally satisfactorily reproduced, although a number of departures of the calculations from field measurements have also been noted. Damage has been simulated in an approximate manner via a continuum approach. This assumption can be considered the main limitation of the performed calculations.

Chapter 5

A nonlocal integral type approach, using the special averaging function from Galavi and Schweiger (2010), has been applied to an elastoplastic model for the objective simulation of localised deformations in stiff clays. From a number of 2D plane strain analyses performed,
relevant aspects of the numerical simulation of localisation have been addressed such as the thickness of the shear band, its orientation and the onset of localisation in BVPs. In addition, the approach proved to be readily transferable to 3D computations.

**Chapter 6**

The nonlocal approach described in chapter 5 has been applied to the simulation of excavations at the MHM URL and, thus, the localised nature of deformations around the drifts has been properly considered. The obtained configuration of the EDZ resembles remarkably the observed fracture networks for the two orientations of the drifts, parallel to the minor horizontal stress and parallel to the major horizontal stresses. Results confirm that ground deformations in the near field are controlled by the EDZ. In addition, the complete mechanism underlying the behaviour of pore water pressures has been described. Together with the initial stress state and the anisotropic stiffness of the clay rock, the configuration and extent of the EDZ plays a major role in the distribution and evolution of water pressures.

**Chapter 7**

Following the simulations described in chapter 6, a sensitivity analysis has been conducted to assess the influence of different parameters on the obtained results. Aspects studied include mechanical anisotropy, strength parameters, excavation size, hydraulic parameters and time dependency. Some of the main aspects affecting the hydromechanical behaviour of the excavations have been identified. For instance, results showed the importance of strength anisotropy and of the particular strength distribution with loading direction.


Amazon (2018). Amazon Elastic Compute Cloud (Amazon EC2).


Andra (2014b). Personal communication.


REFERENCES


REFERENCES


REFERENCES


Appendix A

Numerical simulation of the undrained stability of slopes in anisotropic fine-grained soils

Based on the published manuscript of the following article:

Abstract

The undrained stability of slopes in anisotropic fine-grained soils is studied in this paper using the finite element method (FEM). A constitutive model is presented, able to account for the observed variation of undrained strength with loading direction. The model is able to encompass the different strength distributions observed in normally, slightly overconsolidated and heavily overconsolidated soils. A series of stability analyses have been performed to explore the effect of the type of undrained strength anisotropy on the stability and failure mechanisms of slopes of different inclinations. In addition, a real case study of the failure of an underwater slope is analysed with the numerical approach presented. It suggests that, by considering undrained strength anisotropy, the failure can be satisfactorily explained.

A.1 Introduction

It has long been recognised that soils are generally anisotropic (Casagrande and Carrillo, 1944; Wolf, 1935), with some of their properties varying depending on the direction of loading (e.g. Arthur et al., 1977a; Lade and Kirkgard, 2000; Nishimura et al., 2007; Zdravkovic and Jardine, 2000). In particular, strength anisotropy should be the main concern in relation with the stability assessment of geostructures. Nevertheless, the incorporation of this feature is rarely considered in routine slope stability analyses, in spite of the fact that its absence may lead to an overestimation of the factor of safety (FOS). To include strength anisotropy in slope stability computations two main steps are required: the first one is to establish a failure criterion introducing a dependency with loading direction, able to account for the observed variation of strength. A number of anisotropic failure criteria for soils have been proposed: a review can be found in Mánica et al. (2016b). The second step is to introduce...
the anisotropic criterion into an appropriate methodology for assessing the stability of slopes, such as: limit equilibrium methods, limit analyses or numerical methods. For instance, Chen et al. (1975) used the upper bound technique of limit analysis to establish an expression for the stability number $N_0$, that considered the cohesion variation postulated by Casagrande and Carrillo (1944). The same cohesion variation was included in Bishop’s (1955) simplified method of slices by Al-Karni and Al-Shamrani (2000). Su and Liao (1999) used limit state analysis and a total stress anisotropic strength criterion to calculate an anisotropic FOS. In addition, they provided a simplified approach that can be applied in routine analyses. Another appealing alternative is the use of numerical methods, such as the FEM, which has proved to be a reliable and robust approach for assessing the FOS of slopes (Griffiths and Lane, 1999). Here, no a priori assumptions are made regarding the failure surface that is part of the solution. It is a very versatile tool, allowing complex geometries and material behaviour, spatial variability of properties, or even the possibility to include stabilisation techniques such as piles, bolts or geo-synthetics. Therefore, the use of FEM in combination with an anisotropic constitutive law was a natural step to study the slope stability problem. An example of this approach can be found in Zdravković et al. (2002), where the anisotropic MIT soil model (Whittle and Kavvadas, 1994) was employed for the simulation of a full-scale test embankment brought to failure. Another example is given by Schweiger et al. (2009), where the multilaminate framework is extended to consider inherent strength anisotropy through the microstructure tensor proposed by Pietruszczak and Mroz (2000), and the resulting constitutive model is then applied to the slope stability problem.

A prevailing conclusion in the mentioned works is that the incorporation of strength anisotropy results in a lower FOS, compared to the isotropic analysis using the strength measured with conventional test, when loading is perpendicular to bedding. However, only the case of a monotonic decrease of the strength between the loading perpendicular and parallel to bedding is generally considered. As it will be shown in section A.2, this is a typical behaviour of $K_o$ normally consolidated soils. However, over-consolidated materials may exhibit a quite different behaviour, not yet properly considered in slope stability analyses.

In this paper, the undrained stability of slopes is studied using the FEM. A simple constitutive model is presented, able to account for the different variations of the undrained strength with loading direction that are discussed in section A.2. The model is then employed in a series of stability analyses, whose main objective is to recognise situations where strength anisotropy will play a major role in the stability of slopes, depending on the type of strength distribution. In addition, a real case study of the failure of a 30 m high underwater slope at the Port of San Francisco (Duncan and Buchignani, 1973) was analysed with the present numerical approach. The possibility of explaining the observed failure by including the undrained anisotropy of the San Francisco Bay mud is explored.

A.2 Undrained strength anisotropy of fine grained soils

Skempton and Hutchinson (1969) indicated how the undrained strength of clays varies with the direction of loading (Fig. A.1). They noted that for normally or lightly over-consolidated clays (clay from Welland, San Francisco Bay clay and clay from Surte in Fig. A.1) the undrained strength is highest when the specimen axis (which in turn is parallel to the major
principal stress $\sigma_1$) is perpendicular to bedding, a rather intuitive result. The strength either decreases monotonically with orientation, or there is a minimum value at an intermediate angle, but with a strength just slightly lower than for loading parallel to bedding. On the other hand, heavily over-consolidated materials (London clay from Wraysbury and Ashford sites in Fig. A.1) exhibit a different pattern. The behaviour is similar to the normally consolidated clays at low angles, but then the strength rises quite rapidly so that the value for loading parallel to bedding can be even higher than for loading perpendicular to bedding. Skempton and Hutchinson (1969) interpreted that these high strengths for loading parallel to bedding very probably reflect the high lateral in situ consolidation pressure ($K_o$) in the London clay (Skempton, 1961). These results suggest a progressive evolution of anisotropy with the change in over-consolidation ratio (OCR).

![Diagram](image)

Figure A.1: Normalised undrained strength variation with the loading direction in soils with different OCRs (modified from Skempton and Hutchinson, 1969)

The behaviour for normally or lightly over-consolidated soils has been also confirmed by a series of investigations carried out with the hollow cylinder apparatus (HCA) at the Imperial College of London (Jardine and Menkiti, 1999; Menkiti, 1995; Zdravkovic and Jardine, 2000). This device allows to study the anisotropic characteristics of soils by the rotation of the principal stresses (Hight et al., 1983). The results show a monotonic decrease of the undrained strength with the loading direction, similar to the one exhibited by the clay from Welland in Fig. A.1. In the same way, the behaviour of the natural heavily over-consolidated London clay has been verified during the investigations for the Terminal five of Heathrow Airport (Nishimura et al., 2007), where a similar trend as the Wraysbury and Ashford (Fig. A.1) sites was observed. Nevertheless, this pattern may be disrupted by the presence of fissures (Nishimura et al., 2007). This kind of anisotropy has also been identified in other stiff fine-grained materials. For instance, tests carried out on shale rocks have also shown this strength behaviour (Cho et al., 2012; McLamore and Gray, 1967; Niandou et al., 1997), and a compilation of data by Sayers (2013) suggest that the stiffness is also higher in shale rocks.
when loading is oriented parallel to bedding. Similar conclusions can be drawn about the Opalinus clay sampled at the Mont Terri underground laboratory (Naumann et al., 2007).

It is not clear if the loading history resulting in over-consolidation can explain by itself the observed evolution of anisotropy, or if a more complex interaction of phenomena (including sedimentation, gravitational compaction, unloading and cementation) are the origin of the observed behaviour; more research is needed in this regard. Nevertheless, it seems that it is possible to classify the undrained strength anisotropy of fine-grained soils in three types as shown in Fig. A.2. The convention employed to define the direction of anisotropy with respect to the loading is also depicted in the figure, and will be followed in the entire document. \( \delta \) corresponds to the angle between the normal to bedding and the direction of the applied major principal stress. Therefore, \( \delta = 0^\circ \) and \( \delta = 90^\circ \) correspond to the major principal stress acting perpendicular and parallel to bedding respectively. In addition, \( \Omega \) is defined as,

\[
\Omega(\delta) = \frac{S_u(\delta)}{S_u(0)} \quad \quad (A.1)
\]

The first distribution in Fig. A.2 corresponds to a monotonic decrease of the strength between \( \delta = 0^\circ \) and \( \delta = 90^\circ \). In the other two, the minimum strength is found at an intermediate orientation, but in the second type \( \Omega(90) \leq \Omega(0) \), while in the third one \( \Omega(90) > \Omega(0) \). A constitutive model able to incorporate these strength distributions is presented in the following section.

![Diagram showing three types of strength distributions: type I, type II, type III](image)

Figure A.2: Identified types of undrained strength distributions in fine-grained soils

### A.3 Cross-anisotropic constitutive model

The soil mechanics convention (compression stress and strains are positive) is employed and will be followed in the entire document. Only cross-anisotropy (or transverse isotropy) is considered and, therefore, the existence of a place where properties are the same in all directions. This generally corresponds to the bedding planes in sedimentary materials and will be referred to as the isotropic plane. The model is formulated within the framework of elasto-plasticity. Details about this theory are not given here and can be found elsewhere (e.g. Simo and Hughes, 1998). Only the classical expression relating stress and strain increments
for the elastic perfectly plastic case is presented in Eq. (A.2).

\[ d\sigma = \left(D^e - \frac{D^e (\partial g/\partial \sigma)(\partial f/\partial \sigma)^T D^e}{(\partial f/\partial \sigma)^T D^e (\partial g/\partial \sigma)} \right) \, d\epsilon = D^{ep} \, d\epsilon \quad (A.2) \]

where \( \sigma \) is the column matrix of independent stress components, \( \epsilon \) is the column matrix of engineering strain components, \( f \) is the yield function bounding the elastic domain, \( g \) is the plastic potential function describing the direction of plastic flow, \( D^e \) is the elastic stiffness matrix, and \( D^{ep} \) is the elasto-plastic stiffness matrix.

Inside the yield surface the response is assumed linear elastic, characterised by Hooke’s law. The yield function is based on the Mohr-Coulomb criterion, which for the isotropic case can be expressed in the following way,

\[ f = \left(\cos \theta + \frac{1}{\sqrt{3}} \sin \phi \sin \theta \right) J - p \sin \phi - c \cos \phi \quad (A.3) \]

where \( \phi \) is the friction angle, \( c \) is the cohesion, \( p \) is the mean stress, \( J = \sqrt{J_2} \) where \( J_2 \) is the second invariant of the deviatoric stress tensor \( s \), and \( \theta \) is the Lode’s angle. However, in the present research only the problem of undrained stability of slopes is addressed, and therefore \( \phi = 0^\circ \) and \( c = S_u \) are assumed. In this case Eq. (A.3) reduces to,

\[ f = J \cos \theta - S_u \quad (A.4) \]

corresponding to the Tresca yield function. However, Eq. (A.4) present corners singularities where gradients are not defined; they were smoothed following the Sloan and Booker (1986) procedure. In addition, an associated flow rule is considered in the octahedral plane.

The anisotropic extension of the model is obtained replacing \( S_u \) in Eq. (A.4) by,

\[ S_u^* = \Omega(\delta) S_u(0) \quad (A.5) \]

In this way, a dependency of the strength with the loading direction is introduced. If \( n \) is the vector normal to the isotropic plane, and \( v \) is the direction of the major principal stress, then \( \delta \) can be defined by,

\[ \delta = \cos^{-1} \left| \frac{n \cdot v}{|n| \cdot |v|} \right| \quad (A.6) \]

The direction of \( n \) accounts for situations where the isotropic plane is not horizontal with respect to the global coordinate system. In a three-dimensional (3D) analysis, where the \( z \) axis stands for the depth, the orientation of the isotropic plane can be described according to Fig. A.3a, with \( n \) given by,

\[ n = \begin{bmatrix} \sin \beta \sin \alpha \\ -\cos \alpha \sin \beta \\ \cos \beta \end{bmatrix} \quad (A.7) \]
In a two-dimensional (2D) analysis, where the $y$ axis stands for the depth, and the orientation of the isotropic plane is assumed to vary only around the direction perpendicular to the analysis plane, $\mathbf{n}$ is defined by Eq. (A.8) (Fig. A.3b).

\[
\mathbf{n} = \begin{bmatrix}
-\sin \alpha \\
\cos \alpha \\
0
\end{bmatrix}
\] (A.8)

For the definition of $\mathbf{v}$ the eigenproblem must be solved for the stress tensor. In the present, model this is performed numerically using the Jacobi method (Press et al., 1992).

A function is employed to represent $\Omega$, flexible enough to accommodate the types of strength distributions identified in Fig. A.2. This was achieved by deriving $\Omega$ from the combination of a sigmoid function and its derivative, the first one accounting for the monotonic change of strength between $\delta = 0^\circ$ and $\delta = 90^\circ$, and the second one accounting for a possible minimum strength at an intermediate orientation. In this way, $\Omega$ is defined as,

\[
\Omega = \frac{\hat{A} e^{(\delta_m - \delta)\hat{\alpha}}}{[1 + e^{(\delta_m - \delta)\hat{\alpha}}]^2} + \frac{\hat{B}}{1 + e^{(\delta_m - \delta)\hat{\alpha}}} + \hat{C}
\] (A.9)

where,

\[
\hat{A} = \frac{2(e_1 + 1)(e_2 + 1)(e_1 - e_2 + \Omega_{90} + e_1 e_2 + e_1 \Omega_{90} - e_2 \Omega_{90} - 2e_1 \Omega_m + 2e_2 \Omega_m - e_1 e_2 \Omega_{90} - 1)}{(e_1 - e_2)(e_1 - 1)(e_2 - 1)}
\] (A.10)

\[
\hat{B} = \frac{\Omega_{90} - \frac{\hat{A} e_1}{(e_1 + 1)^2} + \frac{\hat{A} e_2}{(e_2 + 1)^2} - 1}{\frac{1}{e_1 + 1} - \frac{1}{e_2 + 1}}
\] (A.11)

\[
\hat{C} = 1 - \frac{\hat{A} e_2}{(e_2 + 1)^2} - \frac{\hat{B}}{e_2 + 1}
\] (A.12)

Figure A.3: Orientation of the isotropic plane for a) 3D and b) 2D problems
\[ e_1 = e^{\hat{n}(\delta_m - 90)} \]  

\[ e_2 = e^{\hat{n}\delta_m} \]  

and \( \Omega_{90} = \frac{S_u(90)}{S_u(0)} \), \( \Omega_m = \frac{S_u(\delta_m)}{S_u(0)} \), \( \delta_m \) is the orientation at which the centre of the sigmoid function and its derivative occur, and \( \hat{n} \) is a constant controlling the curvature of the function. The graphical interpretation of these parameters with respect to the function \( \Omega \) is depicted in Fig. A.4. It is important to mention that the minimum value of \( \Omega \) does not necessarily occur at \( \delta_m \), and it was not explicitly included in Eq. (A.9). Nevertheless, for a given set of parameters it can be computed as,

\[ \delta_{\text{min}} = \delta_m - \frac{\ln \left( \frac{\hat{A} - \hat{B}}{\hat{A} + \hat{B}} \right)}{\hat{n}} \]  

Figure A.4: Function \( \Omega \) and its parameters

The effect of either the sigmoid function or its derivative can be removed from \( \Omega \) if desired. For instance, if only a monotonic decrease of the strength is sought between \( \delta = 0^\circ \) and \( \delta = 90^\circ \), then \( \delta_m \) must be equal to \( 45^\circ \) and \( \Omega_m \) equal to \( \frac{1 + \Omega_{90}}{2} \). In this case the effect of the sigmoid derivative is deactivated and only \( \Omega_{90} \) and \( \hat{n} \) are required to define \( \Omega \). On the other hand, if \( S_u(0) \approx S_u(90) \) but there is a minimum value at an intermediate orientation, then the effect of the sigmoid function can be removed by assuming \( \Omega_{90} = 1 \).

The gradients of the yield function \( \frac{\partial f}{\partial \sigma} \) in Eq. (A.2) can be obtained in terms of the employed stress invariants in the following way,

\[ \frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial J} \frac{\partial J}{\partial \sigma} + \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial \sigma} + \frac{\partial f}{\partial S_u^*} \frac{\partial S_u^*}{\partial \sigma} \]  

where an additional term appears with respect to the standard definition, since now the undrained strength also depends on stresses. However, this last term involves the computation
of $\partial v / \partial \sigma$, a task that is generally not trivial, requiring special algorithms (e.g. Mills-Curran, 1988; Nelson, 1976). In the present model this was simplified by defining,

$$\frac{\partial S^*_u}{\partial \sigma} = S_u(0) \frac{\partial \Omega}{\partial \sigma}$$  \hspace{1cm} (A.17)$$

and approximating $\partial \Omega / \partial \sigma$ numerically using the central difference method. In the absence of relevant data, the plastic potential was assumed isotropic.

### A.4 Application to slope stability analysis

A series of finite element analyses were performed using the constitutive model described in the previous section, to assess the influence of inherent strength anisotropy on the undrained stability of slopes in fine-grained soils. Three different materials reported in the literature were considered, showing the different types of strength distributions previously defined. The main objective of these analyses is to identify situations where strength anisotropy will play a major role in the stability of the slopes depending on the type of strength distribution.

#### A.4.1 Considered materials

The first material corresponds to the Boston blue clay, an illitic low-plasticity marine clay deposited in the Boston basin during the Pleistocene. Engineering properties of this soil have been extensively studied in the past (Baligh and Levadoux, 1986; Ladd and Varallyay, 1965; Seah, 1990; Sheahan et al., 1996). Here we refer to a particular set of results reported by Seah (1990), where the directional shear cell (DSC) (Arthur et al., 1977a) was employed to study the undrained strength anisotropy in $K_o$ normally-consolidated specimens. As in the HCA, the DSC allows the study of anisotropy by shearing the sample with different orientations of the major principal stresses. The reported strength distribution (normalised with respect to the strength for $\delta = 0^\circ$) is depicted in Fig. A.5. A type I distribution can be clearly identified, where a monotonic decrease of the strength is observed between $\delta = 0^\circ$ and $\delta = 90^\circ$, characteristic of normally-consolidated materials. Therefore, only the effect of the sigmoid function is sufficient to adjust the laboratory data, using only $\Omega_90$ and $\hat{n}$. The adjusted function is also shown in Fig. A.5, the parameters are given in Table A.1.

The second material corresponds to a low plasticity Alaskan silt reported by Fleming and Duncan (1990), retrieved from an offshore site in the Beaufort Sea. The samples were reconstituted from a slurry in a one-dimensional consolidometer under a given vertical pressure. The load was then removed to obtained cylindrical blocks of soil 127 mm in diameter and typically 102 - 127 mm height, from which the 35 mm in diameter triaxial samples were trimmed. Then a series of unconsolidated-undrained triaxial (UU) tests were performed with specimens trimmed with different orientations with respect to bedding. The normalised undrained strength is shown in Fig. A.5, together with the adjusted function. This corresponds to a type II distribution (Fig. A.5).

The third material corresponds to the natural highly over-consolidated London clay at the site of the Heathrow Airport Terminal Five. The London clay is another example of a material whose mechanical properties have been extensively studied in the past (Bishop et al., 1965; Hight et al., 2007; Ward et al., 1965). Here we refer to a set of data from the
study by Nishimura et al. (2007). Fig. A.5 shows the normalised undrained strength variation of samples retrieved from 10.5 m below ground level, and with an OCR estimated around 9 – 12 (Nishimura et al., 2007). It corresponds to a type III distribution, which seems to be associated with highly over-consolidated fine-grained soils. The adjusted function is also depicted in the figure.

![Figure A.5: Observed and computed undrained strength distributions](image)

**Table A.1: Parameters of the adjusted strength distributions**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Boston blue clay</th>
<th>Alaskan silt</th>
<th>London clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega_{90}$</td>
<td>0.56</td>
<td>0.85</td>
<td>1.53</td>
</tr>
<tr>
<td>$\Omega_m$</td>
<td>$\frac{(1 + \Omega_{90})}{2}$</td>
<td>0.73</td>
<td>0.79</td>
</tr>
<tr>
<td>$\delta_m$</td>
<td>45°</td>
<td>45°</td>
<td>45°</td>
</tr>
<tr>
<td>$\hat{n}$</td>
<td>0.08</td>
<td>0.06</td>
<td>0.11</td>
</tr>
</tbody>
</table>

**A.4.2 Main features of the numerical models**

The considered geometry and main boundary conditions are illustrated in Fig. A.6. They correspond to a 2D slope of height $H$ in homogeneous soil, with the firm ground located at a distance $H$ from the toe. Different slope angles $\theta_s$ and different orientations of the isotropic plane $\alpha$ were employed in the analyses. These were carried out using the finite element code Plaxis (Brinkgreve et al., 2017), where the model described in section A.3 was implemented as a user defined soil model. As an example, one of the employed finite element meshes (for the case with $\theta_s = 30^\circ$) is depicted in Fig. A.6. It comprises 1065 triangular 15-noded finite elements with fourth-order interpolation and 12 integration points. Plane strain conditions were considered and the analyses were performed in terms of total stresses and undrained strengths. The strength reduction method was employed to determine the failure condition, as described by Griffiths and Lane (1999), where the FOS is defined as,

$$FOS = \frac{S_u}{S_{u-f}}$$  \hspace{1cm} (A.18)
where $S_{ut}$ is the undrained strength at which failure occurs. To allow direct comparison, the results were then normalised in terms of the stability number $N_o$, defined here as,

$$N_o = \frac{\text{FOS} \gamma_u H}{S_u}$$  \hspace{1cm} (A.19)

where $\gamma_u$ is the unit weight of the soil.

All analyses were first performed without considering anisotropy and the results were compared with Taylor’s (1937) solution, in order to validate the present numerical approach. The strength distribution in Fig. A.5 were then included to assess their effect on the stability analysis. In those cases, $S_u$ and $S_{ut}$ correspond to the values for $\delta = 0^\circ$.

The variations of the failure mechanism are also reported. They are represented by a continuous single line describing the failure plane of the mobilised mechanism. Fig. A.7 shows an example of a slope failure in terms of the deformed mesh (Fig. A.7a) and in terms of the incremental total displacement field (Fig. A.7b). The dashed line representing this mechanism is drawn at the centre of the zone where a high displacement gradient occurs (Fig. A.7b), separating the standing part of the ground and the sliding mass.

**A.4.3 Obtained results**

The stability numbers obtained for different inclinations of the slope are shown in Fig. A.8. Here the orientation of the isotropic plane was assumed horizontal. The solid and dashed black lines represent the isotropic case obtained from the numerical simulation and from
Taylor’s (1937) solution, respectively. A good agreement between both can be noted, validating the employed numerical approach for the slope stability analysis. The other lines correspond to the anisotropic materials, whose strength distributions were shown in Fig. A.5. The variation of $N_o$ with the slope inclination $\theta$ has a similar trend for the isotropic and anisotropic cases, although the magnitude is considerably different. The Boston blue clay lies at the bottom of the graph as the most unfavourable condition, whilst the London clay shows $N_o$ values even higher than the isotropic case for $\theta$ values lower than 50°. For higher inclinations, the London clay and the isotropic case are quite similar. The Alaskan silt is found in-between the isotropic and the Boston clay cases. An important observation is that the effect of anisotropy tends to reduce with $\theta$, so that in the case of a vertical cut ($\theta = 90^\circ$), the effect of anisotropy becomes quite small. The same outcome has been reported by Al-Karni and Al-Shamrani (2000).

![Figure A.8: Variation of the stability number with slope inclination](image)

The failure mechanisms obtained for different slope inclinations are shown in Fig. A.9. As expected, for $\theta = 15^\circ$ and $\theta = 30^\circ$ a well-defined base failure is identified for the isotropic analyses. It can be noted that, despite the fact that in those inclinations the effect of anisotropy on stability number is the highest (see Fig. A.8), it has little effect on the failure mechanism. Only the exit point of the sliding mass for $\theta = 30^\circ$ occurs closer to the toe for London Clay and further away in the Boston clay. The isotropic analysis with $\theta = 50^\circ$ represents a transition between a base and a toe failure. Here we can observe that in the London clay the failure mechanism already corresponds to a toe failure, while for Boston clay and Alaskan silt the base mechanism persists. For the case with $\theta = 70^\circ$; the isotropic case now clearly forms a toe failure, while in the Boston clay case a base mechanism still persists. The Alaskan silt shows an intermediate surface, but it is now closer to a toe mechanism. Finally, with $\theta = 90^\circ$ all materials have moved to a toe mechanism, with a nearly planar slip surface. It can be concluded that the type of anisotropy affects the type failure for intermediate slope angles.

By examining the direction of the major principal stress along the failure surfaces, the decrease of the effect of anisotropy with $\theta$ becomes evident. This is shown in Fig. A.10 for the isotropic case with $\theta = 15^\circ$ and $\theta = 90^\circ$. For a base type mechanism, the major
principal stress direction varies gradually along the failure surface from the sub-vertical to the sub-horizontal orientations (from right to left in Fig. A.10). On the other hand, in a toe failure, the major principal stress barely deviates from the sub-vertical orientation, this corresponding to very low values of $\delta$ (for this case where $\alpha = 0$), where the strength is quite similar for all the considered strength distributions (see Fig. A.5).

$$\theta = 15^\circ$$

$$\theta = 30^\circ$$

$$\theta = 50^\circ$$

$$\theta = 70^\circ$$

$$\theta = 90^\circ$$

Figure A.9: Failure mechanism obtained for different slope inclinations

The relative orientation between the major principal stress and the normal to the failure surface was found to be roughly equal to $45^\circ$ throughout the surface, and in all performed calculations. Therefore, it coincides with Roscoe’s (1970) solution ($45^\circ + \psi/2$) (Mánica et al., 2018a; Potts et al., 1997), since the employed plastic potential yields null volumetric plastic strains at failure, and therefore the dilatancy angle is $\psi = 0^\circ$.

An additional set of analyses was performed for the case with $\theta = 30^\circ$, but with different bedding orientations $\alpha$. Although less frequent, this condition may occur in nature due to cross-bedding or post-depositional deformations. The obtained values of $N_0$ and the obtained failure mechanisms are depicted in Fig. A.11 and A.12 respectively. Values of $0 < \alpha < 90$
correspond to dip slopes, while $90 < \alpha < 180$ correspond to anti-dip slopes. In this case, the failure mechanism is not particularly dependent on variations of the bedding orientation. On the other hand, $N_0$ is significantly affected. The Boston clay shows a wave-like behaviour, with the trough around $55^\circ$ in the dip slope range, and the crest around $145^\circ$ in the anti-dip slope range. The Alaskan silt shows a similar behaviour as the Boston clay in the dip slope range (but with higher values of $N_0$), although in the anti-dip slope zone just a slightly increase of $N_0$ is noticed. On the other hand, London clay shows an opposite behaviour to Boston clay, except for a point near $45^\circ$, where $N_0$ momentarily decreases. The observed behaviour can be clarified by reference to Fig. A.13 where the mean value of $\delta$ along the corresponding failure surface is shown. A very similar variation is obtained in the three materials. The high values of the mean $\delta$ in the dip slope range are associated with low strengths for the Boston clay and the Alaskan silt, but with high strengths for the London clay (see Fig. A.5). On the other hand, for lower values of $\delta$, the strength of the three materials is similar, and therefore the value of $N_0$ tends to be the similar for all them near the bedding orientation corresponding to the lowest mean $\delta$. However, the specific variation of $N_0$ with $\alpha$ is related to the particular strength distribution adopted.

![Figure A.10: Direction of the major principal stress along the failure surface of the isotropic analysis for two slope inclinations](image)

![Figure A.11: Variation of the stability number with the direction of anisotropy](image)
In addition to the synthetic cases presented in the previous section, a real case study was also evaluated with the intention of further stressing the importance of including strength anisotropy in our conventional stability calculations. It corresponds to the failure of a 30 m high underwater slope at the Port of San Francisco (Duncan and Buchignani, 1973). Fig. A.14 shows a cross-section of the slope before failure and the position of the estimated

A.5 Underwater slope failure in San Francisco bay mud

In addition to the synthetic cases presented in the previous section, a real case study was also evaluated with the intention of further stressing the importance of including strength anisotropy in our conventional stability calculations. It corresponds to the failure of a 30 m high underwater slope at the Port of San Francisco (Duncan and Buchignani, 1973). Fig. A.14 shows a cross-section of the slope before failure and the position of the estimated
failure surface. The original short-term design FOS was reported by Duncan and Buchignani (1973) to be 1.17, i.e. it suggested a stable slope (although with a rather low FOS). Revised calculations were later performed with different limit equilibrium programs, confirming this FOS value (Duncan et al., 2014). Nevertheless, a few hours after the excavation of a section about 150 m long, a failure occurred involving a 75 m long portion of the trench. Later, a second failure occurred involving additional 60 m. The discrepancies of the calculated FOS were attributed to a decrease of the undrained strength due to creep deformations (Duncan and Buchignani, 1973). However, it can be argued that due to the very short time between the excavation and failure (just a few hours), significant creep processes would not have had enough time to occur and they may not be the main responsible for the failure.

Here, the possibility of explaining the observed failure by considering the undrained anisotropy of the San Francisco Bay mud is explored. First, an analysis without anisotropy was performed to compare with the original stability calculations. Fig. A.15 shows the employed simplified geometry of the slope, as well as the finite element mesh and boundary conditions used. The debris dike and the soil beneath it at the right of Fig. A.14 were not included in the analysis, since preliminary calculation showed that the failure surface tended to pass beneath the dike. In the real slope failure this did not occur, most likely because the soil beneath the debris dike would have consolidated under the weight of the dike, increasing its undrained strength. Therefore, the lateral boundary conditions at the right of the model were placed where the dike begins, preventing the failure mechanism passing under it. Due to the absence of seepage, it was possible to use the buoyant unit weights instead of total unit weights with external water pressures (Duncan et al., 2014). The average buoyant unit weight of the San Francisco Bay mud was reported to be 5.97 kN/m$^3$ (Duncan, 2000). The observed increase in the undrained strength with depth was also included in the analyses. Fig. A.16 shows the reported (Duncan, 2000) and employed undrained strength profiles. For the anisotropic analysis, data of the undrained strength variation with the loading direction of the San Francisco Bay mud from Lade and Kirkgard (2000) were employed. These results are depicted in Fig. A.17 (normalised with respect to the strength for $\delta = 0^\circ$), together with the adjusted function and its parameters. The strength reduction method, as described by Griffiths and Lane (1999), was again employed to derive the FOS.
Fig. A.15: Geometry and boundary conditions of the analysed underwater slope

Fig. A.16: Undrained strength variation with depth for San Francisco bay mud at the LASH Terminal site (modified from Duncan, 2000)

Fig. A.18a shows the obtained FOS and failure mechanism (in terms of the incremental displacement field) for the isotropic analysis. The FOS of 1.175 confirms the original design value (Duncan and Buchignani, 1973), as well as the revised calculations performed later (Duncan et al., 2014). The failure mechanism is quite similar to the real estimated failure surface (Fig. A.14), and it is practically identical to the critical sliding surface reported in the revised calculations. Therefore, it can be stated that this analysis is analogous to the original design calculations.
Figure A.17: Observed (Lade and Kirkgard, 2000) and computed normalised strength distribution

The anisotropic analysis is identical to the isotropic one, but the undrained strength distribution shown in Fig. A.17 was included. The obtained FOS and failure mechanism are depicted in Fig. A.18b. It is observed that the failure mechanism is not affected by anisotropy, but the FOS is now very close to unity, i.e. very close to an incipient failure condition. Therefore, a more realistic FOS has been obtained just by including in the analysis the undrained strength anisotropy of the San Francisco Bay mud. In the authors’ opinion, this provides a more satisfying explanation for the discrepancies in the FOS than the possible decrease of the strength due to creep deformations is such a rapid failure.

Figure A.18: Obtained failure mechanism and factor of safety for the a) isotropic and b) anisotropic analyses

A.6 Conclusions

In this paper, the FEM was employed to study the effect of strength anisotropy on the undrained stability of slopes. For this purpose, an anisotropic constitutive model has been presented, able to reproduce the undrained strength variations with the loading direction, observed in different fine-grained soils. They include over-consolidated materials where the highest strengths are obtained when loading is parallel to bedding. A series of analysis have
been performed to check the effect of anisotropy on the undrained stability of slopes. For comparison, the isotropic case with the undrained strength obtained under loading perpendicular to bedding has been taken as reference. From the analyses performed, the following conclusions can be drawn:

1. The effect of strength anisotropy decreases when the inclination of the slope increases, so that it becomes quite small in the case of vertical cuts. This occurs because in the nearly planar surface formed in the latter case, the major principal stress barely deviates from the sub-vertical orientation along the slip surface, therefore corresponding to the same strength adopted for the isotropic case. Gentler slopes result in deeper failure mechanisms, where the major principal stress continuously varies along the failure surface, from the sub-vertical to the sub-horizontal directions, and therefore the whole strength distribution is relevant.

2. For horizontal bedding, distributions I and II will always result in $N_\sigma$ lower than the isotropic case. The effect of anisotropy seems negligible for the type III when $\theta^a > 50^\circ$, and for lower inclinations $N_\sigma$ values even higher than the isotropic case can be obtained. Therefore, an isotropic analysis using the strength under loading perpendicular to bedding should be conservative in the latter case. Nevertheless, special care must be paid in the presence of pre-existing fissures, since the strength distribution obtained from a non-fissured sample may not represent the strength of the soil mass, and therefore the FOS may be lower than the isotropic case.

3. Undrained strength anisotropy does not have a very important effect in the failure mechanism obtained. Only close to a transition between a base and a toe failure mechanisms, the strength distribution types I and II will tend towards the former, while type III strength distribution will tend towards the latter.

4. In the case of non-horizontal bedding, the strength distributions I and II always show lower $N_\sigma$ values than the isotropic analysis for all bedding orientations, although the dip slopes represent a more adverse condition than the anti-dip slopes. The opposite occurs for the distribution III, and $N_\sigma$ values lower than the isotropic case can be obtained for anti-dip slopes. This behaviour is related to the average loading angle $\delta$ along the failure plane, which is higher in dip-slopes than for anti-dip slopes.

Finally, a real case failure of an underwater slope was analysed with the numerical approach presented. A more realistic FOS was obtained just by including in the analysis the undrained strength anisotropy of the San Francisco Bay mud, providing a more satisfying explanation for the over estimation of the FOS in the original design calculations.
Appendix B

Richardson’s (1911; 1927) extrapolation

Assuming a general approximation procedure of some desired quantity $U$, we can write,

$$U = U(h) + C h^k + C' h^{k+1} + C'' h^{k+2} + ... \quad (B.1)$$

where $U(h)$ is the approximated value of $U$ using the step size $h$, $k$ is a known constant depending on the particular approximation procedure, and $C$, $C'$, $C''$, ... are some other generally unknown constants. For instance, $k = 2$ for the local truncation error of the forward and backward Euler methods. Using $O(h^{k+1})$ to account for the sum of terms of order $h^{k+1}$ or higher we get,

$$U = U(h) + C h^k + O(h^{k+1}) \quad (B.2)$$

In fact Eq. (B.2) is a different equation for different step sizes. If we take for instance half of $h$,

$$U = U(h/2) + C(h/2)^k + O(h^{k+1}) \quad (B.3)$$

By solving Eq. (B.2) and (B.3) for $U$ we get,

$$U = \frac{2^k U(h/2) - U(h)}{2^k - 1} + O(h^{k+1}) \quad (B.4)$$

and if we name,

$$X(h) = \frac{2^k U(h/2) - U(h)}{2^k - 1} \quad (B.5)$$

then,

$$U = X(h) + O(h^{k+1}) \quad (B.6)$$

Here, $X(h)$ represents an improved approximation of $U$, with an error order $k + 1$ (one order higher than $U(h)$). Therefore, Richardson’s extrapolation allows to obtained a higher order solution from a single approximation procedure, by solving the problem with two different step sizes. Alternatively, we can use the higher order solution to estimate an error. The
error estimation for $U(h/2)$ reads,

$$error(h/2) = U - U(h/2)$$

(B.7)

therefore,

$$error(h/2) = C(h/2)^k + O(h^{k+1})$$

(B.8)

By solving Eq. (B.2) and (B.3) for $C$,

$$C = \frac{U(h/2) - U(h)}{h^k (1 - \frac{1}{2^k})} + O(h)$$

(B.9)

and substituting in Eq. (B.8),

$$error(h/2) = \frac{U(h/2) - U(h)}{2^k - 1} + O(h^{k+1})$$

(B.10)

We generally assume that the higher order terms are small and drop $O(h^{k+1})$. Here, we stay with the original lower order solution, but with an error estimation, which can be the basis for a sub-stepping algorithm.
Appendix C

Derivatives of the constitutive law

B.1 Stress invariants

\[ p = \frac{1}{3} \text{tr} \sigma \]  \hspace{1cm} (C.1)

\[ J_2 = \frac{1}{2} \text{tr} \sigma^2 \]  \hspace{1cm} (C.2)

\[ J_3 = \text{det} \sigma \]  \hspace{1cm} (C.3)

\[ \theta = -\frac{1}{3} \sin^{-1} \left( \frac{3 \sqrt{3} J_3}{2 J_2^{3/2}} \right) \]  \hspace{1cm} (C.4)

C.2 Derivatives of stress invariants with respect to stresses

\[ \frac{\partial p}{\partial \sigma} = \frac{1}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \]  \hspace{1cm} (C.5)

\[ \frac{\partial J_2}{\partial \sigma} = \begin{bmatrix} s_{xx} \\ s_{yy} \\ s_{zz} \\ 2\sigma_{xy} \\ 2\sigma_{yz} \\ 2\sigma_{xz} \end{bmatrix} \]  \hspace{1cm} (C.6)
\[ \frac{\partial J_3}{\partial \sigma} = \begin{bmatrix} s_{xx}^2 + s_{xy}^2 + s_{xz}^2 - \frac{2J_3}{3} \\ s_{xy}^2 + s_{yy}^2 + s_{yz}^2 - \frac{2J_3}{3} \\ s_{xz}^2 + s_{yz}^2 + s_{zz}^2 - \frac{2J_3}{3} \\ 2s_{xx}s_{xy}^2 + 2s_{yy}s_{xy}^2 + 2s_{yz}s_{xz}^2 \\ 2s_{xy}^2s_{yz}^2 + 2s_{zz}s_{yz}^2 + 2s_{xy}s_{xz}^2 \\ 2s_{xx}s_{xz}^2 + 2s_{zz}s_{xz}^2 + 2s_{xy}s_{yz}^2 \end{bmatrix} \quad (C.7) \]

\[ \frac{\partial \theta}{\partial \sigma} = -\tan(3\theta) \frac{\partial J_2}{\partial \sigma} + \frac{\tan(3\theta)}{2J_2} \frac{\partial J_3}{\partial \sigma} + \frac{\tan(3\theta)}{3J_3} \frac{\partial J_3}{\partial \sigma} \quad (C.8) \]

### C.3 Second derivatives of stress invariants with respect to stresses

\[ \frac{\partial^2 p}{\partial \sigma^2} = 0 \quad (C.9) \]

\[ \frac{\partial^2 J_2}{\partial \sigma^2} = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad (C.10) \]

\[ \frac{\partial^2 J_3}{\partial \sigma^2} = \begin{bmatrix} \frac{2}{3}s_{xx} & \frac{2}{3}s_{zz} & \frac{2}{3}s_{yy} & \frac{2}{3}s_{xy} & -\frac{4}{3}s_{yz} & \frac{2}{3}s_{xz} \\ \frac{2}{3}s_{zz} & \frac{2}{3}s_{yy} & \frac{2}{3}s_{xx} & \frac{2}{3}s_{xy} & \frac{2}{3}s_{yz} & -\frac{4}{3}s_{xz} \\ \frac{2}{3}s_{yy} & \frac{2}{3}s_{xx} & \frac{2}{3}s_{zz} & -\frac{4}{3}s_{xy} & \frac{2}{3}s_{yz} & \frac{2}{3}s_{xz} \\ \frac{2}{3}s_{xy} & \frac{2}{3}s_{yy} & -\frac{4}{3}s_{xz} & -2s_{zz} & 2s_{xz} & 2s_{yz} \\ -\frac{4}{3}s_{yz} & \frac{2}{3}s_{xy} & \frac{2}{3}s_{yy} & 2s_{xx} & -2s_{xx} & 2s_{xy} \\ \frac{2}{3}s_{xz} & -\frac{4}{3}s_{xz} & \frac{2}{3}s_{xx} & 2s_{xy} & 2s_{yz} & -2s_{yy} \end{bmatrix} \quad (C.11) \]

\[ \frac{\partial^2 \theta}{\partial \sigma^2} = -\frac{\tan(3\theta)}{2J_2} \frac{\partial^2 J_2}{\partial \sigma^2} + \frac{\partial J_3}{\partial \sigma} \left[ -3 - 3\tan^2(3\theta) \frac{\partial \theta}{\partial \sigma} + \frac{\tan(3\theta)}{2J_2} \frac{\partial J_3}{\partial \sigma} \right] \quad (C.12) \]
C.4 Derivative of the yield function with respect to stresses

\[ f = -\left(\Omega^c c_0^* + p \Omega^\phi \tan \phi_0^*\right) + \sqrt{\frac{J_2}{f_2(\theta)}} \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)^2 \]  \hspace{1cm} (C.13)

\[ \frac{\partial f}{\partial \sigma} = -\Omega^\phi \tan \phi_0^* \frac{\partial p}{\partial \sigma} + \frac{\partial f}{\partial J_2} \frac{\partial J_2}{\partial \sigma} + \frac{\partial f}{\partial f_2} \frac{\partial f_2}{\partial \sigma} + \frac{\partial f}{\partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \sigma} + \hat{f} \]  \hspace{1cm} (C.14)

\[ \frac{\partial f}{\partial J_2} = \frac{1}{2f_2 \sqrt{(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} \]  \hspace{1cm} (C.15)

\[ \frac{\partial f}{\partial f_2} = -\frac{J_2}{2f_2^2 \sqrt{(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} \]  \hspace{1cm} (C.16)

\[ \frac{\partial f_2}{\partial \theta} = 3\beta^\theta \alpha^\theta n^\theta \cos(3\theta) \left[ \beta^\theta \sin(3\theta) + 1 \right]^{n^\theta-1} \]  \hspace{1cm} (C.17)

\[ \frac{\partial f}{\partial \tan \phi_0^*} = \frac{\Omega^c p_0 \Omega^\phi \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)}{\sqrt{\frac{J_2}{f_2} + \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)^2}} - p \Omega^\phi \]  \hspace{1cm} (C.18)

\[ \frac{\partial f}{\partial c_0^*} = \frac{\Omega^c \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)}{\sqrt{\frac{J_2}{f_2} + \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)^2}} - \Omega^c \]  \hspace{1cm} (C.19)

\[ \frac{\partial f}{\partial p_0} = \frac{\Omega^c \Omega^\phi \tan \phi_0^* \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)}{\sqrt{\frac{J_2}{f_2} + \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)^2}} \]  \hspace{1cm} (C.20)

\[ \frac{\partial f}{\partial \Omega^\phi} = \frac{\Omega^c p_0 \tan \phi_0^* \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)}{\sqrt{\frac{J_2}{f_2} + \left(\Omega^c c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^*\right)^2}} - p \tan \phi_0^* \]  \hspace{1cm} (C.21)
\[
\frac{\partial f}{\partial \bar{F}} = \left( c_0^* + p_0 \Omega^\phi \tan \phi_0^* \right) \left( \Omega^\epsilon c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^* \right) - c_0^* \sqrt{\frac{J_2}{f_2} + \left( \Omega^\epsilon c_0^* + \Omega^c p_0 \Omega^\phi \tan \phi_0^* \right)^2} - c_0^* 
\]  
(C.22)

C.5 Derivative of the yield function with respect to state variables

\[
\frac{\partial f}{\partial \epsilon_p} = \frac{\partial f}{\partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon_p} + \frac{\partial f}{\partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon_p} + \frac{\partial f}{\partial p_0^*} \frac{\partial p_0^*}{\partial \epsilon_p} 
\]  
(C.23)

\[
\frac{\partial f}{\partial \epsilon_{eq}^c} = 0 
\]  
(C.24)

C.6 Derivative of the plastic potential with respect to stresses

\[
f^{iso} = - \left( c_0^* + p \tan \phi_0^* \right) + \sqrt{\frac{J_2}{f_2(\theta)}} + \left( c_0^* + p_0^* \tan \phi_0^* \right)^2 
\]  
(C.25)

\[
\frac{\partial g}{\partial \sigma} = \omega \left( - \tan \phi_0^* \frac{\partial p}{\partial \sigma} + \frac{\partial f^{iso}}{\partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \sigma} + \frac{\partial f^{iso}}{\partial c_0^*} \frac{\partial c_0^*}{\partial \sigma} + \frac{\partial f^{iso}}{\partial p_0^*} \frac{\partial p_0^*}{\partial \sigma} \right) + \frac{\partial f^{iso}}{\partial J_2} \frac{\partial J_2}{\partial \sigma} + \frac{\partial f^{iso}}{\partial \theta} \frac{\partial \theta}{\partial \sigma} 
\]  
(C.26)

\[
\frac{\partial f^{iso}}{\partial \tan \phi_0^*} = \frac{p_0 \left( c_0^* + p_0^* \tan \phi_0^* \right)}{\sqrt{(c_0^* + p_0^* \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - p 
\]  
(C.27)

\[
\frac{\partial f^{iso}}{\partial c_0^*} = \frac{2c_0^* + 2p_0^* \tan \phi_0^*}{2 \sqrt{(c_0^* + p_0^* \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - 1 
\]  
(C.28)

\[
\frac{\partial f^{iso}}{\partial p_0^*} = \frac{\tan \phi_0^* \left( c_0^* + p_0^* \tan \phi_0^* \right)}{\sqrt{(c_0^* + p_0^* \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} 
\]  
(C.29)

\[
\frac{\partial f^{iso}}{\partial J_2} = \frac{1}{2f_2 \sqrt{(c_0^* + p_0^* \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} 
\]  
(C.30)
\[ \frac{\partial J_{\text{iso}}}{\partial f_2} = \frac{-J_2}{2f_2^2 \sqrt{(e_0^t + p_0 \tan \phi_0^t)^2 + \frac{J_2}{f_2}}} \]  

(C.31)

C.7 Second derivative of the plastic potential with respect to stresses

\[ \frac{\partial^2 g}{\partial \sigma^2} = \omega \frac{\partial \text{aux}^{\text{vol}}}{\partial \sigma} + \text{aux}^{\text{vol}} \frac{\partial \omega}{\partial \sigma} + \frac{\partial f_{\text{iso}}}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} + \frac{\partial J_2}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} + \frac{\partial f_{\text{iso}}}{\partial \sigma} \frac{\partial f_2}{\partial \theta} \frac{\partial^2 \theta}{\partial \sigma^2} + \frac{\partial \theta}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \theta \partial \sigma} \]  

(C.32)

\[ \text{aux}^{\text{vol}} = -\tan \phi_0^t \frac{\partial p}{\partial \sigma} + \frac{\partial f_{\text{iso}}}{\partial \sigma} \frac{\partial \tan \phi_0^t}{\partial \sigma} + \frac{\partial f_{\text{iso}}}{\partial \tau_0} \frac{\partial \phi}{\partial \sigma} + \frac{\partial f_{\text{iso}}}{\partial \tau_0} \frac{\partial p_0}{\partial \sigma} \]  

(C.33)

\[ \frac{\partial \text{aux}^{\text{vol}}}{\partial \sigma} = -\frac{\partial p}{\partial \sigma} \tan \frac{\phi_0^t}{\partial \tan \phi_0^t} + \frac{\partial f_{\text{iso}}}{\partial \sigma} \frac{\partial \tan \phi_0^t}{\partial \sigma^2} + \frac{\partial \tan \phi_0^t}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} + \frac{\partial \tan \phi_0^t}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} \]  

(C.34)

\[ \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^t \partial \sigma} = -\frac{\partial p}{\partial \sigma} + \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} \frac{\partial \tau_0}{\partial \sigma} + \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} \frac{\partial \phi_0^t}{\partial \sigma} \]  

(C.35)

\[ \frac{\partial^2 f_{\text{iso}}}{\partial \tau_0 \partial \sigma} = \frac{\partial^2 f_{\text{iso}}}{\partial \tau_0 \partial \sigma} \frac{\partial \tau_0}{\partial \sigma} + \frac{\partial^2 f_{\text{iso}}}{\partial \sigma^2} \frac{\partial \phi_0^t}{\partial \sigma} \]  

(C.36)

\[ \frac{\partial^2 f_{\text{iso}}}{\partial p_0 \partial \sigma} = \frac{\partial^2 f_{\text{iso}}}{\partial p_0 \partial \sigma} \frac{\partial \tau_0}{\partial \sigma} + \frac{\partial^2 f_{\text{iso}}}{\partial p_0 \partial \sigma} \frac{\partial \phi_0^t}{\partial \sigma} \]  

(C.37)

\[ \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \sigma} = \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \sigma} \frac{\partial \tau_0}{\partial \sigma} + \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \sigma} \frac{\partial \phi_0^t}{\partial \sigma} \]  

(C.38)
\[
\frac{\partial^2 f_{iso}}{\partial \theta \partial \sigma} = \frac{\partial f_{iso}}{\partial f_2} \frac{\partial^2 f_2}{\partial \theta \partial \sigma} + \frac{\partial f_2}{\partial \theta} \frac{\partial^2 f_{iso}}{\partial f_2 \partial \sigma} \tag{C.39}
\]

\[
\frac{\partial^2 f_2}{\partial \theta \partial \sigma} = \frac{\partial^2 f_2}{\partial \theta^2} \frac{\partial \theta}{\partial \sigma} \tag{C.40}
\]

\[
\frac{\partial^2 f_{iso}}{\partial f_2 \partial \sigma} = \frac{\partial^2 f_{iso}}{\partial f_2^2} \frac{\partial f_2}{\partial \theta} \frac{\partial \theta}{\partial \sigma} + \frac{\partial^2 f_{iso}}{\partial f_2 \partial \sigma} \frac{\partial \tan \phi_0^*}{\partial \theta} \frac{\partial \tan \phi_0^*}{\partial \sigma} + \frac{\partial^2 f_{iso}}{\partial f_2 \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \sigma} + \frac{\partial^2 f_{iso}}{\partial f_2 \partial \sigma} \frac{\partial \tan \phi_0^*}{\partial \sigma} \tag{C.41}
\]

\[
\frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial J_2} = -\frac{p_0 (c_0^* + p_0 \tan \phi_0^*)}{2f_2 \left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.42}
\]

\[
\frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial f_2} = \frac{J_2 p_0 (c_0^* + p_0 \tan \phi_0^*)}{2f_2 \left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.43}
\]

\[
\frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial c_0^*} = \frac{p_0^2}{\sqrt{(c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - \frac{2p_0^2 (c_0^* + p_0 \tan \phi_0^*)^2}{\left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.44}
\]

\[
\frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial p_0} = \frac{p_0}{\sqrt{(c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - \frac{p_0 (2c_0^* + 2p_0 \tan \phi_0^*) (c_0^* + p_0 \tan \phi_0^*)}{2 \left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.45}
\]

\[
\frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial J_2} = \frac{c_0^* + p_0 \tan \phi_0^*}{\sqrt{(c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} \frac{p_0 \tan \phi_0^*}{\sqrt{(c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - \frac{2p_0 \tan \phi_0^*}{\left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.46}
\]

\[
\frac{\partial^2 f_{iso}}{\partial c_0^* \partial J_2} = -\frac{2c_0^* + 2p_0 \tan \phi_0^*}{4f_2 \left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} \tag{C.47}
\]
\[ \frac{\partial^2 f_{iso}}{\partial c_0^* \partial f_2} = \frac{J_2 (2c_0^* + 2p_{t0} \tan \phi_0^*)}{4f_2^2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.48)

\[ \frac{\partial^2 f_{iso}}{\partial c_0^* \partial \tan \phi_0^*} = \frac{\partial^2 f_{iso}}{\partial \tan \phi_0^* \partial c_0^*} \]  
(C.49)

\[ \frac{\partial^2 f_{iso}}{\partial c_0^2} = \frac{1}{\left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{1/2}} - \frac{(2c_0^* + 2p_{t0} \tan \phi_0^*)^2}{4 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.50)

\[ \frac{\partial^2 f_{iso}}{\partial c_0^* \partial p_{t0}} = \frac{\tan \phi_0^*}{\sqrt{(c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - \frac{\tan \phi_0^* (2c_0^* + 2p_{t0} \tan \phi_0^*) (c_0^* + p_{t0} \tan \phi_0^*)}{2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.51)

\[ \frac{\partial^2 f_{iso}}{\partial p_{t0} \partial J_2} = -\frac{\tan \phi_0^* (c_0^* + p_{t0} \tan \phi_0^*)}{2f_2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.52)

\[ \frac{\partial^2 f_{iso}}{\partial p_{t0} \partial f_2} = \frac{J_2 \tan \phi_0^* (c_0^* + p_{t0} \tan \phi_0^*)}{2f_2^2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.53)

\[ \frac{\partial^2 f_{iso}}{\partial p_{t0} \partial \tan \phi_0^*} = \frac{\partial f_{iso}}{\partial \tan \phi_0^* \partial p_{t0}} \]  
(C.54)

\[ \frac{\partial^2 f_{iso}}{\partial p_{t0} \partial c_0^*} = \frac{\partial^2 f_{iso}}{\partial c_0^* \partial p_{t0}} \]  
(C.55)

\[ \frac{\partial^2 f_{iso}}{\partial p_{t0}^2} = \frac{\tan^2 \phi_0^*}{\sqrt{(c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2}}} - \frac{\tan^2 \phi_0^* (c_0^* + p_{t0} \tan \phi_0^*)^2}{2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.56)

\[ \frac{\partial^2 f_{iso}}{\partial J_2^2} = -\frac{1}{4f_2^2 \left( (c_0^* + p_{t0} \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right)^{3/2}} \]  
(C.57)
\[
\frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial f_2} = \frac{J_2}{4f_2^3 \left[ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} \right]^{3/2}} - \frac{1}{2f_2^2 \sqrt{ (c_0^* + p_0 \tan \phi_0^*)^2 + \frac{J_2}{f_2} }} \tag{C.58}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \tan \phi_0^*} = \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial J_2} \tag{C.59}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial c_0^*} = \frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial J_2} \tag{C.60}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial p_{00}} = \frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial J_2} \tag{C.61}
\]

### C.8 Second derivative of the plastic potential with respect to stresses and state variables

\[
\frac{\partial^2 g}{\partial \sigma \partial \epsilon^p} = \omega \frac{\partial \text{aux}^{\text{vol}}}{\partial \epsilon^p} + \text{aux}^{\text{vol}} \frac{\partial \omega}{\partial \sigma} + \frac{\partial J_2}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \epsilon^p} + \frac{\partial f_2}{\partial \theta} \frac{\partial^2 f_{\text{iso}}}{\partial \theta \partial J_2} + \frac{\partial f_2}{\partial \epsilon} \frac{\partial^2 f_{\text{iso}}}{\partial \epsilon \partial J_2} \tag{C.62}
\]

\[
\frac{\partial \text{aux}^{\text{vol}}}{\partial \epsilon^p} = - \frac{\partial p}{\partial \sigma} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial f_{\text{iso}}}{\partial \tan \phi_0^*} \frac{\partial^2 \tan \phi_0^*}{\partial \sigma \partial \epsilon^p} + \frac{\partial \tan \phi_0^*}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial \epsilon^p} + \frac{\partial f_{\text{iso}}}{\partial c_0^*} \frac{\partial^2 c_0^*}{\partial \sigma \partial \epsilon^p} + \frac{\partial c_0^*}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial \epsilon^p} + \frac{\partial f_{\text{iso}}}{\partial p_{00}} \frac{\partial^2 p_{00}}{\partial \sigma \partial \epsilon^p} + \frac{\partial p_{00}}{\partial \sigma} \frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial \epsilon^p} \tag{C.63}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \epsilon^p} = \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial J_2 \partial p_{00}} \frac{\partial p_{00}}{\partial \epsilon^p} \tag{C.64}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial f_2 \partial \epsilon^p} = \frac{\partial^2 f_{\text{iso}}}{\partial f_2 \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial f_2 \partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial f_2 \partial p_{00}} \frac{\partial p_{00}}{\partial \epsilon^p} \tag{C.65}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial \epsilon^p} = \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial \tan \phi_0^* \partial p_{00}} \frac{\partial p_{00}}{\partial \epsilon^p} \tag{C.66}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial \epsilon^p} = \frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial c_0^* \partial p_{00}} \frac{\partial p_{00}}{\partial \epsilon^p} \tag{C.67}
\]

\[
\frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial \epsilon^p} = \frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial \tan \phi_0^*} \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial c_0^*} \frac{\partial c_0^*}{\partial \epsilon^p} + \frac{\partial^2 f_{\text{iso}}}{\partial p_{00} \partial p_{00}} \frac{\partial p_{00}}{\partial \epsilon^p} \tag{C.68}
\]
C.9 Derivatives of the function $\omega$

\[
\frac{\partial \omega}{\partial \sigma} = \zeta \frac{\partial \dot{\omega}}{\partial \sigma} + \dot{\omega} \frac{\partial \zeta}{\partial \sigma}
\]  

\[
\frac{\partial \dot{\omega}}{\partial \sigma} = \begin{cases} 
0 & \left( p + \frac{J}{\sqrt{3}} < 0 \right) \\
\frac{\partial \dot{\omega}}{\partial p} \frac{\partial p}{\partial \sigma} + \frac{\partial \dot{\omega}}{\partial J_2} \frac{\partial J_2}{\partial \sigma} & \left( 0 \leq p + \frac{J}{\sqrt{3}} \leq p_{nodil} + \frac{J}{\sqrt{3}} \right) \\
0 & (p > p_{nodil})
\end{cases}
\]  

\[
\frac{\partial \dot{\omega}}{\partial p} = \frac{\pi \sin \left[ \frac{\pi \left( p + \frac{\sqrt{3}J_2}{3} \right)}{p_{nodil} + \frac{\sqrt{3}J_2}{3}} \right]}{2 \left( p_{nodil} + \frac{\sqrt{3}J_2}{3} \right)} (\omega_{res} - 1)
\]  

\[
\frac{\partial \dot{\omega}}{\partial J_2} = \frac{2}{6 \sqrt{J_2} \left( p_{nodil} + \frac{\sqrt{3}J_2}{3} \right)} \left[ \frac{\pi \sqrt{3}}{6 \sqrt{J_2} \left( p_{nodil} + \frac{\sqrt{3}J_2}{3} \right)^2} - \frac{\pi \sqrt{3} \left( p + \frac{\sqrt{3}J_2}{3} \right)}{6 \sqrt{J_2} \left( p_{nodil} + \frac{\sqrt{3}J_2}{3} \right)^2} \right] (\omega_{res} - 1)
\]  

\[
\frac{\partial \zeta}{\partial \sigma} = \begin{cases} 
0 & (\dot{\varepsilon}_p \leq \xi_2) \\
\frac{\partial \zeta}{\partial \tan \phi_0^G} & (\dot{\varepsilon}_p > \xi_2)
\end{cases}
\]  

\[
\frac{\partial \zeta}{\partial \tan \phi_0^G} = \tan \phi_{peak}^G - \tan \phi_{res}^G
\]  

\[
\frac{\partial \omega}{\partial \varepsilon_p} = \dot{\omega} \frac{\partial \zeta}{\partial \varepsilon_p}
\]
\[ \frac{\partial \zeta}{\partial \epsilon^p} = \begin{cases} 0 & (\epsilon^p \leq \xi_2) \\ \frac{\partial \zeta}{\partial \tan \phi_0^*} & (\epsilon^p > \xi_2) \end{cases} \] (C.77)

C.10 Derivatives of the strength parameters with respect to stresses

\[ \frac{\partial \tan \phi_0^*}{\partial \sigma} = \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \sigma} \] (C.78)

\[ \frac{\partial c_0^*}{\partial \sigma} = \frac{\partial c_0^*}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \sigma} \] (C.79)

\[ \frac{\partial p_0}{\partial \sigma} = \frac{\partial p_0}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \sigma} \] (C.80)

\[ \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} = \begin{cases} \frac{1}{a_{\text{hard}} + \frac{\epsilon^p}{\epsilon^p_{\text{aux}}}} - \frac{\epsilon^p}{\epsilon^p_{\text{aux}} a_{\text{hard}} + \frac{\epsilon^p}{\epsilon^p_{\text{aux}}}} \xi_2 \tan \phi^*_{\text{peak}} - \tan \phi^*_{\text{ini}} - a_{\text{hard}} \xi_2 \tan \phi^*_{\text{peak}} - \tan \phi^*_{\text{ini}} - a_{\text{hard}} & (\epsilon^p \leq \xi_2) \\ b_{\text{res}} e_{\text{res}} \xi_2 (\tan \phi^*_\text{res} - \tan \phi^*_\text{peak}) \xi_2 \tan \phi^*_\text{peak} - \tan \phi^*_\text{ini} - a_{\text{hard}} & (\epsilon^p > \xi_2) \end{cases} \] (C.81)

\[ a_{\text{aux}} = \frac{\xi_2}{\tan \phi^*_\text{peak} - \tan \phi^*_\text{ini} - a_{\text{hard}}} \] (C.82)

\[ \frac{\partial c_0^*}{\partial \epsilon^p} = \begin{cases} 0 & (\epsilon^p \leq \xi_2) \\ -b_{\text{res}} e_{\text{res}} \xi_2 (c^*_\text{ini} - c^*_\text{post}) e_{\text{post}} \xi_2 - \xi_2 e_{\text{post}} (\xi_2 - \xi_{\text{ini}}) & (\epsilon^p > \xi_2) \end{cases} \] (C.83)

\[ \frac{\partial p_0}{\partial \epsilon^p} = \begin{cases} 0 & (\epsilon^p \leq \xi_2) \\ -b_{\text{res}} p_{\text{post}} e_{\text{post}} \xi_2 (p_{\text{ini}} - p_{\text{post}}) e_{\text{post}} \xi_2 - \xi_2 e_{\text{post}} (\xi_2 - \xi_{\text{ini}}) & (\epsilon^p > \xi_2) \end{cases} \] (C.84)

C.11 Derivatives of the strength parameters with respect to state variables

\[ \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} = \frac{\partial \tan \phi_0^*}{\partial \epsilon^p} \frac{\partial \epsilon^p}{\partial \epsilon^p} \] (C.85)
\[
\frac{\partial c_0^*}{\partial \epsilon_p} = \frac{\partial c_0^*}{\partial \epsilon^p_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \epsilon_p} = \frac{\partial c^*_0}{\partial \epsilon_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \epsilon_p}
\]
\(\text{(C.86)}\)

\[
\frac{\partial p_0}{\partial \epsilon_p} = \frac{\partial p_0}{\partial \epsilon^p_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \epsilon_p} = \frac{\partial p_0}{\partial \epsilon_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \epsilon_p}
\]
\(\text{(C.87)}\)

C.12 Second derivatives of the strength parameters with respect to stresses

\[
\frac{\partial^2 \tan \phi^*_0}{\sigma^2} = \frac{\partial^2 \tan \phi^*_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} + \frac{\partial^2 \epsilon^p_{eq}}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.88)}\)

\[
\frac{\partial^2 c^*_0}{\sigma^2} = \frac{\partial^2 c^*_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} + \frac{\partial^2 \epsilon^p_{eq}}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.89)}\)

\[
\frac{\partial^2 p_0}{\sigma^2} = \frac{\partial^2 p_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} + \frac{\partial^2 \epsilon^p_{eq}}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \sigma}{\partial \epsilon^p_{eq}} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.90)}\)

\[
\frac{\partial^2 \tan \phi^*_0}{\partial \epsilon^p_{eq} \partial \sigma} = \frac{\partial^2 \tan \phi^*_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.91)}\)

\[
\frac{\partial^2 c^*_0}{\partial \epsilon^p_{eq} \partial \sigma} = \frac{\partial^2 c^*_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.92)}\)

\[
\frac{\partial^2 p_0}{\partial \epsilon^p_{eq} \partial \sigma} = \frac{\partial^2 p_0}{\partial \epsilon^p_{eq} \partial \sigma} \frac{\partial \epsilon^p_{eq}}{\partial \sigma}
\]
\(\text{(C.93)}\)

\[
\frac{\partial^2 \tan \phi^*_0}{\partial \epsilon^p_{eq}^2} = \begin{cases} 
\frac{2 \epsilon^p_{eq}}{\text{aux}^2} \left( a_{\text{hard}} + \frac{\epsilon^p_{eq}}{\text{aux}^2} \right)^2 \frac{2}{\text{aux}^2} & (\epsilon^p_{eq} \leq \xi_2) \\
- b_{\text{res}} e^{b_{\text{res}} (\xi_2 - \epsilon^p_{eq})} \left( \tan \phi^*_{\text{res}} - \tan \phi^*_{\text{peak}} \right) & (\epsilon^p_{eq} > \xi_2)
\end{cases}
\]
\(\text{(C.94)}\)

\[
\frac{\partial^2 c^*_0}{\partial \epsilon^p_{eq}^2} = \begin{cases} 
0 & (\epsilon^p_{eq} \leq \xi_2) \\
b_{\text{post}}^2 (c^*_{\text{ini}} - c^*_{\text{post}}) e^{b_{\text{post}} (\xi_2 - \epsilon^p_{eq})} + b_{\text{res}}^2 c^*_{\text{post}} e^{b_{\text{res}} (\xi_2 - \epsilon^p_{eq})} & (\epsilon^p_{eq} > \xi_2)
\end{cases}
\]
\(\text{(C.95)}\)
\[
\frac{\partial^2 p_{t0}}{\partial \hat{\epsilon}_{eq}^2} = \begin{cases} 
0 & (\hat{\epsilon}_{eq}^p \leq \xi_2) \\
\hat{b}^2_{\text{post}} (p_{\text{ini}} - p_{\text{post}}) e^{b_{\text{post}} (\xi_2 - \hat{\epsilon}_{eq}^p)} + \hat{b}^2_{\text{res}} p_{\text{post}} e^{b_{\text{res}} (\xi_2 - \hat{\epsilon}_{eq}^p)} & (\hat{\epsilon}_{eq}^p > \xi_2)
\end{cases}
\]

(C.96)

C.13 Second derivatives of the strength parameters with respect to stresses and state variables

\[
\frac{\partial^2 \tan \phi^*_0}{\partial \sigma \partial \hat{\epsilon}^p} = \frac{\partial \hat{\epsilon}_{eq}^p}{\partial p} \frac{\partial^2 \tan \phi^*_0}{\partial \sigma \partial \hat{\epsilon}_{eq}^p \partial \hat{\epsilon}^p} + \frac{\partial \tan \phi^*_0}{\partial \sigma} \frac{\partial^2 \hat{\epsilon}_{eq}^p}{\partial \hat{\epsilon}^p} 
\]

\[
\frac{\partial^2 c^*_0}{\partial \sigma \partial \hat{\epsilon}^p} = \frac{\partial \hat{\epsilon}_{eq}^p}{\partial p} \frac{\partial^2 c^*_0}{\partial \sigma \partial \hat{\epsilon}_{eq}^p \partial \hat{\epsilon}^p} + \frac{\partial c^*_0}{\partial \sigma} \frac{\partial^2 \hat{\epsilon}_{eq}^p}{\partial \hat{\epsilon}^p} 
\]

\[
\frac{\partial^2 p_{t0}}{\partial \sigma \partial \hat{\epsilon}^p} = \frac{\partial \hat{\epsilon}_{eq}^p}{\partial p} \frac{\partial^2 p_{t0}}{\partial \sigma \partial \hat{\epsilon}_{eq}^p \partial \hat{\epsilon}^p} + \frac{\partial p_{t0}}{\partial \sigma} \frac{\partial^2 \hat{\epsilon}_{eq}^p}{\partial \hat{\epsilon}^p} 
\]

(C.98)

(C.99)

(C.100)

(C.101)

(C.102)

C.14 Derivatives of \(\hat{\epsilon}_{eq}^p\)

\[
\frac{\partial \hat{\epsilon}_{eq}^p}{\partial p} = \begin{cases} 
- \frac{2 \hat{m}^2 p \epsilon_{eq}^p}{p_{\text{atm}}^2 \left( \frac{\hat{m}^2 p_{\text{eq}}^2}{p_{\text{atm}}^2} + 1 \right)} & (\hat{\epsilon}_{eq}^p \leq \xi_2) \\
\frac{2 \hat{m}^2 p \xi_2}{p_{\text{atm}}^2} & (\hat{\epsilon}_{eq}^p > \xi_2)
\end{cases}
\]

(C.103)
\[
\frac{\partial^2 \hat{\epsilon}_p}{\partial p^2} = \begin{cases} 
8 \hat{m}^4 p^2 \hat{\epsilon}^p_{eq} & (\hat{\epsilon}^p_{eq} \leq \xi_2) \\
\frac{p_{atm}^4 \left( \frac{\hat{m}^2 p^2}{p_{atm}^2} + 1 \right)}{p_{atm}^2 \left( \frac{\hat{m}^2 p^2}{p_{atm}^2} + 1 \right)}^3 - \frac{2 \hat{m}^2 \hat{\epsilon}^p_{eq}}{p_{atm}^2 \left( \frac{\hat{m}^2 p^2}{p_{atm}^2} + 1 \right)} & (\hat{\epsilon}^p_{eq} > \xi_2)
\end{cases}
\]

(C.104)

\[
\frac{\partial \hat{\epsilon}^p_{eq}}{\partial \hat{\epsilon}^p_{eq}} = \begin{cases} 
1 & (\hat{\epsilon}^p_{eq} \leq \xi_2) \\
\frac{1}{\hat{m}^2 p^2 \left( \frac{\hat{m}^2 p^2}{p_{atm}^2} + 1 \right)} & (\hat{\epsilon}^p_{eq} > \xi_2)
\end{cases}
\]

(C.105)

\[
\frac{\partial^2 \hat{\epsilon}^p_{eq}}{\partial p \partial \hat{\epsilon}^p_{eq}} = \begin{cases} 
\frac{2 \hat{m}^2 p}{p_{atm}^2 \left( \frac{\hat{m}^2 p^2}{p_{atm}^2} + 1 \right)} & (\hat{\epsilon}^p_{eq} \leq \xi_2) \\
0 & (\hat{\epsilon}^p_{eq} > \xi_2)
\end{cases}
\]

(C.106)

\[
\frac{\partial^2 \hat{\epsilon}^p_{eq}}{\partial p \partial \sigma} = \frac{\partial^2 \hat{\epsilon}^p_{eq}}{\partial p^2} \frac{\partial p}{\partial \sigma}
\]

(C.107)

\[
\frac{\partial \hat{\epsilon}^p_{eq}}{\partial \epsilon^p} = \frac{\partial \hat{\epsilon}^p_{eq}}{\partial \hat{\epsilon}^p_{eq}} \frac{\partial \hat{\epsilon}^p_{eq}}{\partial \epsilon^p}
\]

(C.108)

\[
\frac{\partial \hat{\epsilon}^p_{eq}}{\partial \epsilon^p} = \frac{\partial \hat{\epsilon}^p_{eq}}{\partial \hat{\epsilon}^p_{eq}} \frac{\partial \hat{\epsilon}^p_{eq}}{\partial \epsilon^p}
\]

(C.109)

\[
\frac{\partial \hat{\epsilon}^p_{eq}}{\partial \epsilon^p} = \begin{bmatrix}
\hat{\epsilon}^p_{xx} \\
\hat{\epsilon}^p_{xy} \\
\hat{\epsilon}^p_{yx} \\
\hat{\epsilon}^p_{yy} \\
\hat{\epsilon}^p_{xz} \\
\hat{\epsilon}^p_{yz} \\
\hat{\epsilon}^p_{yz} \\
\hat{\epsilon}^p_{zz} \\
\end{bmatrix}
\]

(C.110)
C.15 Derivatives of state variables

\[
\frac{\partial \chi}{\partial \epsilon^p} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]  
(C.111)

\[
\frac{\partial \chi}{\partial \epsilon^c} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
\epsilon_{xx}^c & \epsilon_{xx}^c & \epsilon_{xx}^c & \epsilon_{xx}^c & \epsilon_{xx}^c & \epsilon_{xx}^c \\
\epsilon_{eq} & \epsilon_{eq} & \epsilon_{eq} & \epsilon_{eq} & \epsilon_{eq} & \epsilon_{eq}
\end{bmatrix}
\]  
(C.112)
Appendix D

Script of the constitutive law

D.1 File - main.for

```
1 ************************************************************************
2 * AHW (ARGILLACEOUS HARD SOILS - WEAK ROCKS) *
3 * Constitutive model implemented as part of the PhD Thesis "Analysis *
4 * of underground excavations in argillaceous hard soils - weak rocks" *
5 * By: Miguel Angel Manica Malcom *
6 * Supervisors: Antonio Gens & Jean Vaunat *
7 * Technical University of Catalonia, 2018 *
8 ************************************************************************

9 Subroutine const_law(IDTask, iMod, IsUndr,
10   * iStep, iter, iEl, Int,
11   * X, Y, Z,
12   * Time0, dTime,
13   * Props, Sig0, Swp0, StVar0,
14   * dEps, D, BulkN,
15   * Sig, Swp, StVar, ipl,
16   * nStat,
17   * NonSym, iStrsDep, iTimeDep, iTang,
18   * iPrjDir, iPrjLen, iAbort)

20 ! Depending on IDTask, 1 : Initialise state variables
21 ! 2 : calculate stresses,
22 ! 3 : calculate material stiffness matrix
23 ! 4 : return number of state variables
24 ! 5 : inquire matrix properties
25 ! 6 : calculate elastic material stiffness matrix
26 ! return switch for non-symmetric D-matrix
27 ! stress/time dependent matrix

29 ! Arguments:
30 ! I/O Type          :
31 ! IDTask   I I    : see above
32 ! iMod     I I    : model number (1..10)
33 ! IsUndr   I I    : -1 for undrained, 0 otherwise
34 ! iStep    I I    : Global step number
35 ! iter     I I    : Global iteration number
36 ! iel      I I    : Global element number
37 ! Int      I I    : Global integration point number
38 ! X        I R    : X-Position of integration point
39 ! Y        I R    : Y-Position of integration point
40 ! Z        I R    : Z-Position of integration point
```
! Time0 I R : Time at start of step
! dTime I R : Time increment
! Props I R() : List with model parameters
! Sig0 I R() : Stresses at start of step
! Swp0 I R : Excess pore pressure start of step
! StVar0 I R() : State variable at start of step
! dEps I R() : Strain increment
! D I/O R(,) : Material stiffness matrix
! BulkW I/O R : Bulk modulus for water (undrained only)
! Sig O R() : Resulting stresses
! Swp O R : Resulting excess pore pressure
! StVar O R() : Resulting values state variables
! ipl O I : Plasticity indicator
! nStat O I : Number of state variables
! NonSym O I : Non-Symmetric D-matrix ?
! iStrsDep O I : =1 for stress dependent D-matrix
! iT imeDep O I : =1 for time dependent D-matrix
! iAbort O I : =1 to force stopping of calculation

Implicit Double Precision (A-H, O-Z)

! Arguments
Dimension Props(*), Sig0(6), StVar0(8), dEps(6), Sig(6)
Dimension StVar(8)
Dimension D(6,6)
Dimension iPrjDir(*)

! Local variables
Dimension Ctrl(3), dSig(6)
Dimension Sig0_1(6), StVar0_1(7), dEps_1(6), Sig_1(6), StVar_1(7)
Dimension Sig0_2(6), StVar0_2(7), dEps_2(6), Sig_2(6), StVar_2(7)
Dimension StVar0_it(7)
Character *255 PrjDir, File1, File2, File3, File4, File5, File6
Character *255 File7, File8, File9, File10, File11
Logical check
Save iGauss, iphase, i1stele, i1steleflag

!----------------------------------------------------------------------!
! IDTask = 0 (Check consistency of parameters) !
!----------------------------------------------------------------------!
! No negative parameters
Do i=1,32
  If (Props(i) .Lt. 0.) Then
    Call Ok_messagebox(’Only 33. weak elem can have a negative value’)
  End if
End do
Do i=34,40
  If (Props(i) .Lt. 0.) Then
    Call Ok_messagebox(’Only 33. weak elem can have a negative value’)
  End if
End do

! Elastic parameters
If (Props(1) .Eq. 0. .or. Props(2) .Eq. 0.) Then
  Call Ok_messagebox(’Stiffness parameter missing’)

Stop
102           Else
103               If (Props(3) .Eq. 0. .And. Props(4) .Eq. 0. .And. Props(5) .Eq. 0.) Then
104                   Props(3) = Props(1)
105                   Props(4) = Props(2)
106                   Props(5) = Props(1)/2./(1.+Props(2))
107               Else If (Props(3) .Eq. 0. .or. Props(4) .Eq. 0. .or. Props(5) .Eq. 0.) Then
108                   Call Ok_messagebox('Stiffness parameter missing')
109                   Stop
110               End if
111           End if
112           If ((Props(2) .Gt. 0.499) .or. (Props(4) .Gt. 0.499)) Then
113               Call Ok_messagebox('02. nu_1 or 04. nu_2 cannot be greater than 0.499')
114               Stop
115           End if
116
117 ! Strength parameters
118           If (Props(8) .Gt. Props(9)) Then
119               Call Ok_messagebox('08. phi_ini cannot be greater than 09. phi_p.eak')
120               Stop
121           End if
122           If (Props(10) .Gt. Props(9)) Then
123               Call Ok_messagebox('10. phi_res cannot be greater than 09. phi_p.eak')
124               Stop
125           End if
126           If (Props(13) .Gt. 1.) Then
127               Call Ok_messagebox('13. r_post only takes values between 0 and 1')
128               Stop
129           End if
130
131 ! Plastic potential
132           If (Props(15) .Gt. 1.) Then
133               Call Ok_messagebox('15. omega only takes values between 0 and 1')
134               Stop
135           End if
136
137 ! Hardening
138           If ((Props(08) .Lt. Props(09)) .And. (Props(16) .Eq. 0.)) Then
139               Call Ok_messagebox('16. xi_2 cannot be equal to zero')
140               Stop
141           End if
142           If ((Props(08) .Lt. Props(09)) .And. (Props(18) .Eq. 0.)) Then
143               Call Ok_messagebox('18. a_hard cannot be equal to zero')
144               Stop
145           End if
146
147 ! Strength anisotropy
148           If (Props(21) .Eq. 0. .And. Props(22) .Eq. 0. .And. Props(24) .Eq. 0. .And. Props(23) .Eq. 0.) Then
149               Props(21) = 1.
150               Props(22) = 1.
151               Props(24) = 45.
152               Props(23) = 1.
153           Else If (Props(21) .Eq. 0.) Then
Call Ok_messagebox('21. Omega_90 cannot be equal to zero')
Stop
Else If (Props(22) .Eq. 0.) Then
Call Ok_messagebox('22. Omega_m cannot be equal to zero')
Stop
Else If (Props(23) .Eq. 0.) Then
Call Ok_messagebox('23. delta_m cannot be equal to zero')
Stop
Else If (Props(24) .Eq. 0.) Then
Call Ok_messagebox('24. n cannot be equal to zero')
Stop
End If

! Perzyna
If (Props(25) .Eq. 0. .And. Props(26) .Eq. 0.) Then
Props(25) = 1.
Props(26) = 1.e-3
Else If (Props(25) .Eq. 0.) Then
Call Ok_messagebox('25. N cannot be equal to zero')
Stop
Else If (Props(26) .Eq. 0.) Then
Call Ok_messagebox('26. eta_pz cannot be equal to zero')
Stop
End If

! Creep
If ((Props(28) .Gt. 0.) .Or. (Props(29) .Gt. 0.) .Or.
. (Props(30) .Gt. 0.)) Then
If (Props(27) .Eq. 0.) Then
Call Ok_messagebox('27. gamma^c cannot be equal to zero')
Stop
End if
End if
If (Props(28) .Gt. 1.) Then
Call Ok_messagebox('28. psi^c only takes values between 0 and 1')
Stop
End if

! Nonlocal model
nlflag = Props(31)

! Control parameters
If (Props(34) .Eq. 0) Then
Call Ok_messagebox('34. ctrl p_atm must be always equal to 100 K
.N/m2 in the current units')
Stop
End if
If (Props(35) .Eq. 0.) Props(35) = 1.e-8
If (Props(36) .Eq. 0.) Props(36) = 30
If (Props(37) .Eq. 0.) Props(37) = 3
If (Props(38) .Eq. 0.) Props(38) = 1.e-3
If (Props(39) .Eq. 0.) Props(39) = 1.e-99
If (Props(40) .Eq. 1.) Props(7) = 0.

!----------------------------------------------------------------------!

! IDTask = 1 (Initialise state variables) !
!----------------------------------------------------------------------!
It is not necessary to initialise history variables

Write Gauss points information at the beginning of a phase for the nonlocal model

If (nlflag .Eq. 1) Then
  iGauss = iGauss+1
  Write(2,Rec=iGauss) X, Y, Z, StVar0(8)
If(Int .Eq. 1) Write(3,Rec=iel) iGauss
If (i1steleflag .Eq. 0) i1stele = iel
i1steleflag = 1
End if

End If ! IDTask = 1

!----------------------------------------------------------------------!

! IDTask = 2 (Calculate constitutive stresses Sig and Swp)
!----------------------------------------------------------------------!

If (IDTask .Eq. 2) Then
  iPhase = IDTask
End if

iphase = IDTask

! Equilibrium recalculation is avoided between phases
If (((dEps(1) .Eq. 0.) .And. (dEps(2) .Eq. 0.) .And. (dEps(3) .Eq. 0.) .And. (dEps(4) .Eq. 0.) .And. (dEps(5) .Eq. 0.) .And. (dEps(6) .Eq. 0.)) .Or. (dtime .Eq. 0.)) Then
  Do i=1,iPrjLen
    PrjDir(i:i) = Char(iPrjDir(i))
  End Do
  File3 = PrjDir(:iPrjLen)\'file3.txt'
  File4 = PrjDir(:iPrjLen)\'file4.txt'
  File5 = PrjDir(:iPrjLen)\'file5.txt'
  File6 = PrjDir(:iPrjLen)\'file6.txt'
  File7 = PrjDir(:iPrjLen)\'file7.txt'
  File8 = PrjDir(:iPrjLen)\'nGausspoints.txt'
  Open(Unit=4, File=File3, iostat=ios, Status='Unknown', Access='Direct', Recl=2, Form='Unformatted')
  Open(Unit=5, File=File4, iostat=ios, Status='Unknown', Access='Direct', Recl=20000, Form='Unformatted')
  Open(Unit=6, File=File5, iostat=ios, Status='Unknown', Access='Direct', Recl=40000, Form='Unformatted')
  Open(Unit=7, File=File6, iostat=ios, Status='Unknown', Access='Direct', Recl=2, Form='Unformatted')
  Open(Unit=8, File=File7, iostat=ios, Status='Unknown', Access='Direct', Recl=2, Form='Unformatted')
  Call Nonlocal1(Props, iGauss)
End if

Equilibrium recalculation is avoided between phases
If (((dEps(1) .Eq. 0.) .And. (dEps(2) .Eq. 0.) .And. (dEps(3) .Eq. 0.) .And. (dEps(4) .Eq. 0.) .And. (dEps(5) .Eq. 0.) .And. (dEps(6) .Eq. 0.)) .Or. (dtime .Eq. 0.)) Then
  Do i=1,6
    Sig(i) = Sig0(i)
  End do
  Do i=1,8
    StVar(i) = StVar0(i)
  End do
Goto 101
End if
! Calculate nonlocal state variable (at the beginning of a step)
If (nlflag .Eq. 1).And.(iel .Eq. i1stele).And.(Int .Eq. 1)) Then
  Call Nonlocal2(Props, iGauss)
End if

! Calculate new pore pressure
If (IsUndr.Eq.1) Then
  dEpsV = dEps(1) + dEps(2) + dEps(3)
  dSwp = BulkW * dEpsV
  Swp = Swp0 + dSwp
Else
  Swp = Swp0
End If

! Soil mechanics sign convention
Do i=1,6
  Sig0(i) = -Sig0(i)
  dEps(i) = -dEps(i)
End do

! Control parameters
Ctrl(1) = Props(35) !tol1
Ctrl(2) = Props(36) !nNRmax
!Ctrl(3) !nNRflag
nM = Props(37)
tol2 = Props(38)
dTmin = Props(39)
zero = 1.e-10

! Stress integration algorithm with automatic time step control
! Initialise variables
T = 0.
dT = 1.
Do i=1,7
  StVar0_it(i) = StVar0(i)
End do

! Start iterations
100 Do while(T .Lt. 1.)
  If (dT .Lt. dTmin) Then
    Call Ok_messagebox('Max time step reduction reached')
    Stop
  End if
  Do i=1,6
    Sig0_1(i) = Sig0(i)
    Sig0_2(i) = Sig0(i)
    dEps_1(i) = dEps(i)*dT
    dEps_2(i) = dEps(i)*dT/nM
  End do
  Do i=1,7
    StVar0_1(i) = StVar0_it(i)
    StVar0_2(i) = StVar0_it(i)
  End do
  dTime_1 = dTime*dT
  dTime_2 = dTime*dT/nM
  ! Calculate Sig_1
  Call SPA(Props, Sig0_1, StVar0_1, dEps_1, D, Sig_1, StVar_1,
    Ctrl, dTime_1, iel, Int, nlflag)
  If (Ctrl(3) .Eq. 1) Then
APPENDICES

346          dT = 0.5*dT
347          Goto 100
348          End if
349
350          ! Calculate Sig_2
351          Do i=1,nM
352             Call SPA(Props, Sig0_2, StVar0_2, dEps_2, D, Sig_2, StVar_2,
353                Ctrl, dTime_2, iel, Int, nlflag)
354             If (Ctrl(3) .Eq. 1) Then
355                dT = 0.5*dT
356                Goto 100
357             End if
358          Do j=1,6
359             Sig0_2(j) = Sig_2(j)
360          End do
361          Do j=1,7
362             StVar0_2(j) = StVar_2(j)
363          End do
364          End do
365
366          ! Estimate error
367          aux1 = 0.
368          aux2 = 0.
369          aux3 = 0.
370          Do i=1,6
371             aux1 = (Sig_2(i)-Sig_1(i))/(nM**2-1)
372             aux2 = aux2+aux1**2
373             aux3 = aux3+Sig_2(i)**2
374          End do
375          rE = sqrt(aux2)/sqrt(aux3)
376          rE = max(rE,Epsilon(rE))
377
378          ! If the step fails
379          If (rE .Gt. tol2) Then
380             xQ = 0.8*sqrt(tol2/rE)
381             dT = max(xQ*dT,0.1*dT)
382             Goto 100
383          End if
384
385          ! If the step succeeds
386          T = T+dT
387          Do i=1,6
388             Sig0(i) = Sig_2(i)
389          End do
390          Do i=1,7
391             StVar0_it(i) = StVar_2(i)
392          End do
393
394          ! Update variables
395          Do i=1,6
396             Sig(i) = -Sig_2(i)
397             Sig0(i) = -Sig0(i) !Return to PLAXIS sign convention
398             dEps(i) = -dEps(i) !Return to PLAXIS sign convention
399          End do
Do i=1,7
   StVar(i) = StVar_2(i)
End do
StVar(8) = sqrt((StVar(1)**2+StVar(2)**2+StVar(3)**2
               +0.5*StVar(4)**2+0.5*StVar(5)**2+0.5*StVar(6)**2))
If (StVar(8) .Eq. StVar0(8)) Then
   ipl = 0
Else
   ipl = 1
End if

! Write resulting state variable for the nonlocal model
If (nlflag .Eq. 1) Then
   Read(3,Rec=iel) naux1
   naux2 = naux1+(Int-1)
   Write(7,Rec=naux2) StVar(8)
End if
101 Continue
End If ! IDTask = 2

!----------------------------------------------------------------------!
! IDTask = 3 (Create effective material stiffness matrix D)  
! IDTask = 6 (Create elastic material stiffness matrix De)    
!----------------------------------------------------------------------!
If ( IDTask .Eq. 3 .Or. 
   * IDTask .Eq. 6 ) Then
   ! Calculate stiffness matrix D
   Call Stiff_mat(Props, D)
End If ! IDTask = 3 or 6

!----------------------------------------------------------------------!
! IDTask = 4 (Return number of state parameters) 
!----------------------------------------------------------------------!
If (IDTask .Eq. 4) Then
   nStat = 8
End If ! IDTask = 4

!----------------------------------------------------------------------!
! IDTask = 5 (Return matrix attributes) 
!----------------------------------------------------------------------!
If (IDTask .Eq. 5) Then
   ! Matrix attributes
   NonSym = 0 ! 1 for non-symmetric D-matrix
   iStrsDep = 0 ! 1 for stress dependent D-matrix
   iTang = 0 ! 1 for tangent D-matrix
   iTimeDep = 0 ! 1 for time dependent D-matrix
   ! Open files to write Gauss points information for the nonlocal model
If (nlflag .Eq. 1) Then
   Do i=1,iPrjLen
      PrjDir(i:i) = Char(iPrjDir(i))
   End Do
   File1 = PrjDir(:iPrjLen)//'file1.txt'
   File2 = PrjDir(:iPrjLen)//'file2.txt'
   Open(Unit=2, File=File1, iostat=ios, Status='Unknown',
       Access='Direct', Recl=8, Form='Unformatted')
   Open(Unit=3, File=File2, iostat=ios, Status='Unknown',
       Access='Direct', Recl=2, Form='Unformatted')
   End if
iGauss = 0
i1steleflag = 0

! Read and write strength distribution file
If (Props(33) .Eq. -1) Then
   Call Ok_messagebox('Copy strg. distribution file - file9.txt')
   Do i=1,iPrjLen
      PrjDir(i:i) = Char(iPrjDir(i))
   End Do
   File9 = PrjDir(:iPrjLen)//'file9.txt'
   File10 = PrjDir(:iPrjLen)//'file10.txt'
   Open(Unit= 9,File=File9, iostat=ios, Status='Old')
   If (ios .GT. 0) Then
      Call Ok_messagebox('file9.txt could not be opened')
      Stop
   End if
   Open(Unit=10, File=File10, iostat=ios, Status='Unknown',
       Access='Direct', Recl=2, Form='Unformatted')
   Read(9,*) ingauss
   Do i=1,ingauss
      Read(9,*) strg_factor
      Write(10,Rec=i) strg_factor
   End do
   Close(9)
End if ! IDTask = 5

!----------------------------------------------------------------------!
Return
End ! const_law

!----------------------------------------------------------------------!
Subroutine Stiff_mat
! Calculates the elasticstiffness matrix with transverse isotropy
!----------------------------------------------------------------------!
Subroutine Stiff_mat(Props, D)

Implicit Double Precision (A-H,O-Z)

! Arguments
Dimension Props(*)
Dimension D(6,6)

! Local variables
Dimension D_loc(6,6), T_eps(6,6), T_eps_t(6,6)

! Parameters
pi = 3.141592653589793
\[ E_1 = \text{Props}(1) \]
\[ x\text{Nu1} = \text{Props}(2) \]
\[ E_2 = \text{Props}(3) \]
\[ x\text{Nu2} = \text{Props}(4) \]
\[ G_2 = \text{Props}(5) \]
\[ \alpha = \text{Props}(6) \cdot \pi/180. \]
\[ \beta = \text{Props}(7) \cdot \pi/180. \]

! Calculate local stiffness matrix \( D_{\text{loc}} \)
\[ x_n = E_1/E_2 \]
\[ x_m = 1.-x\text{Nu1}-2.\cdot x_n\cdot x\text{Nu2}^2 \]
If \( x_m \leq 0. \)
   Call Ok_messagebox('1-x\text{Nu1}-2\cdot x_n\cdot x\text{Nu2}^2=0')
Stop
Endif
\[ D_{\text{loc}} = \begin{bmatrix} 0. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \end{bmatrix} \]
If \( \text{Props(40)} \leq 1. \)
   For 2D analyses
   \[ D_{\text{loc}} = 0. \]
   \[ D_{\text{loc}}(1,1) = E_1\cdot(1.-x_n\cdot(x\text{Nu2})^2)/(1.+x\text{Nu1})/x_m \]
   \[ D_{\text{loc}}(1,2) = E_1\cdot(x\text{Nu1}+x_n\cdot x\text{Nu2}^2)/(1.+x\text{Nu1})/x_m \]
   \[ D_{\text{loc}}(1,3) = E_1\cdot x\text{Nu2}/x_m \]
   \[ D_{\text{loc}}(2,1) = D_{\text{loc}}(1,2) \]
   \[ D_{\text{loc}}(2,2) = D_{\text{loc}}(1,1) \]
   \[ D_{\text{loc}}(2,3) = D_{\text{loc}}(1,3) \]
   \[ D_{\text{loc}}(3,1) = D_{\text{loc}}(1,3) \]
   \[ D_{\text{loc}}(3,2) = D_{\text{loc}}(1,1) \]
   \[ D_{\text{loc}}(3,3) = E_2\cdot(1.-x\text{Nu1})/x_m \]
   \[ D_{\text{loc}}(4,4) = E_1/2./\left(1.+x\text{Nu1}\right) \]
   \[ D_{\text{loc}}(5,5) = G_2 \]
   \[ D_{\text{loc}}(6,6) = D_{\text{loc}}(5,5) \]
End if

! Calculate strain transformation matrix \( T_{\text{eps}} \)
\[ x_{l1} = \cos(\alpha) \]
\[ x_{l2} = -\sin(\alpha)\cdot\cos(\beta) \]
\[ x_{l3} = \sin(\alpha)\cdot\sin(\beta) \]
\[ x_{m1} = \sin(\alpha) \]
\[ x_{m2} = \cos(\alpha)\cdot\cos(\beta) \]
\[ x_{m3} = -\cos(\alpha)\cdot\sin(\beta) \]
\[ x_{n1} = 0. \]
\[ x_{n2} = \sin(\beta) \]
\[ x_{n3} = \cos(\beta) \]
\[ T_{\text{eps}}(1,1) = x_{l1}^2 \]
\[ T_{\text{eps}}(2,1) = x_{l2}^2 \]
\[ T_{\text{eps}}(3,1) = x_{l3}^2 \]
\[ T_{\text{eps}}(4,1) = 2.\cdot x_{l1}\cdot x_{l2} \]
\[ T_{\text{eps}}(5,1) = 2.\cdot x_{l2}\cdot x_{l3} \]
\[ T_{\text{eps}}(6,1) = 2.\cdot x_{l1}\cdot x_{l3} \]
\[ T_{\text{eps}}(1,2) = x_{m1}^2 \]
\[ T_{\text{eps}}(2,2) = x_{m2}^2 \]
\[ T_{\text{eps}}(3,2) = x_{m3}^2 \]
\[ T_{\text{eps}}(4,2) = 2 \cdot x_{m1} \cdot x_{m2} \]
\[ T_{\text{eps}}(5,2) = 2 \cdot x_{m2} \cdot x_{m3} \]
\[ T_{\text{eps}}(6,2) = 2 \cdot x_{m1} \cdot x_{m3} \]
\[ T_{\text{eps}}(1,3) = x_{n1}^2 \]
\[ T_{\text{eps}}(2,3) = x_{n2}^2 \]
\[ T_{\text{eps}}(3,3) = x_{n3}^2 \]
\[ T_{\text{eps}}(4,3) = 2 \cdot x_{n1} \cdot x_{n2} \]
\[ T_{\text{eps}}(5,3) = 2 \cdot x_{n2} \cdot x_{n3} \]
\[ T_{\text{eps}}(6,3) = 2 \cdot x_{n1} \cdot x_{n3} \]
\[ T_{\text{eps}}(1,4) = x_{l1} \cdot x_{m1} \]
\[ T_{\text{eps}}(2,4) = x_{l2} \cdot x_{m2} \]
\[ T_{\text{eps}}(3,4) = x_{l3} \cdot x_{m3} \]
\[ T_{\text{eps}}(4,4) = x_{l1} \cdot x_{m2} + x_{l2} \cdot x_{m1} \]
\[ T_{\text{eps}}(5,4) = x_{l2} \cdot x_{m3} + x_{l3} \cdot x_{m2} \]
\[ T_{\text{eps}}(6,4) = x_{l3} \cdot x_{m1} + x_{l1} \cdot x_{m3} \]
\[ T_{\text{eps}}(1,5) = x_{m1} \cdot x_{n1} \]
\[ T_{\text{eps}}(2,5) = x_{m2} \cdot x_{n2} \]
\[ T_{\text{eps}}(3,5) = x_{m3} \cdot x_{n3} \]
\[ T_{\text{eps}}(4,5) = x_{m1} \cdot x_{n2} + x_{m2} \cdot x_{n1} \]
\[ T_{\text{eps}}(5,5) = x_{m2} \cdot x_{n3} + x_{m3} \cdot x_{n2} \]
\[ T_{\text{eps}}(6,5) = x_{m3} \cdot x_{n1} + x_{m1} \cdot x_{n3} \]
\[ T_{\text{eps}}(1,6) = x_{l1} \cdot x_{n1} \]
\[ T_{\text{eps}}(2,6) = x_{l2} \cdot x_{n2} \]
\[ T_{\text{eps}}(3,6) = x_{l3} \cdot x_{n3} \]
\[ T_{\text{eps}}(4,6) = x_{l1} \cdot x_{n2} + x_{l2} \cdot x_{n1} \]
\[ T_{\text{eps}}(5,6) = x_{l2} \cdot x_{n3} + x_{l3} \cdot x_{n2} \]
\[ T_{\text{eps}}(6,6) = x_{l3} \cdot x_{n1} + x_{l1} \cdot x_{n3} \]

\[ \text{! Calculate } T_{\text{eps}} \text{ transpose} \]
\[ T_{\text{eps}}_{\text{t}} = \text{Transpose}(T_{\text{eps}}) \]

\[ \text{! Calculate global stiffness matrix } D \]
\[ D = 0. \]
\[ D = \text{Matmul(}\text{Matmul}(T_{\text{eps}}_{\text{t}}, D_{\text{loc}}), T_{\text{eps}}) \]

\[ \text{Return} \]
\[ \text{End} \]

\[ \text{!----------------------------------------------------------------------!} \]

\[ \text{! Subroutine SPA} \]
\[ \text{! Stress point algorithm - Backward Euler method} \]
\[ \text{!----------------------------------------------------------------------!} \]

```fortran
Subroutine SPA(Props, Sig0, StVar0, dEps, D, Sig, StVar, Ctrl, dtime, iel, Int, nlflag)
    Implicit Double Precision (A-H, O-Z)
    ! Arguments
    Dimension Props(*), Sig0(6), StVar0(7), dEps(6), D, Sig, StVar,
    Ctrl, dtime, iel, Int, nlflag)
    ! Implicit Double Precision (A-H, O-Z)
    ! Arguments
    Dimension Props(*), Sig0(6), StVar0(7), dEps(6), D, Sig, StVar,
    Ctrl, dtime, iel, Int, nlflag)
    ! Local variables
    Dimension dEpsp(6), dEpse(6), index(14), res(14), dFdSig(6)
    Dimension dFdepshis(6), dGdSig(6), dSig(6), dStVar(7), csr(6)
    Dimension dcsrdepshis2(6), depshis2dEps(6)
    Dimension d2GdSig2(6,6), d2Gdsigdepshis(6,6), dcsrdsig(6,6)
```

\[ \text{Return} \]
\[ \text{End} \]

\[ \text{!----------------------------------------------------------------------!} \]
Dimension xJac(14,14)

! Parameters

  tol1 = Ctrl(1)
  nNRmax = Ctrl(2)
  eta = Props(26)
  patm = Props(34)
  xNN = Props(25)

! Elastic trial

dSig = Matmul(D,dEps)
Do i=1,6
  Sig = Sig0 + dSig
End do

! Check yield criterion and calculate plastic parameters (if applicable)

  Call HMC(Props, Sig, StVar0, F, dFdSig, dfdepshis, dGdSig,
  .  d2GdSig2, d2Gdsigdepshis, dFdlamb, Ctrl, dtime, iel,
  .  Int, nlflag)

! Calculate creep strain rates and its derivatives (if applicable)

  Call Creep_st(Props, Sig, StVar0, F, dtime, csr, dcsrdsig,
  .  dcsrdepshis2, depshis2dEpsc)

! Calculate Jacobian

dlamb = 0.
  dStVar = 0.
  Call Jacobian(D, dFdSig, dfdepshis, dGdSig, d2GdSig2,
  .  d2Gdsigdepshis, dlamb, dFdlamb, dtime, csr,
  .  dcsrdsig, dcsrdepshis2, dEpsc, xJac,
  .  Props, F)

! Calculate opposite of residuals

  res = 0.
Do i=1,6
  dEpse(i) = dEps(i)-dtime*csr(i)
End do
  res(1:6) = matmul(D,dEpse)
Do i=1,6
  res(i) = res(i)-dSig(i)
  res(i+6) = dtime*csr(i)
End do
Do i=1,6
  res(13) = res(13)+depshis2dEpsc(i)*dtime*csr(i)
End do
  res(14) = -F

! Start Newton-Raphson iterations

  nNR = 0
  Ctrl(3)= 0
  aux1 = toll+toll
  Do while((aux1 .gt. toll) .or. (aux2 .gt. toll)) .or.
    .  (aux3 .gt. toll) .or. (aux4.gt.toll))
  nNR = nNR+1
If (nNR .Gt. nNRmax) Then
  Ctrl(3) = 1
  Return
End if

! Calculate corrections

  Call ludcmp(xJac, 14, indx, dd)
Call Lubksb(xJac, 14, indx, res)

! Update variables
Do i=1,6
   dSig(i) = dSig(i)+res(i)
   Sig(i) = Sig(i)+res(i)
End do
Do i=1,7
   dStVar(i) = dStVar(i)+res(i+6)
   StVar(i) = StVar0(i)+dStVar(i)
End do
dlamb = dlamb+res(14)

! Calculate plastic parameters
Call HMC(Props, Sig, StVar, F, dFdSig, dFdepshis, dGdSig,
   d2GdSig2, d2Gdsigdepshis, dFdlamb, Ctrl, dtime, iel,
   Int, niflag)

! Calculate creep strain rates and its derivatives
Call Creep_st(Props, Sig, StVar, F, dtime, csr, dcsrdsig,
   dcsrdepshis2, depshis2dEpse)

! Calculate Jacobian
Call Jacobian(D, dFdSig, dFdepshis, dGdSig, d2GdSig2,
   d2Gdsigdepshis, dlamb, dFdlamb, dtime, csr,
   dcsrdsig, dcsrdepshis2, depshis2dEpse, xJac,
   Props, F)

! Calculate opposite of residuals
Do i=1,6
   dEpsp(i) = dGdSig(i)*dlamb
   dEpse(i) = dEps(i)-dEpsp(i)-dtime*csr(i)
End do
res(1:6) = matmul(D,dEpse)
Do i=1,6
   res(i) = res(i)-dSig(i)
End do
Do i=1,6
   res(i+6) = dEpsp(i)+dtime*csr(i)-dStVar(i)
End do
res(13) = -dStVar(7)
Do i=1,6
   res(13) = res(13)+depshis2dEpsc(i)*dtime*csr(i)
End do
res(14) = -F+dlamb*eta/dtime/((F/patm)**xNN)
If (Abs(F) .lt. tol1) res(14) = 0.
If (dlamb .lt. 0.) dlamb = 0.

! Check convergence
aux1 = 0.
aux2 = 0.
Do i=1,6
   aux1 = aux1+res(i)**2
   aux2 = aux2+res(i+6)**2
End do
aux1 = Sqrt(aux1)
aux2 = Sqrt(aux2)
aux3 = Abs(res(13))
aux4 = Abs(res(14))

! End Newton-Raphson iterations
End do
Subroutine Jacobian

Calculates the Jacobian matrix for the Newton-Raphson method.

Subroutine Jacobian(D, dFdSig, dDepshis, dGdSig, d2GdSig2, dcsr.
d2Gdsigdepshis, dlamb, dFdlamb, dtime, csr, dcrsdsig, dcsrdepshis2, depshis2dEpsc, xJac, Props, F)

Implicit Double Precision (A-H,O-Z)

Arguments
Dimension dFdSig(6), dDepshis(6), dGdSig(6), csr(6)
Dimension dcsrdepshis2(6), depshis2dEpsc(6)
Dimension D(6,6), d2Gdsig2(6,6), d2Gdsigdepshis(6,6)
Dimension dcsrdsig(6,6), xJac(14,14)
Dimension Props(*)

Local variables
Dimension aux1(6,6)

Initialise variables
xJac = 0.

Parameters
eta = Props(26)
patm = Props(34)
xNN = Props(25)

Calculation of drsigdsig
Do i=1,6
    Do j=1,6
        aux1(i,j) = dlamb*d2Gdsig2(i,j)+dtime*dcsrdsig(i,j)
    End do
End do

Calculation of drsigdxi
xJac(1:6,7:12) = Matmul(D, aux1)
Do i=1,6
    xJac(i,7:12) = xJac(i,7:12) + aux1(i,7:12)
End do

Calculation of drsigdlamb
xJac(1:6,14) = Matmul(D,dGdSig)

! Calculation of drxidsig
Do i=1,6
Do j=1,6
   xJac(i+6,j) = -dlamb*d2GdSig2(i,j)-dtime*dcsrdsig(i,j)
End do
End do

! Calculation of drxidxi
Do i=1,6
Do j=1,6
   xJac(i+6,j+6) = -dlamb*d2Gdsigdepshis(i,j)
End do
End do
Do i=1,6
   xJac(i+6,i+6) = 1.+xJac(i+6,i+6)
End do

! Calculation of drxidxi2
Do i=1,6
   xJac(i+6,13) = -dtime*dcsrdepshis2(i)
End do

! Calculation of drxidlamb
Do i=1,6
   xJac(i+6,14) = -dGdSig(i)
End do

! Calculation of drxi2dsig
xJac(13,1:6) = Matmul(depshis2dEpsh, dcsrdsig)
Do i=1,6
   xJac(13,i) = -dtime*xJac(13,i)
End do

! Calculation of drxi2dxj = 0
!drxi2dxj = 0

! Calculation of drxi2dxj2
Do i=1,6
   xJac(13,13) = xJac(13,13)+depshis2dEpsh(i)*dcsrdepshis2(i)
End do
xJac(13,13) = 1.-dtime*xJac(13,13)

! Calculation of drxi2dxi = 0
!drxi2dxi = 0

! Calculation of drxi2dxj2

! Calculation of dF/2dF = 1.+xNN*eta*dlamb/dtime/patm/((F/patm)**(xNN+1.))
If (F .Eq. 0.) dF2dF = 0.
Do j=1,6
   xJac(14,j) = dF2dF*dFdsig(j)
End do

! Calculation of dF/2dxi
Do j=1,6
   xJac(14,j+6) = dF2dF*dFdepshis(j)
End do

! Calculation of dF/2dxi2
!dFdxj2 = 0
Calculation of $dF/d\lambda$

\[
x_{Jac}(14,14) = -\eta/d_{time}/((F/p_{atm})^{xNN})
\]

If $F = 0.$

\[
x_{Jac}(14,14) = 1.
\]

Return

End

!----------------------------------------------------------------------!

! Subroutine HMC !
! Hyperbolic Mohr-Coulomb - Verification of the yield condition and !
! calculation of plastic parameters !
!----------------------------------------------------------------------!

Subroutine HMC(Props, Sig, epshis, F, dFdSig, dFdepshis, dGdSig,
.
.  d2GdSig2, d2Gdsigdepshis, dFdlamb, Ctrl, dtime,
.
.  iel, Int, niflag)

Implicit Double Precision (A-H,O-Z)

! Arguments

Dimension Props(*), Sig(6), epshis(7), dFdSig(6), dFdepshis(6)
Dimension dGdSig(6), Ctrl(3)
Dimension d2GdSig2(6,6), d2Gdsigdepshis(6,6)

! Local variables

Dimension dev(6), aux(6), dpdsig(6), dxJ2dsig(6), dxJ3dsig(6)
Dimension dthetadsig(6), d2Fdpdsig(6), d2FxJ2dsig(6)
Dimension dphidsig(6), dcohdsig(6), dptdsig(6)
Dimension dphidepshis(6), dcohdepshis(6), dptdepshis(6)
Dimension d2FdF2dsig(6), d2F2dthetadsig(6), d2F2dthetadsig(6)
Dimension d2Fdp2phidsig(6), d2Fdcohdsig(6), d2Fdptdsig(6)
Dimension d2Fdpdepshis(6), d2FxJ2depshis(6), d2FdF2depshis(6)
Dimension d2F2depshis(6), d2F2dcohdepshis(6), d2F2dptdepshis(6)
Dimension domegasig(6), auxvol(6), domegaphidsig(6)
Dimension domegacohdsig(6), dzetadsig(6), dzetadepshis(6)
Dimension domegacohdsig(6), domeg2dsig(6), domeg2depshis(6)
Dimension d2xJ2dsig2(6,6), d2xJ3dsig2(6,6), d2thetadsig2(6,6)
Dimension d2phidsig2(6,6), d2cohdsig2(6,6), d2ptdsig2(6,6)
Dimension d2thphidsigdepshis(6,6), d2cohdsigdepshis(6,6)
Dimension d2ptdsigdepshis(6,6), dauxvoldepshis(6,6)

! Initialise variables

dFdSig = 0.
dFdepshis = 0.
dGdSig = 0.
d2GdSig2 = 0.
d2Gdsigdepshis = 0.
dFdlamb = 0.

! Parameters

pi = 3.141592653589793
alpha = Props(14) ! van Eekelen (1980)
beta = 0.85*sqrt(alpha) ! van Eekelen (1980)
xN = -0.229 ! van Eekelen (1980)
toll = Ctrl(1)
tksil = Props(16)
tphipeak = tan(Props(9)*pi/180.)
tphires = tan(Props(10)*pi/180.)
omega = Props(15)
eta = Props(26)

!omegaphi_90
!omegaphi_crit
!xphi
omegacoh_90 = Props(21)
omegacoh_crit = Props(22)
xcOH = Props(24)
delta_crit = Props(23)

! Stress invariants and its derivatives
Call Stress_inva(Sig, dev, aux, p, xJ, xJ2, xJ3, theta)
Call Stress_inva_dev(Sig, dev, aux, p, xJ, xJ2, xJ3, theta, dpdsig, dxJ2dsig, dxJ3dsig, dthetadsig)
Call Stress_inva_2dev(Sig, dev, aux, p, xJ, xJ2, xJ3, theta, dpdsig, dxJ2dsig, dxJ3dsig, dthetadsig, d2xJ2dsig2, d2xJ3dsig2, d2thetadsig2)

! Strength parameters and derivatives of evolution laws
Call Mob_strg(Props, epshis, p, dpdsig, tphi, coh, pt, dtphidsig, dcohdsig, dptdsig, d2tphidsig2, d2cohdsig2, d2ptdsig2, iel, Int, nlflag, epseq2)

! Strength anisotropy variables
!Call Fomega(xnphi, omegaphi_90, omegaphi_crit, delta_crit, Props, Sig, omegaphi)
omegaphi = 1.0
Call Fomega(xncoh, omegacoh_90, omegacoh_crit, delta_crit, Props, Sig, omegacoh)

! Yield condition
aux1 = 3.*theta
aux2 = omegacoh*coh+omegacoh*pt*omegaphi*tphi
aux3 = aux2**2
F2 = alpha*(1.+beta*sin(aux1))**xN
F = -(omegacoh*coh+p*omegaphi*tphi)+sqrt(xJ2/F2+aux3)
If (F .lt. -tol1) Then
F = 0.
dFdlamb = 1.
Return
End if

! Strength anisotropy variables derivatives
!Call Fomega_dev(xnphi, omegaphi_90, omegaphi_crit, delta_crit, Props, Sig, omegaphi)
domegaphidsig = 0.0
Call Fomega_dev(xncoh, omegacoh_90, omegacoh_crit, delta_crit, Props, Sig, omegacoh)

! Derivative of the yield function with respect to stresses
dFdp = -omegaphi*tphi
dFDxJ2 = 1./(2.*F2*sqrt(aux3+(xJ2/F2)))
dFDF2 = -xJ2/(2.*F2**2*sqrt(aux3+(xJ2/F2)))
dF2dtheta = 3.*beta*alpha*xN*cos(aux1)*((beta*sin(aux1)+1.)*xN-1.)
dFdtphi = omegacoh*pt*omegaphi+aux2/sqrt(aux3+(xJ2/F2))-p*
          omegaphi
\[
dFdcoh = \omega_{coh}*(\omega_{coh}\cdot coh + \omega_{coh}\cdot pt\cdot \omega_{phi}\cdot tphi)/\sqrt{aux3+(xJ2/F2)} - \omega_{coh}
\]
\[
dFpt = \omega_{coh} \cdot \omega_{phi} \cdot tphi \cdot aux2/sqrt(aux3+(xJ2/F2))
\]
\[
dF domegaphi = (coh+pt\cdot \omega_{phi}\cdot tphi)\cdot aux2/sqrt(aux3+(xJ2/F2)) - coh
\]
\[
\text{Do } i=1,6
\]
\[
dFdSig(i) = dFdp\cdot dpdsig(i)+dFdxJ2\cdot dxJ2dsig(i)+dFdF2\cdot dF2dtheta\cdot dthetadsig(i)+dFdphi\cdot dtphidsig(i)+dFdcoh\cdot dcohdsig(i)+dFdpt\cdot dptdsig(i)+dFdomegaphi\cdot domegaphidsig(i)
\]
\[
\text{End do}
\]
\[
\text{Derivative of the yield function with respect to history variable}
\]
\[
\text{Do } i=1,6
\]
\[
dFdepshis(i) = dFdtphi\cdot dtphidepshis(i)+dFdcoh\cdot dcohdepshis(i)+dFdpt\cdot dptdepshis(i)
\]
\[
\text{End do}
\]
\[
\text{Derivative of the yield function with respect to the plastic multiplier}
\]
\[
dFdlamb = -\eta/dtime
\]
\[
\text{Non-associativity function - dependency with the mean stress}
\]
\[
\text{If } ((p+xJ/sqrt(3.)) \Lt. 0.) \text{ Then}
\]
\[
\text{omega} = 1.
\]
\[
\text{End if}
\]
\[
\text{Else if } ((p+xJ/sqrt(3.)) \Lt. (pnodil+xJ/sqrt(3.))) \text{ Then}
\]
\[
\text{omega} = 0.5*((1.+omegares)+(1.-omegares)*cos(pi*(p+xJ/sqrt(3.))/sqrt(3.)))/sqrt(3.))
\]
\[
\text{domegadp} = pi*sin(pi*(p+xJ/sqrt(3.))/sqrt(3.))/(pnodil+xJ*sqr(sqrt(3.)))*sqrt(3.3.)
\]
\[
\text{domegadxJ2} = sin(pi*(p+xJ/sqrt(3.)))*sqrt(3.)/sqrt(3.)*sqrt(3.)/sqrt(3.3.)
\]
\[
\text{Else}
\]
\[
\text{omega} = omegares
\]
\[
\text{domegadp} = 0.
\]
\[
\text{End if}
\]
\[
\text{Do } i=1,6
\]
\[
\text{domegadsig(i) = domegadp\cdot dpdsig(i)+domegadxJ2\cdot dxJ2dsig(i)}
\]
\[
\text{End do}
\]
\[
\text{Do } i=1,6
\]
\[
\text{domega2dsig(i) = zeta \cdot domegadsig(i) + omega \cdot dzetadsig(i) + dzetadepshis(i) \cdot dtphidesig(i) + dzetadepshis(i) \cdot domegaphis(i)}
\]
\[
\text{End do}
\]
\[
\text{Non-associativity function - critical state}
\]
\[
\text{If } (epseq2 \Lt. xksil) \text{ Then}
\]
\[
\text{zeta} = 1.
\]
\[
\text{Else}
\]
\[
\text{zeta} = (tphi-tphires)/(tphipeak-tphires)
\]
\[
\text{dzetadepshis(i) = dzetadepshis(i)}
\]
\[
\text{End if}
\]
\[
\text{Do } i=1,6
\]
\[
\text{domegad2dsig(i) = zeta \cdot domegadsig(i) + omega \cdot dzetadsig(i) + domegad2dsig(i) \cdot domegadeps2(i) + omega \cdot dzetadepshis(i)}
\]
\[
\text{End do}
\]
\[
\text{End do}
\]
\begin{verbatim}
1078  omega2 = omega
1079  Do i=1,6
1080     domega2dsig(i) = 0.
1081     domega2depshis(i) = 0.
1082  End do
1083
1084 ! Derivative of the plastic potential with respect to stresses
1085  aux2 = coh+pt*tphi
1086  aux3 = aux2**2
1087  aux4 = aux3+(xJ2/F2)
1088  dFdp = -tphi
1089  dFxJ2 = 1./2.*F2*sqrt(aux3+(xJ2/F2))
1090  dFdepshis = -xJ2/(2.*F2*aux2*sqrt(aux3+(xJ2/F2)))
1091  dF2dsig = xJ2*aux4/(aux3+(xJ2/F2))
1092
1093  auxvol(i) = dFdp*dpdsig(i)+dFdepshis*dtphidsig(i)+
1094     dF2dsig(i)*aux2dsig(i)
1095  dGdSig(i) = omega2*auxvol(i)+dFdxJ2*dxJ2dsig(i)+
1096     dF2dtheta*dxJ2dsig(i)
1097  End do
1098
1099 ! Second derivative of the plastic potential with respect to stresses
1100  d2FdxJ22 = -1./(4.*F2**2*aux4**(3./2.))
1101  d2FdxJ2dF2 = xJ2/(4.*F2**3*aux4**(3./2.))-1./(2.*F2**2*
1102     sqrt(aux4))
1103  d2FdF22 = xJ2/(F2**3*sqrt(aux4))-xJ2**2/(4.*F2**4*aux4**
1104     (3./2.))
1105  d2F2dtheta2 = 9.*beta**2*alpha*xN*(cos(aux1))**2*(xN-1.)*
1106     (beta*sin(aux1)+1.)*((xN-2.)-9.*beta*alpha*xN*
1107     sin(aux1)}(beta*sin(aux1)+1.)*((xN-1.)
1108  d2Fdtphidp = -1.
1109  d2FdtphidxJ2 = -pt*aux2/2./F2/(aux3+(xJ2/F2))+aux2*sqrt(aux4))
1110  d2FdtphidF2 = xJ2*pt*aux2/2./F2*aux3+(xJ2/F2))**2/*(xJ2/F2)**(3./2.)
1111
1112 Do i=1,6
1113     d2Fdpdsig(i) = dFdepshis*dtphidsig(i)+dF2dsig(i)*aux2dsig(i)
1114 End do
\end{verbatim}
. d2FdF2dsig(i) = d2FdF22 *dF2dtheta*dthetadsig(i)+d2FdxJ2dF2* dxJ2dsig(i)+d2FdphidF2*dphidsig(i)+
  . dFdcohdF2*dcohdsig(i)+d2FdptdF2*dptdsig(i)
  . d2Fd2thetadsig(i) = d2Fd2thetah2*dthetadsig(i)
  . d2Fdthetadsig(i) = d2FdF2*d2F2dthetadsig(i)+dF2d2theta*
  . d2Fd2Sig(i) = d2Fd2Sig(l)
  . d2Fdphidbsig(i) = d2Fdphidp*dpdsig(i)+d2FdphidxJ2*
  . dxJ2dsig(i)+d2FdphidF2*dphidsig(i)+
  . d2dtphidsig(i) + d2Fdtphidpt*
  . dptdsig(i)
  . d2Fdtphidbsig(i) = d2Fdtphidp*dpdsig(i)+d2FdphidxJ2*
  . dFdxJ2dbsig(i)+d2FdphidF2*dphidsig(i)+
  . d2Fdtphidbsig(i) + d2Fdtphidpt*
  . dptdsig(i)
  . d2Fdtphidbsig(i) = d2Fdtphidp*dpdsig(i)+d2FdphidxJ2*
  . d2Fdphidbsig(i) + d2Fdtphidpt*
  . dptdsig(i)
  . d2Fdcohdbsig(i) = d2Fdcohdp*dpdsig(i)+d2FdcohdxJ2*dxJ2dsig(i)+
  . d2Fc2ohdcoh*cohdbsig(i)+d2Fdcohdpt*  
  . d2Fdcohdbsig(i) + d2Fdcohdpt*
  . dptdsig(i)
  . d2Fdptdsig(i) = d2Fdptdp*dpdsig(i)+d2FdptdxJ2*dxJ2dsig(i)+
  . d2Fdptdbsig(i) + d2Fdpt2*dptdsig(i)
  . dptdsig(i)

End do

Do i=1,6  
  Do j=1,6
  dauxvoldsig(i,j) = dpdsig(i)*d2Fdpdsig(j)+
  . dFdtphi+d2tphidsig2(i,j)+dphidsig(i)+
  . d2Fdtphidbsig(j)+d2Fc2ohdbsig2(i,j)+
  . dcohdbsig(i)+d2Fc2ohdbsig(i)+dFdtphi*
  . d2ptdsig2(i,j)+dptdsig(i)*d2Fdptdsig(j)
End do

End do

Do i=1,6  
  Do j=1,6
  d2Gdsig2(i,j) = omega2*dauxvoldsig(i,j)+auxvol(i)*domega2dsig(j)+
  . dFdxJ2+d2xJ2dsig2(i,j)+dxJ2dsig(i)+
  . d2Fd2sig2(i,j)+d2Fd2theta*
End do

End do

End do

Do i=1,6
  d2Fdpdeph(i) = d2Fdphidp*dphideph(i)
End do

Do i=1,6
  d2FdxJ2deph(i) = d2FdphidxJ2*dphideph(i)+d2FdcohdxJ2*
End do

Do i=1,6
  d2FdF2deph(i) = d2FdphidF2*dphideph(i)+d2FdcohdF2*
End do

Do i=1,6
  d2Fdphideph(i) = d2Fdphidp*dphideph(i)+d2FdphidxJ2*
End do

Do i=1,6
  d2Fc2oheph(i) = d2Fcohdh2*dcoheph(i)+d2Fcohdpt*
End do

Do i=1,6
  d2Fdptdeph(i) = d2Fdphidp*dphideph(i)+d2Fdcohdp*
End do

Do i=1,6  
  Do j=1,6
  dauxvoldeph(i,j) = dpdsig(i)*d2Fdpdeph(j)+dFdtphi*
End do

Do i=1,6
  d2Fdtphideph(i) = d2Fdtphidp*dphideph(i)+d2Fdtphidpt*
End do

End do
APPENDICES

1200 .
1201 .
1202 .
1203 .
1204 End do
1205 End do
1206 Do i=1,6
1207 Do j=1,6
1208 d2Gdsigdepshis(i,j) = omega2*dauxvoldepshis(i,j)+auxvol(i)**
1209 domegadepshis(j)+dxJ2dsig(i) *
1210 d2FdxJ2depshis(j)+dF2dtheta *
1211 dthetadsig(i)*d2FdF2depshis(j)
1212 End do
1213 End do
1214 Return
1215 End
1216
1217 !----------------------------------------------------------------------!
1218 ! Subroutine Mob_strg !
1219 ! Mobilised strength parameters and derivatives of evolution laws !
1220 !----------------------------------------------------------------------!
1221 Subroutine Mob_strg(Props, epshis, p, dpdsig, tphi, coh, pt,
1222 . dtphidsig, dcohdsig, dptdsig, d2tphidsig2,
1223 . d2cohdsig2, d2ptdsig2, dthphidepshis,
1224 . dcohdepshis, dptdepshis, d2tphidsigdepshis,
1225 . d2cohdsigdepshis, d2ptdsigdepshis, iel, Int,
1226 . d2tphidsigdepshis, d2cohdsigdepshis, d2ptdsigdepshis)
1227 Implicit Double Precision (A-H,O-Z)
1228 ! Arguments
1229 Dimension Props(*), epshis(7), dpdsig(6), dtphidsig(6)
1230 Dimension dcohdsig(6), dptdsig(6), dthphidepshis(6)
1231 Dimension dcohdepshis(6), dptdepshis(6)
1232 Dimension d2tphidsig2(6,6), d2cohdsig2(6,6), d2ptdsig2(6,6)
1233 Dimension d2tphidsigdepshis(6,6), d2cohdsigdepshis(6,6)
1234 Dimension d2ptdsigdepshis(6,6)
1235 ! Local variables
1236 ! Parameters
1237 pi = 3.141592653589793
1238 xksi1 = Props(16)
1239 xm = Props(17)
1240 patm = Props(34)
1241 a = Props(18)
1242 b = Props(20)
1243 b2 = Props(19)
1244 tphiini = tan(Props(8)*pi/180.)
1245 tphipeak = tan(Props(9)*pi/180.)
1246 tphires = tan(Props(10)*pi/180.)
cini = Props(11)
ptini = -Props(12)
r_post = Props(13)
zero = 1.e-10
naux3 = 0

! Standard weak element
If ((Props(33) .Ne. 0) .And. (iel .Eq. Props(33))) Then
tphiini = tan(Props(8) *pi/180.)*0.20
tphipeak = tan(Props(9) *pi/180.)*0.20
tphires = tan(Props(10) *pi/180.)*0.20
cini = Props(11)*0.20
ptini = -Props(12)*0.20
End if

! Given strength distribution
If (Props(33) .Eq. -1) Then
Read(3,Rec=iel) naux1
naux2 = naux1+(Int-1)
Read(10,Rec=naux2) strg_factor
cini = Props(11) *strg_factor
ptini = -Props(12)*strg_factor
End if

! Stress dependent history variable
epseq = sqrt(epshis(1)**2+epshis(2)**2+epshis(3)**2
   +0.5*epshis(4)**2+0.5*epshis(5)**2+0.5*epshis(6)**2)
pp = p
If (pp .Le. 0.) pp = 0.
epseq2 = epseq/(1+(pp/patm)**2+xm**2)
If ((nlflag .Eq. 1) .And. (epseq2 .Ge. xksi1)) Then
Read(3,Rec=iel) naux1
naux2 = naux1+(Int-1)
Read(8,Rec=naux2) epseq
epseq2 = epseq/(1+(pp/patm)**2+xm**2)
aux3 = 1
End if
If (epseq2 .Lt. xksi1) Then
depseq2dp = -2.*xm**2*pp*epseq/patm**2/((xm**2*pp**2/patm**2)+1.)
   .**2
d2epseq2dp2 = 8.*xm**4*pp**2*epseq/patm**4/((xm**2*pp**2/patm**2)
   .+1.)*3-2.*xm**2*epseq/patm**2/((xm**2*pp**2/patm**2)
   .2)+1.)***2
depseq2depseq = 1./((xm**2*pp**2/patm**2)+1.)
If (naux3 .Eq. 1) depseq2depseq = 0.
d2epseq2ddepseq = -2.*xm**2*pp/patm**2/((xm**2*pp**2/patm**2)+1.)
   .**2
If (naux3 .Eq. 1) d2epseq2ddepseq = 0.
Else
epseq2 = epseq-xksi1*(pp/patm)**2*xm**2
depseq2dp = -2.*xm**2*pp*xksi1/patm**2
d2epseq2dp2 = -2.*xm**2*xksi1/patm**2
depseq2ddepseq = 1.
If (naux3 .Eq. 1) depseq2ddepseq = 0.
d2epseq2ddepseq = 0.
End If
Do i=1,3
depseq2dpsig(i) = d2epseq2dp2*dpsig(i)
depseqdpephish(i) = epshis(i)/epseq
If(epseq.Gt.-zero).And.(epseq.Lt.zero) depseqdpephish(i) = 0.
depseq2dpephish(i) = depseq2ddepseq*depseqdpephish(i)
\[ d2epseq2dpdepshis(i) = d2epseq2dpdepseq*depseqdepshis(i) \]
End do

Do i=4,6
\[ \text{depseq2dpdsig}(i) = d2epseq2dp2*dpdsig(i) \]
\[ \text{depseqdepshis}(i) = \frac{epshis(i)}{2.*epseq} \]
If((epseq.Gt.-zero).And.(epseq.Lt.zero)) depseqdepshis(i) = 0.
\[ \text{depseq2depshis}(i) = \text{depseq2depseq} * \text{depseqdepshis}(i) \]
\[ d2epseq2dpdepshis(i) = d2epseq2dpdepseq * \text{depseqdepshis}(i) \]
End do

! Friction angle evolution and its derivatives
If (epseq2 .Lt. xksi1) Then
\[ \text{deltaphi} = \frac{xksi1}{(xksi1/(\text{tphipeak}-\text{tphiini}))-a} \]
\[ \text{tphi} = \text{tphiini} + \text{epseq2}/(a+\text{epseq2}/\text{deltaphi}) \]
\[ \text{dtphidepseq2} = 1.((a+\text{epseq2}/\text{deltaphi}))-\text{epseq2}/\text{deltaphi}/ \]
\[ \text{d2tphidepseq22} = \frac{2.*\text{epseq2}}{((a+\text{epseq2}/\text{deltaphi})**2)} \]
End if

Else
\[ \text{tphi} = \text{tphipeak}-(\text{tphipeak}-\text{tphires})*(1.-\exp\left(-b*\text{epseq2}-xksi1\right)) \]
\[ \text{dtphidepseq2} = b*\exp\left(b*(xksi1-\text{epseq2})\right) \]
\[ \text{d2tphidepseq22} = -b**2*\exp\left(b*(xksi1-\text{epseq2})\right) \]
End if

! Cohesion evolution and its derivatives
If (epseq2 .Lt. xksi1) Then
\[ \text{coh} = \text{cini} \]
\[ \text{dcohdepseq2} = 0. \]
\[ \text{d2cohdepseq22} = 0. \]
Else
\[ \text{cpost} = \text{cini}*r_post \]
\[ \text{coh} = (\text{cini}-\text{cpost})\exp\left(-b*(\text{epseq2}-xksi1)\right) + cpost*\exp\left(-b* \right) \]
\[ \text{dcohdepseq2} = -b*\text{cpost}\exp\left(b*(xksi1-\text{epseq2})\right)-b2*(\text{cini}-\text{cpost})* \]
\[ \exp\left(b2*(xksi1-\text{epseq2})\right) \]
\[ \text{d2cohdepseq22} = b2**2*(\text{cini}-\text{cpost})\exp\left(b2*(xksi1-\text{epseq2})\right)+ \]
\[ b2**2*\text{cpost}\exp\left(b*(xksi1-\text{epseq2})\right) \]
End if

! Isotropic tensile strength strength and its derivatives
If (epseq2 .Lt. xksi1) Then
\[ \text{pt} = \text{ptini} \]
\[ \text{dptdepseq2} = 0. \]
\[ \text{d2ptdepseq22} = 0. \]
Else
\[ \text{ptpost} = \text{ptini}*r_post \]
\[ \text{pt} = (\text{ptini}-\text{ptpost})\exp\left(-b*(\text{epseq2}-xksi1)\right)+ \text{ptpost}\exp\left(-b* \right) \]
\[ \exp\left(\text{epseq2}-xksi1\right) \]
\[ \text{dptdepseq2} = -b*\text{ptpost}\exp\left(b*(\text{epseq2})\right)-b2*(\text{ptini}-\text{ptpost})* \]
\[ \exp\left(b2*(\text{epseq2})\right) \]
\[ \text{d2ptdepseq22} = b2**2*(\text{ptini}-\text{ptpost})\exp\left(b2*(\text{xksi1-epseq2})\right)+ \]
\[ b2**2*\text{ptpost}\exp\left(b*(\text{xksi1-epseq2})\right) \]
End if
! Derivative of strength parameters with respect to stresses
Do i=1,6
  dtphidsig(i) = dtphidepseq2*depseq2dp*dpdsig(i)
  dcohdsig(i) = dcohdepseq2*depseq2dp*dpdsig(i)
  dptdsig(i) = dptdepseq2*depseq2dp*dpdsig(i)
  d2tphidepseq2dsig(i) = d2tphidepseq22*depseq2dp*dpdsig(i)
  d2cohdepseq2dsig(i) = d2cohdepseq22*depseq2dp*dpdsig(i)
  d2ptdepseq2dsig(i) = d2ptdepseq22*depseq2dp*dpdsig(i)
End do
Do i=1,6
  Do j=1,6
    d2tphidsig2(i,j) = d2tphidepseq2dsig(i)*depseq2dp*dpdsig(j)+
                    depseq2dpdsig(i)*dtphidepseq2*dpdsig(j)
    d2cohdsig2(i,j) = d2cohdepseq2dsig(i)*depseq2dp*dpdsig(j)+
                    depseq2dpdsig(i)*dcohdepseq2*dpdsig(j)
    d2ptdsig2(i,j) = d2ptdepseq2dsig(i)*depseq2dp*dpdsig(j)+
                    depseq2dpdsig(i)*dptdepseq2*dpdsig(j)
  End do
End do

! Derivative of strength parameters with respect to history variable
Do i=1,6
  dtphidepshis(i) = dtphidepseq2*depseq2depshis(i)
  dcohdepshis(i) = dcohdepseq2*depseq2depshis(i)
  dptdepshis(i) = dptdepseq2*depseq2depshis(i)
  d2tphidepseq2depshis(i) = d2tphidepseq22*depseq2depshis(i)
  d2cohdepseq2depshis(i) = d2cohdepseq22*depseq2depshis(i)
  d2ptdepseq2depshis(i) = d2ptdepseq22*depseq2depshis(i)
End do
Do i=1,6
  Do j=1,6
    d2tphidsigdepshis(i,j) = depseq2dp*dpdsig(i)*
                           d2tphidepseq2depshis(j)+
                           depseq2dpdsig(i)*dtphidepseq2*dpdsig(j)
    d2cohdsigdepshis(i,j) = depseq2dp*dpdsig(i)*
                           d2cohdepseq2depshis(j)+
                           depseq2dpdsig(i)*dcohdepseq2*dpdsig(j)
    d2ptdsigdepshis(i,j) = depseq2dp*dpdsig(i)*
                           d2ptdepseq2depshis(j)+
                           depseq2dpdsig(i)*dptdepseq2*dpdsig(j)
  End do
End do

Return
End

!----------------------------------------------------------------------!

! Subroutine Creep_st
! Calculation of the creep strain rates and its derivatives
Subroutine Creep_st(Props, Sig, StVar, F, dtime, csr, dcsrdsig,
  dcsrdepshis2, depshis2dEpsc)
Implicit Double Precision (A-H,O-Z)
! Arguments
Dimension Props(*), Sig(6), StVar(7), csr(6), dcsrdepshis2(6)
Dimension depshis2dEpsc(6)
Dimension dcsrdsig(6,6)

! Local variables
Dimension dev(6), xIp(6), dEpsc(6)
Dimension xIdpdsig(6,6), ddevdsig(6,6)

! Initialise variables
epshis2 = StVar(7)
csr = 0.
dcsrdsig = 0.
dcsrdepshis2 = 0.
depshis2dEpsc = 0.

! Parameters
epseqmin = Props(30)
gama = Props(27)
psi = Props(28)
c = Props(29)

! Check if creep has been activated
epseq = sqrt((StVar(1)**2+StVar(2)**2+StVar(3)**2 +0.5*StVar(4)**2+0.5*StVar(5)**2+0.5*StVar(6)**2))
If ((epseq .Lt. epseqmin) .And. (epshis2 .Eq. 0.)) Return
If (gama .Eq. 0.) Return

! Identity matrix times invariant p
xIp = 0.
Do i=1,3
   xIp(i) = (Sig(1)+Sig(2)+Sig(3))/3.
End do

! Identity matrix times derivative of p with respect to stresses
xIdpdsig = 0.
Do i=1,3
   Do j=1,3
      xIdpdsig(i,j) = 1./3.
   End do
End do

! Deviatoric stress tensor
Do i=1,3
   dev(i) = Sig(i)-(Sig(1)+Sig(2)+Sig(3))/3.
End do
Do i=4,6
   dev(i) = Sig(i)
End do

! Derivative of the deviatoric stress tensor with respect to stresses
ddevdsig = 0.
Do i=1,3
   Do j=1,3
      ddevdsig(i,j) = -1./3.
   End do
End do
Do i=4,6
   ddevdsig(i,i) = 2./3.
End do
Do i=1,3
   ddevdsig(i,i) = 1.
! Creep strain rates
aux1 = gama*exp(-c*epshis2)
Do i=1,6
csr(i) = aux1*(dev(i)+psi*xIp(i))
End do
Do i=4,6
csr(i) = 2.*csr(i)
End do

! Derivative of creep strain rates with respect to stresses
Do i=1,6
Do j=1,6
dcsrdsig(i,j) = aux1*(ddevdsig(i,j)+psi*xIdpdsig(i,j))
End do
End do
Do i=4,6
dcsrdsig(i,i) = 2.*dcsrdsig(i,i)
End do

! Derivative of creep strain rates with respect to the creep history variable
Do i=1,6
dcsrdepshis2(i) = -c*aux1*(dev(i)+psi*xIp(i))
End do
Do i=4,6
dcsrdepshis2(i) = 2.*dcsrdepshis2(i)
End do

! Derivative of creep history variable with respect to creep strains
Do i=1,6
dEpsc(i) = csr(i)*dtime
End do
aux2 = sqrt((dEpsc(1)**2+dEpsc(2)**2+dEpsc(3)**2+0.5*dEpsc(4)**2+0.5*dEpsc(5)**2+0.5*dEpsc(6)**2))
Do i=1,3
depshis2dEpsc(i) = dEpsc(i)/aux2
End do
Do i=4,6
depshis2dEpsc(i) = dEpsc(i)/2./aux2
End do

Return
End

!----------------------------------------------------------------------!

Subroutine Stress_inva !
Calculation of stress invariants !----------------------------------------------------------------------!

Subroutine Stress_inva(Sig, dev, aux, p, xJ, xJ2, xJ3, theta)
Implicit Double Precision (A-H,O-Z)
Arguments
Dimension Sig(*), dev(6), aux(6)
Parameters
zero = 1.e-10
! Invariant p
1566  p = (Sig(1)+Sig(2)+Sig(3))/3.

! Invariant xJ & xJ2
1570  Do i=1,3
1571     dev(i) = Sig(i)-p
1572     aux(i) = dev(i)*dev(i)
1573  End do
1574  Do i=4,6
1575     dev(i) = Sig(i)
1576     aux(i) = dev(i)*dev(i)
1577  End do
1578  xJ2 = 0.5*(aux(1)+aux(2)+aux(3))+aux(4)+aux(5)+aux(6)
1579  xJ = sqrt(xJ2)

! Invariant xJ3
1582  aux1 = dev(1)*dev(2)*dev(3)
1583  aux2 = 2*dev(4)*dev(5)*dev(6)
1584  aux3 = dev(1)*aux(5)+dev(2)*aux(6)+dev(3)*aux(4)
1585  xJ3 = aux1+aux2-aux3

! Invariant theta
1588  If (xJ .gt. zero) Then
1589     aux1 = -1.5*sqrt(3.)*xJ3/(xJ*xJ2)
1590  If (aux1 .lt. -1.) Then
1591     aux1 = -1.
1592  Elseif (aux1 .gt. 1.) Then
1593     aux1 = 1.
1594  End if
1595  theta = asin(aux1)/3.
1596  Else
1597     theta = 0.
1598  End if

! Identify volumetric loading
1600  If (xJ .Lt. zero) Then
1602  xJ = 0.
1603  xJ2 = 0.
1604  xJ3 = 0.
1605  End if
1606  Return
1607  End

!----------------------------------------------------------------------!
1610
!----------------------------------------------------------------------!

Subroutine Stress_inva_dev
1614  Calculation of derivatives of stress invariants
1618 !----------------------------------------------------------------------!
Subroutine Stress_inva_dev(Sig, dev, aux, p, xJ, xJ2, xJ3, theta,
1619     dpdsig, dxJ2dsig, dxJ3dsig, dthetadsig)
1621 ! Arguments
1622     Dimension Sig(*), dev(*), aux(*), dpdsig(6), dxJ2dsig(6)
1623     Dimension dxJ3dsig(6), dthetadsig(6)
1624 ! Parameters
1626     zero = 1.e-10
! Derivative of invariant $p$

\begin{verbatim}
1627 pi   = 3.141592653589793
1628
1629 ! Derivative of invariant $p$
1630 Do i=1,3
1631 dpdsig(i) = 1./3.
1632 End do
1633 Do i=4,6
1634 dpdsig(i) = 0.
1635 End do
1636
1637 ! Derivative of invariant $x_J^2$
1638 Do i=1,3
1639 dxJ2dsig(i) = dev(i)
1640 End do
1641 Do i=4,6
1642 dxJ2dsig(i) = 2.*dev(i)
1643 End do
1644
1645 ! Derivative of invariant $x_J^3$
1646 dxJ3dsig(1) = aux(1)+aux(4)+aux(6)-2.*xJ2/3.
1647 dxJ3dsig(2) = aux(4)+aux(2)+aux(5)-2.*xJ2/3.
1648 dxJ3dsig(3) = aux(6)+aux(5)+aux(3)-2.*xJ2/3.
1649 dxJ3dsig(4) = 2.*dev(1)*dev(4)+2.*dev(2)*dev(4)+2.*dev(5)*dev(6)
1650 dxJ3dsig(5) = 2.*dev(4)*dev(6)+2.*dev(2)*dev(5)+2.*dev(3)*dev(5)
1651 dxJ3dsig(6) = 2.*dev(1)*dev(6)+2.*dev(4)*dev(5)+2.*dev(3)*dev(6)
1652
1653 ! Derivative of invariant $\theta$
1654 theta3max = 89.9*pi/180.
1655 theta3min = -theta3max
1656 If (theta .gt. theta3max) Then
1657 theta3 = theta3max
1658 Else if (theta .lt. theta3min) Then
1659 theta3 = theta3min
1660 Else
1661 theta3 = 3.*theta
1662 End if
1663
1664 If (xJ .gt. zero) Then
1665 aux1 = -tan(theta3)/2./xJ**2
1666 aux2 = tan(theta3)/3./xJ3
1667 Do i=1,6
1668 dthetadsig(i) = aux1*dxJ2dsig(i)+aux2*dxJ3dsig(i)
1669 End do
1670 Else
1671 Do i=1,6
1672 dthetadsig(i) = 0.
1673 End do
1674 End if
1675
1676 ! Identify volumetric loading
1677 If (xJ .gt. zero) Then
1678 dxJ2dsig = 0.
1679 dxJ3dsig = 0.
1680 End if
1681 Return
1682 End
\end{verbatim}

Subroutine Stress_inva_2dev(Sig, dev, aux, p, xJ, xJ2, xJ3, theta,
                        dpdsig, dxJ2dsig, dxJ3dsig,
                        dthetadsig, d2xJ2dsig2, d2xJ3dsig2,
                        d2thetadsig2)

Implicit Double Precision (A-H,O-Z)

! Arguments
Dimension Sig(*), dev(*), aux(*), dpdsig(6), dxJ2dsig(6)
Dimension dxJ3dsig(6), dthetadsig(6)
Dimension d2xJ2dsig2(6,6), d2xJ3dsig2(6,6), d2thetadsig2(6,6)

! Local variables
Dimension A(6), B(6)

! Parameters
zero = 1.e-10
pi = 3.141592653589793

! Second derivate of p = 0
! Second derivative of xJ2
Do i=1,3
  Do j=1,3
    d2xJ2dsig2(i,j) = -1./3.
  End do
End do
Do i=1,3
  d2xJ2dsig2(i,i) = 2./3.
  d2xJ2dsig2(i+3,i+3) = 2.
End do

! Second derivative of xJ3
aux1 = 2./3.
aux2 = -4./3.
aux3 = -2.
aux4 = 2.

Do i=1,6
  d2xJ3dsig2(i,1) = aux1*dev(1)
  d2xJ3dsig2(i,2) = aux1*dev(3)
  d2xJ3dsig2(i,3) = aux1*dev(2)
  d2xJ3dsig2(i,4) = aux1*dev(4)
  d2xJ3dsig2(i,5) = aux2*dev(5)
  d2xJ3dsig2(i,6) = aux1*dev(6)
End do

Do i=1,3
  d2xJ3dsig2(i,i) = 2./3.
d2xJ3dsig2(i+3,i+3) = 2.
End do
do i=1,6
    do j=i+1,6
        d2xJ3dsig2(j,i)=d2xJ3dsig2(i,j)
    enddo
enddo

! Second derivative of invariant theta
theta3max = 89.9*pi/180.
theta3min = -theta3max
If (theta .gt. theta3max) Then
    theta3 = theta3max
Else if (theta .lt. theta3min) Then
    theta3 = theta3min
Else
    theta3 = 3.*theta
End if
If (xJ .gt. zero) Then
    aux1 = tan(theta3)
    aux2 = aux1*aux1
    Do i=1,6
        A(i) = -3.*(1.+aux2)*dthetadsig(i)/2./xJ2+aux1*dxJ2dsig(i)/2./
               xJ2**2
        B(i) = (1.+aux2)*dthetadsig(i)/xJ3-aux1*dxJ3dsig(i)/3./xJ3**2
    End do
    Do i=1,6
        Do j=1,6
            d2thetadsig2(i,j) = -aux1*d2xJ2dsig2(i,j)/2./xJ2+dxJ2dsig(i)/2./
                                xJ2**2
                                *A(i)+aux1*d2xJ3dsig2(i,j)/3./xJ3+
                                dxJ3dsig(j)*B(i)
        End do
    End do
Else
    d2thetadsig2=0
End if
!
Identify volumetric loading
If (xJ .Lt. zero) Then
    d2xJ2dsig2 = 0.
    d2xJ3dsig2 = 0.
End if
Return
End

!----------------------------------------------------------------------!

Subroutine ludcmp
LU decomposition of a square matrix [Press et al., 1992]

Subroutine ludcmp(a, n, indx, d)

Integer n, indx(n), NMAX
Real(8) d, a(n,n), TINY
Parameter (NMAX = 500,TINY = 1.0e-20)
Integer i, imax, j, k
Real(8) aamax, dum, sum, vv(NMAX)

d = 1.
Do i = 1,n
    Do j = 1,n
If (Abs(a(i,j)) .gt. aamax) aamax = Abs(a(i,j))
End do
If (aamax .eq. 0.) Then
  Call Ok_messagebox('Singular matrix in Ludcmp')
  Stop
End if
vv(i) = 1./aamax
End do
Do j = 1,n
  Do i = 1,j-1
    sum = a(i,j)
    Do k = 1,i-1
      sum = sum-a(i,k)*a(k,j)
    End do
    a(i,j) = sum
  End do
  aamax = 0.
  Do i = j,n
    sum = a(i,j)
    Do k = 1,j-1
      sum = sum-a(i,k)*a(k,j)
    End do
    a(i,j) = sum
dum = vv(i)*Abs(sum)
If (dum .ge. aamax) Then
  imax = i
  aamax = dum
End if
End do
If (j .ne. imax) Then
  Do k = 1,n
    dum = a(imax,k)
    a(imax,k) = a(j,k)
    a(j,k) = dum
  End do
d = -d
vv(imax) = vv(j)
End if
 indexed(j) = imax
If (a(j,j) .eq. 0.) a(j,j) = TINY
If (j .ne. n) Then
  dum = 1./a(j,j)
  Do i = j+1,n
    a(i,j) = a(i,j)*dum
  End do
End if
End do
End
!--------------------------------------------------------------------------------!
! Subroutine Lubksb !
! Solves the set of n linear equations A X = B from the results of !
! the LU decomposition [Press et al., 1992] !
!--------------------------------------------------------------------------------!
Subroutine Lubksb(a, n, indx, b)
Integer n, indx(n)
Real(8) a(n,n), b(n)
integer i, ii, j, ll
real(8) sum
ii = 0
do i = 1, n
ll = indx(i)
sum = b(ll)
b(ll) = b(i)
if (ii .ne. 0) then
  do j = ii, i-1
    sum = sum - a(i,j) * b(j)
  end do
else if (sum .ne. 0.) then
  ii = i
  end if
  b(i) = sum
end do
do i = n, 1, -1
sum = b(i)
doi = i+1, n
sum = sum - a(i,j) * b(j)
end do
b(i) = sum / a(i,i)
end do
return
end

!----------------------------------------------------------------------!

subroutine fomega
! Calculation of Omega that controls strength anisotropy
!----------------------------------------------------------------------!
subroutine fomega(xno, omega90, omegacrit, delcrit, props, sig, omega)
implicit double precision (a-h,o-z)
!
! arguments
dimension props(*), sig(6)
!
! parameters
pi = 3.141592653589793
if (omegacrit .eq. 1.) omegacrit = .99999
!
! auxiliary exponential functions
el = exp(45.*xno)
e2 = exp(deltcrit*xno)
e3 = exp(-45.*xno)
e4 = exp((-deltcrit-90.)*xno)
e5 = exp((deltcrit-90.)*xno)
!
! a, b, c constants
aux1 = 1./(e3+1.)-1./(el+1.)
aux2 = omegacrit*(omegacrit-1.)/(el+1.)
aux3 = aux1-1.
aux4 = aux2+aux1-1.
aux5 = aux3+(aux4-aux3)/(el+1.)/(el+1.)/(el+1.)/(el+1.)
!
$C = aux2/aux5$
B = (omega90+C*aux4-C*aux3-1.)/aux1
A = C*aux3-B/(e1+1.)+1.

! Angle delta
Call Delta(Props, Sig, adel)

! Factor omega
omega = A+B/(1.+exp((45.-adel)*xno))-C*exp((delcrit-adel)*xno)/
. (1.+exp((delcrit-adel)*xno))**2

Return
End

!----------------------------------------------------------------------!

Subroutine Fomega_dev
! First derivative of Omega with respect to stresses (central difference)
!----------------------------------------------------------------------!
Subroutine Fomega_dev(xno, omega90, omegacrit, delcrit, Props, Sig, domegadsig)

Implicit Double Precision (A-H,O-Z)

! Arguments
Dimension Props(*), Sig(6), domegadsig(6)

! Local variables
Dimension Sigh(6)
Dimension omegah(6,2)

! Optimum step size
h = epsilon(sig(1))**(1./3.)

! Function evaluations
Do i=1,6
Sigh = Sig
Sigh(i) = Sig(i)+h
Call Fomega(xno, omega90, omegacrit, delcrit, Props, Sigh, omega)
.
omegah(i,1) = omega
End do
Do i=1,6
Sigh = Sig
Sigh(i) = Sig(i)-h
Call Fomega(xno, omega90, omegacrit, delcrit, Props, Sigh, omega)
.
omegah(i,2) = omega
End do

! First derivative (central difference, 2 points)
Do i=1,6
domegadsig(i) = (omegah(i,1)-omegah(i,2))/2./h
End do

Return
End

!----------------------------------------------------------------------!
Subroutine Delta(Props, Sig, del)

Implicit Double Precision (A-H,O-Z)

! Arguments
Dimension Props(*), Sig(6)

! Local variables
Dimension xn(3), eval(3), v1(3)
Dimension Sig_T(3,3), R(3,3), Rz(3,3), Rx(3,3), evec(3,3)

! Initialise variables
R = 0.
Rz = 0.
Rx = 0.
xn = 0.
xn(3) = 1.

If (Props(40) .Eq. 1.) Then ! For 2D analyses
xn = 0.
xn(2) = 1.
End if

! Parameters
pi = 3.141592653589793
alpha = Props(6)*pi/180.
beta = Props(7)*pi/180.

! Rotation matrix
Rz(1,1) = cos(alpha)
Rz(2,2) = cos(alpha)
Rz(3,3) = 1.
Rz(1,2) = -sin(alpha)
Rz(2,1) = sin(alpha)
Rx(1,1) = 1.
Rx(2,2) = cos(beta)
Rx(3,3) = cos(beta)
Rx(2,3) = -sin(beta)
Rx(3,2) = sin(beta)
R = matmul(Rz,Rx)

! Normal to the isotropic plane
xn = matmul(R,xn)

! Major principal stress direction
Sig_T(1,1) = Sig(1)
Sig_T(2,2) = Sig(2)
Sig_T(3,3) = Sig(3)
Sig_T(1,2) = Sig(4)
Sig_T(2,3) = Sig(5)
Sig_T(1,3) = Sig(6)
Sig_T(2,1) = Sig(4)
Sig_T(3,2) = Sig(5)
Sig_T(3,1) = Sig(6)
Call Eigen(Sig_T, 3, 3, eval, evec, nrot)
Call Eigart(eval, evec, 3, 3)
If (Abs(eval(1)) .Gt. Abs(eval(3))) Then
   Do i=1,3
v1(i) = evec(i,1)
End do
Else
  Do i=1,3
    v1(i) = evec(i,3)
  End do
End if

! Angle delta
aux1 = abs(xn(1)*v1(1)+xn(2)*v1(2)+xn(3)*v1(3))
aux2 = sqrt(xn(1)**2+xn(2)**2+xn(3)**2)
aux3 = sqrt(v1(1)**2+v1(2)**2+v1(3)**2)
del = acos(aux1/aux2/aux3)*180./pi

Return
End

!----------------------------------------------------------------------!

! Subroutine Eigen !
! Calculates all eigenvalues and eigenvectors of a real symmetric !
!----------------------------------------------------------------------!

Subroutine Eigen(a,n,np,d,v,nrot)

Integer n,np,nrot,NMAX
Real(8) a(np,np),d(np),v(np,np)
Parameter (NMAX=500)
Integer i,ip,iq,j
Real(8) c,g,h,s,sm,t,tau,theta,tresh,b(NMAX),z(NMAX)

Do ip=1,n
  Do iq=1,n
    v(ip,iq) = 0.
  End do
  v(ip,ip) = 1.
End do
Do ip=1,n
  b(ip) = a(ip,ip)
  d(ip) = b(ip)
  z(ip) = 0.
End do
nrot = 0
Do i=1,50
  sm = 0.
  Do ip=1,n-1
    Do iq=ip+1,n
      g = 100.*Abs(a(ip,iq))
      If((i .Gt. 4) .And. (Abs(d(ip))+g .Eq. Abs(d(ip)))}
And. (Abs(d(iq)) + g . Eq. Abs(d(iq))) Then
a(ip, iq) = 0.
Else If(Abs(a(ip, iq)) . Gt. thresh) Then
h = d(iq) - d(ip)
If(Abs(h) + g . Eq. Abs(h)) Then
t = a(ip, iq) / h
Else
theta = 0.5 * h / a(ip, iq)
t = 1. / (Abs(theta) + Sqrt(1. + theta**2))
If(theta . Lt. 0.) t = -t
End if
c = 1. / Sqrt(1 + t**2)
s = t * c
tau = s / (1 + c)
h = t * a(ip, iq)
z(ip) = z(ip) - h
z(iq) = z(iq) + h
d(ip) = d(ip) - h
d(iq) = d(iq) + h
a(ip, iq) = 0.
Do j=1, ip-1
  g = a(j, ip)
  h = a(j, iq)
  a(j, ip) = g - s * (h + g * tau)
  a(j, iq) = h + s * (g - h * tau)
End do
Do j=ip+1, iq-1
  g = a(ip, j)
  h = a(j, iq)
  a(ip, j) = g - s * (h + g * tau)
  a(j, iq) = h + s * (g - h * tau)
End do
Do j=iq+1, n
  g = a(ip, j)
  h = a(iq, j)
  a(ip, j) = g - s * (h + g * tau)
  a(iq, j) = h + s * (g - h * tau)
End do
Do j=1, n
  g = v(j, ip)
  h = v(j, iq)
  v(j, ip) = g - s * (h + g * tau)
  v(j, iq) = h + s * (g - h * tau)
End do
End if
End do
End do
Do ip=1, n
b(ip) = b(ip) + z(ip)
d(ip) = b(ip)
z(ip) = 0.
End do
End do
Call Ok_messagebox(‘too many iterations in Eigen’)
Stop
Return
End
Subroutine Eigsrt

Subroutine eigsrt(d,v,n,np)

Integer n,np
Real(8) d(np),v(np,np)
Integer i,j,k
Real(8) p

Do i=1,n-1
  k = i
  p = d(i)
  Do j=i+1,n
    If(d(j) .Ge. p) Then
      k = j
      p = d(j)
    End if
  End do
  If(k .Ne. i) Then
    d(k) = d(i)
    d(i) = p
    Do j=1,n
      p = v(j,i)
      v(j,i) = v(j,k)
      v(j,k) = p
    End do
  End if
End do
Return
End

Subroutine Nonlocal1

Subroutine Nonlocal1(Props, iGauss)

Implicit Double Precision (A-H,O-Z)

! Arguments
Dimension Props(*)

! Local variables
Dimension ngp(5000)
Dimension ngpnl(5000,20000), radnl(5000,20000)
Double precision, Allocatable, Dimension(:, :) :: afile1

! Allocate memory
Allocate (afile1(4,iGauss), STAT=istat)
If (istat .Ne. 0) Then
  Call Ok_messagebox('Error: not enough memory')
  Stop
End if

! Parameters
plength = Props(32)
radius = plength*2.

! Read Gauss points information
Do i=1,igauss
   Read(2,Rec=i) afile1(1,i),afile1(2,i),afile1(3,i),afile1(4,i)
End do

! Find points within the interaction radius and create required files
ibegin = 1
iend = 5000
Do while (ibegin .Le. iGauss)
   ngp = 0
   radnl = 0
   ngpnl = 0
   Do i=ibegin,iend
      ipos = i-ibegin+1
      X = afile1(1,i)
      Y = afile1(2,i)
      Z = afile1(3,i)
      StVar0 = afile1(4,i)
      Do j=1,iGauss
         X2 = afile1(1,j)
         Y2 = afile1(2,j)
         Z2 = afile1(3,j)
         dist = sqrt((X2-X)**2+(Y2-Y)**2+(Z2-Z)**2)
         If (dist .Le. radius) Then
            ngp(ipos) = ngp(ipos)+1
            If (ngp(ipos).Ge.20000) Then
               Call Ok_messagebox('Error: more than 20000 Gauss points within the interaction radius')
               Stop
            End if
            ngpnl(ipos,ngp(ipos))= j
            radnl(ipos,ngp(ipos))= dist
         End if
      End do
   End do
ibegin = ibegin + 5000
iend = iend + 5000
End do

Return
End
Implicit Double Precision (A-H, O-Z)

! Arguments
Dimension Props(*)

! Local variables
Dimension radnl(20000)
Dimension ngpnl(20000)

! Parameters
plength = Props(32)
zero = 1.e-10

! Calculate and write nonlocal state variable
Do i=1,iGauss
  Read(7,Rec=i) StVar0
  If (StVar0 .Gt. zero) Then
    Sumweight = 0.
    StVarnl = 0.
    Read(4,Rec=i) ngp
    Read(5,Rec=i) (ngpnl(k),k=1,ngp)
    Read(6,Rec=i) (radnl(k),k=1,ngp)
    Do j=1,ngp
      Read(7,Rec=ngpnl(j)) StVar0
      aux1 = (radnl(j)/plength)*Exp(-((radnl(j)/plength)**2))
      aux2 = aux1*StVar0
      Sumweight = sumweight+aux1
      StVarnl = StVarnl+aux2
      End do
    End if
  End do
Return
End

!----------------------------------------------------------------------!
D.2 File - perm.for

```fortran
!----------------------------------------------------------------------!
! Subroutine perm !
! Replace saturated permeability !
!----------------------------------------------------------------------!
subroutine perm(kv, ki, kp, mv, mp, ksat)

!DEC$ ATTRIBUTES DLLEXPORT,STDCALL,REFERENCE :: perm
implicit none

double precision, dimension(*), intent(IN) :: kv, ki, kp, mp

double precision, dimension(*), intent(INOUT) :: mv

double precision, dimension(3), intent(OUT) :: ksat

double precision :: epseq, beta, kfact

! Parameters
epseq = kv(308) ! State variable from the mechanical model
beta = mp(1) ! Parameter for the permeability model

! Compute permeability factor
kfact = beta*epseq**3

! Update permeability
ksat(1) = (1.0d0 + kfact) * kp(1)
ksat(2) = (1.0d0 + kfact) * kp(2)
ksat(3) = (1.0d0 + kfact) * kp(3)

end subroutine perm

!----------------------------------------------------------------------!
```
Subroutine User_Mod ( IDTask, iMod, IsUndr,
   * iStep, iTer, iEl, Int,
   * X, Y, Z,
   * Time0, dTime,
   * Props, Sig0, Swp0, StVar0,
   * dEps, D, BulkW,
   * Sig, Swp, StVar, ipl,
   * nStat, NonSym, iStrsDep, iTimeDep, iTang,
   * iplDir, iPljLen, iAbort )

Implicit Double Precision (A-H, O-Z)
Dimension Props(*), Sig0(*), StVar0(*), dEps(*), D(6,6), Sig(*)
Dimension StVar(*), iPljDir(*)

!DEC$ ATTRIBUTES DLLExport, StdCall, Reference :: User_Mod

! For debugging purposes
Character*255 Dbg_Name
Data iDbg / 0 /
If (iDbg.Eq.0) then
   Dbg_Name='C://debug.txt'
   Open(Unit = 1, File = Dbg_Name, Status = 'Unknown')
iDbg=iDbg+1
End if

Select Case (iMod)
   Case (1) ! PRO
      Call const_law(IDTask, iMod, IsUndr, iStep, iTer, iEl, Int,
      * X, Y, Z, Time0, dTime,
      * Props, Sig0, Swp0, StVar0,
      * dEps, D, BulkW, Sig, Swp, StVar, ipl,
      * nStat, NonSym, iStrsDep, iTimeDep, iTang,
      * iPljDir, iPljLen, iAbort)
   Case Default
      Stop 'invalid model number in UsrMod'
iAbort=1
Return
End Select ! iMod
Return
End ! User_Mod
! include 'main.for'
Subroutine GetModelCount(nMod)

  Integer (Kind=4) nMod

  nMod = 2 ! Maximum model number (iMod) in current DLL

  Return

End

Subroutine GetModelName( iMod , ModelName )

  Integer iMod
  Character (Len= *) ModelName

  Character (Len=255) tName

  Select Case (iMod)
    Case (1)
      tName = 'AHW_model'
    Case (2)
      tName = 'perm'
    Case Default
      tName = 'not in DLL'
  End Select

  LT = Len_Trim(tName)
  ModelName= Char(LT) // tName(1:LT)

  Return

End

Subroutine GetParamCount( iMod , nParam )

  Select Case (iMod)
    Case ( 1 )
      nParam = 40
    Case Default
      nParam = 0
  End Select

  Return

End

Subroutine GetModelCount(nMod)

!----------------------------------------------------------------------!
! Subroutine GetModelCount
! Return the maximum model number (iMod) in this DLL
!----------------------------------------------------------------------!
Subroutine GetModelCount(nMod)

Integer (Kind=4) nMod

!DEC$ ATTRIBUTES DLLExport, StdCall, reference :: GetModelCount

  nMod = 2 ! Maximum model number (iMod) in current DLL

  Return

End

!----------------------------------------------------------------------!
! Subroutine GetModelName
! Return the name of the different models
!----------------------------------------------------------------------!
Subroutine GetModelName( iMod , ModelName )

  Integer iMod
  Character (Len= *) ModelName

  Character (Len=255) tName

  Select Case (iMod)
    Case (1)
      tName = 'AHW_model'
    Case (2)
      tName = 'perm'
    Case Default
      tName = 'not in DLL'
  End Select

  LT = Len_Trim(tName)
  ModelName= Char(LT) // tName(1:LT)

  Return

End

!----------------------------------------------------------------------!
! Subroutine GetParamCount
! Return the number of parameters of the different models
!----------------------------------------------------------------------!
Subroutine GetParamCount( iMod , nParam )

  Select Case (iMod)
    Case ( 1 )
      nParam = 40
    Case Default
      nParam = 0
  End Select

  Return

End

!----------------------------------------------------------------------!
Subroutine GetParamName( iMod, iParam, ParamName )

Character (Len=255) ParamName, Units

Call GetParamAndUnit(iMod,iParam,ParamName,Units)

Return

End

Subroutine GetParamUnit( iMod, iParam, Units )

Character (Len=255) ParamName, Units

Call GetParamAndUnit(iMod,iParam,ParamName,Units)

Return

End

Subroutine GetParamAndUnit( iMod, iParam, ParamName, Units )

Character (Len=255) ParamName, Units, tName

Select Case (iMod)

Case (1)

! ModName = 'DP'

Select Case (iParam)

Case (1)

ParamName = '01. E_1#'; Units = 'F/L^2#'

Case (2)

ParamName = '02. n_1#'; Units = '-'

Case (3)

ParamName = '03. E_2#'; Units = 'F/L^2#'

Case (4)

ParamName = '04. @a#'; Units = 'deg'

Case (5)

ParamName = '05. @b#'; Units = 'deg'

Case (6)

ParamName = '06. @a#'; Units = 'deg'

Case (7)

ParamName = '07. @b#'; Units = 'deg'

Case (8)
ParamName = '08. @f^*#_ini' ; Units = 'deg'

Case (9)

ParamName = '09. @f^*#_peak' ; Units = 'deg'

Case (10)

ParamName = '10. @f^*#_res' ; Units = 'deg'

Case (11)

ParamName = '11. c^*#_0 ini' ; Units = 'F/L^2#'

Case (12)

ParamName = '12. p_t0 ini' ; Units = 'F/L^2#'

Case (13)

ParamName = '13. r_post' ; Units = '-'

Case (14)

ParamName = '14. 0a^0q' ; Units = '-'

Case (15)

ParamName = '15. 0w' ; Units = '-'

Case (16)

ParamName = '16. 0x^2' ; Units = '-'

Case (17)

ParamName = '17. m' ; Units = '-'

Case (18)

ParamName = '18. a_hard' ; Units = '-'

Case (19)

ParamName = '19. b_post' ; Units = '-'

Case (20)

ParamName = '20. b_res' ; Units = '-'

Case (21)

ParamName = '21. @W^90' ; Units = '-'

Case (22)

ParamName = '22. @W^m' ; Units = '-'

Case (23)

ParamName = '23. @d^m' ; Units = '-'

Case (24)

ParamName = '24. n' ; Units = '-'

Case (25)

ParamName = '25. N' ; Units = '-'

Case (26)

ParamName = '26. @h^pz(FT/L^2#)' ; Units = '-'

Case (27)

ParamName = '27. @g^c(L^2#/F/T)' ; Units = '-'

Case (28)

ParamName = '28. @y^c' ; Units = '-'

Case (29)

ParamName = '29. a^c' ; Units = '-'

Case (30)

ParamName = '30. @e^c_thr' ; Units = '-'

Case (31)

ParamName = '31. nonlocal flag y(1) n(0)' ; Units = '-'

Case (32)

ParamName = '32. l_s' ; Units = 'L'

Case (33)

ParamName = '33. weak element?' ; Units = '-'

Case (34)

ParamName = '34. ctrl - p_atm' ; Units = 'F/L^2#'

Case (35)

ParamName = '35. ctrl - tol yield' ; Units = '-'

Case (36)

ParamName = '36. ctrl - max NR iter' ; Units = '-'

Case (37)

ParamName = '37. ctrl - num subinc' ; Units = '-'

Case (38)

ParamName = '38. ctrl - rel tol error' ; Units = '-'

ParamName = '08. @f^*#_ini' ; Units = 'deg'

Case (9)

ParamName = '09. @f^*#_peak' ; Units = 'deg'

Case (10)

ParamName = '10. @f^*#_res' ; Units = 'deg'

Case (11)

ParamName = '11. c^*#_0 ini' ; Units = 'F/L^2#'

Case (12)

ParamName = '12. p_t0 ini' ; Units = 'F/L^2#'

Case (13)

ParamName = '13. r_post' ; Units = '-'

Case (14)

ParamName = '14. 0a^0q' ; Units = '-'

Case (15)

ParamName = '15. 0w' ; Units = '-'

Case (16)

ParamName = '16. 0x^2' ; Units = '-'

Case (17)

ParamName = '17. m' ; Units = '-'

Case (18)

ParamName = '18. a_hard' ; Units = '-'

Case (19)

ParamName = '19. b_post' ; Units = '-'

Case (20)

ParamName = '20. b_res' ; Units = '-'

Case (21)

ParamName = '21. @W^90' ; Units = '-'

Case (22)

ParamName = '22. @W^m' ; Units = '-'

Case (23)

ParamName = '23. @d^m' ; Units = '-'

Case (24)

ParamName = '24. n' ; Units = '-'

Case (25)

ParamName = '25. N' ; Units = '-'

Case (26)

ParamName = '26. @h^pz(FT/L^2#)' ; Units = '-'

Case (27)

ParamName = '27. @g^c(L^2#/F/T)' ; Units = '-'

Case (28)

ParamName = '28. @y^c' ; Units = '-'

Case (29)

ParamName = '29. a^c' ; Units = '-'

Case (30)

ParamName = '30. @e^c_thr' ; Units = '-'

Case (31)

ParamName = '31. nonlocal flag y(1) n(0)' ; Units = '-'

Case (32)

ParamName = '32. l_s' ; Units = 'L'

Case (33)

ParamName = '33. weak element?' ; Units = '-'

Case (34)

ParamName = '34. ctrl - p_atm' ; Units = 'F/L^2#'

Case (35)

ParamName = '35. ctrl - tol yield' ; Units = '-'

Case (36)

ParamName = '36. ctrl - max NR iter' ; Units = '-'

Case (37)

ParamName = '37. ctrl - num subinc' ; Units = '-'

Case (38)

ParamName = '38. ctrl - rel tol error' ; Units = '-'
Case (39)
  ParamName = '"39. ctrl - rel min dt'  ; Units = '-'
Case (40)
  ParamName = '"40. ctrl - 2D? y(1) n(0)' ; Units = '-'
Case Default
  ParamName = '"???'  ; Units = '"???'
End Select
Case Default
  ! model not in DLL
  ParamName = ' N/A '  ; Units = ' N/A '
End Select

!----------------------------------------------------------------------!

Subroutine GetStateVarCount ( iMod, nVar )

Select Case (iMod)
Case (1)
  nVar = 8
Case Default
  nVar = 0
End Select

Return
End

!----------------------------------------------------------------------!

Subroutine GetStateVarName ( iMod, iVar, Name )

Character (Len=255) Name, Unit

Call GetStateVarNameAndUnit( iMod, iVar, Name, Unit )

End

!----------------------------------------------------------------------!
Subroutine GetStateVarUnit( iMod , iVar, Unit )

Character (Len=255) Name, Unit

Call GetStateVarNameAndUnit( iMod , iVar, Name, Unit )

End

Subroutine GetStateVarNameAndUnit( iMod , iVar, Name, Unit )

Character (Len=255) Name, Unit, tName

Select Case (iMod)
    Case (1)
        Select Case (iVar)
            Case (1)
                Name = '@e#ˆP#_xx' ; Unit = '-'
            Case (2)
                Name = '@e#ˆP#_yy' ; Unit = '-'
            Case (3)
                Name = '@e#ˆP#_zz' ; Unit = '-'
            Case (4)
                Name = '@g#ˆP#_xy' ; Unit = '-'
            Case (5)
                Name = '@g#ˆP#_yz' ; Unit = '-'
            Case (6)
                Name = '@g#ˆP#_xz' ; Unit = '-'
            Case (7)
                Name = '@e#ˆc#_eq' ; Unit = '-'
            Case (8)
                Name = '@e#ˆp#_eq' ; Unit = '-'
            Case Default
                Name='N/A' ; Unit = '?'
        End Select
    Case Default
        Name='N/A' ; Unit = '?'
End Select

Name = Name
Name = Char(LT) // tName(1:LT)

Unit = Unit
Unit = Char(LT) // tName(1:LT)

Return

End
D.5  File - okmsg.for

1  !-------------------------------------------------------------------------!
2  ! Subroutine Ok_messagebox !
3  ! Display a messagebox with an OK button !
4  !-------------------------------------------------------------------------!
5     Subroutine Ok_messagebox(t)
6  
7     use dfwin
8     use dfwinty
9     integer (kind=Int_Ptr_Kind()) hWnd
10    character(*) t
11    character(len=256) :: msg, title
12
13    msg = Trim(t) // char(0)
14    title = 'CSM Model' // char(0)
15
16    hWnd = 0
17
18    iret = MessageBox( hWnd,
19        * msg,
20        * title,
21        * MB_OK )
22
23    Return
24
25  !-------------------------------------------------------------------------!