

When Gas Builds Up, Do Clay-Rich Rocks (Re)Fracture?

Insights From Hydro-Mechanical Modelling for Nuclear Waste Repositories

Gilles CORMAN & Frédéric COLLIN

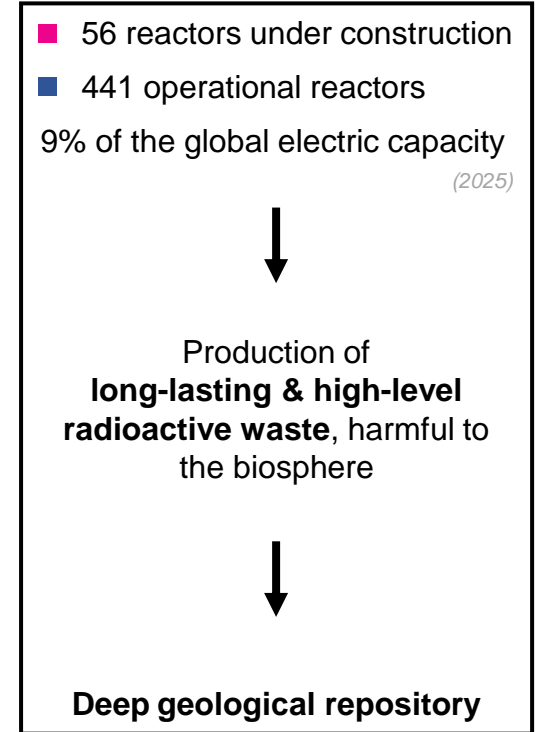
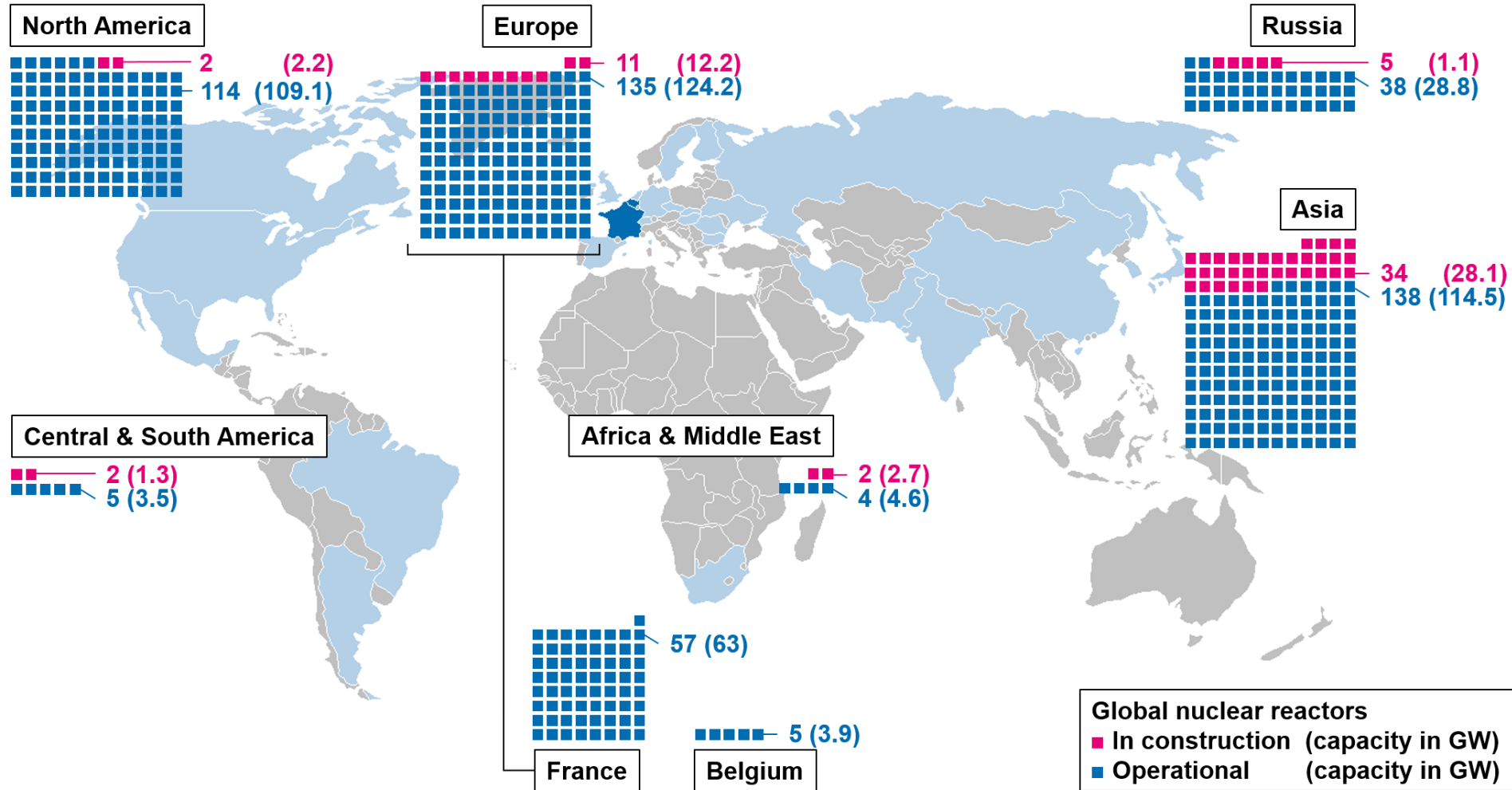
May 28, 2026 • Mines Paris (France)



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n° 847593.

Introduction

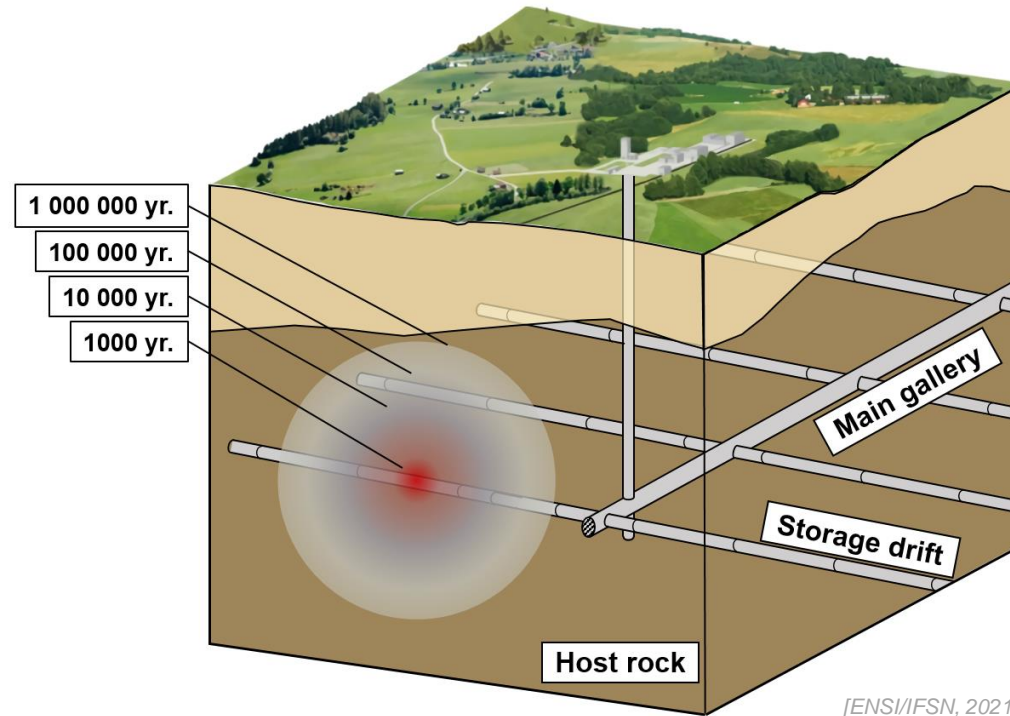
A story of energy



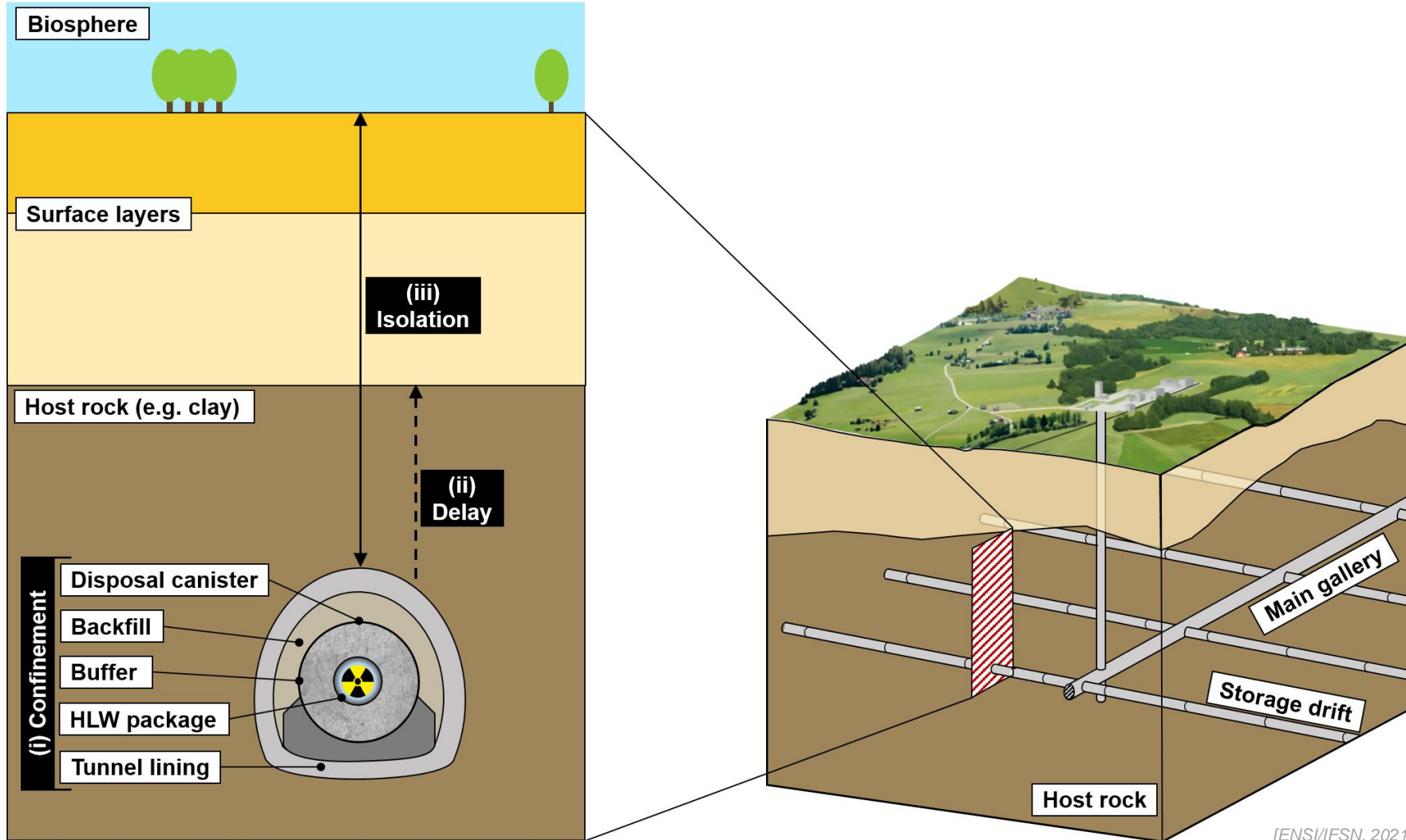
Global nuclear reactors
■ In construction (capacity in GW)
■ Operational (capacity in GW)

Data collected from [IAEA, 2025]

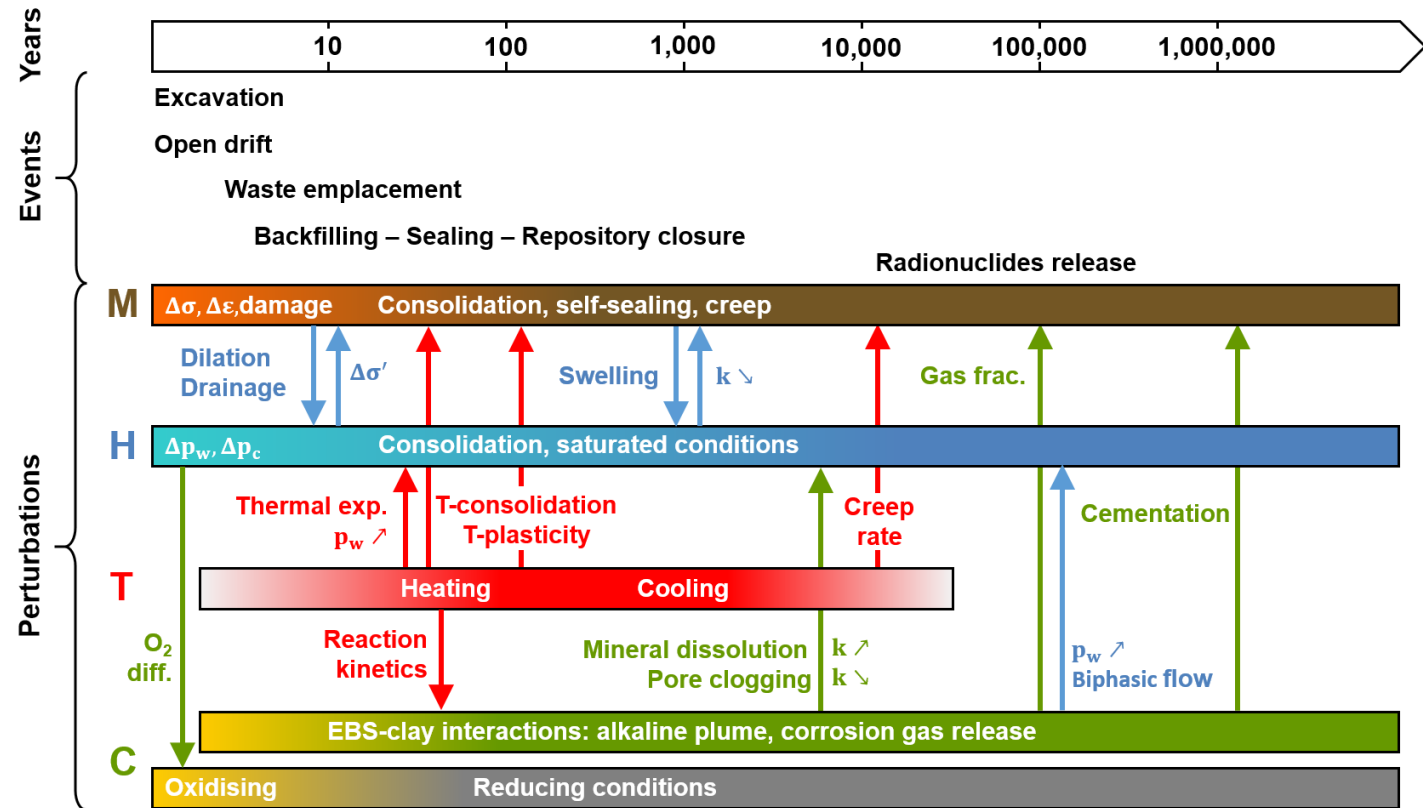
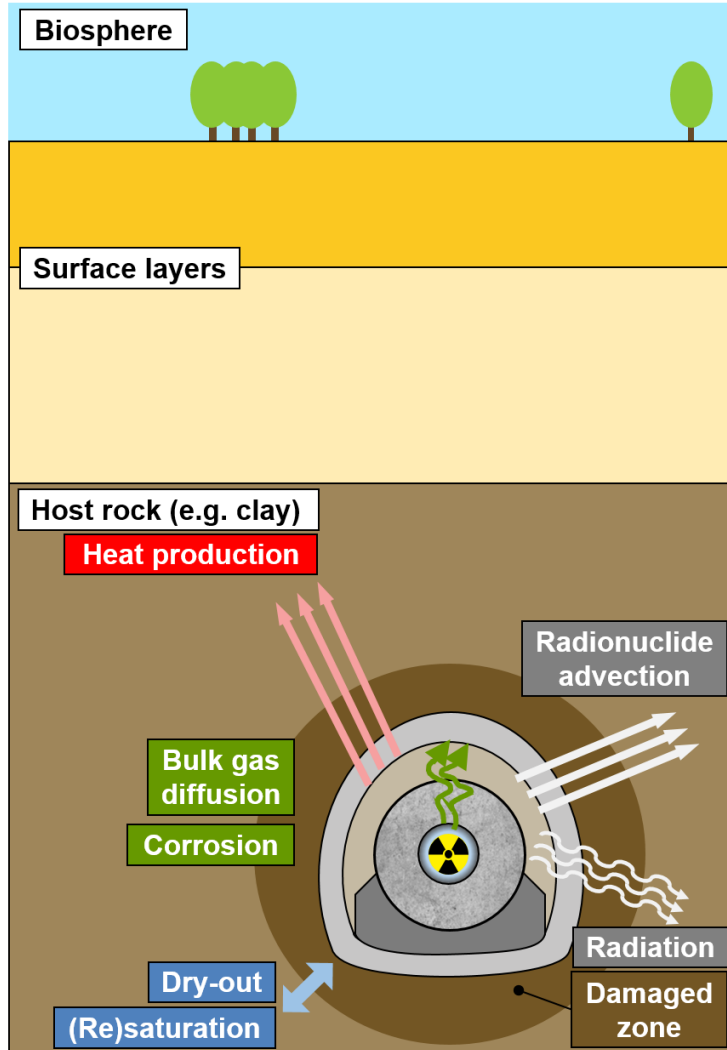
Deep geological repository



Deep geological repository

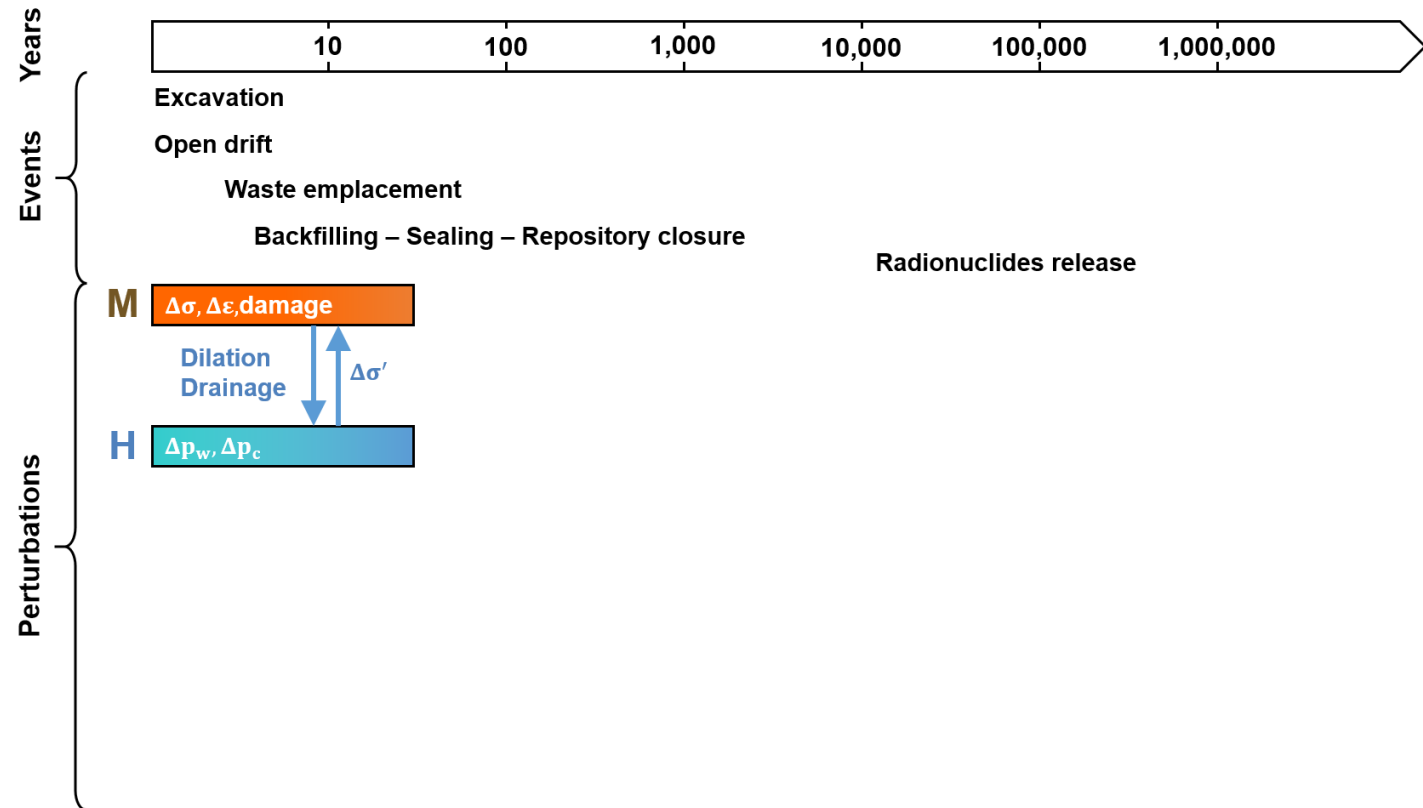
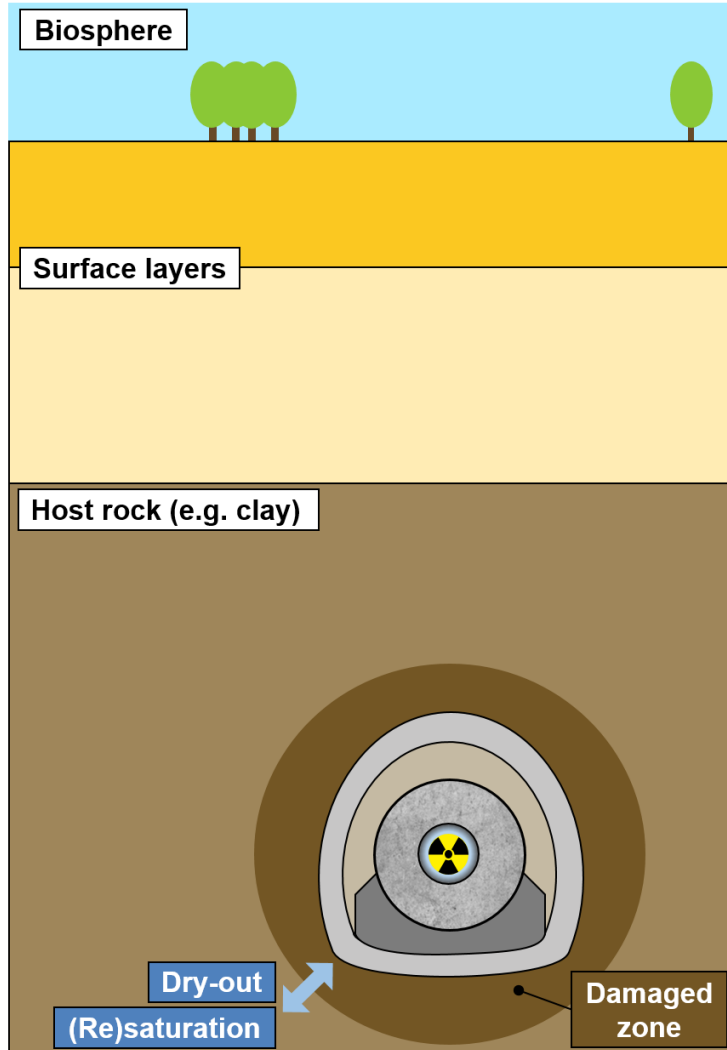


Deep geological repository



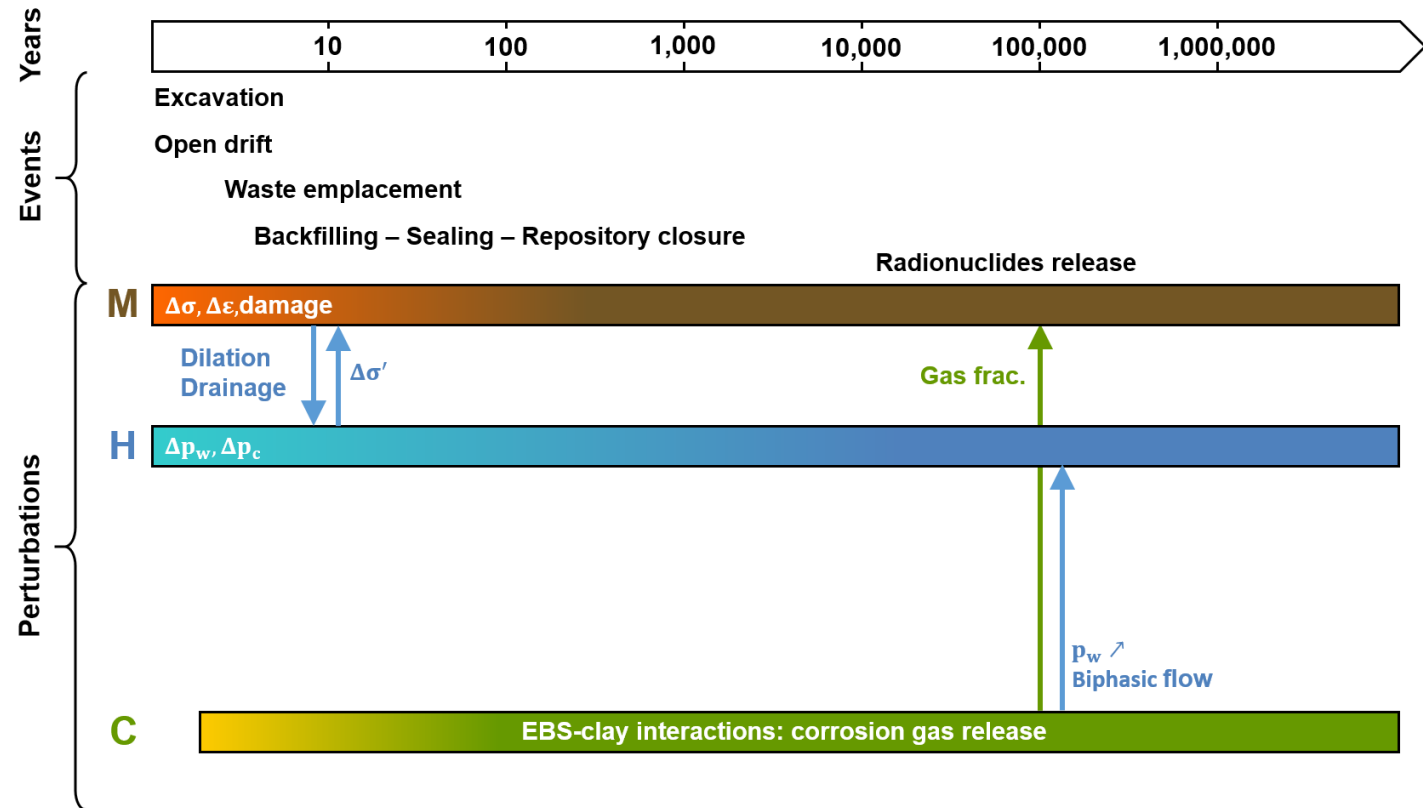
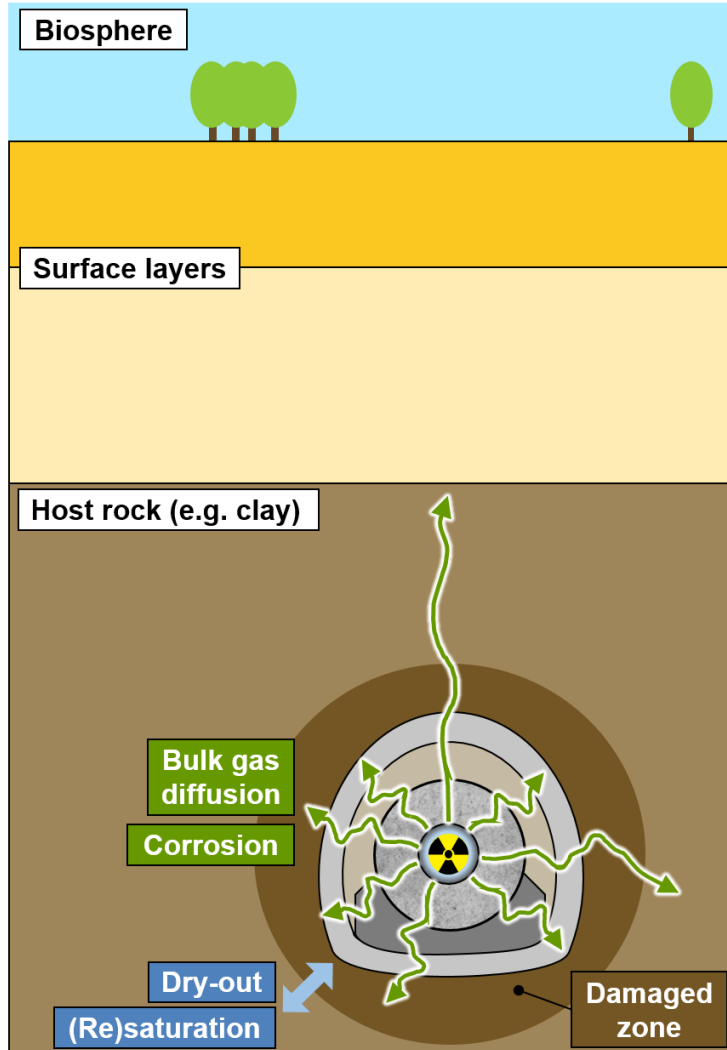
[Sillen, 2012]

Deep geological repository



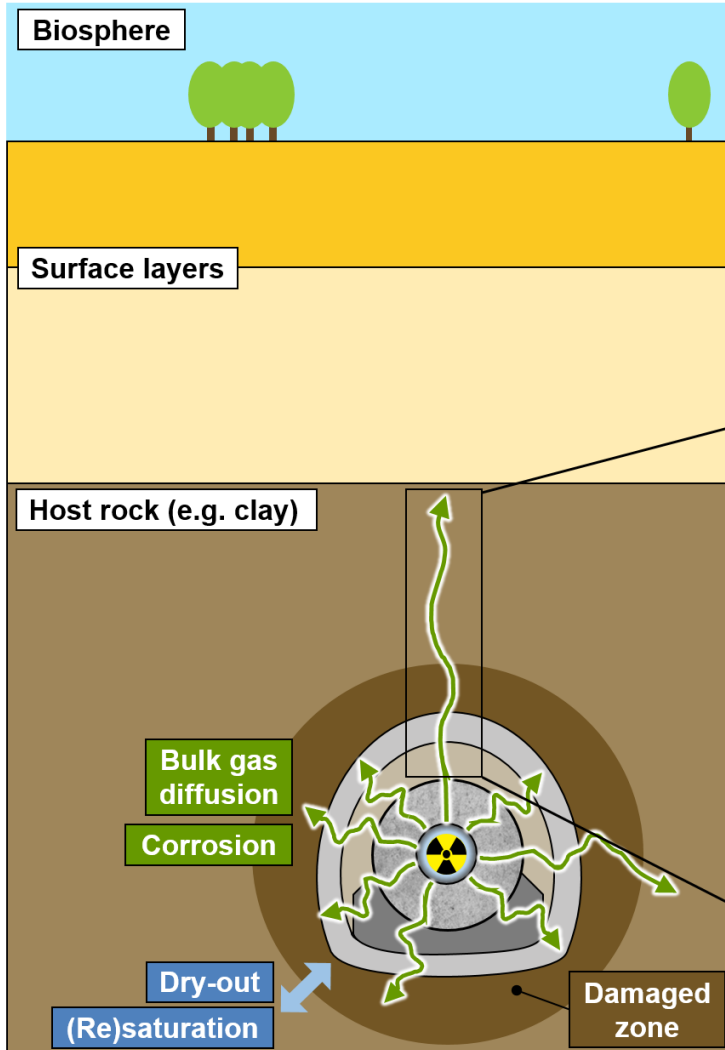
[Sillen, 2012]

Deep geological repository



[Sillen, 2012]

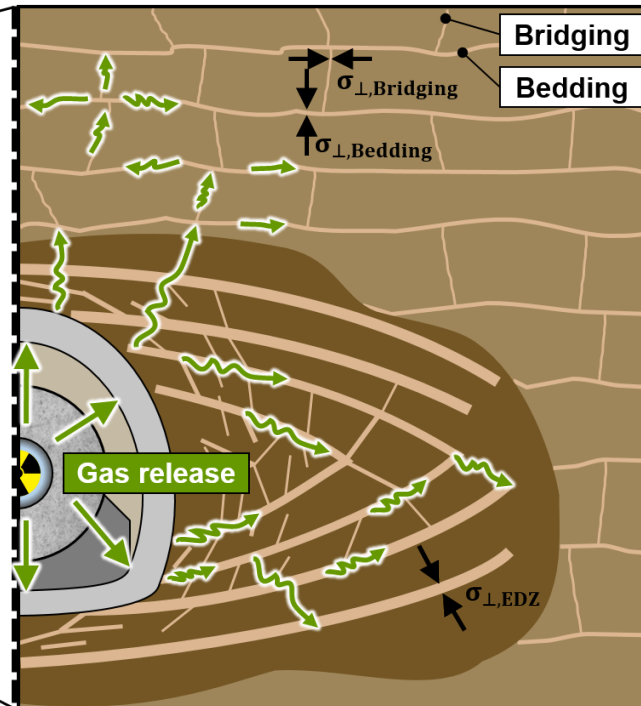
Work objectives



When gas builds up, do clay-rich rocks (re)fracture?



Numerical models of gas transport modes



Zones of interest



Sound rock

[Corman et al., 2025]

Excavation Damaged Zone (EDZ)

[Corman et al., 2022]

01

**Characterisation of gas
transport processes**

Introduction

02

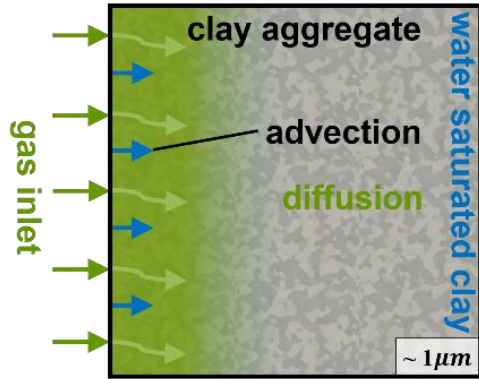
**Modelling gas transport
in the EDZ**

Conclusion

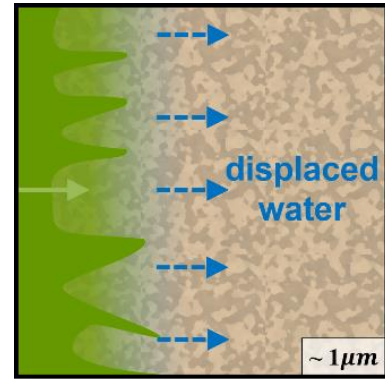
03

**Modelling gas transport
in sound rocks**

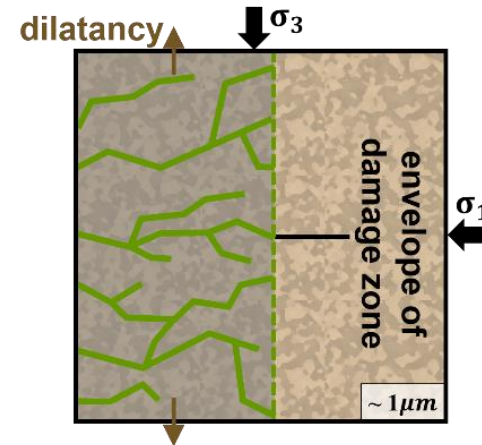
Experimental insights for HM modelling



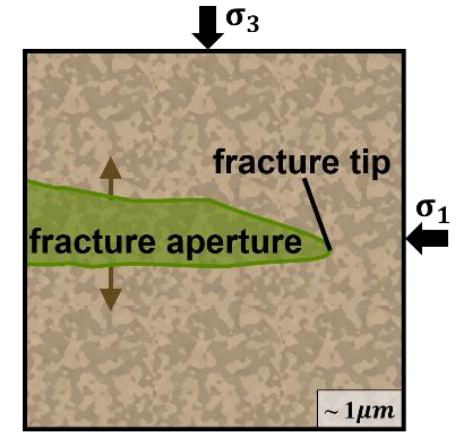
(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow



(iii) Gas flow in preferential pathways

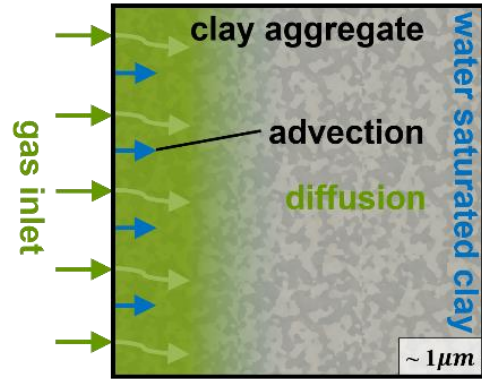


(iv) Gas flow in macroscopic fractures

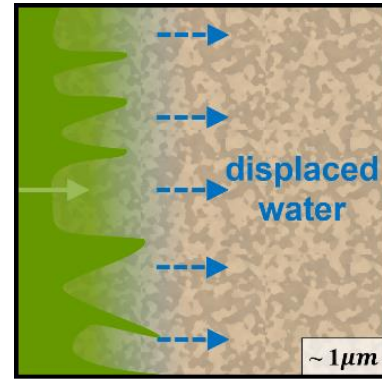
[Marshall et al., 2005]

Gas pressure

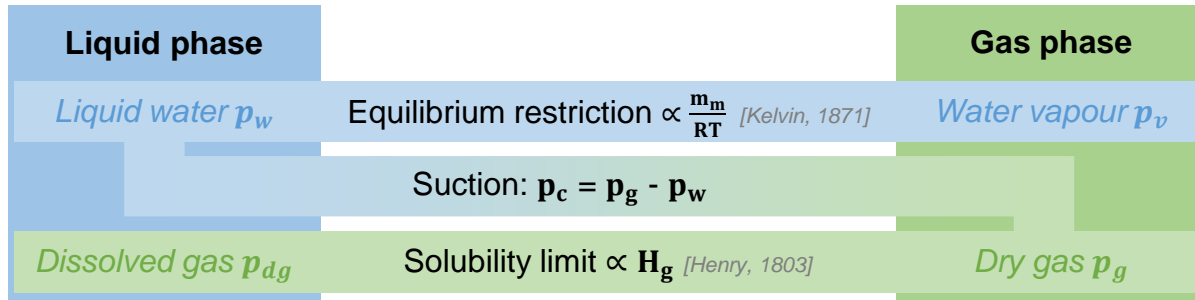
Experimental insights for HM modelling



(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow



Diffusive transport mode

[Fick, 1855]

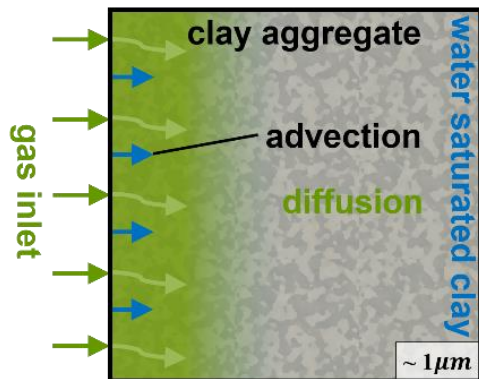
$$\mathbf{i} \propto \bar{\tau} D_e \nabla \left(\frac{\rho_{dg}}{\rho_w} \right)$$

Advective transport mode

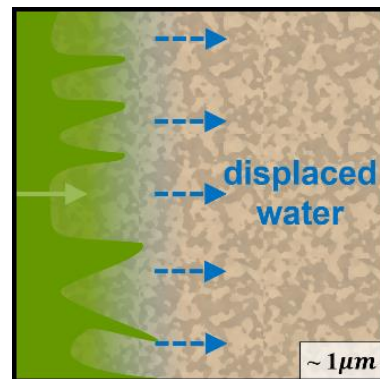
[Darcy, 1856]

$$\mathbf{q} \propto \frac{k}{\mu} (\nabla p - \rho \mathbf{g})$$

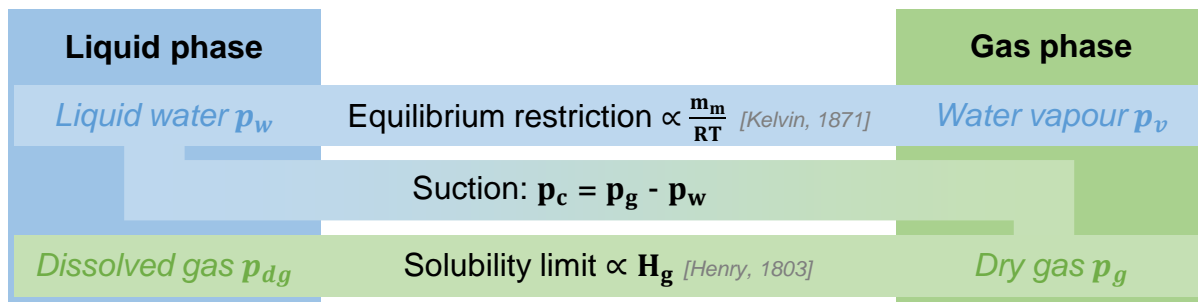
Experimental insights for HM modelling



(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow



Diffusive transport mode

[Fick, 1855]

$$\mathbf{i} \propto \bar{\tau} D_e \nabla \left(\frac{\rho_{dg}}{\rho_w} \right)$$

Retention curve

[van Genuchten, 1980]

$$S_{r,w} = f(p_c, P_e)$$

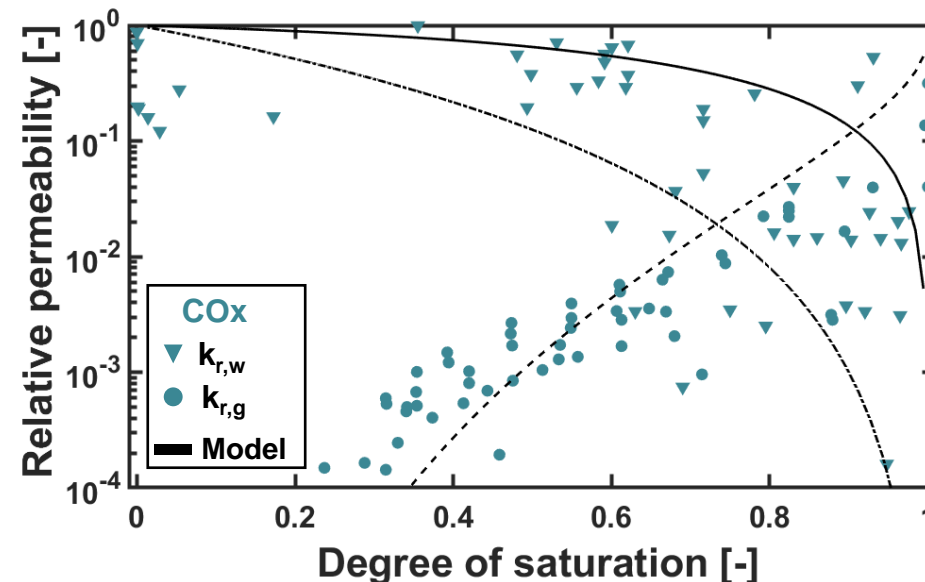
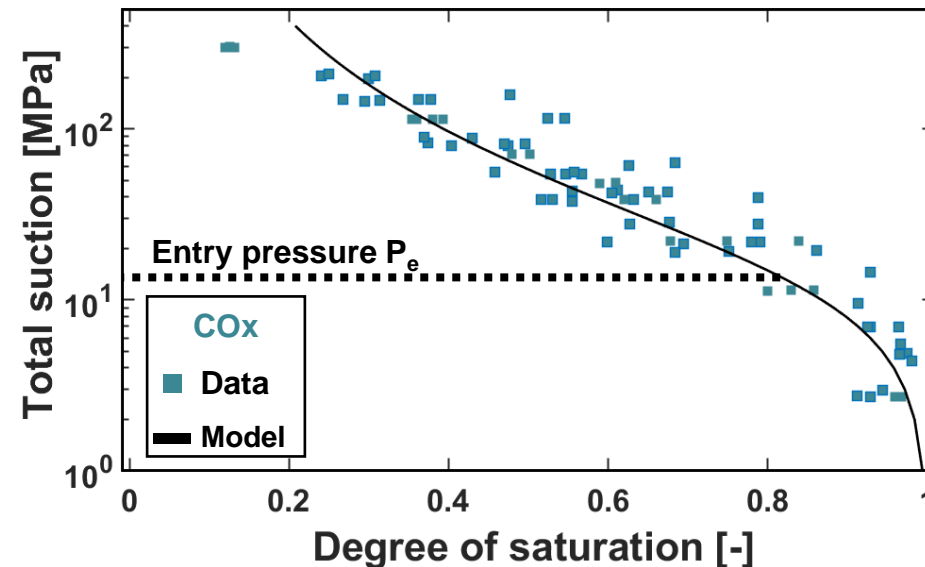
Advective transport mode

[Darcy, 1856]

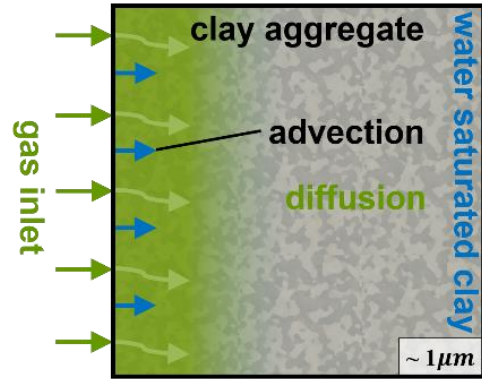
$$\mathbf{q} \propto \frac{k_{int} k_r}{\mu} (\nabla p - \rho \mathbf{g})$$

Relative permeability curves

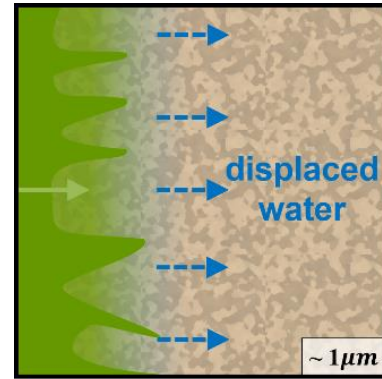
$$k_r = f(S_{r,w})$$



Experimental insights for HM modelling



(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow

Liquid phase

Gas phase

Liquid water p_w

Equilibrium restriction $\propto \frac{m_m}{RT}$ [Kelvin, 1871]

Water vapour p_v

Suction: $p_c = p_g - p_w$

Dissolved gas p_{dg}

Solubility limit $\propto H_g$ [Henry, 1803]

Dry gas p_g

Diffusive transport mode

[Fick, 1855]

$$\mathbf{i} \propto \bar{\tau} D_e \nabla \left(\frac{\rho_{dg}}{\rho_w} \right)$$

Retention curve

[van Genuchten, 1980]

$$S_{r,w} = f(p_c, P_e)$$

Advective transport mode

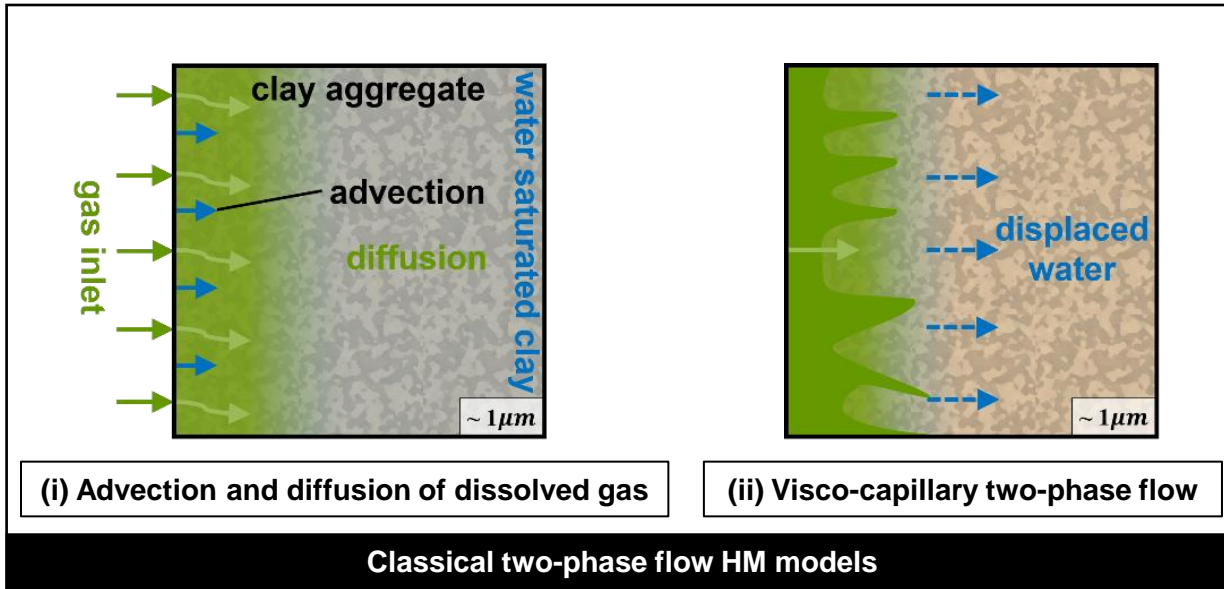
[Darcy, 1856]

$$\mathbf{q} \propto \frac{k_{int} k_r}{\mu} (\nabla p - \rho g)$$

Relative permeability curves

$$k_r = f(S_{r,w})$$

Experimental insights for HM modelling

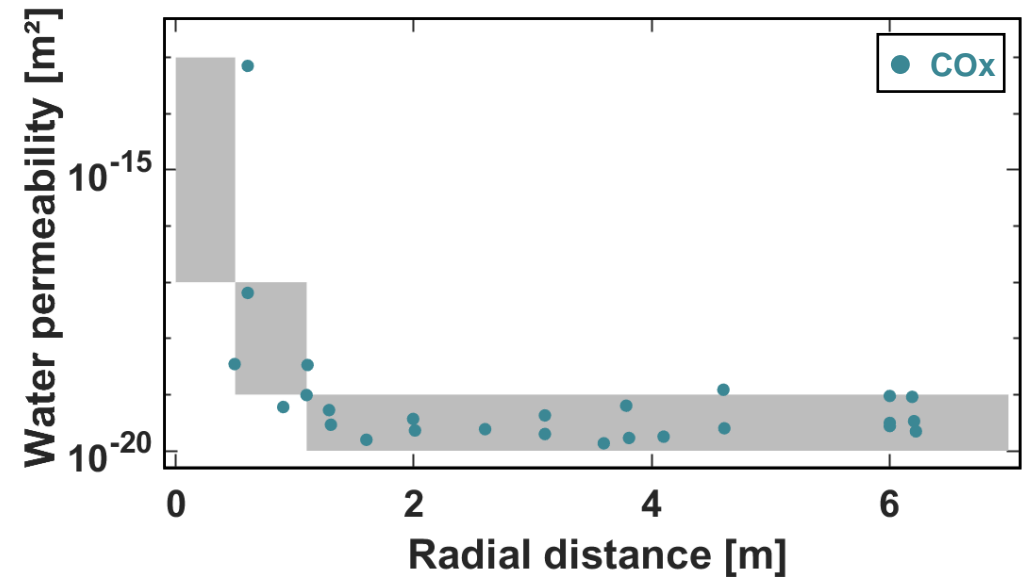
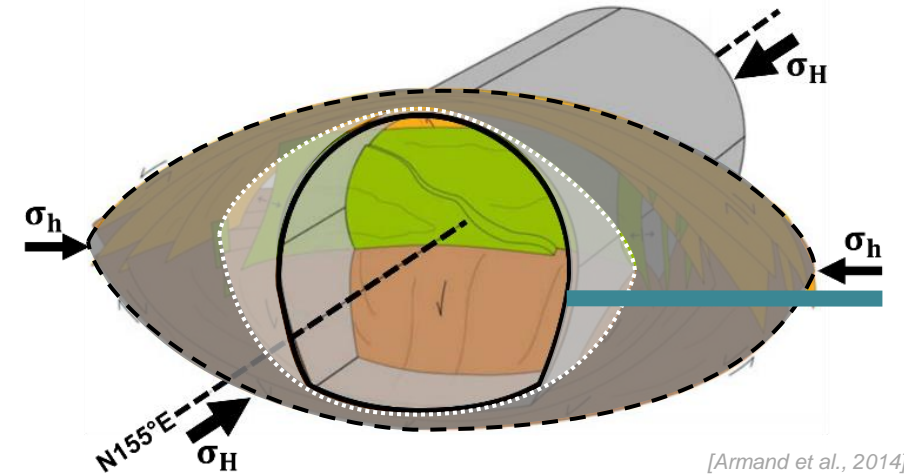


Excavation process in clay rocks creates an EDZ, characterised by:

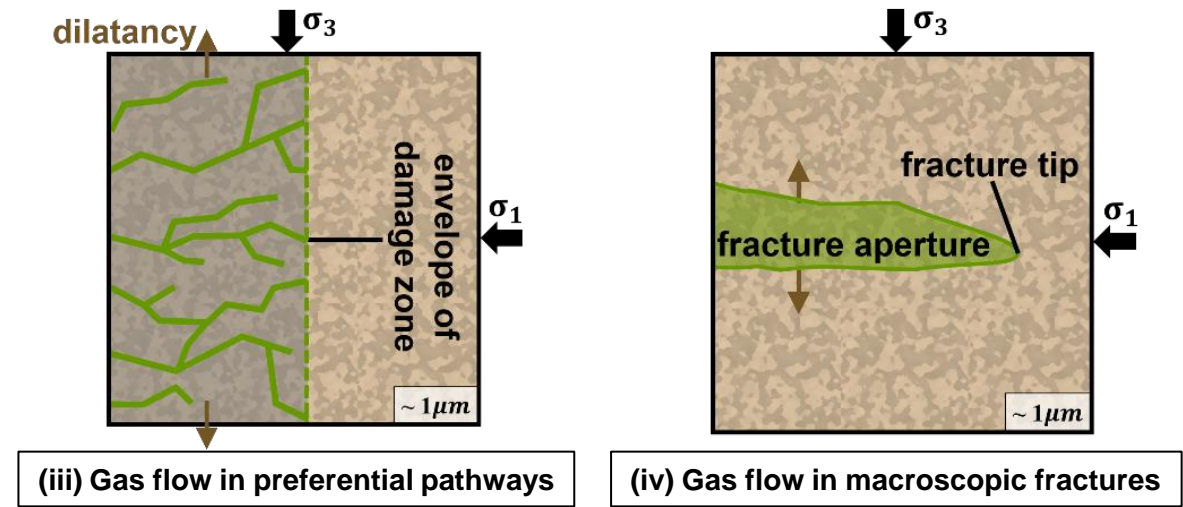
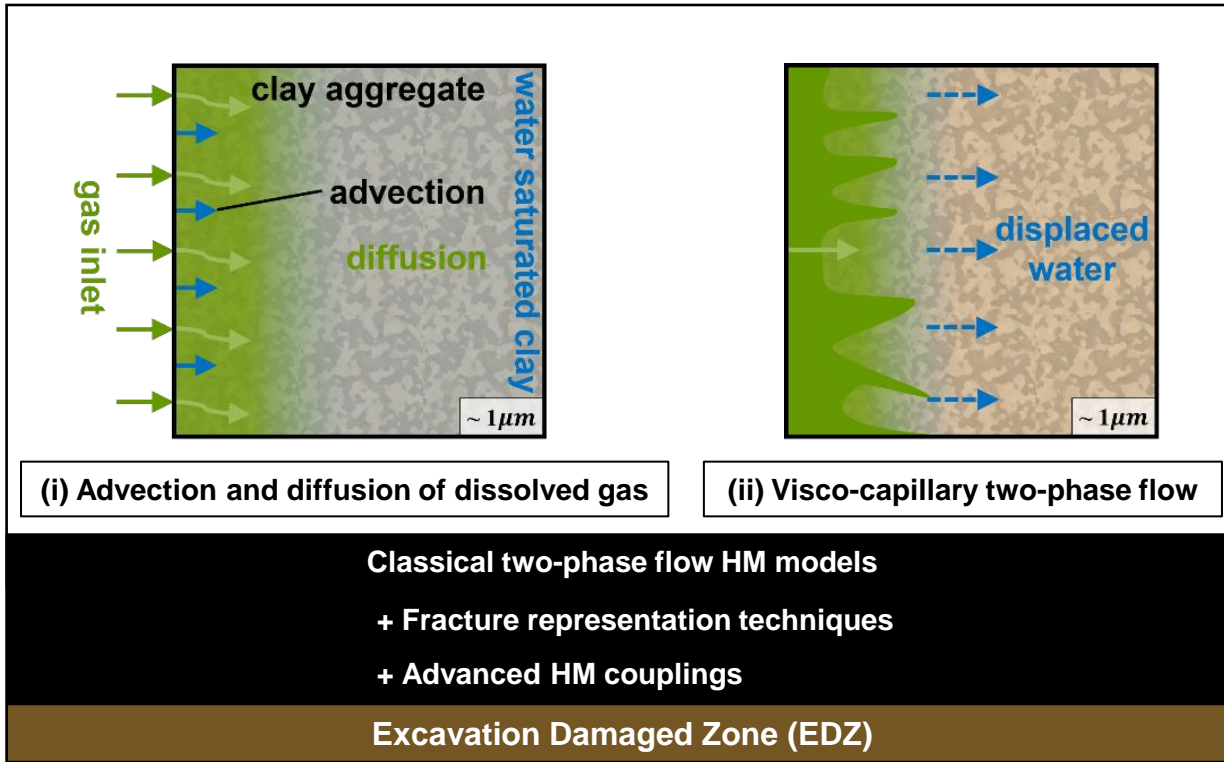
- + Fracture geometry and patterns
- + Transport properties evolution

Modelling needs:

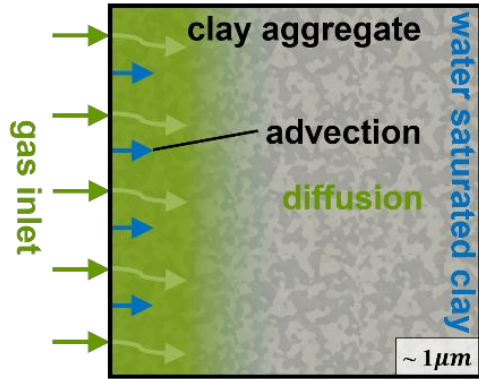
- + Fracture representation techniques
- + Advanced HM couplings ($k_w, P_r = f(\varepsilon)$)



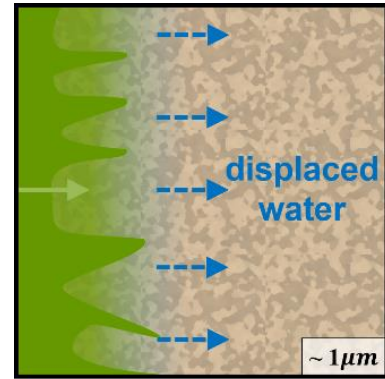
Experimental insights for HM modelling



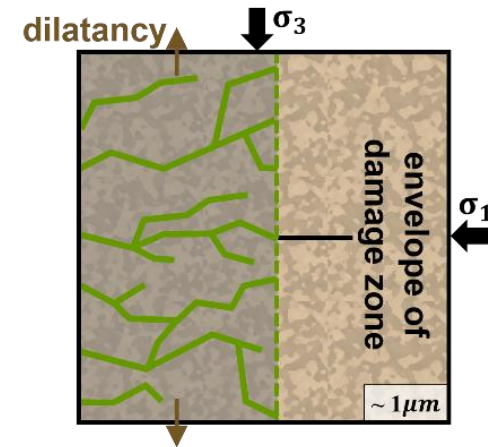
Experimental insights for HM modelling



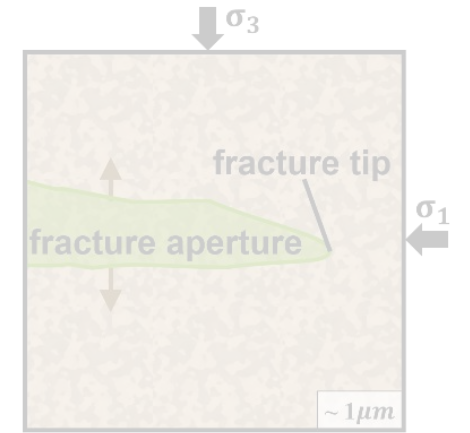
(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow



(iii) Gas flow in preferential pathways



(iv) Gas flow in macroscopic fractures

Classical two-phase flow HM models

+ Fracture representation techniques

+ Advanced HM couplings

Excavation Damaged Zone (EDZ)

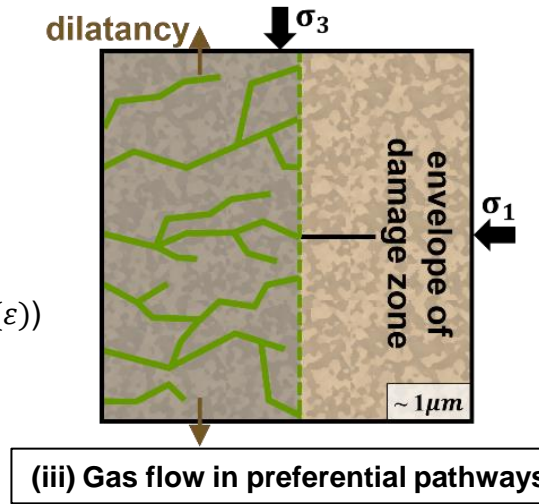
Experimental insights for HM modelling

Discrete gas-filled pathways
in sound rocks, driven by:

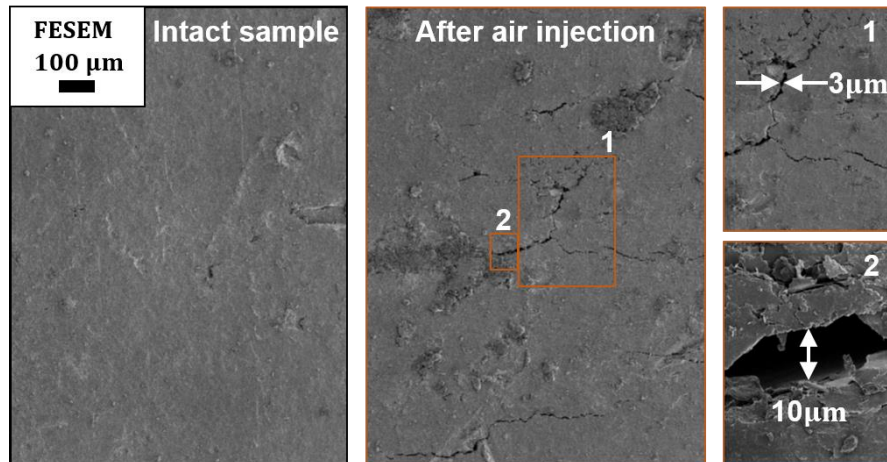
- + Natural heterogeneities & spatial variability of HM properties
- + Transport properties evolution

Modelling needs:

- + Microstructure-informed techniques
- + Advanced HM couplings ($k_w, P_r = f(\varepsilon)$)

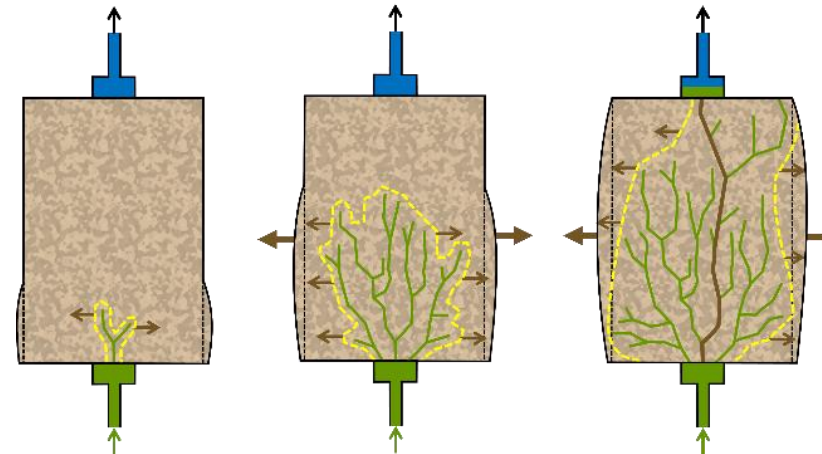


Boom clay



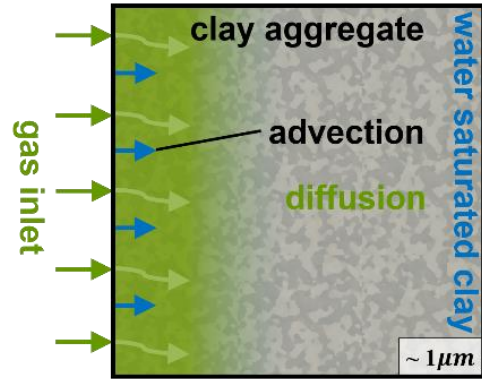
[Gonzalez-Blanco et al. 2022]

Callovo-Oxfordian claystone

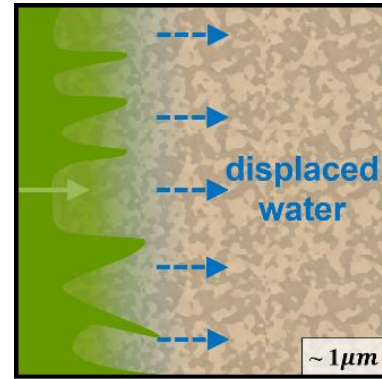


[Cuss et al. 2014]

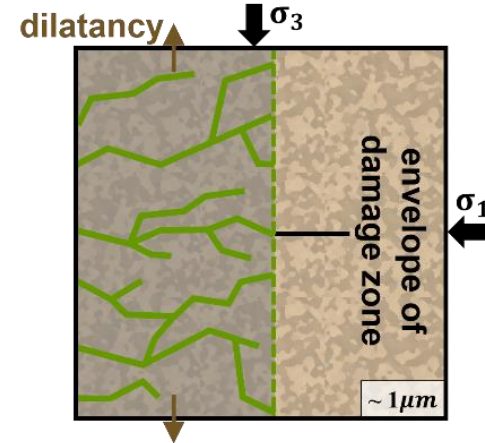
Experimental insights for HM modelling



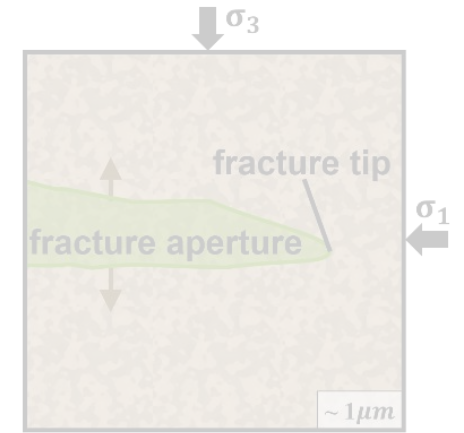
(i) Advection and diffusion of dissolved gas



(ii) Visco-capillary two-phase flow



(iii) Gas flow in preferential pathways



(iv) Gas flow in macroscopic fractures

Classical two-phase flow HM models
 + Fracture representation techniques
 + Advanced HM couplings

Excavation Damaged Zone (EDZ)

Localised two-phase flow HM models
 + Microstructure-informed techniques
 + Advanced HM couplings

Sound rock

01

**Characterisation of gas
transport processes**

Introduction

02

**Modelling gas transport
in the EDZ**

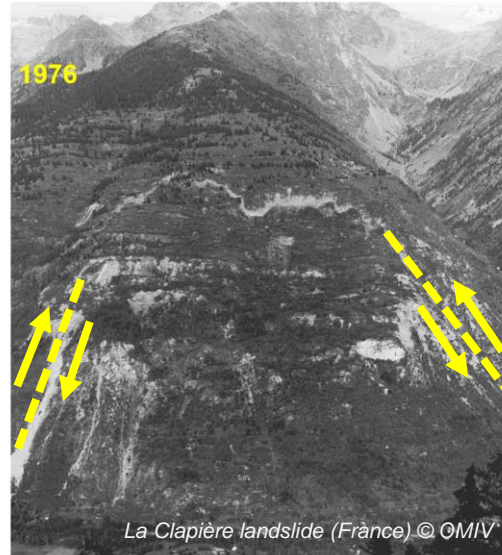
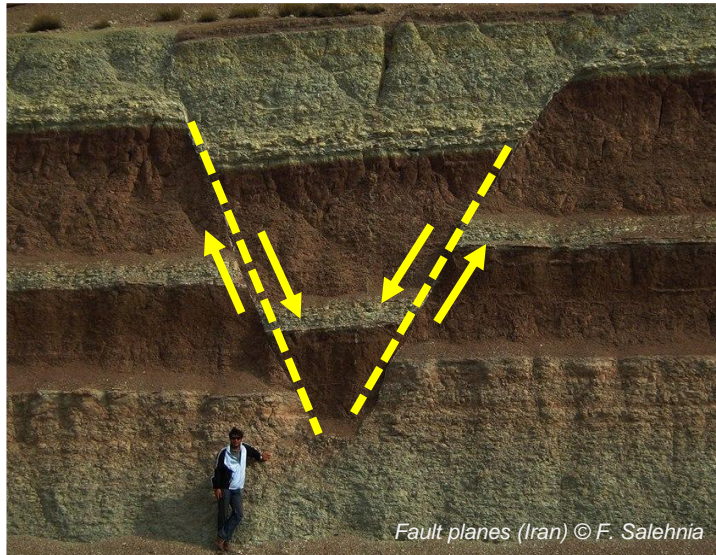
Conclusion

03

**Modelling gas transport
in sound rocks**

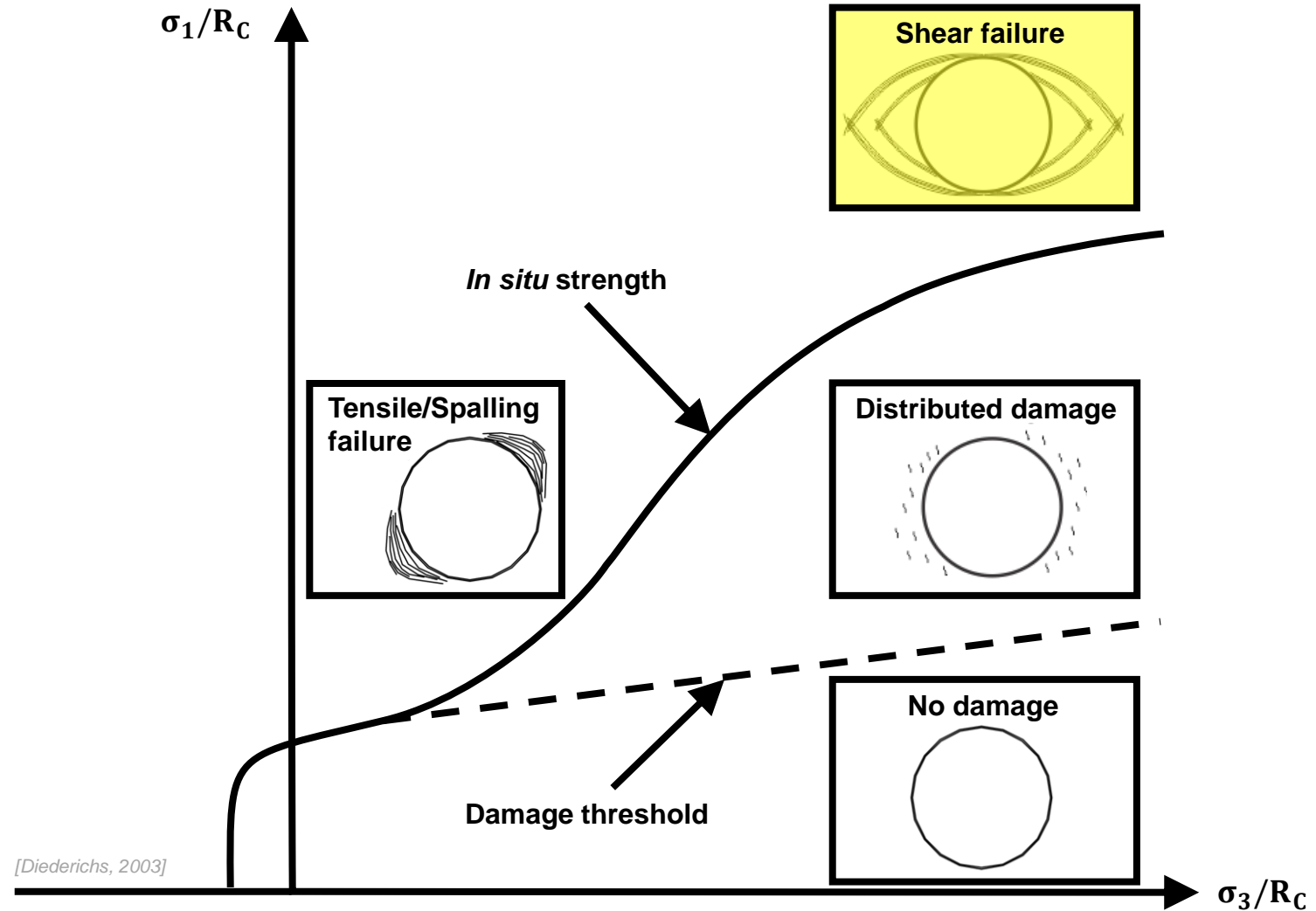
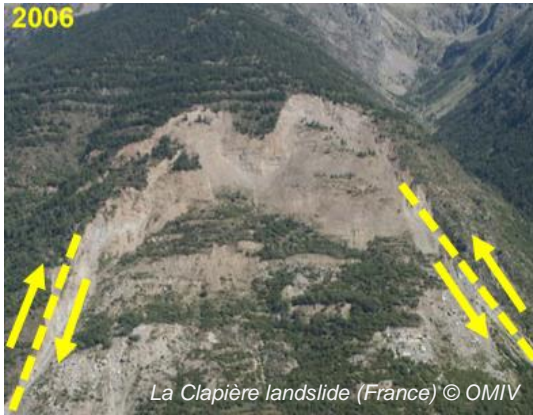
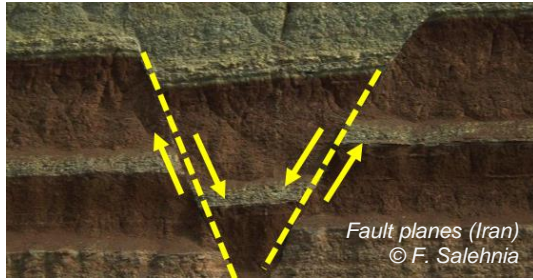
Fracturing process

From geomaterials failure...



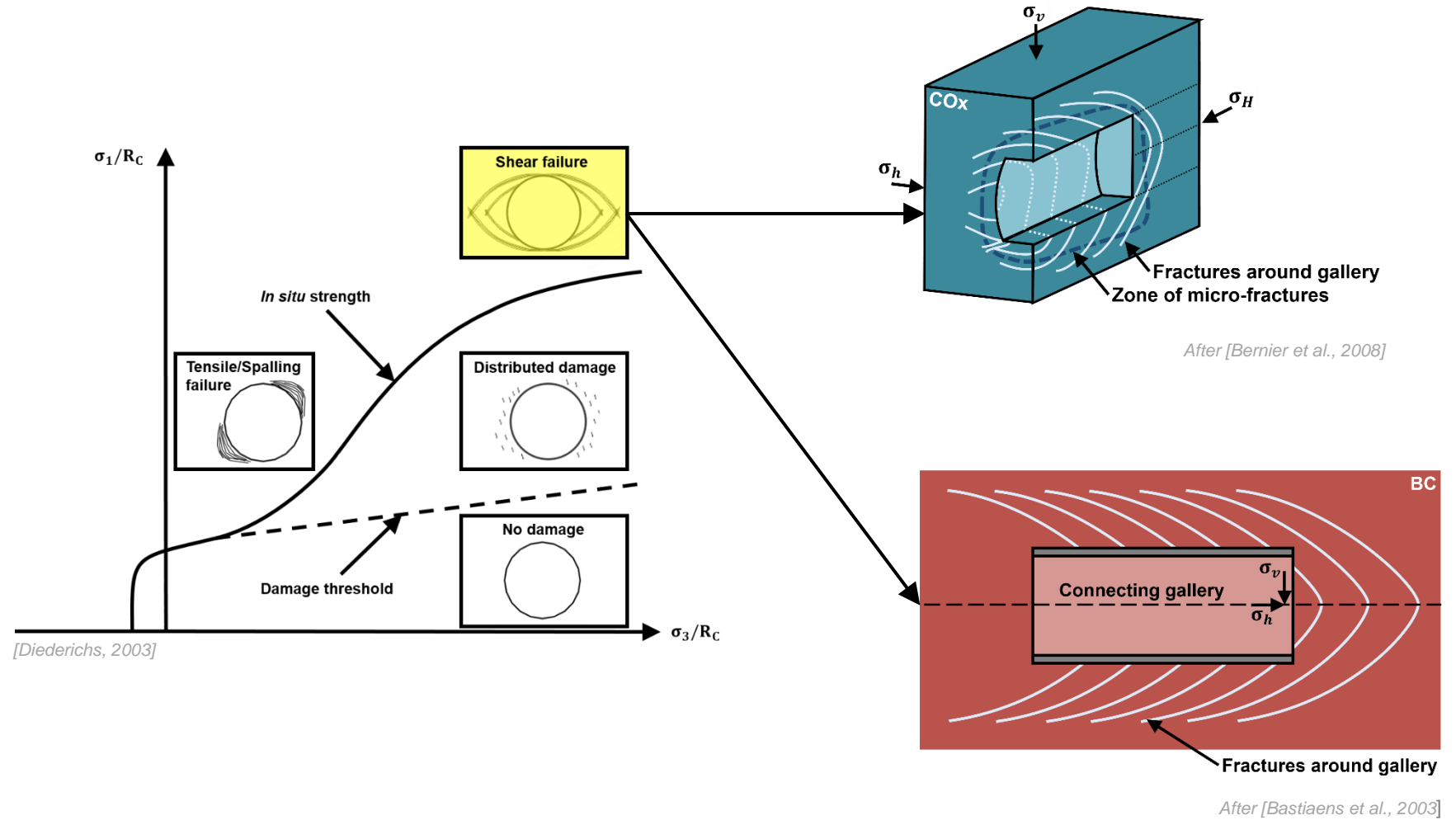
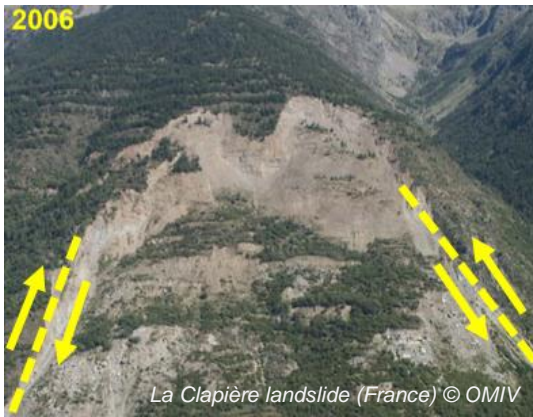
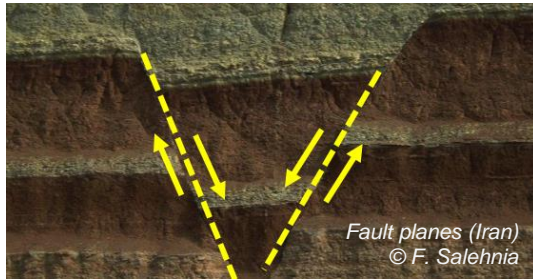
Fracturing process

From geomaterials failure to the drilling of underground galleries...



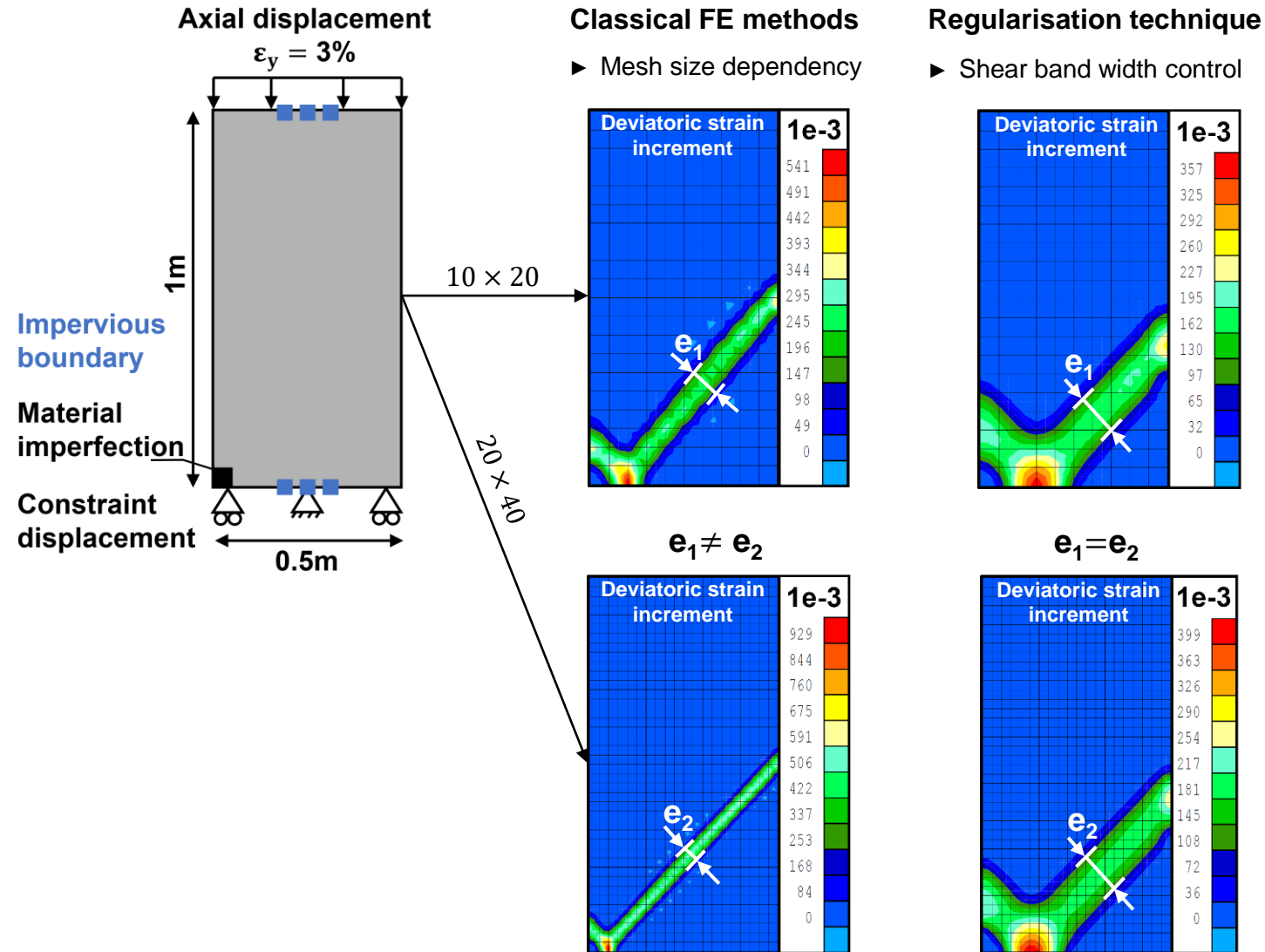
Fracturing process

From geomaterials failure to the drilling of underground galleries in clay host formations

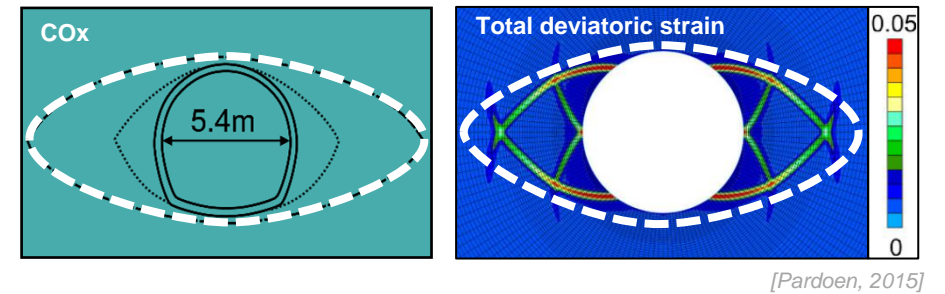
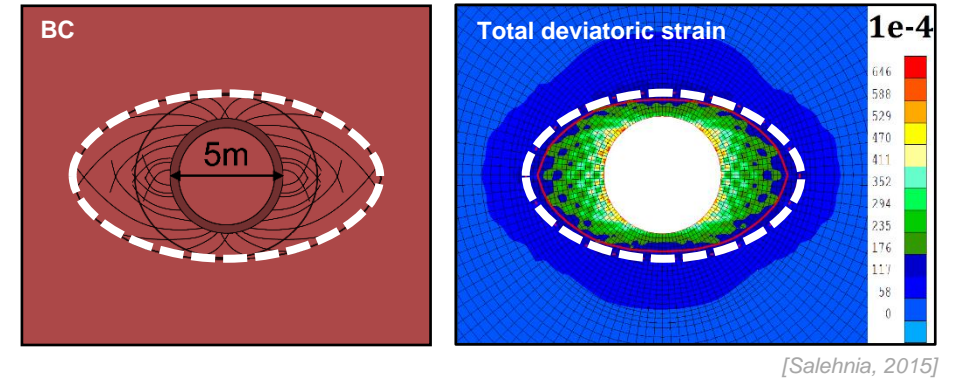


Second gradient H²M model

Shear strain localisation modelling

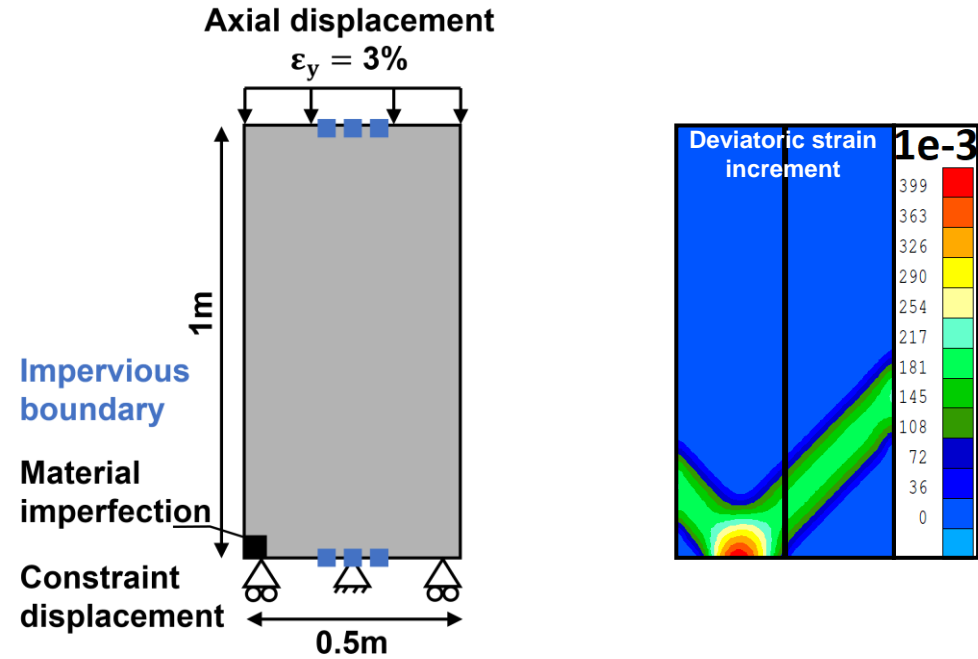


Numerical vs conceptual extension of the EDZ



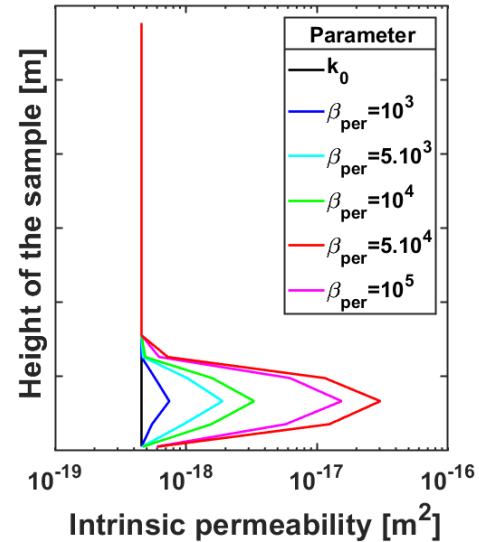
Second gradient H²M model

Advanced HM couplings



Intrinsic permeability

[Pardoen et al., 2014]



$$k_{ij} = k_{ij,0} (1 + \beta_{per} (YI - YI^{thr}) \hat{\epsilon}_{eq}^3)$$

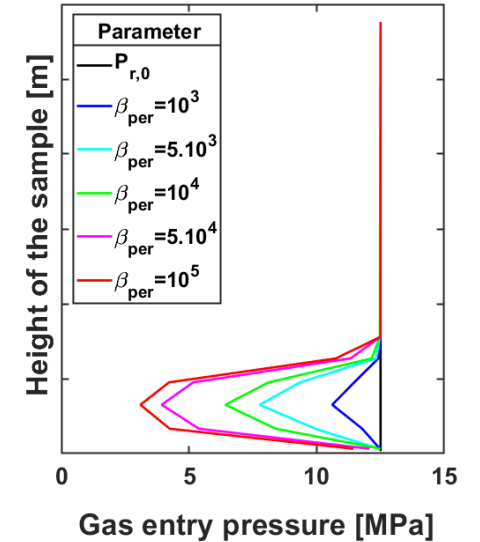
$\hat{\epsilon}_{eq}$: Von Mises' equivalent deviatoric plastic strain

β_{per} : evolution parameter

YI: yield index

Retention behaviour

[Olivella, 2008]

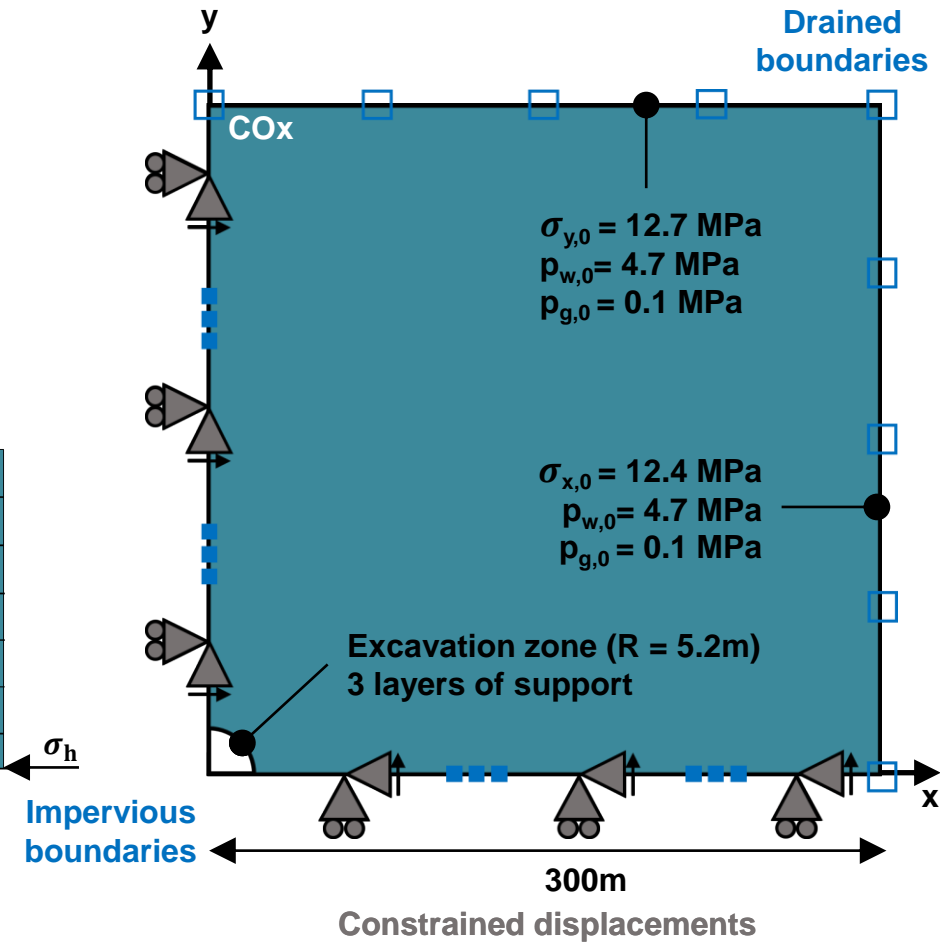
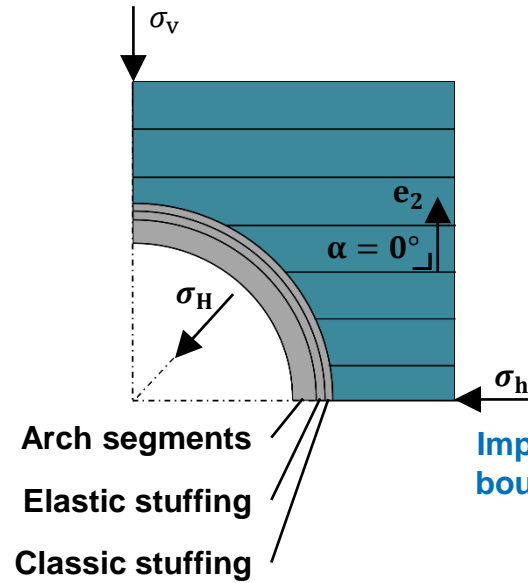
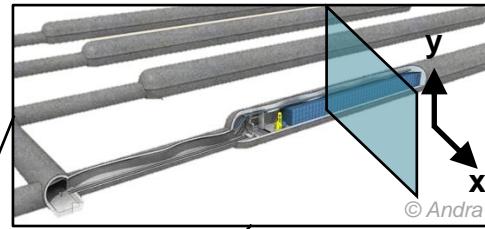
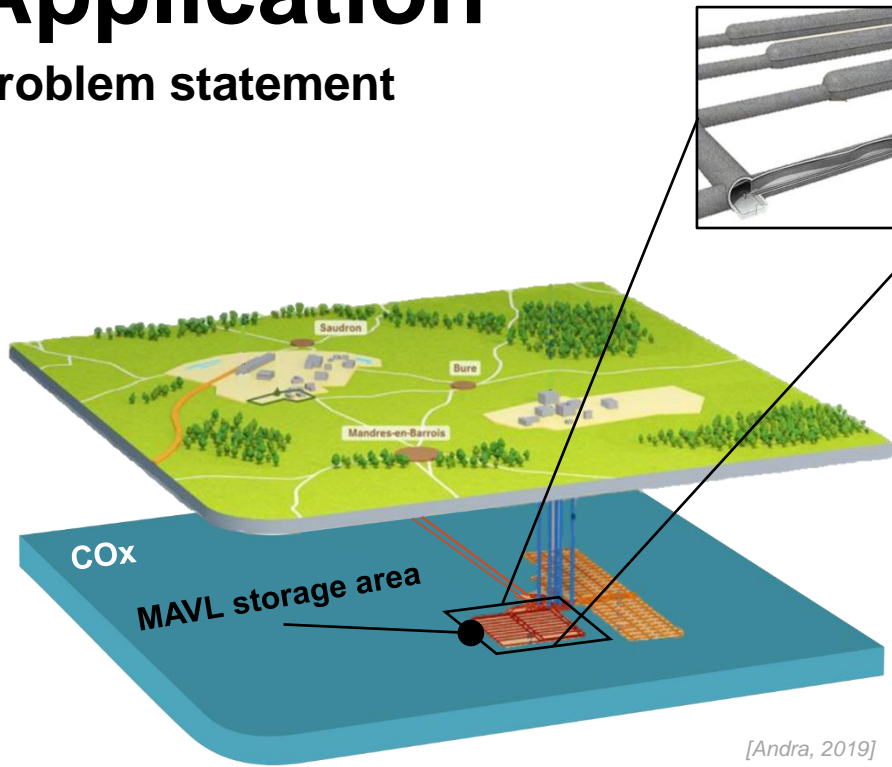


$$P_r = P_{r,0} \frac{\sqrt[3]{k_{ij,0}}}{\sqrt[3]{k_{ij}}}$$

P_r : van Genuchten's parameter identified as the entry pressure

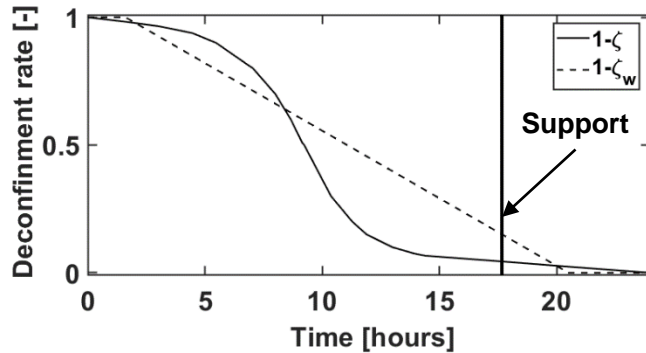
Application

Problem statement

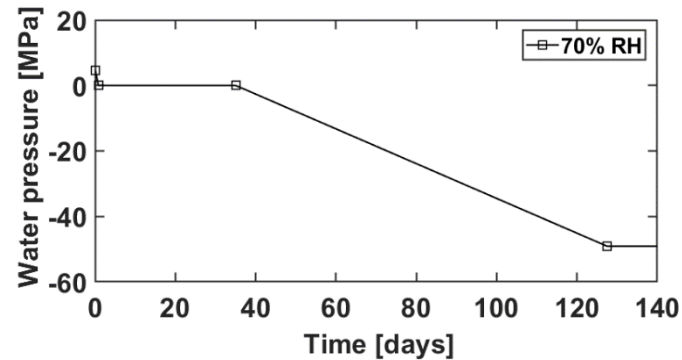


Three-step simulations

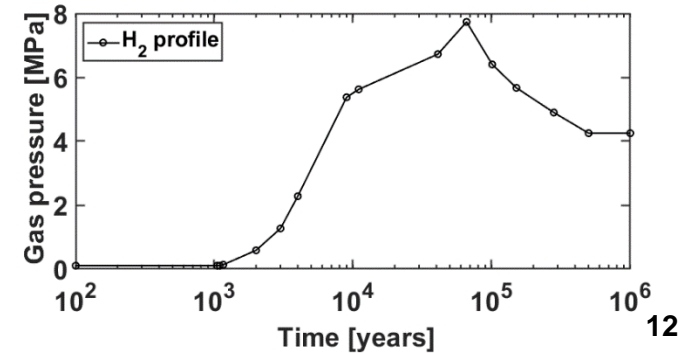
1 Excavation phase



2 Operation phase

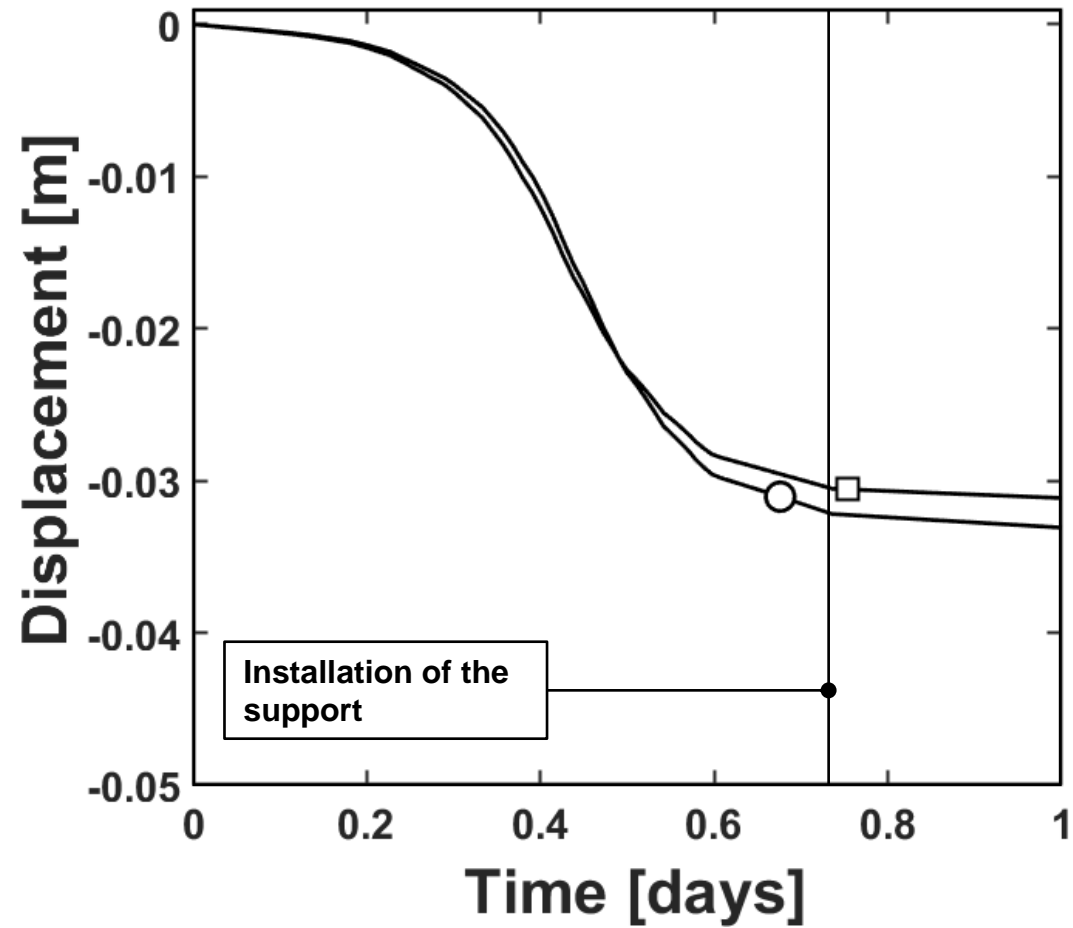


3 Gas migration phase



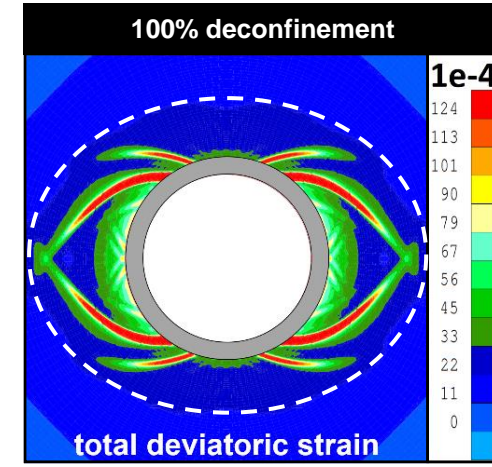
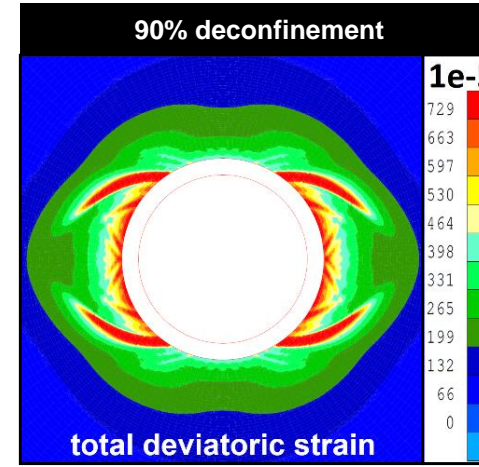
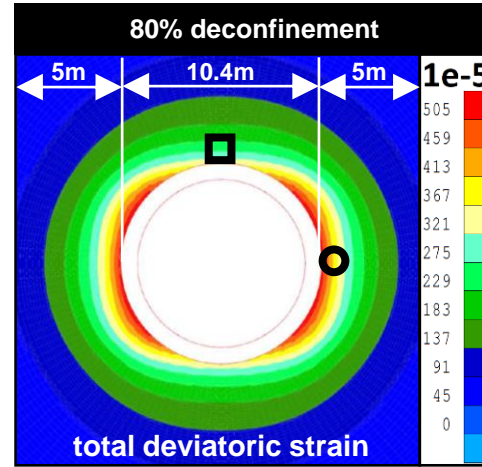
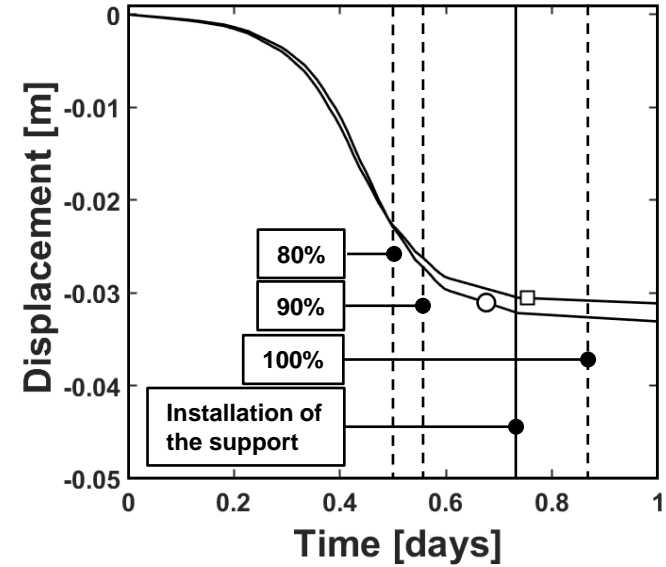
Application

Convergence of the rock mass



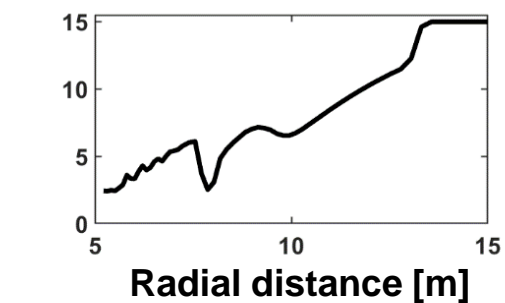
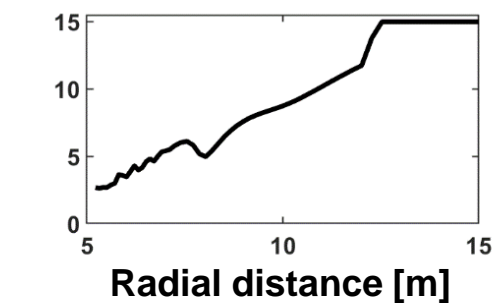
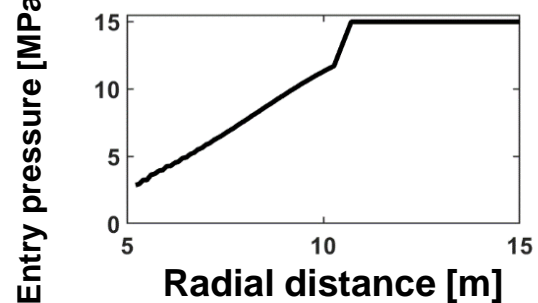
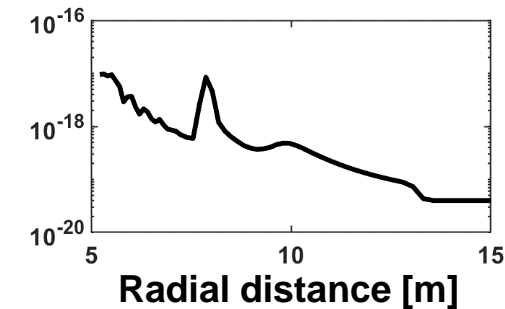
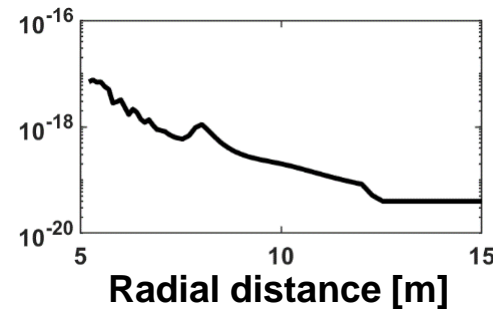
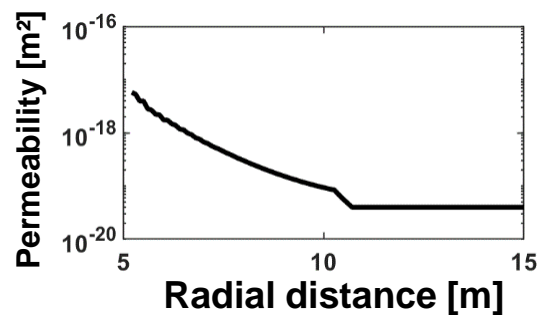
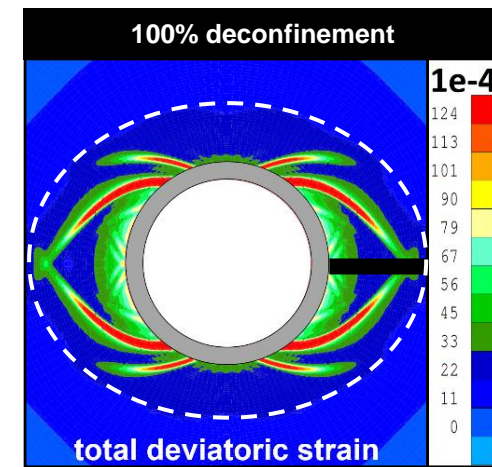
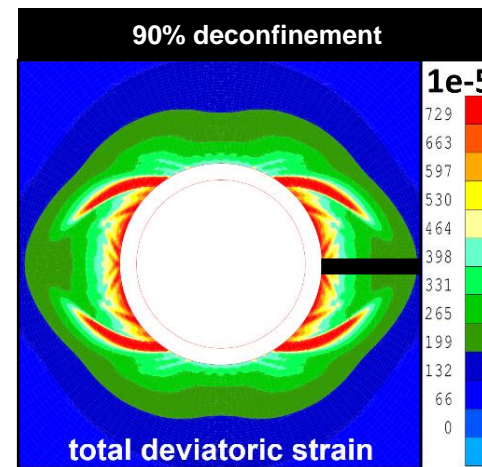
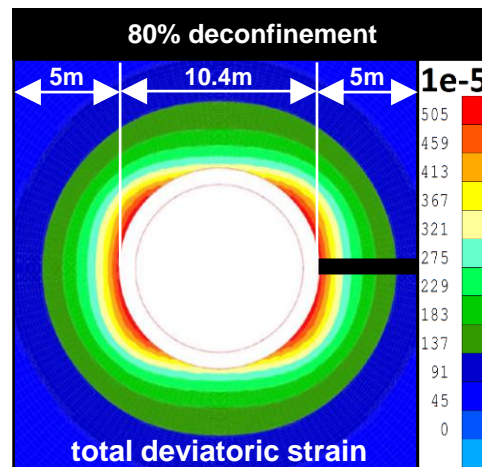
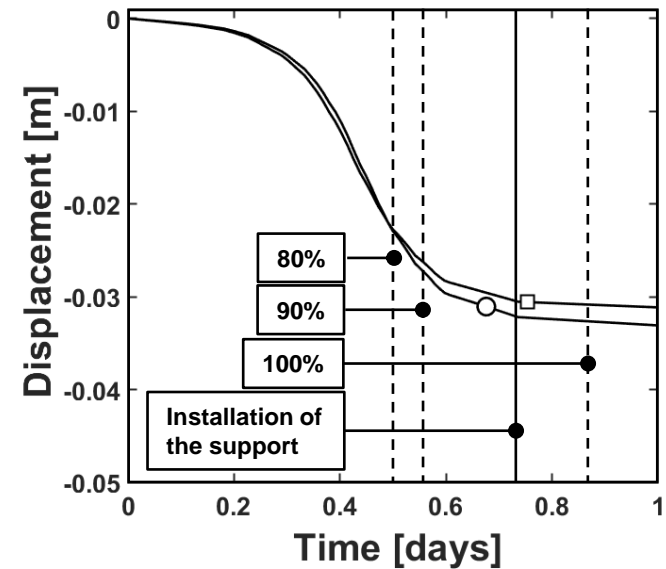
Application

Development of plasticity in the near field



Application

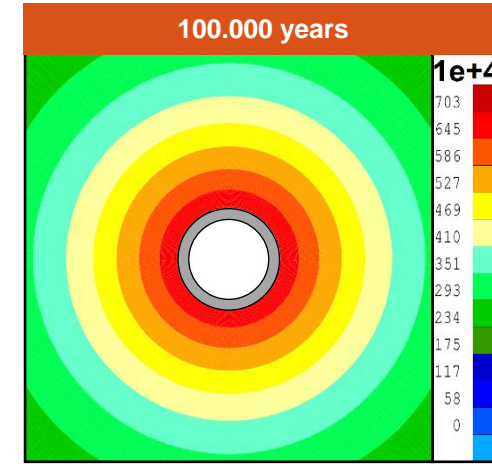
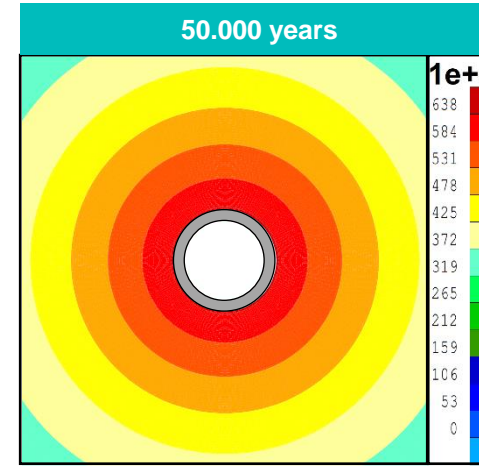
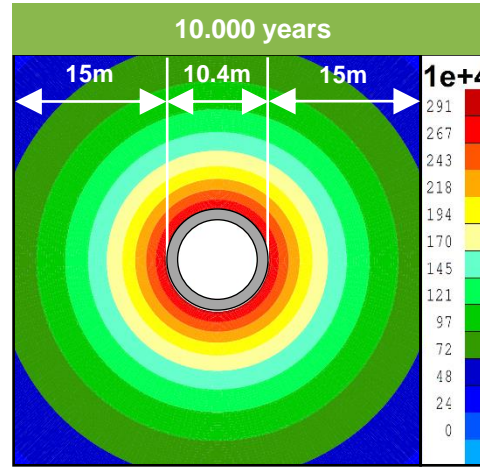
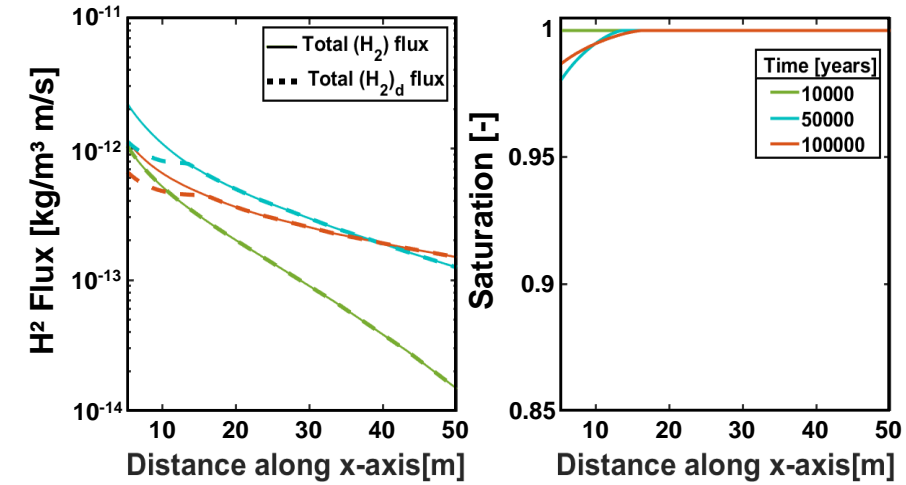
Development of plasticity in the near field



Application

Maps of gas (H_2) pressure evolution

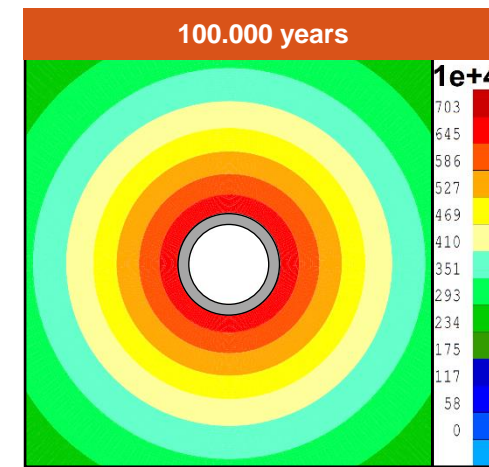
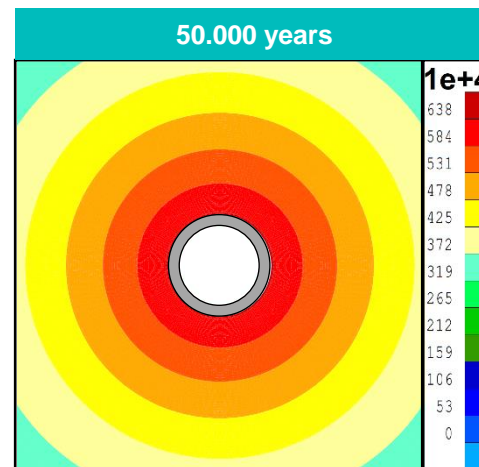
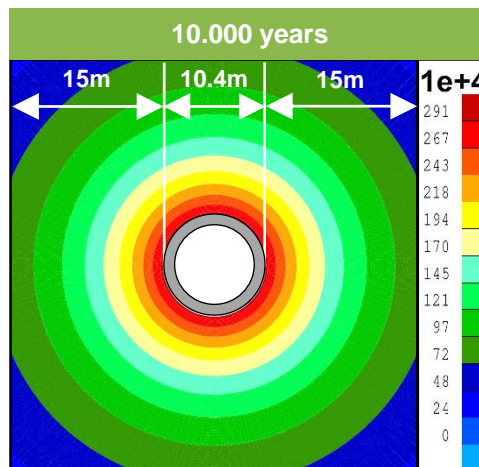
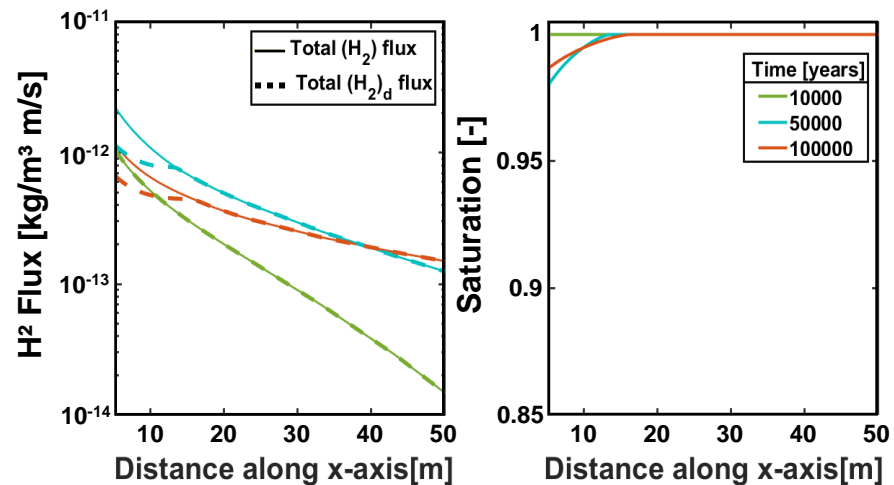
No evolution of transfer properties



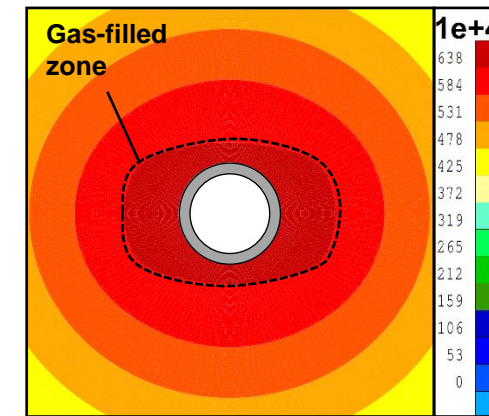
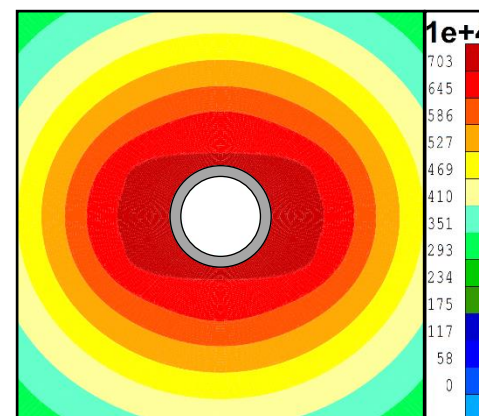
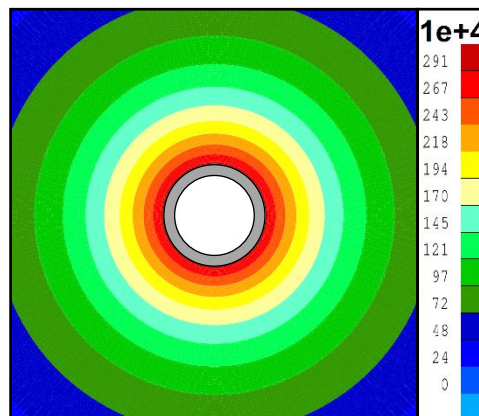
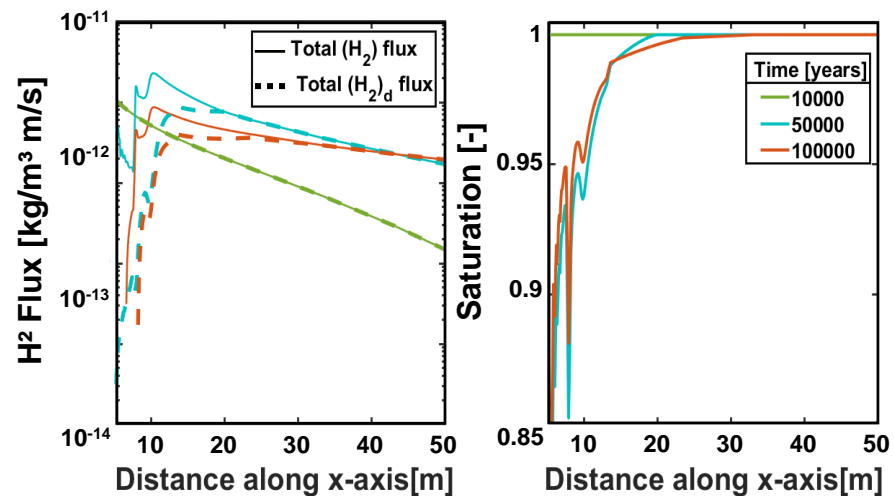
Application

Maps of gas (H_2) pressure evolution

No evolution of transfer properties



Evolution of transfer properties with strains



01

**Characterisation of gas
transport processes**

Introduction

02

**Modelling gas transport
in the EDZ**

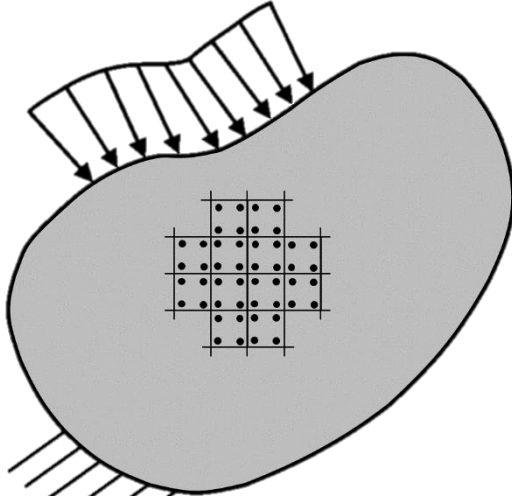
Conclusion

03

**Modelling gas transport
in sound rocks**

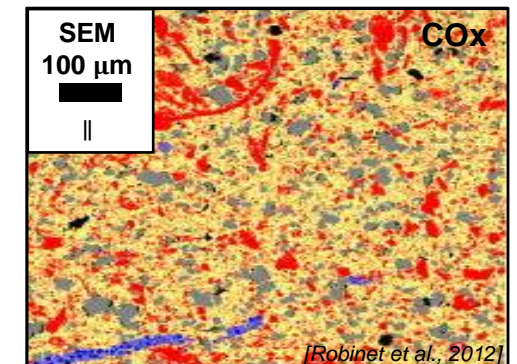
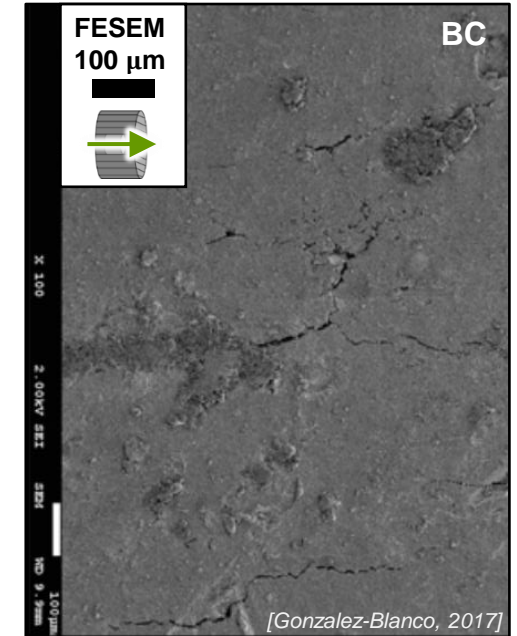
Hydro-mechanical multi-scale model

Macro-scale



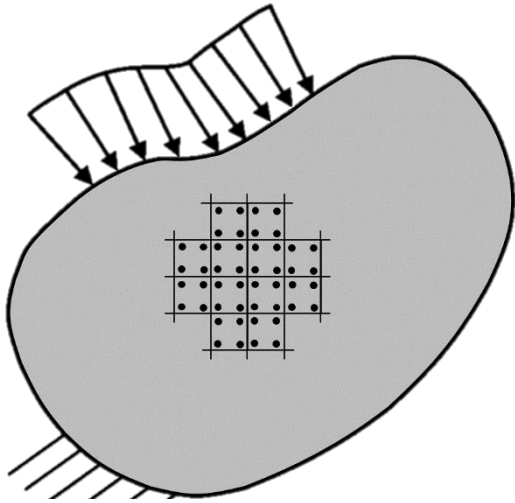
Micro-scale

Data-supported microstructure



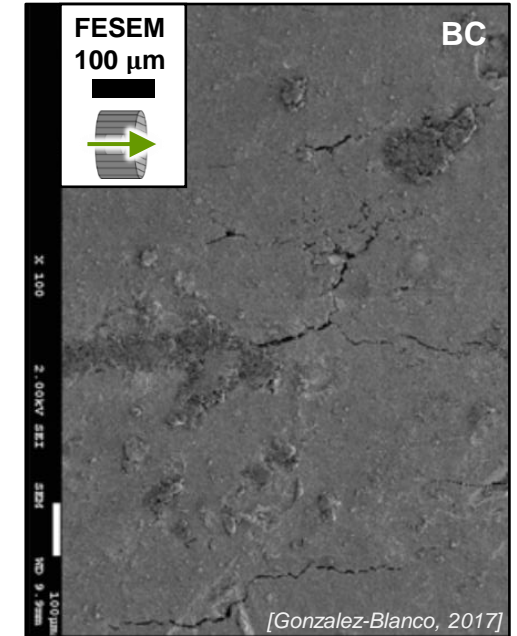
Hydro-mechanical multi-scale model

Macro-scale

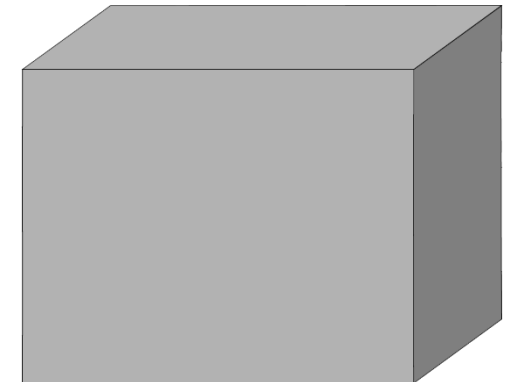


Micro-scale

Data-supported microstructure

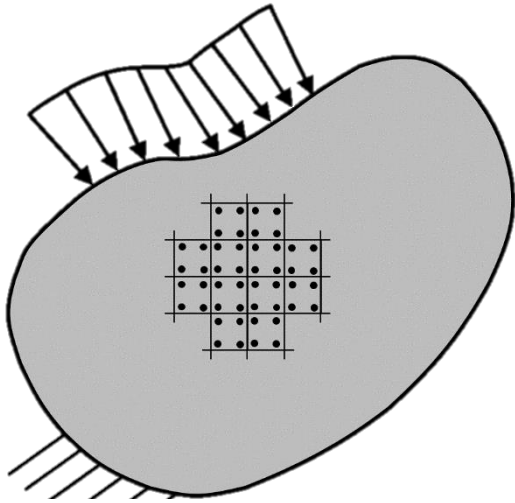


Physical idealisation



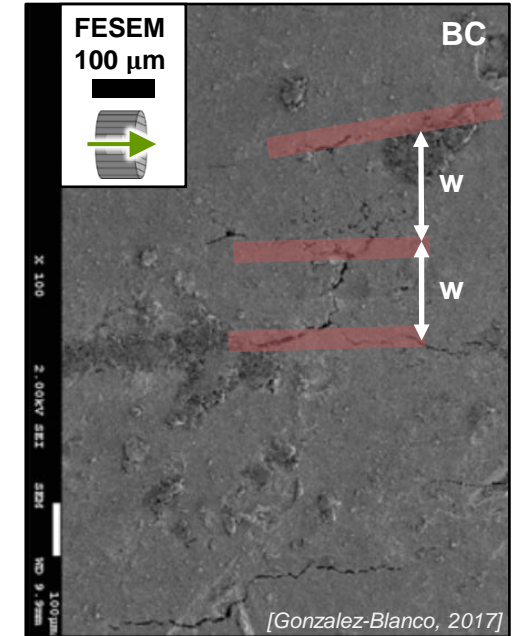
Hydro-mechanical multi-scale model

Macro-scale

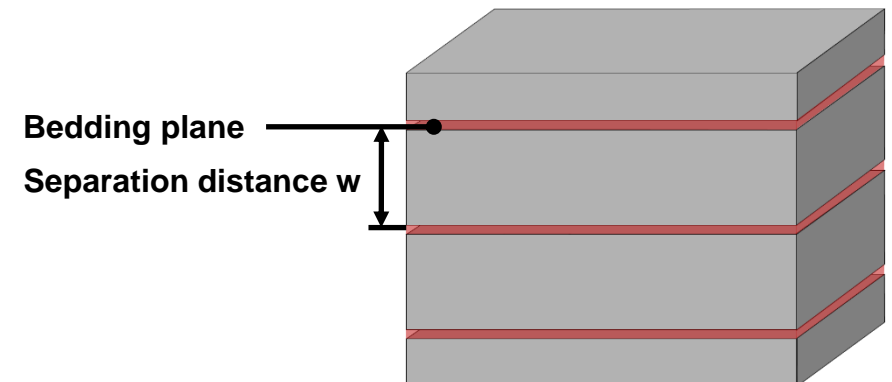


Micro-scale

Data-supported microstructure

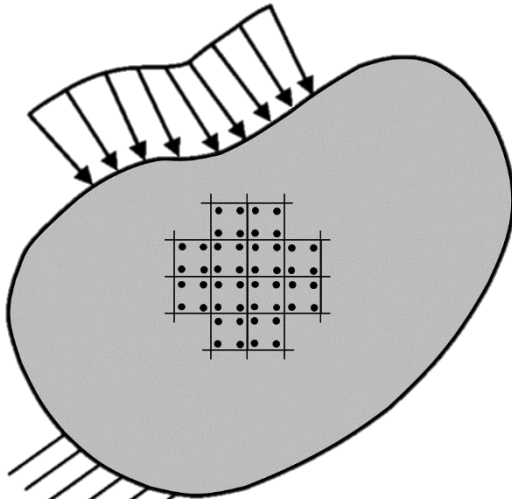


Physical idealisation



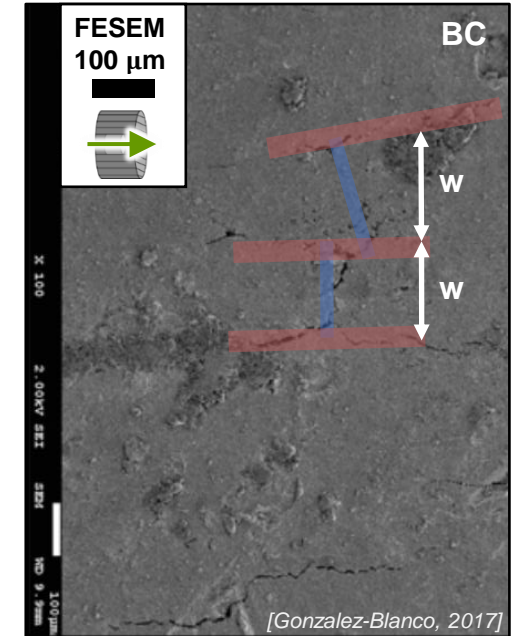
Hydro-mechanical multi-scale model

Macro-scale

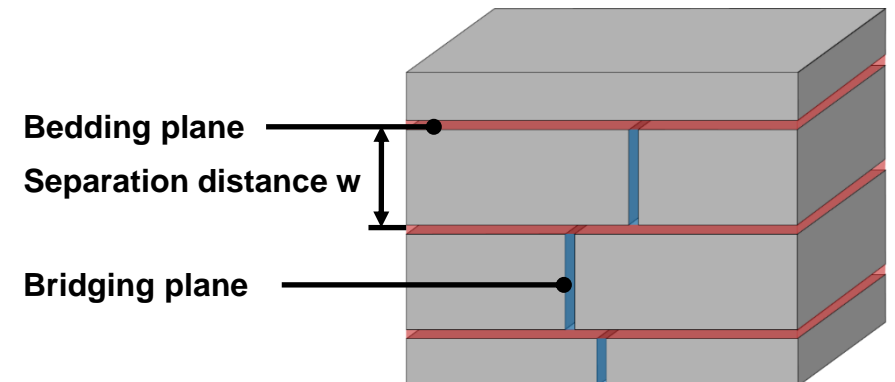


Micro-scale

Data-supported microstructure

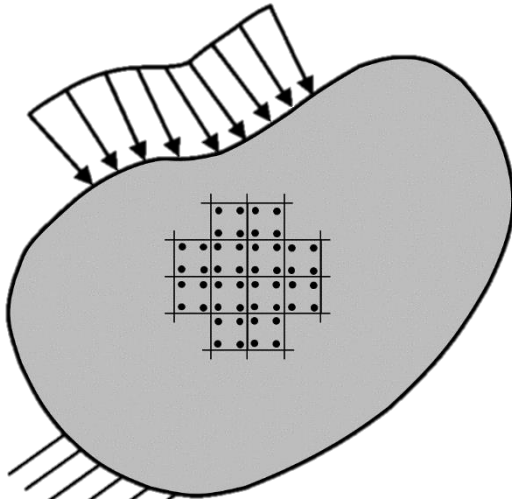


Physical idealisation



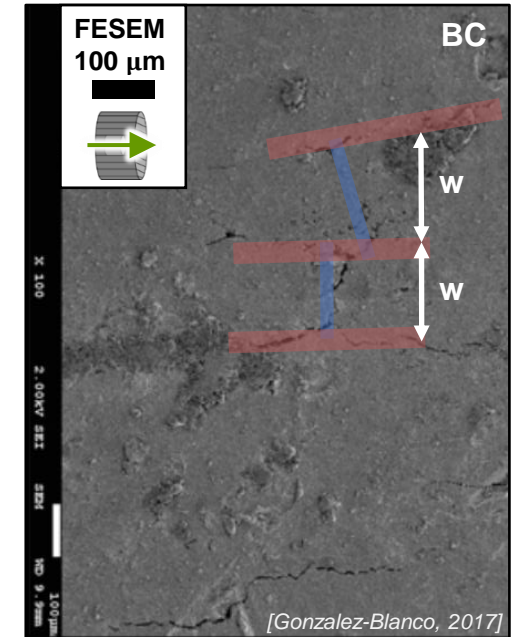
Hydro-mechanical multi-scale model

Macro-scale

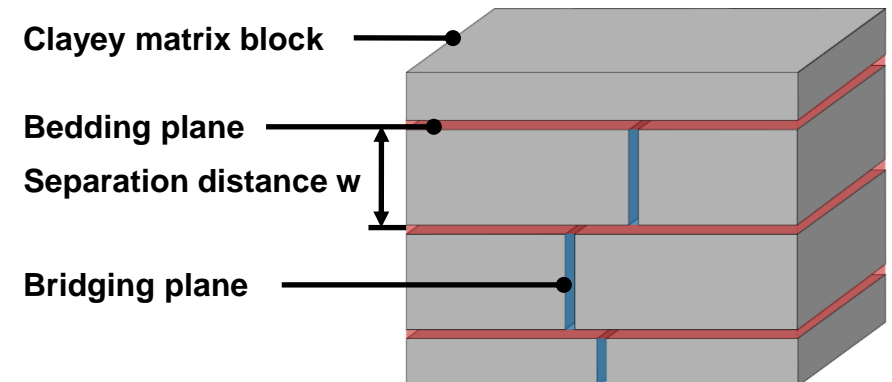


Micro-scale

Data-supported microstructure

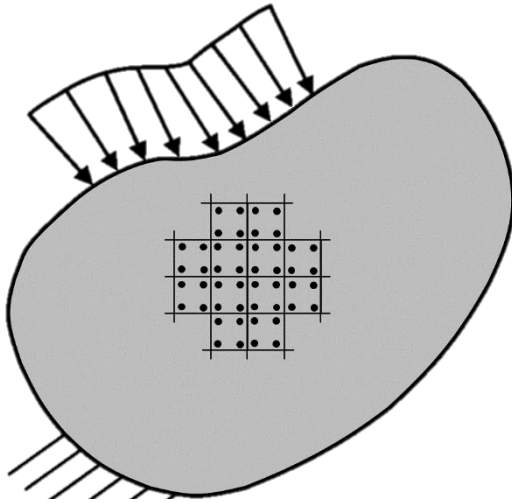


Physical idealisation

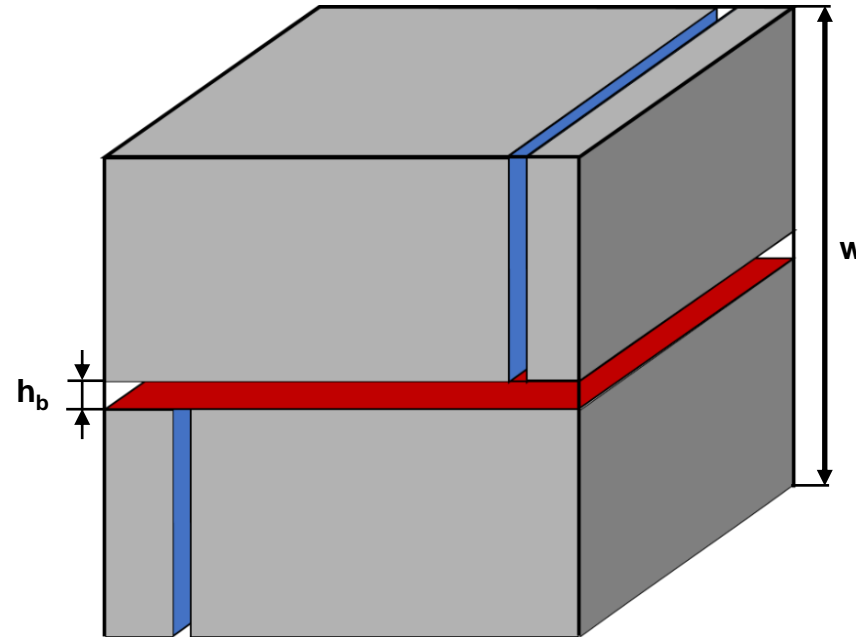


Hydro-mechanical multi-scale model

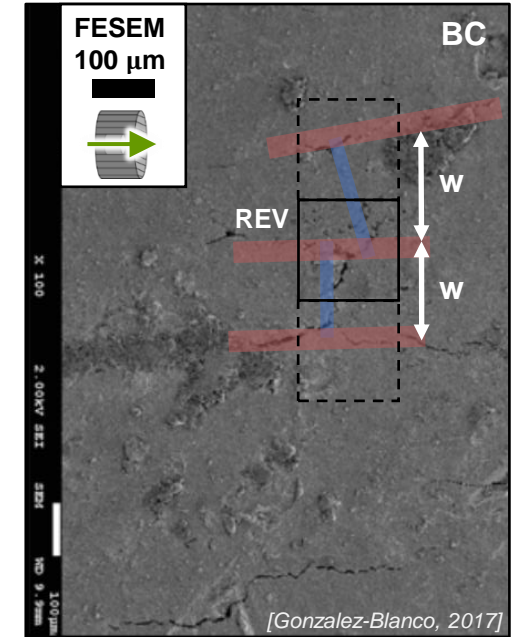
Macro-scale



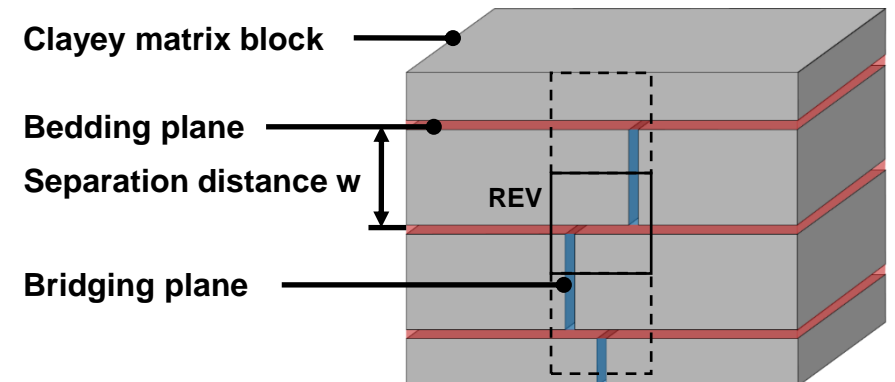
Micro-scale (REV)



Data-supported microstructure



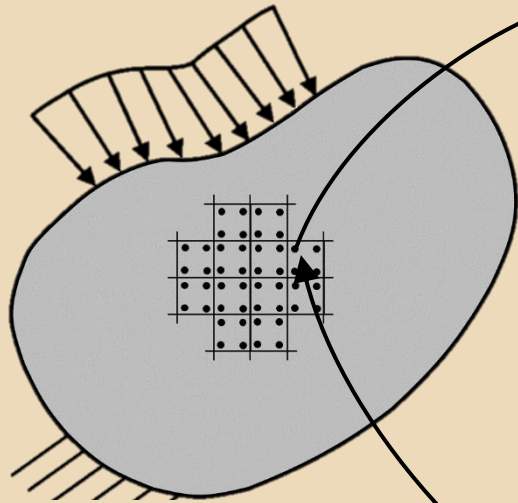
Physical idealisation



Hydro-mechanical multi-scale model

Macro-scale

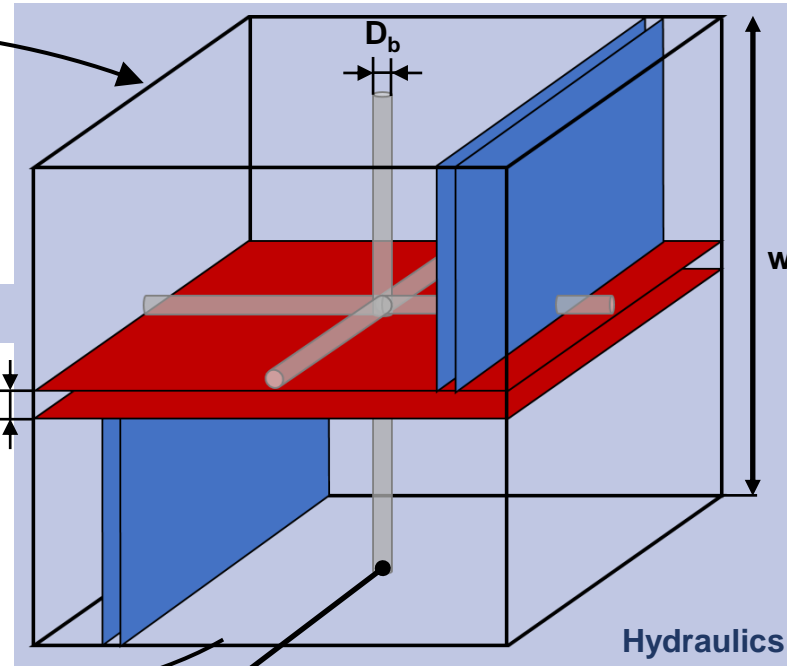
Mechanics



4. Macro-scale FE computations

1. Localisation

Micro-scale (REV)

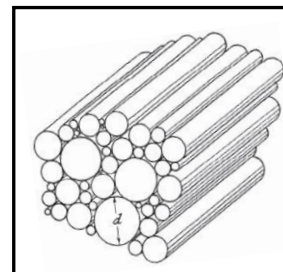


HM couplings

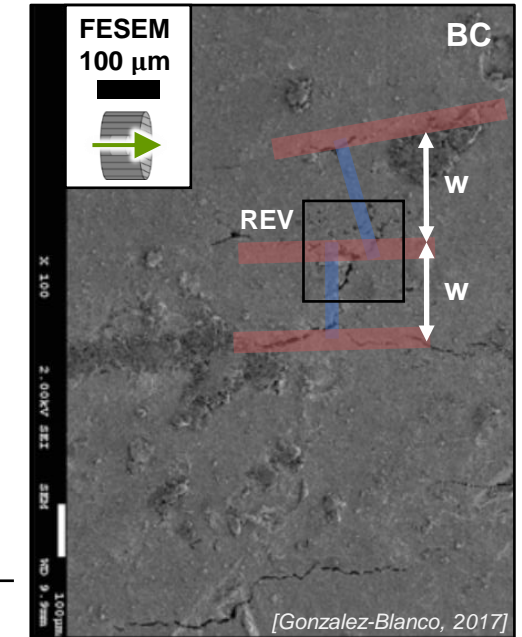
2. Resolution of the hydraulic system

3. Homogenisation

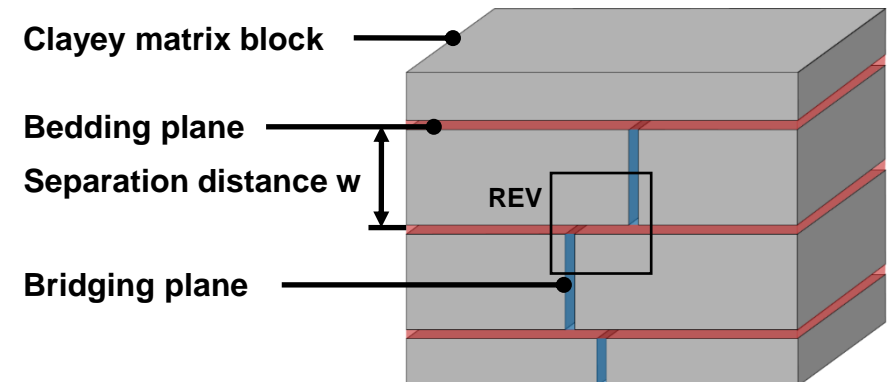
Equivalent bundle of tubes



Data-supported microstructure

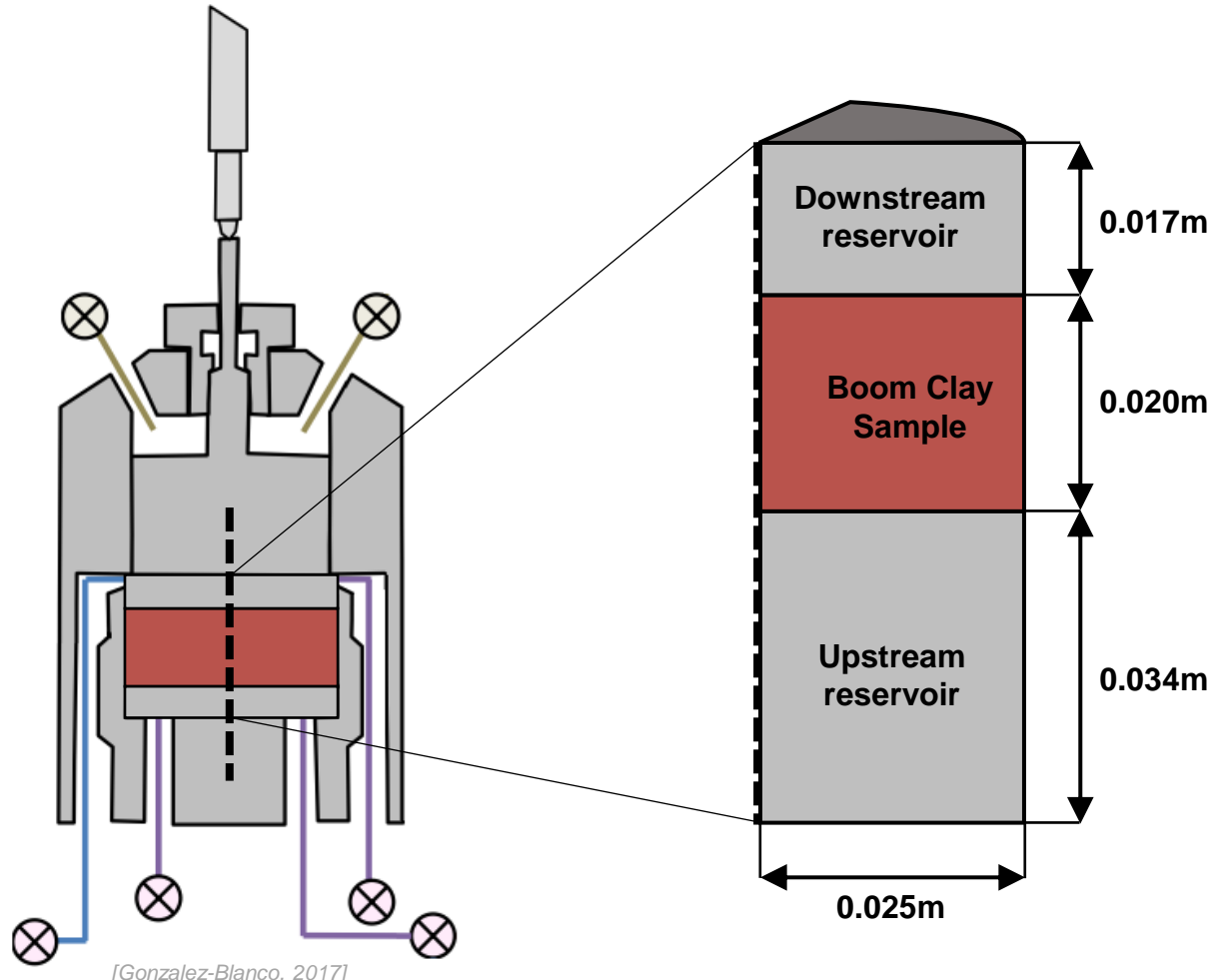


Physical idealisation



Gas injection test modelling

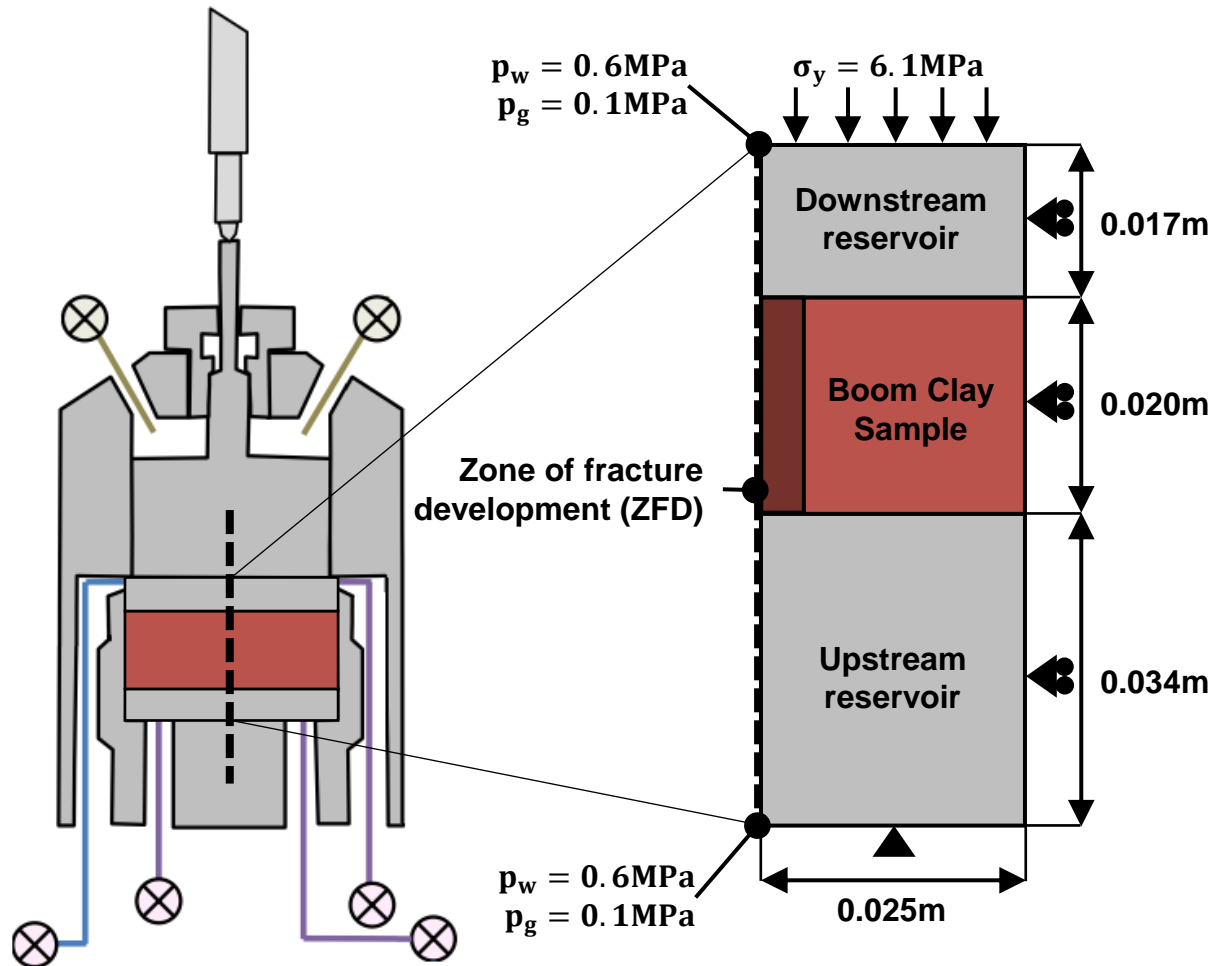
Problem statement



[Gonzalez-Blanco, 2017]

Gas injection test modelling

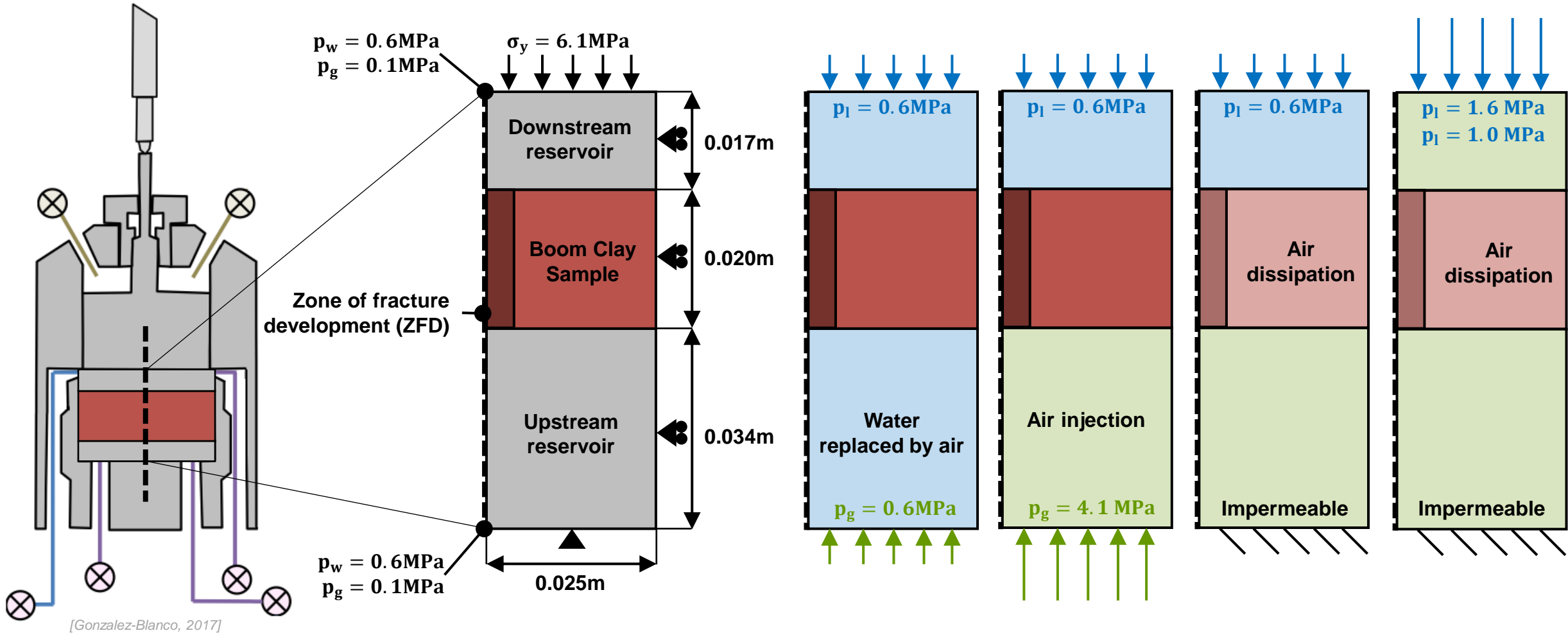
Problem statement



[Gonzalez-Blanco, 2017]

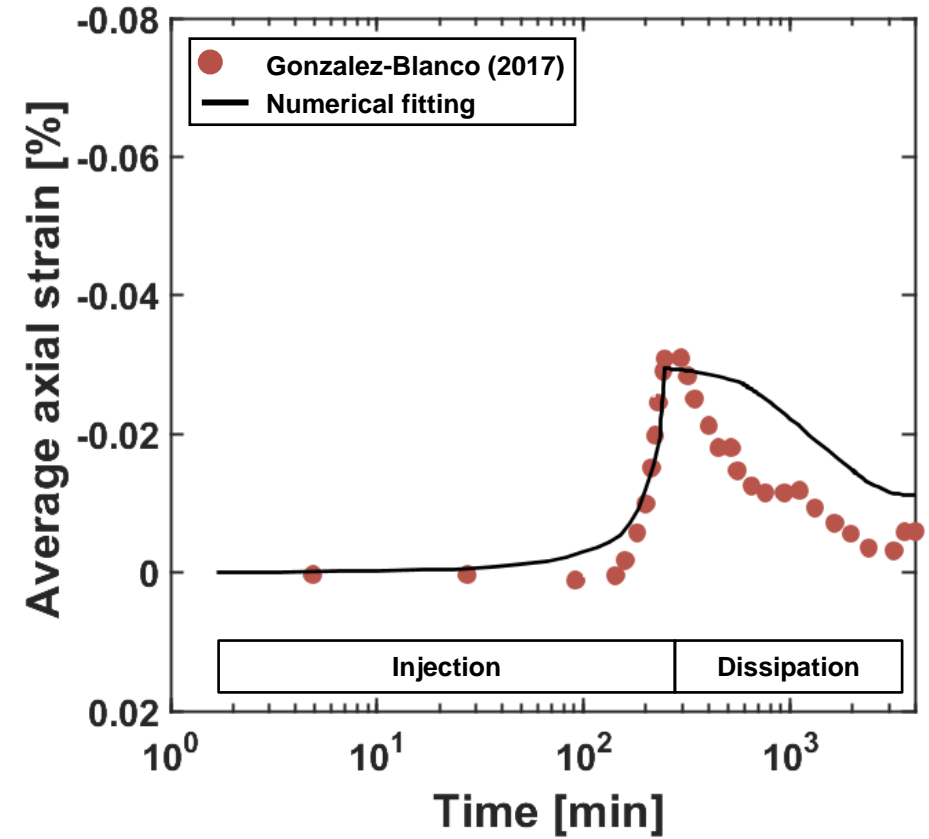
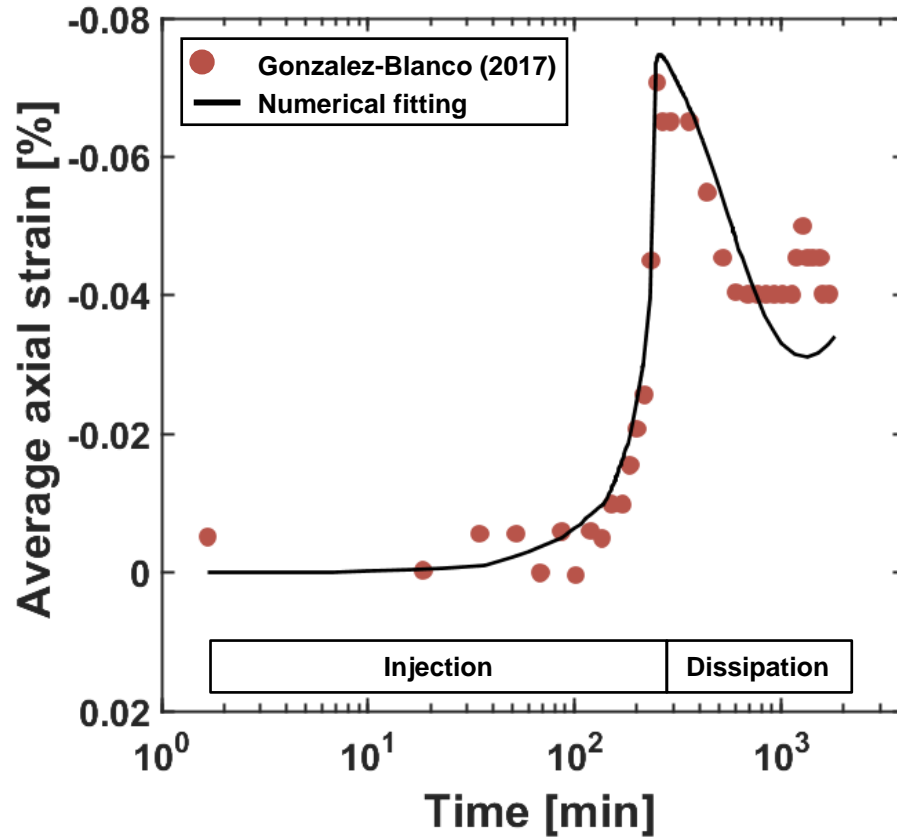
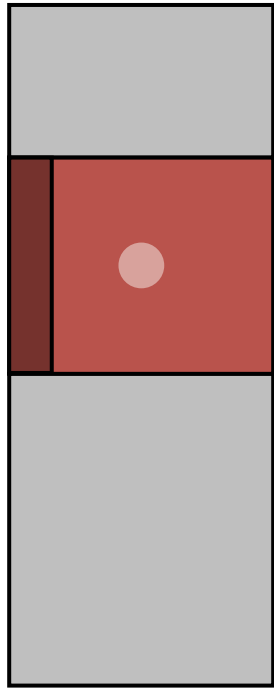
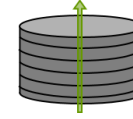
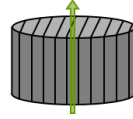
Gas injection test modelling

Problem statement



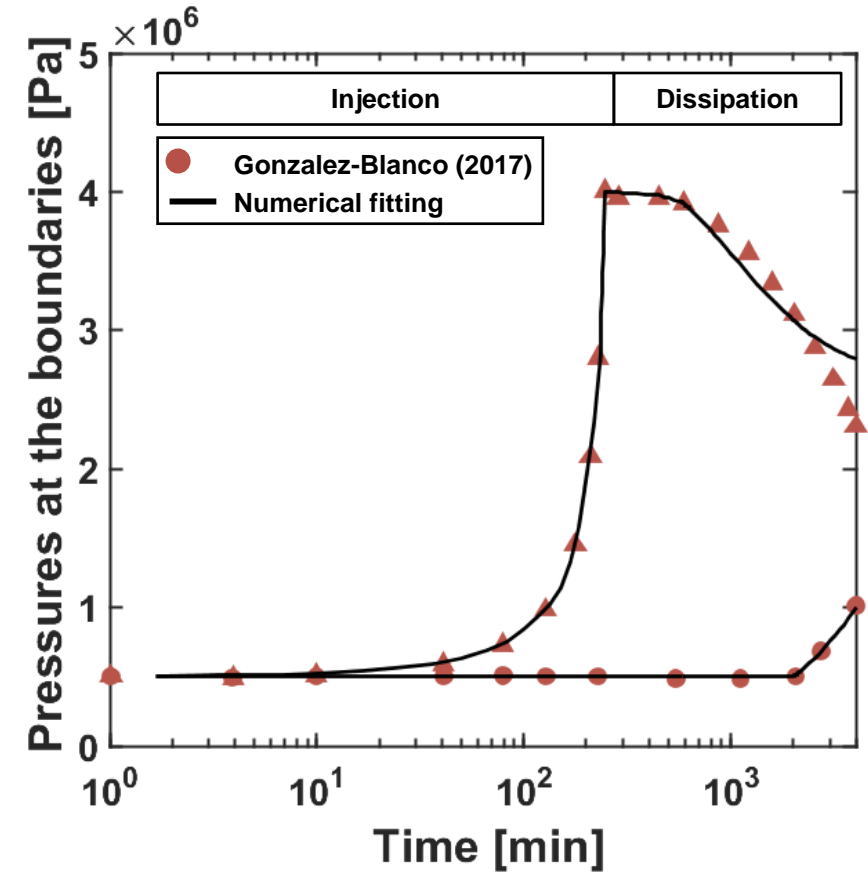
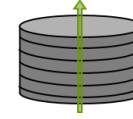
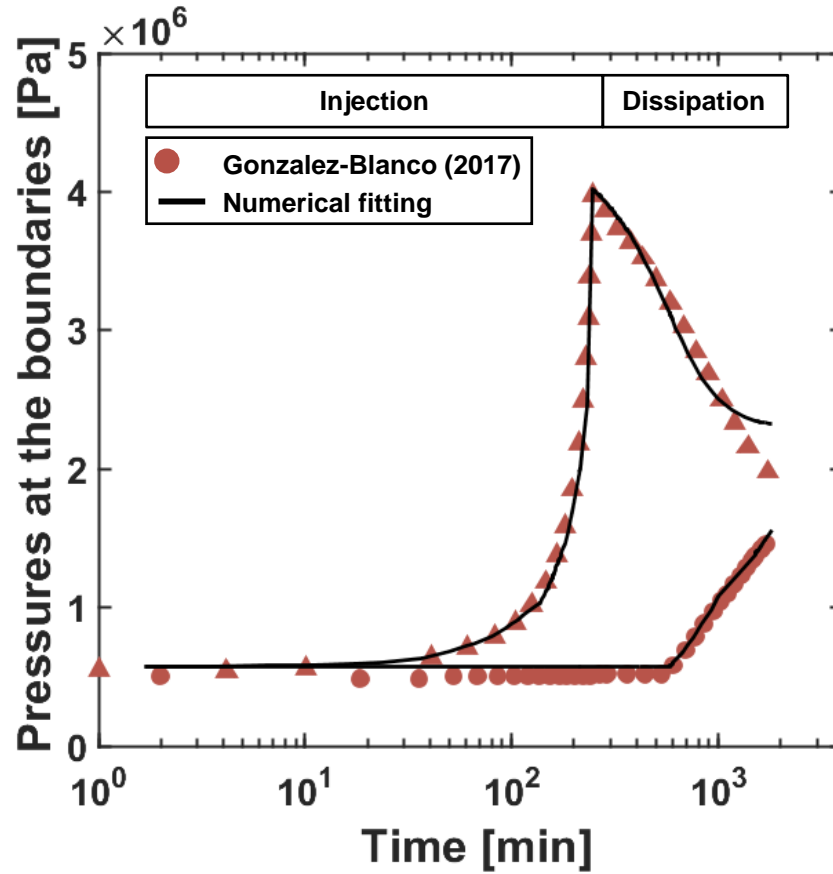
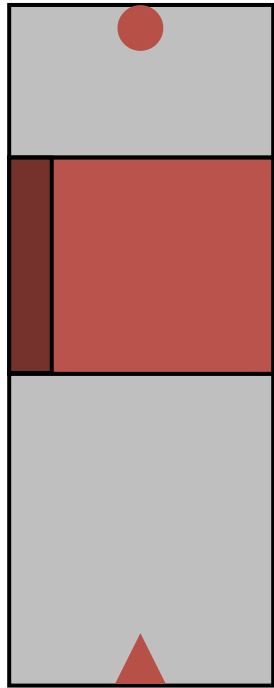
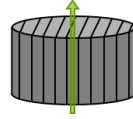
Gas injection test modelling

Average axial strain



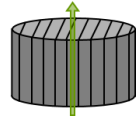
Gas injection test modelling

Injection and recovery pressure

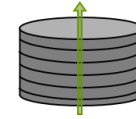
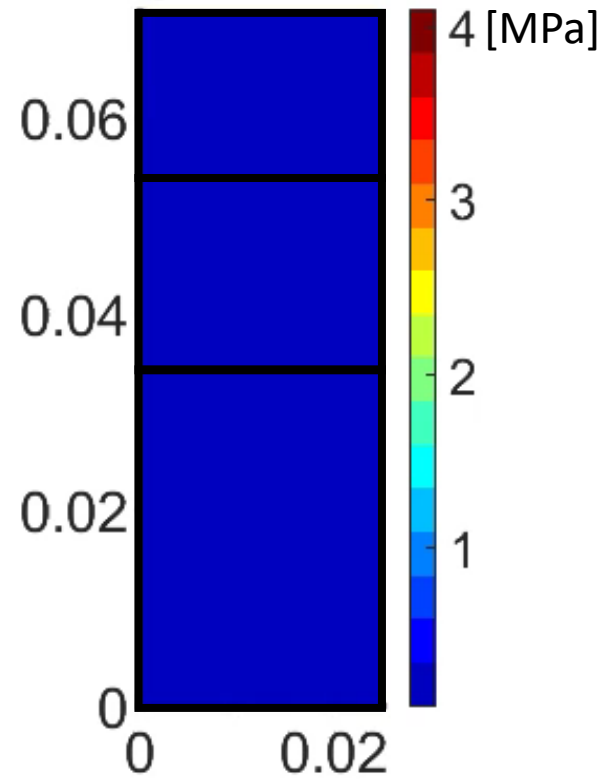


Gas injection test modelling

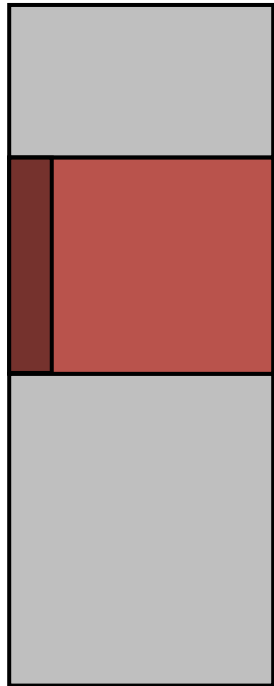
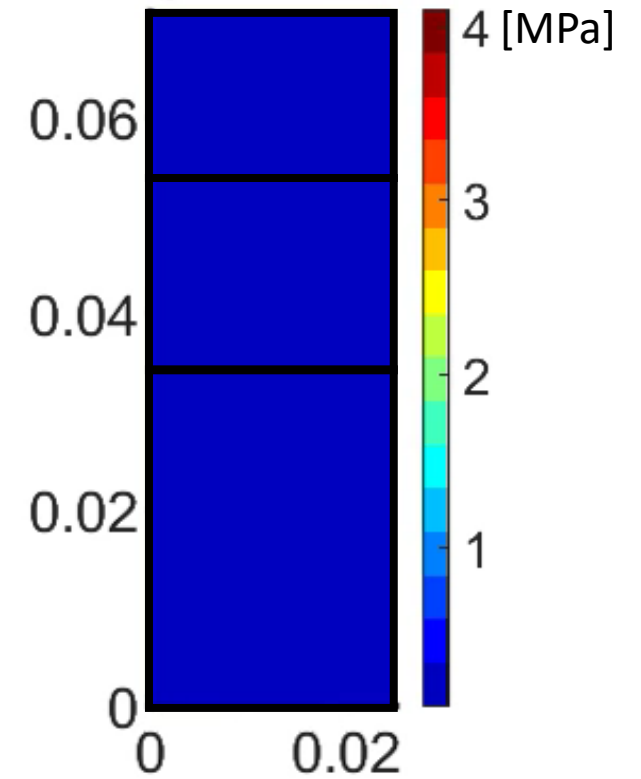
Maps of gas pressure



P_g at 100s.

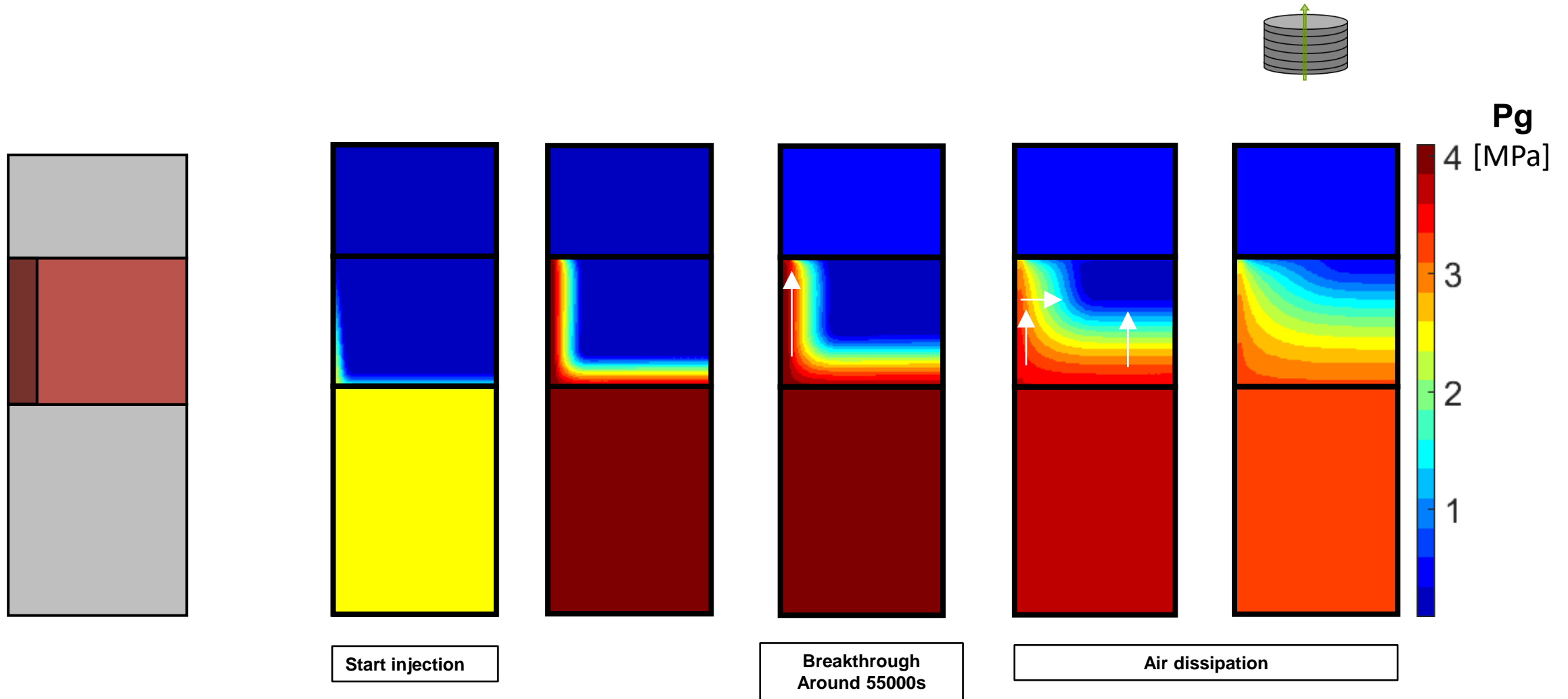


P_g at 100s.



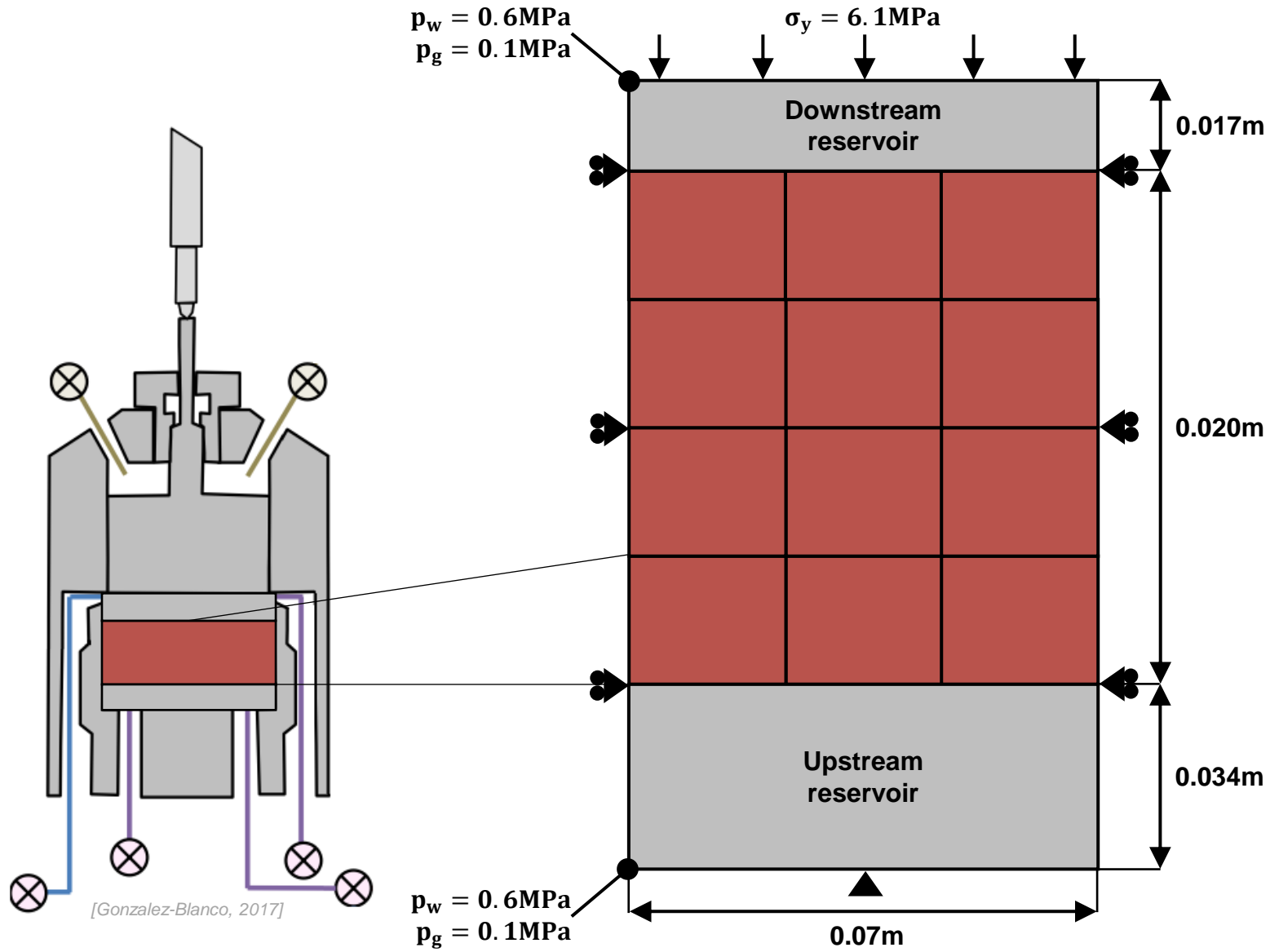
Gas injection test modelling

Maps of gas pressure



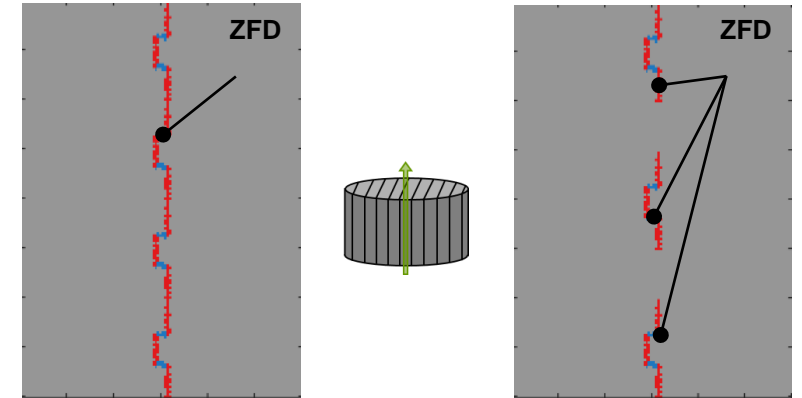
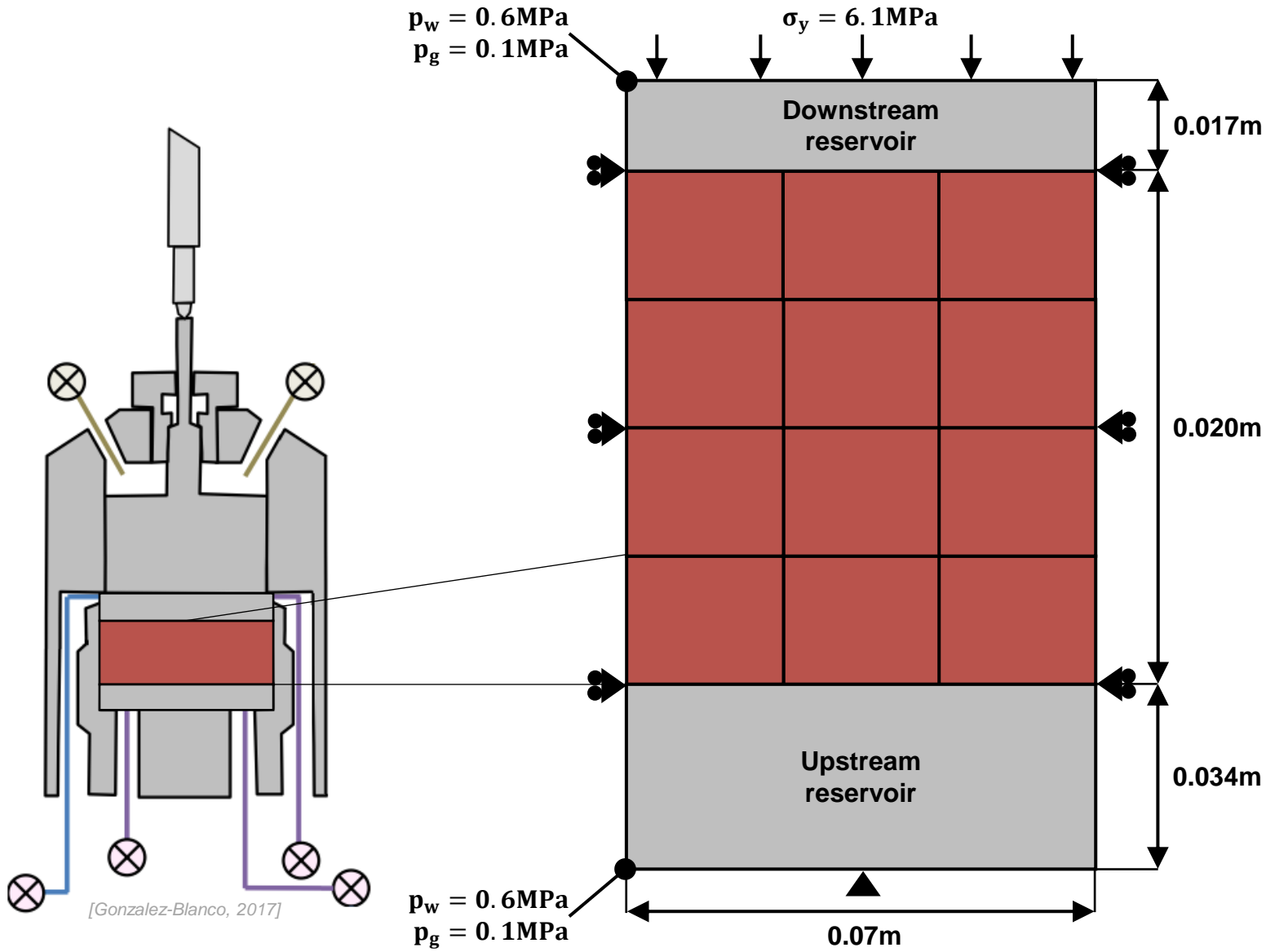
Up-scaled configuration modelling

Problem statement



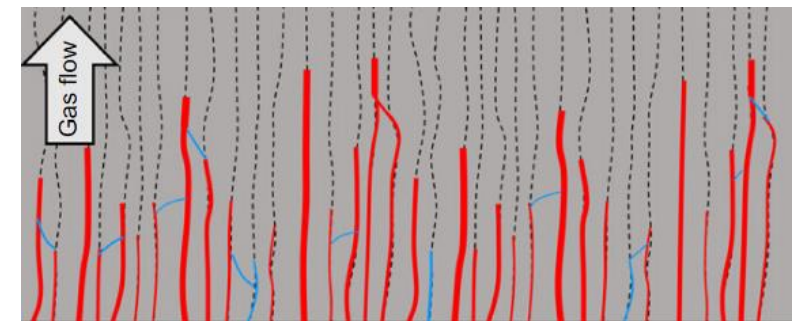
Up-scaled configuration modelling

Problem statement



- Undisturbed Boom Clay
- Disturbed bridging planes
- Disturbed bridging planes
- ⋯ Undamaged planes

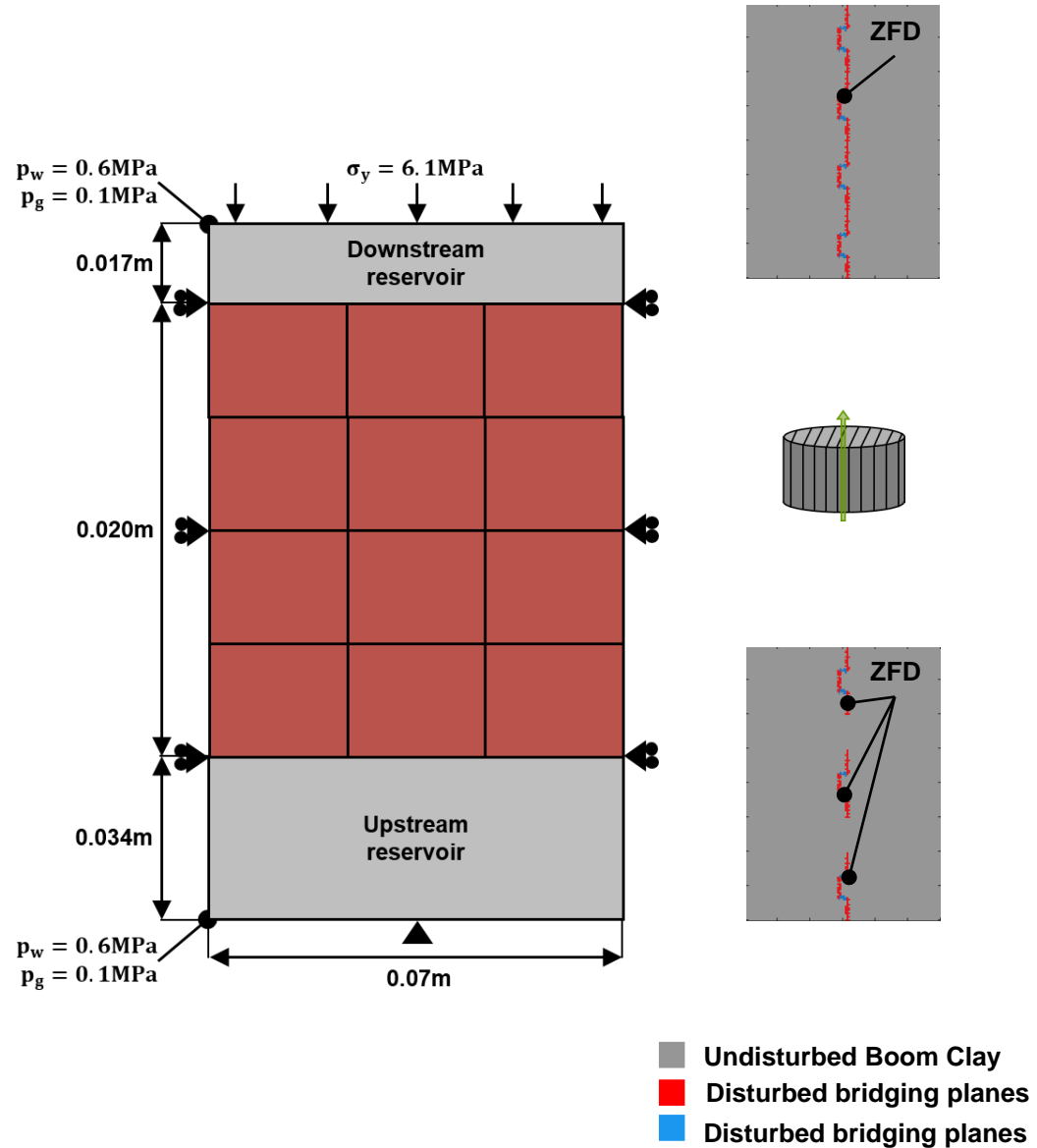
Conceptualisation



[Gonzalez-Blanco, 2017]

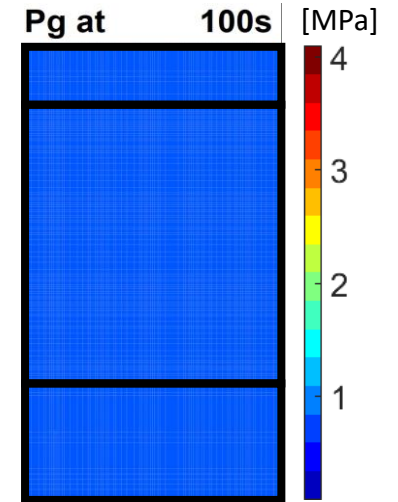
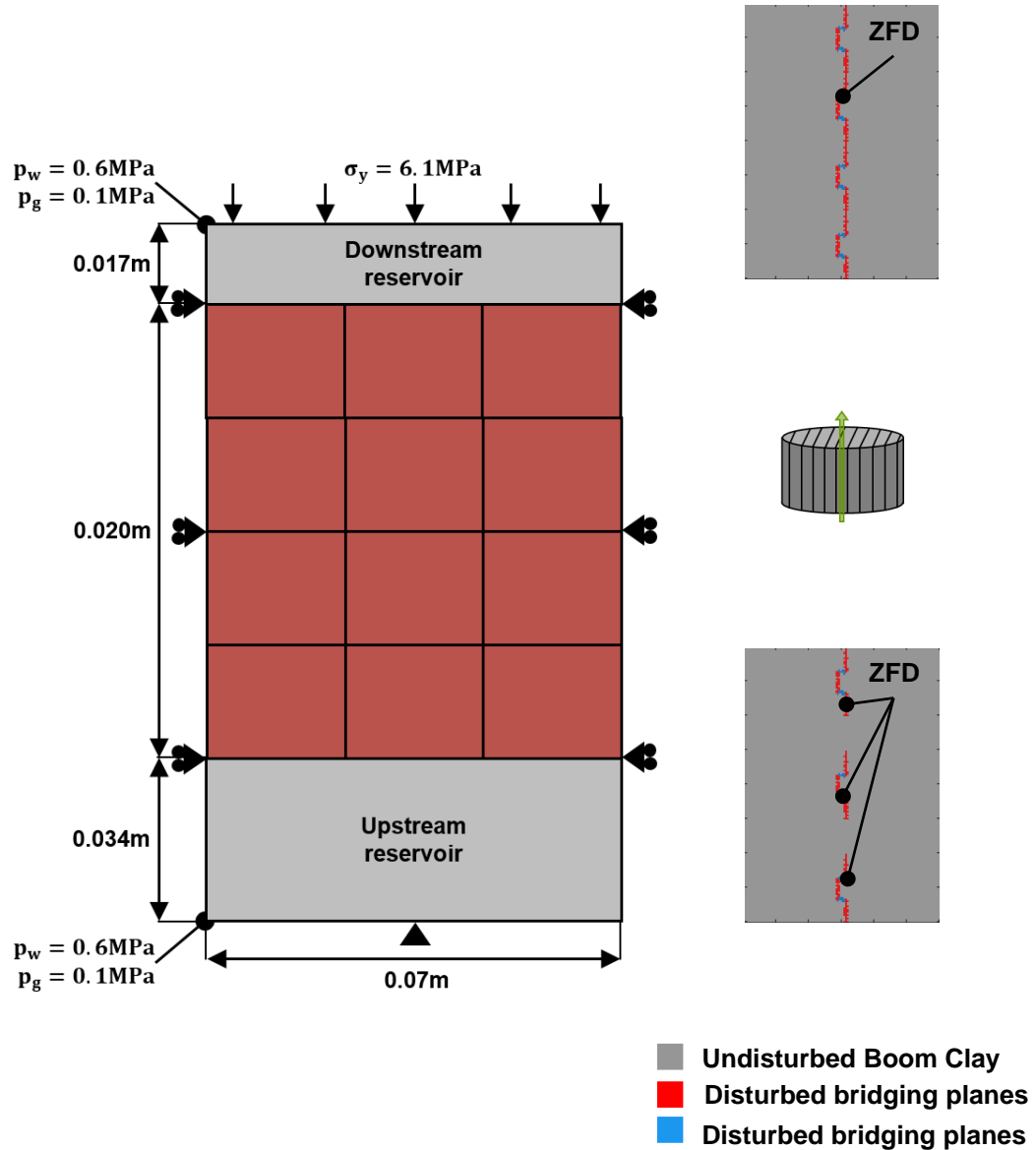
Up-scaled configuration modelling

Maps of gas pressure



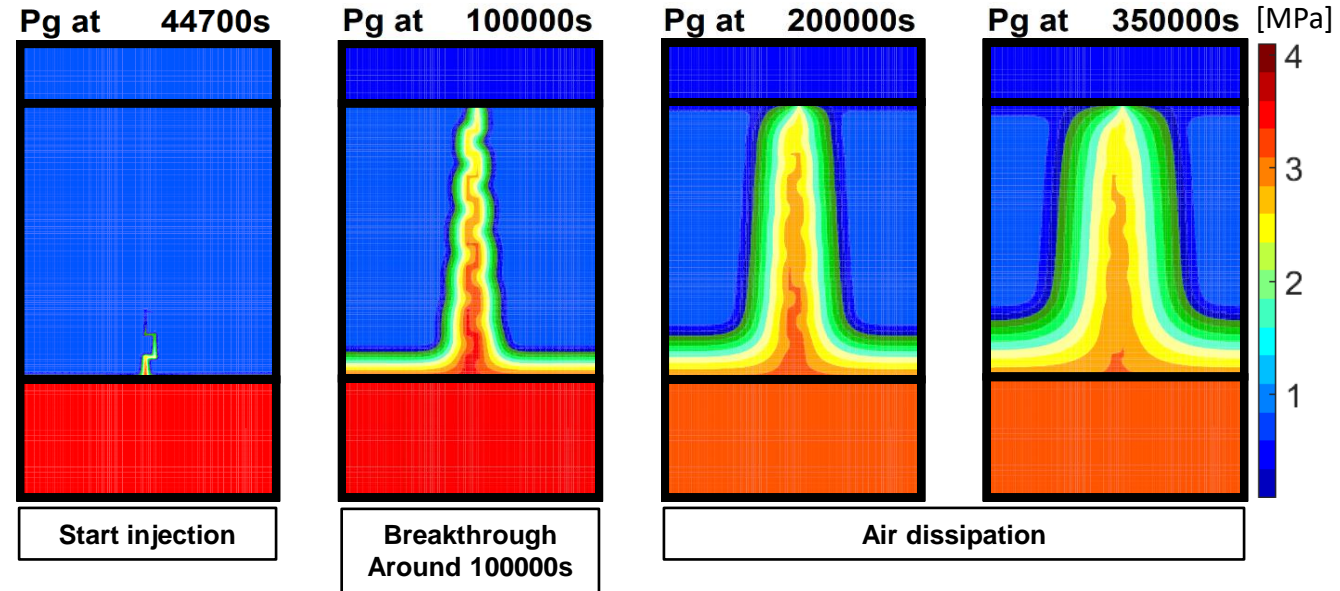
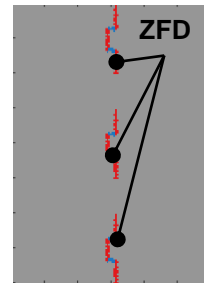
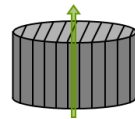
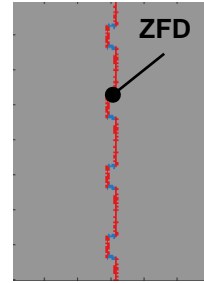
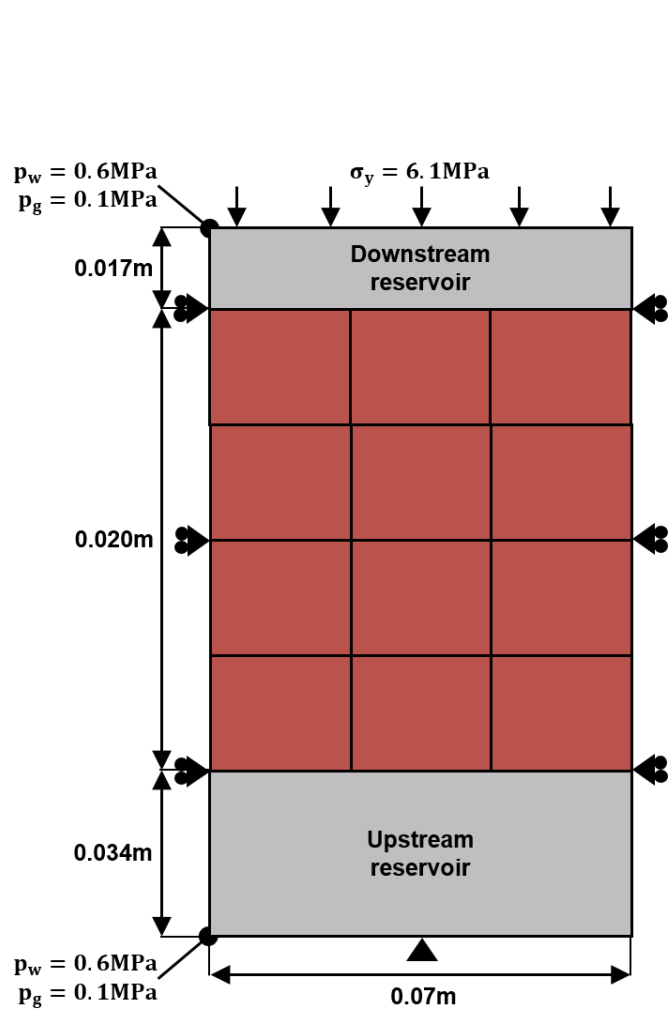
Up-scaled configuration modelling

Maps of gas pressure



Up-scaled configuration modelling

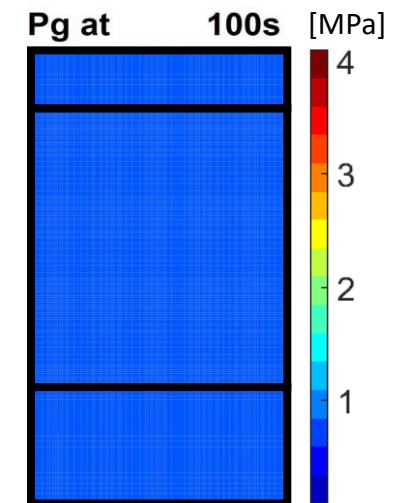
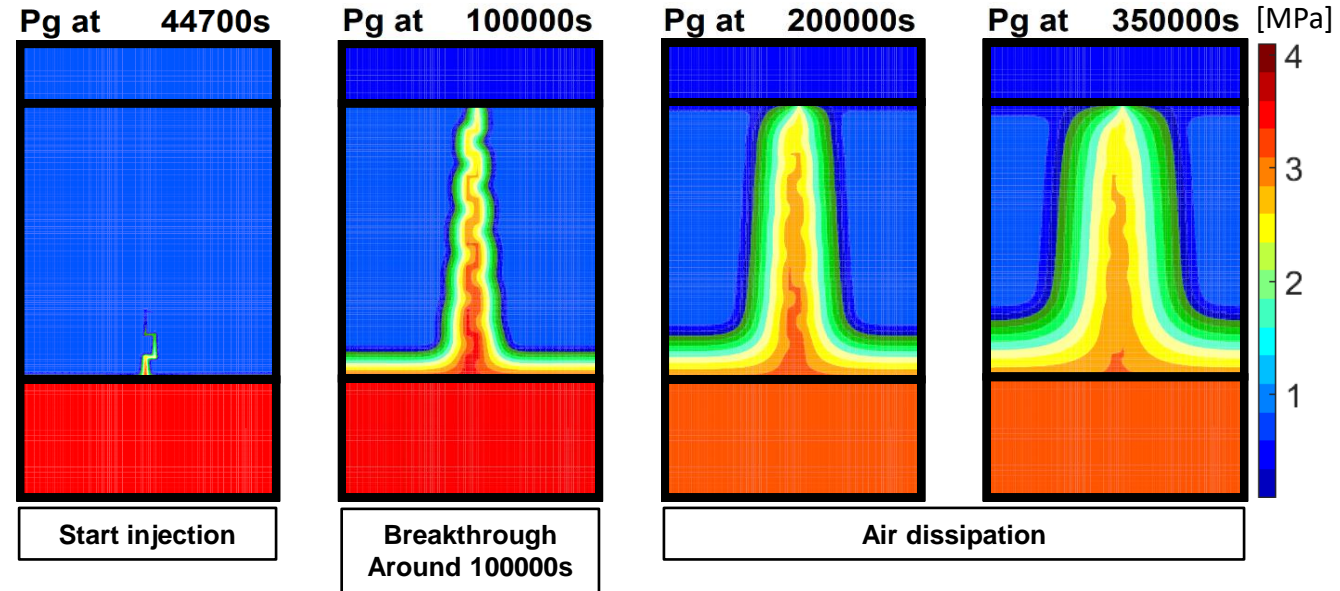
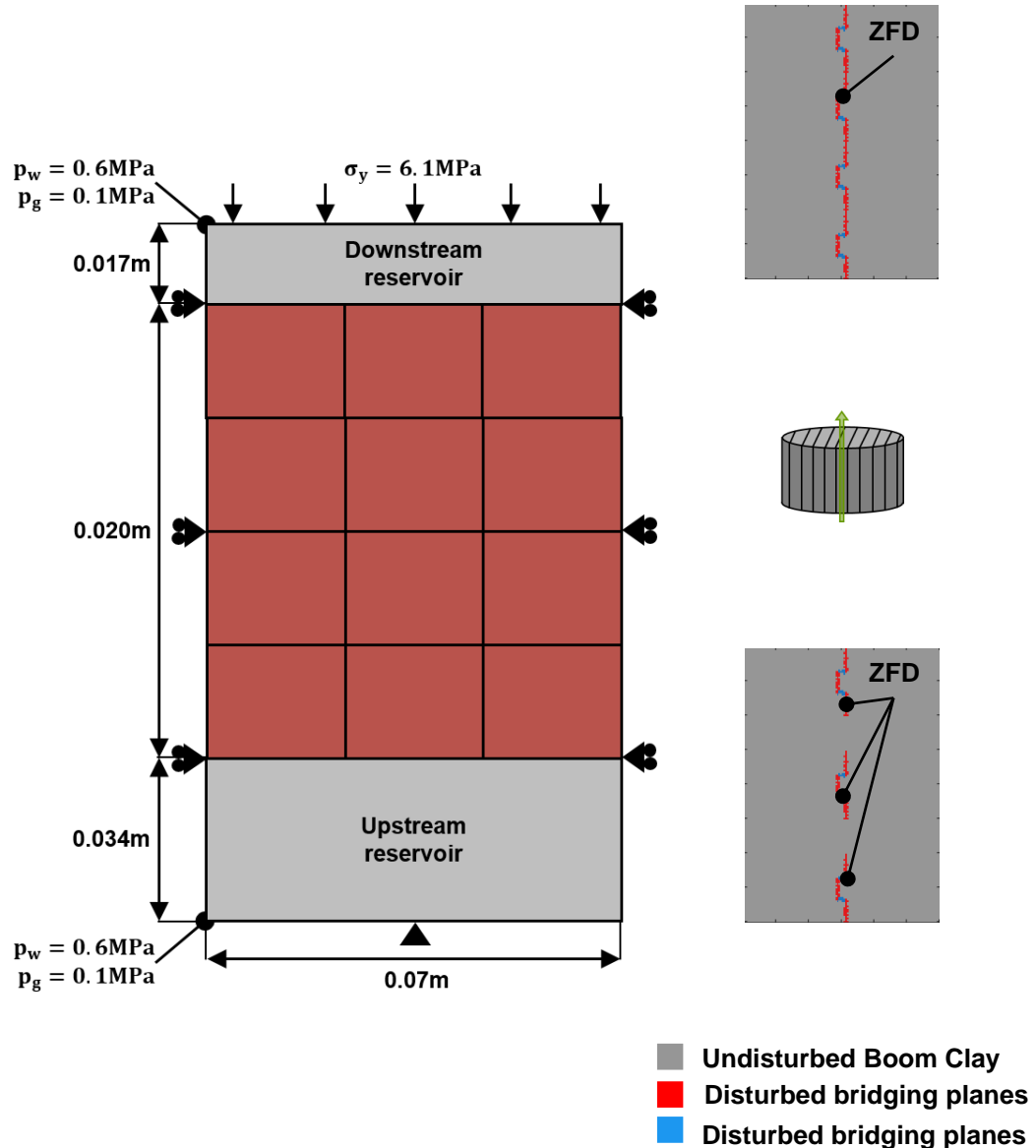
Maps of gas pressure



- Undisturbed Boom Clay
- Disturbed bridging planes
- Disturbed bridging planes

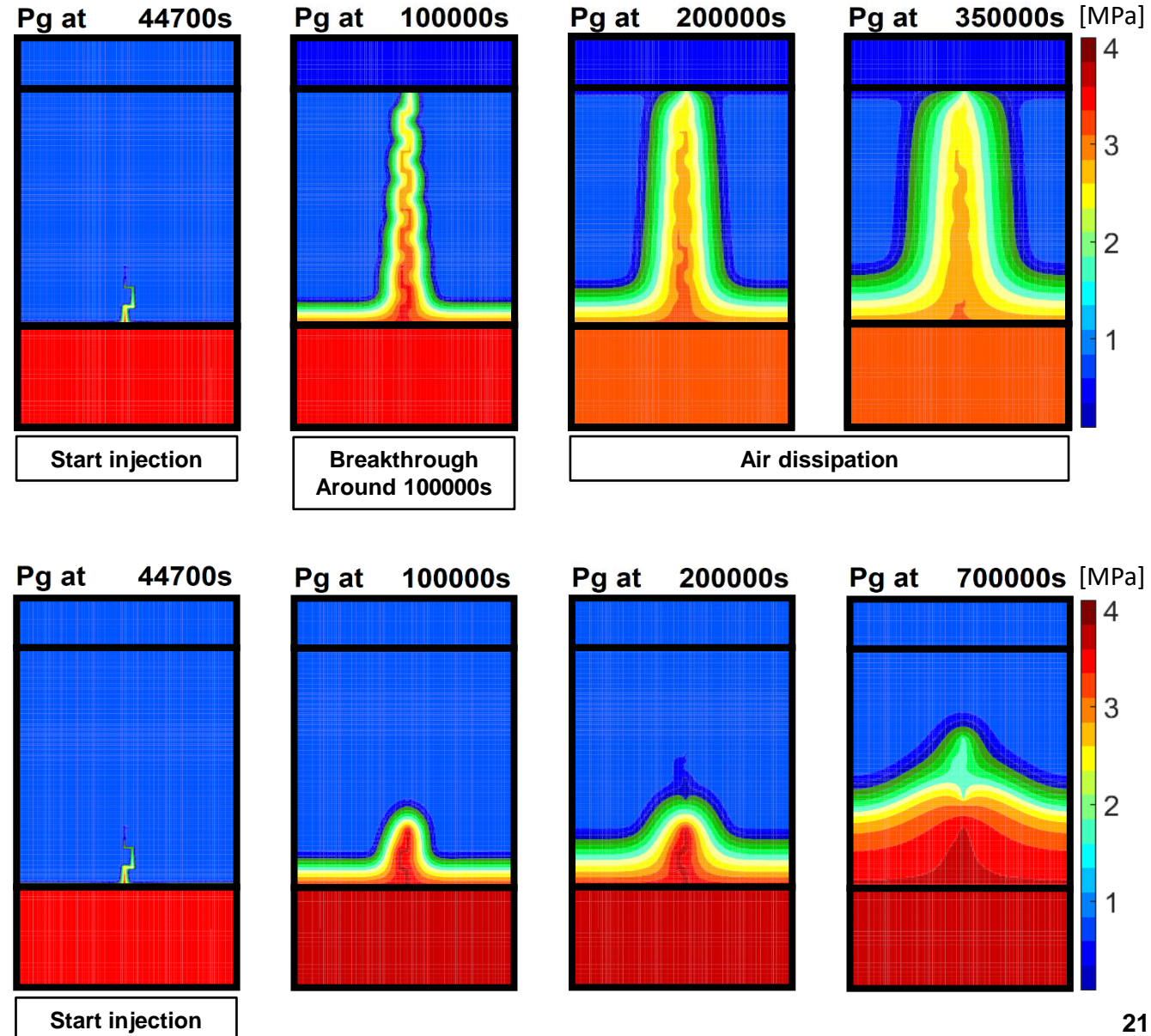
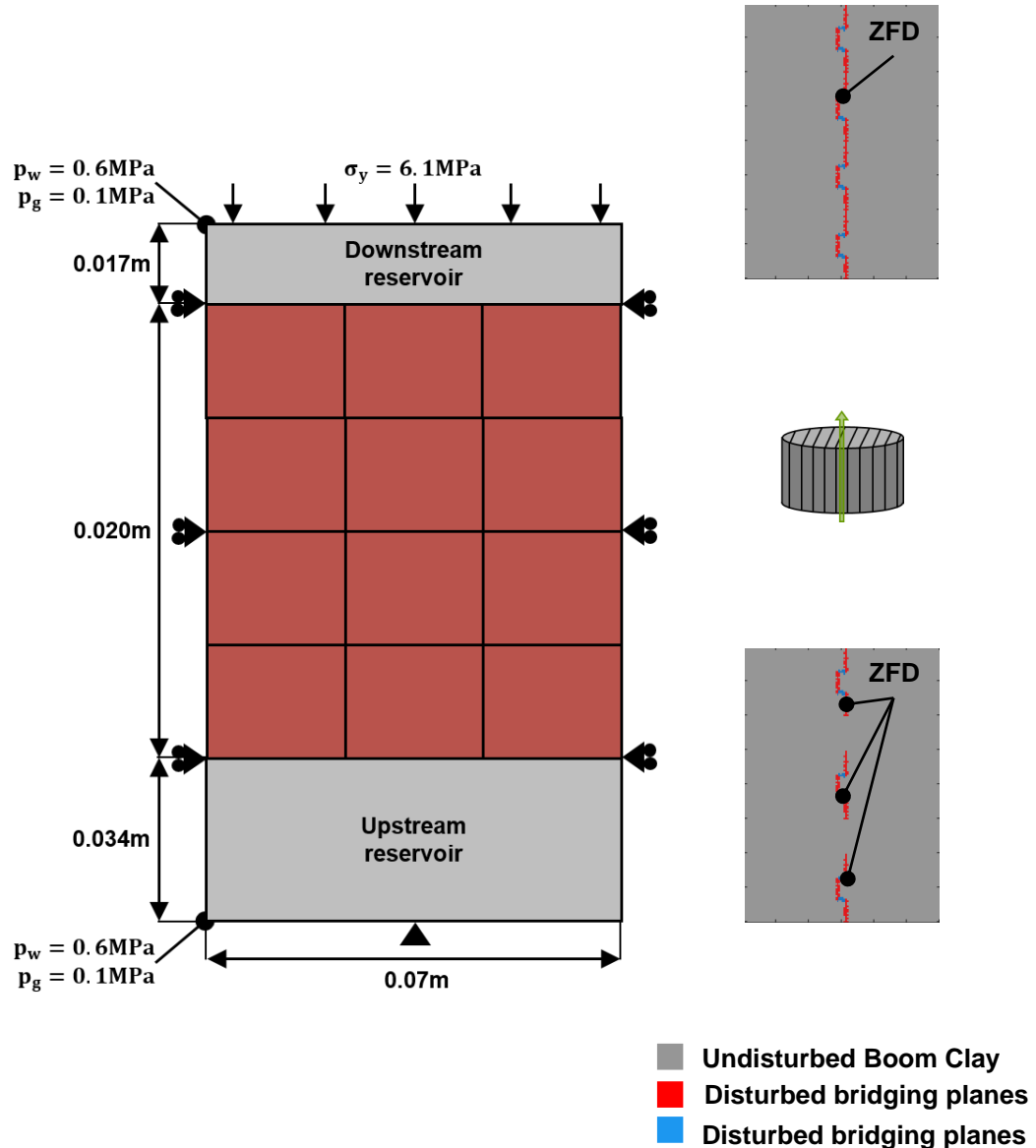
Up-scaled configuration modelling

Maps of gas pressure



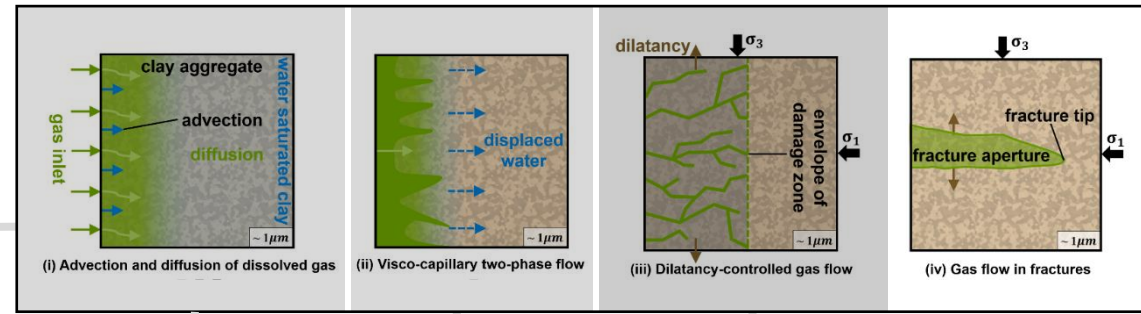
Up-scaled configuration modelling

Maps of gas pressure



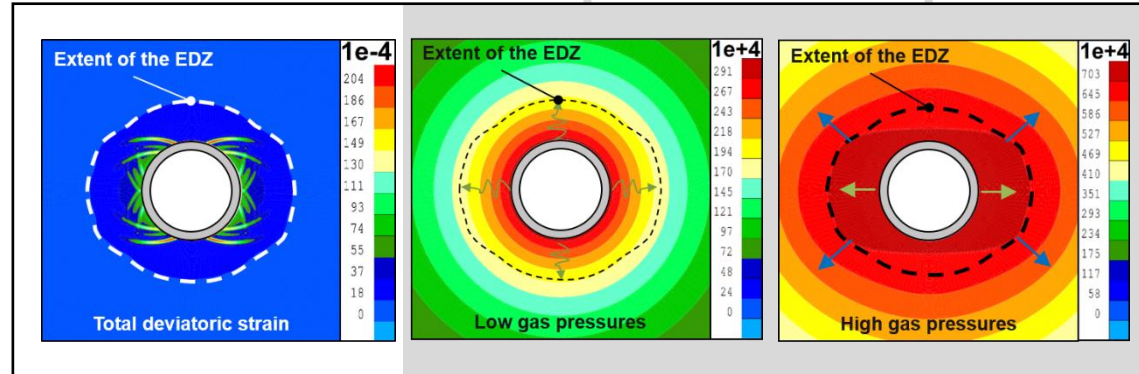
Conclusion

When gas builds up, do clay-rich rocks (re)fracture?



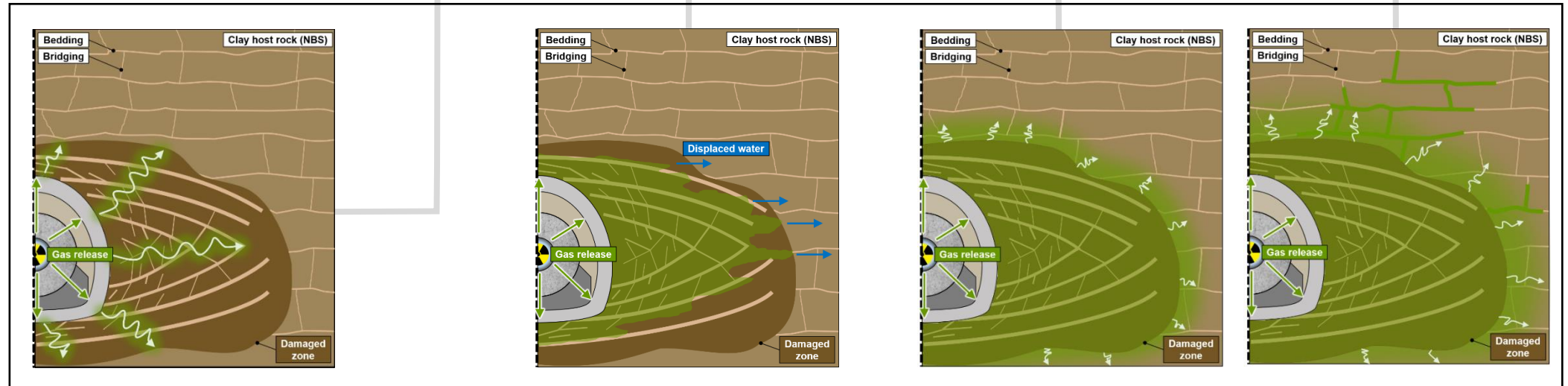
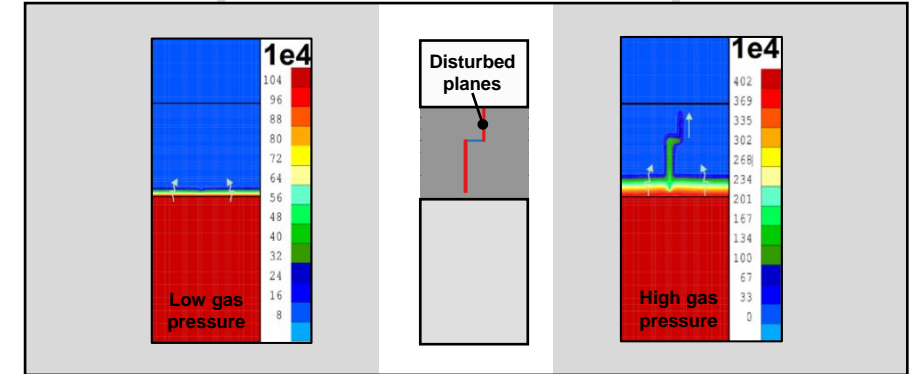
Phenomenological description

Second gradient H^2M model



Numerical implementation

Multi-scale HM model



Repository-scale conceptualisation

Thank you for your attention

When gas builds up,
do clay-rich rocks (re)fracture?

Gilles CORMAN & Frédéric COLLIN
gilles.corman@uliege.be

May 28, 2026 • Mines Paris (France)



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n° 847593.

References I

- [BP, 2022] BP (2022). BP Statistical Review of World Energy 2022. Technical report, BP, London, The United Kingdom.
- [Smil, 2016] Smil, V. (2016). Energy Transitions: Global and National Perspectives, 2nd Edition. Online, Praeger Edition.
- [IAEA, 2021] IAEA (2021). Energy, Electricity and Nuclear Power Estimates for the Period up to 2050. Reference data series No. 1, 2021 Edition. Technical report, International Atomic Energy Agency, Vienna, Austria.
- [IPCC, 2022] IPCC (2022). Mitigation pathways compatible with long-term goals. In *IPCC, 2022: Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*. Cambridge University Press.
- [IAEA, 2023] PRIS – The Database on Nuclear Power Reactors, Online, Accessed 18 December 2023.
- [IAEA, 2009] IAEA (2009). Classification of Radioactive Waste. General Safety Guide No. GSG-1. Technical report, International Atomic Energy Agency, Vienna, Austria.
- [KASAM, 1998] KASAM (1998). Nuclear Waste. State-of-the-art reports 1998. Technical report, Report from the Swedish National Council for Nuclear Waste, Stockholm, Sweden.
- [ENSI/IFSN, 2021] ENSI/IFSN (2021). Geologische Tiefenlager – Radioaktive Abfälle Sicher Entsorgen. Informationsbroschüre from the Swiss Federal Nuclear Safety Inspectorate, Brugg, Switzerland.
- [Sillen, 2012] Sillen, X. (2012). Keynote on repository-induced perturbations of the host rock, in the context of the safety case for the geological disposal of VHLW and SF in clay formations. In *Proceedings of the European Commission TIMODAZ-THERESA International Conference*, pages 159–171, Brussels, Belgium.
- [Marschall et al., 2005] Marschall, P., Horseman, S., and Gimmi, T. (2005). Characterisation of Gas Transport Properties of the Opalinus Clay, a Potential Host Rock Formation for Radioactive Waste Disposal. *Oil & Gas Science and Technology – Rev. IFP*, 60(1):121–139.
- [Henry, 1803] Henry, W. (1803). Experiments on the quantity of gases absorbed by water, at different temperatures, and under different pressures. *Society*, 93:29–274.
- [Fick, 1855] Fick, A. (1855). Über Diffusion [Translated: On liquid diffusion]. *Poggendorff's Annalen der Physik und Chemie*, 170(1):59–86.

References II

- [Jacops et al., 2013] Jacops, E., Volckaert, G., Maes, N., Weetjens, E., and Govaerts, J. (2013). Applied Clay Science Determination of gas diffusion coefficients in saturated porous media : He and CH4 diffusion in Boom Clay. *Applied Clay Science*, 83-84:217–223.
- [Jacops et al., 2015] Jacops, E., Wouters, K., Volckaert, G., Moors, H., Maes, N., Bruggeman, C., Swennen, R., and Littke, R. (2015). Measuring the effective diffusion coefficient of dissolved hydrogen in saturated Boom Clay. *Applied Geochemistry*, 61:175–184.
- [Jacops et al., 2016] Jacops, E., Maes, N., Bruggeman, C., and Grade, A. (2016). Measuring diffusion coefficients of dissolved He and Ar in three potential clay host formations: Boom Clay, Callovo-Oxfordian Clay and Opalinus Clay. *Geological Society Special Publication*, 443(1):349–360.
- [Darcy, 1856] Darcy, H. (1856). *Les fontaines publiques de la ville de Dijon*. Librairie des Corps Impériaux des Ponts et Chaussées et des Mines, Paris, France.
- [Kelvin, 1871] Thomson, W. (1871). On the equilibrium of vapour at a curved surface of liquid. *Philosophical Magazine, series 4*, 42 (282) : 448-452.
- [Clapeyron, 1834] Clapeyron, E. (1834). Mémoire sur la Puissance Motrice de la Chaleur. *Journal de l'École polytechnique*, 23:153–191.
- [van Genuchten, 1980] van Genuchten, M. (1980). Predicting the hydraulic conductivity of unsaturated soils. *Soil. Sci. Soc. Am. J*, 44(5):892–898.
- [Brooks and Corey, 1964] Brooks, R. H. and Corey, A. (1964). Hydraulic properties of porous media and their relation to drainage design. *Transactions of the ASAE*, 7(1):26–28.
- [Armand et al., 2014] Armand, G., Leveau, F., Nussbaum, C., de La Vaissiere, R., Noiret, A., Jaeggi, D., Landrein, P., and Righini, C. (2014). Geometry and properties of the excavation-induced fractures at the Meuse/Haute-Marne URL drifts. *Rock Mechanics and Rock Engineering*, 47(1):21–41.
- [Mertens et al., 2004] Mertens, J., Bastiaens, W., and Dehandschutter, B. (2004). Characterisation of induced discontinuities in the Boom Clay around the underground excavations (URF, Mol, Belgium). *Applied Clay Science*, 26:413–428.
- [Wiseall et al., 2015] Wiseall, A. C., Cuss, R. J., Graham, C. C., and Harrington, J. F. (2015b). The visualization of flow paths in experimental studies of clay-rich materials. *Mineralogical Magazine*, 79(6):1335–1342.
- [Cuss et al., 2014a] Cuss, R., Harrington, J., Giot, R., and Auvray, C. (2014a). Experimental observations of mechanical dilation at the onset of gas flow in Callovo-Oxfordian claystone. *Geological Society Special Publication*, 400(1):507–519.

References III

- [Gonzalez-Blanco et al., 2022] Gonzalez-Blanco, L., Romero, E., Marschall, P., and Levasseur, S. (2022). Hydro - mechanical Response to Gas Transfer of Deep Argillaceous Host Rocks for Radioactive Waste Disposal. *Rock Mechanics and Rock Engineering*, 55(3):1159–1177.
- [Corman et al., 2022] Corman, G., Vu, M., and Collin, F. (2022). Numerical investigation of the couplings between strain localisation processes and gas migrations in clay materials. *International Journal of Solids and Structures*, 256(June):111974.
- [Diederichs, 2003] Diederichs, M. S. (2003). Rock Fracture and Collapse Under Low Confinement Conditions. *Rock Mechanics and Rock Engineering*, 36(5):339–381.
- [Wileveau and Bernier, 2008] Wileveau, Y. and Bernier, F. (2008). Similarities in the hydromechanical response of Callovo-Oxfordian clay and Boom Clay during gallery excavation. *Physics and Chemistry of the Earth*, 33(SUPPL. 1):343–349.
- [Bastiaens et al., 2003] Bastiaens, W., Bernier, F., Buyens, M., Demarche, M., Li, X. L., Linotte, J. M., and Verstricht, J. (2003). The connecting gallery-the extension of the HADES underground research facility at Mol, Belgium. Technical report, European Underground Research Infrastructure for Disposal of nuclear waste in Clay Environment (EURIDICE), Mol, Belgium.
- [Chambon et al., 1998] Chambon, R., Caillerie, D., and El Hassan, N. (1998). One-dimensional localisation studied with a second grade model. *European Journal of Mechanics, A/Solids*, 17(4):637–656.
- [Pardoen, 2015] Pardoen, B. (2015). Hydro-mechanical analysis of the fracturing induced by the excavation of nuclear waste repository galleries using shear banding. PhD thesis, University of Liège.
- [Salehnia, 2015] Salehnia, F. (2015). From some obscurity to clarity in Boom Clay behavior : Analysis of its coupled hydro-mechanical response in the presence of strain localization. PhD thesis, University of Liège.
- [Pardoen et al., 2014] Pardoen, B., Levasseur, S., and Collin, F. (2014). Excavation damaged zone modelling including hydraulic permeability evolution in unsaturated argillaceous rock. *Unsaturated Soils: Research and Applications - Proceedings of the 6th International Conference on Unsaturated Soils, UNSAT 2014*, (Desrues):1387–1393.
- [Olivella and Alonso, 2008] Olivella, S. and Alonso, E. E. (2008). Gas flow through clay barriers. *Géotechnique*, 58(3):157–176.

References IV

- [Volckaert et al., 1995] Volckaert, G., Ortiz, L., Canniere, P. D., Put, M., Horseman, S. T., Harrington, J. F., Fioravante, V., and Impey, M. (1995). MEGAS: modelling and experiments on GAS migration in repository host rocks. Final report phase 1. Technical report, Eur. Comm., [Rep.] EUR 16235 EN.
- [Corman et al., 2024] Corman, G., Gonzalez-Blanco, L., Levasseur, S. and Collin, F. (2024, under review). Hydro-mechanical modelling of gas transport processes in clay materials using a multi-scale approach. *Computers and Geotechnics*.
- [Gonzalez-Blanco, 2017] Gonzalez-Blanco, L. (2017). Gas migration in deep argillaceous formations : Boom Clay and indurated clays. PhD thesis, Universitat Politècnica de Catalunya (UPC).
- [Bertrand et al., 2019] Bertrand, F., Buzzi, O., Collin, F. (2019). Cleat-scale modelling of the coal permeability evolution due to sorption-induced strain. *International Journal of Coal Geology*, 216, 103320.
- [Jing et al., 2016] Jing, Y., Armstrong, R. T., Ramandi, H. L., and Mostaghimi, P. (2016). Coal cleat reconstruction using micro-computed tomography imaging. *Fuel*, 181:286–299.
- [Gerard et al., 2014] Gerard, P., Harrington, J., Charlier, R., and Collin, F. (2014). Modelling of localised gas preferential pathways in claystone. *International Journal of Rock Mechanics and Mining Sciences*, 67:104–114.
- [van den Eijnden et al., 2016] van den Eijnden, A. P., Bésuelle, P., Chambon, R., and Collin, F. (2016). A FE2 modelling approach to hydromechanical coupling in cracking-induced localization problems. *International Journal of Solids and Structures*, 97-98:475–488.
- [Robinet et al., 2012] Robinet, J. C., Sardini, P., Coelho, D., Parneix, J. C., Prt, D., Sammartino, S., Boller, E., and Altmann, S. (2012). Effects of mineral distribution at mesoscopic scale on solute diffusion in a clay-rich rock: Example of the Callovo-Oxfordian mudstone (Bure, France). *Water Resources Research*, 48(5):1–17.
- [Bishop, 1959] Bishop, A. W. (1959). The principle of effective stress. *Teknisk Ukeblad*, 39:859–863.
- [Yuster, 1951] Yuster, S. (1951). Theoretical considerations of multiphase flow in idealized capillary systems.pdf. *Proceedings of the 3rd World Petroleum Congress, Section II*, The Hague, 2:437–445.
- [Goodman, 1976] Goodman, R. (1976). *Methods of geological engineering in Discontinuous Rocks*. West Publishing Co.

References V

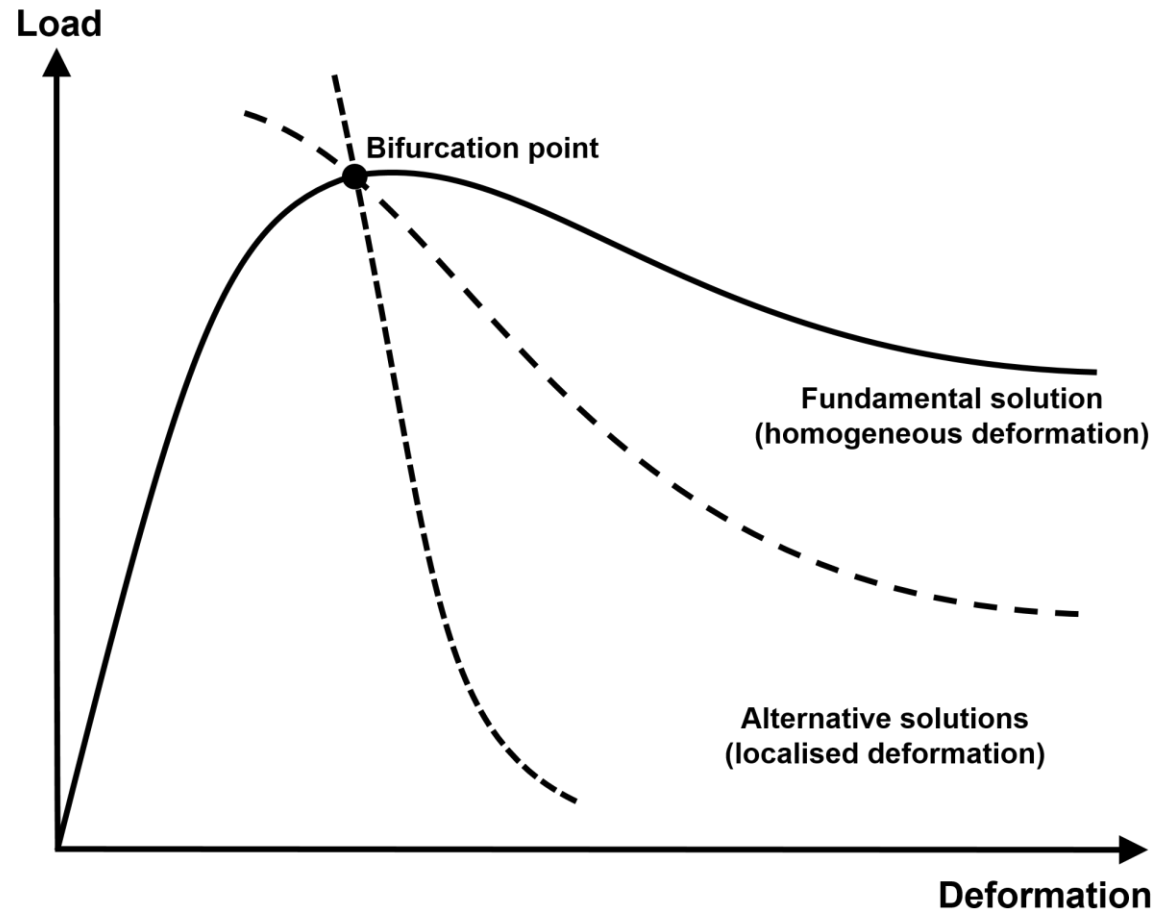
- [Bandis et al., 1983] Bandis, S. C., Lumsden, A. C., and Barton, N. R. (1983). Fundamentals of rock joint deformation. *International Journal of Rock Mechanics and Mining Sciences & Geomechanics Abstracts*, 20(6):249–268.
- [Hill, 1965] Hill, R. (1965). A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, 13(4):213–222.
- [Mandel, 1966] Mandel, J. (1966). Conditions de Stabilité et Postulat de Drucker. In Kravtchenko, J. and Sirieys, P., editors, *Rheology and Soil Mechanics / Rhéologie et Mécanique des Sols*, pages 58–68. International Union of Theoretical and Applied Mechanics. Springer, Berlin, Germany.
- [Bésuelle et al., 2014] Bésuelle, P., Viggiani, G., Desrues, J., Coll, C., and Charrier, P. (2014). A laboratory experimental study of the hydromechanical behavior of boom clay. *Rock Mechanics and Rock Engineering*, 47(1):143–155.

Appendices

Model 1

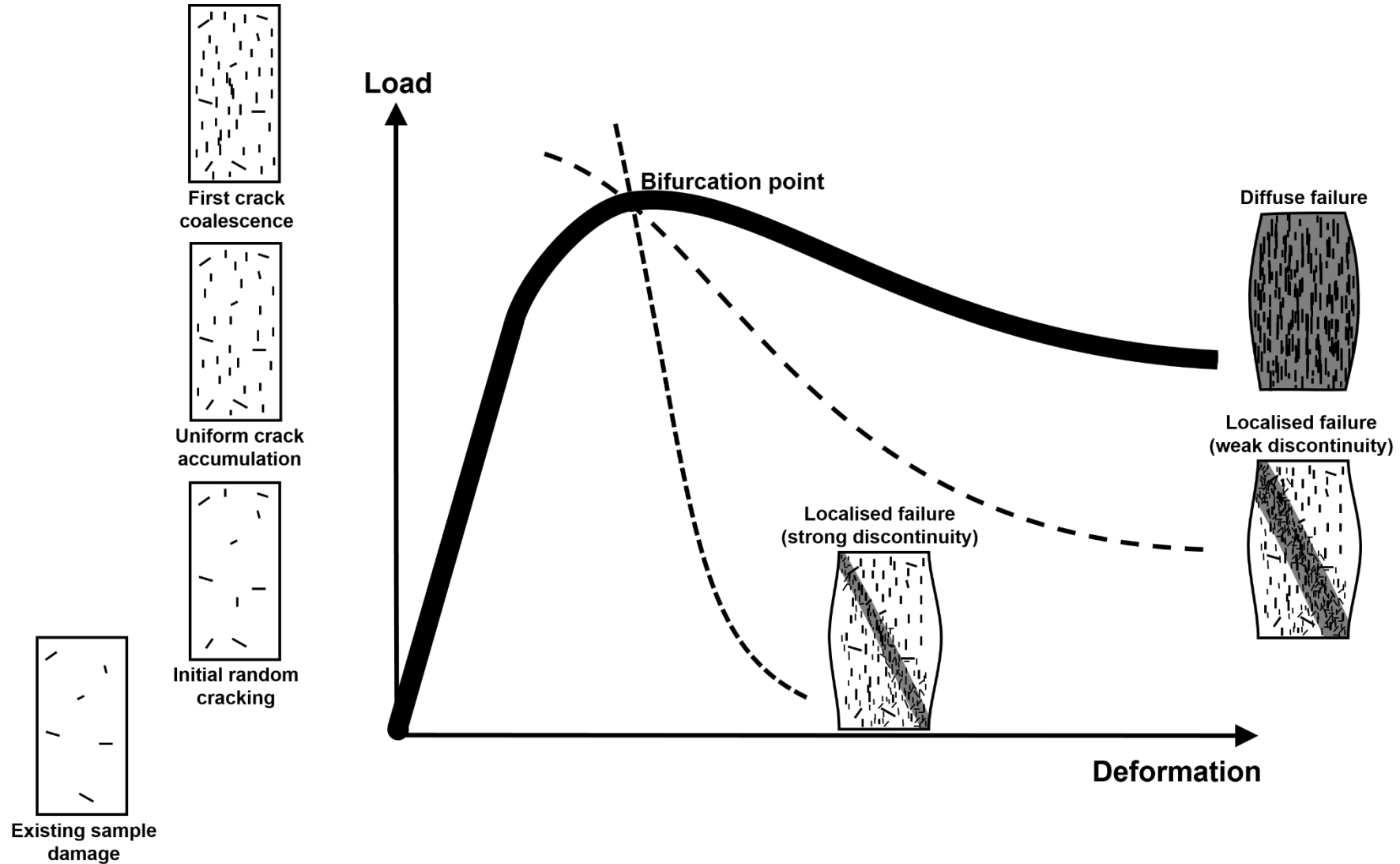
Representation of fracturing

Shear strain localisation conceptualisation



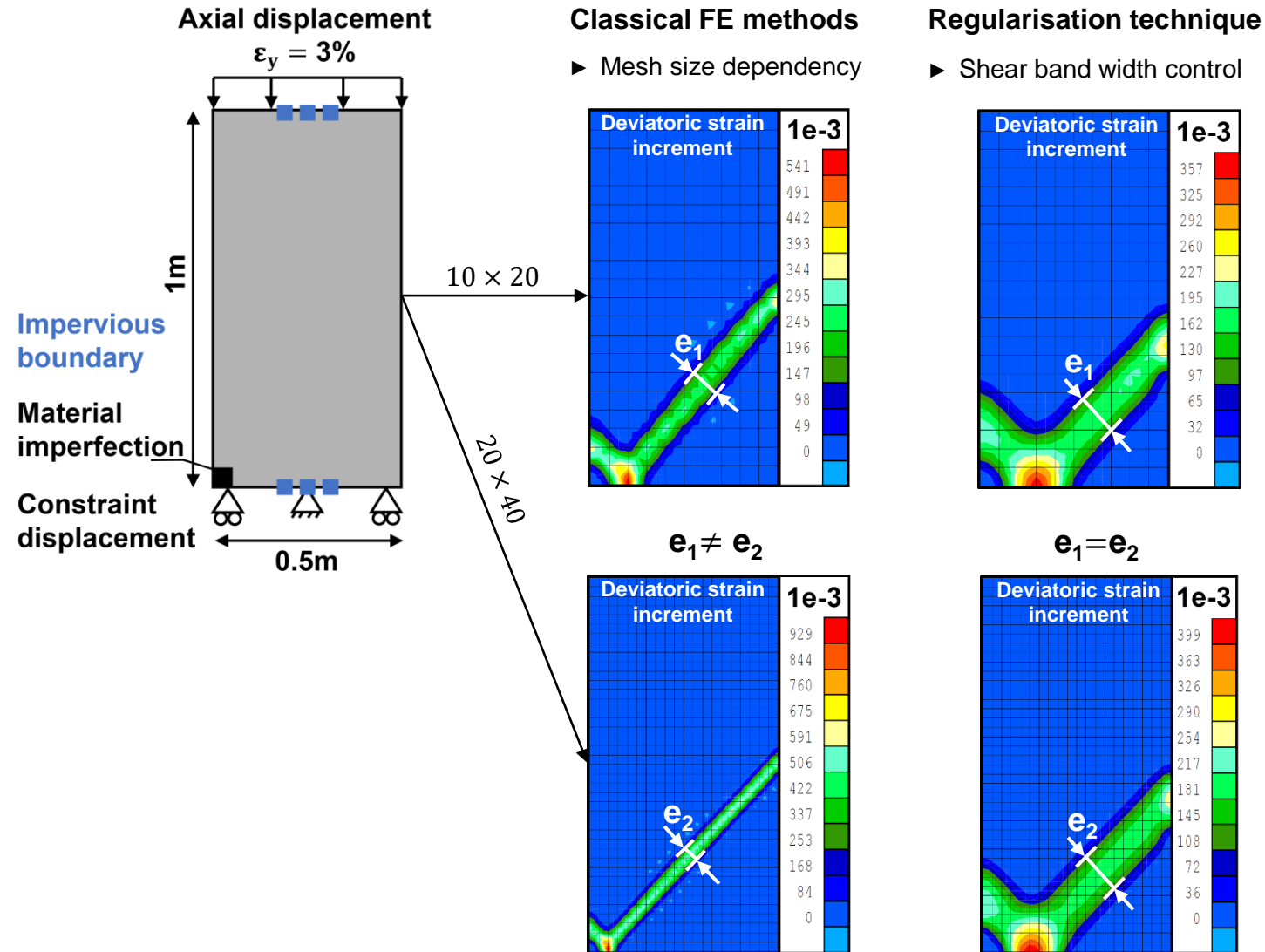
Representation of fracturing

Shear strain localisation conceptualisation



Representation of fracturing

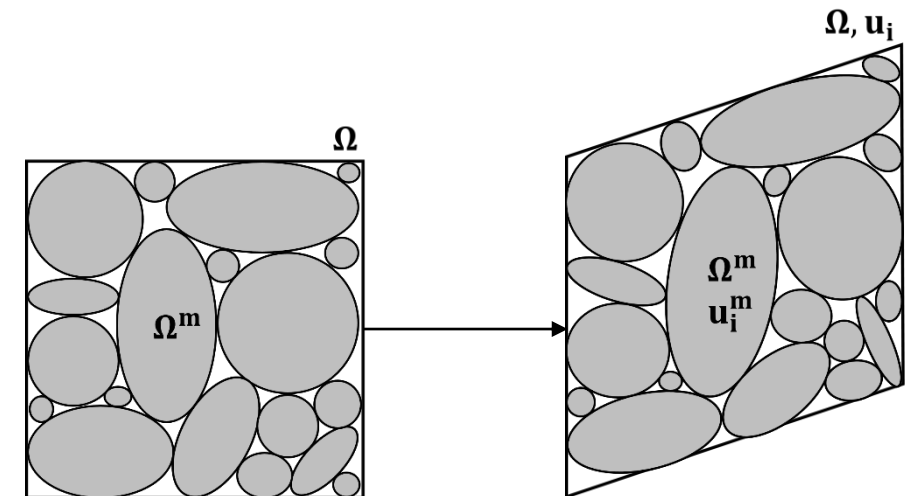
Shear strain localisation modelling



Enrichment of the kinematics with microstructure effects

2nd gradient type [Chambon et al., 1998]

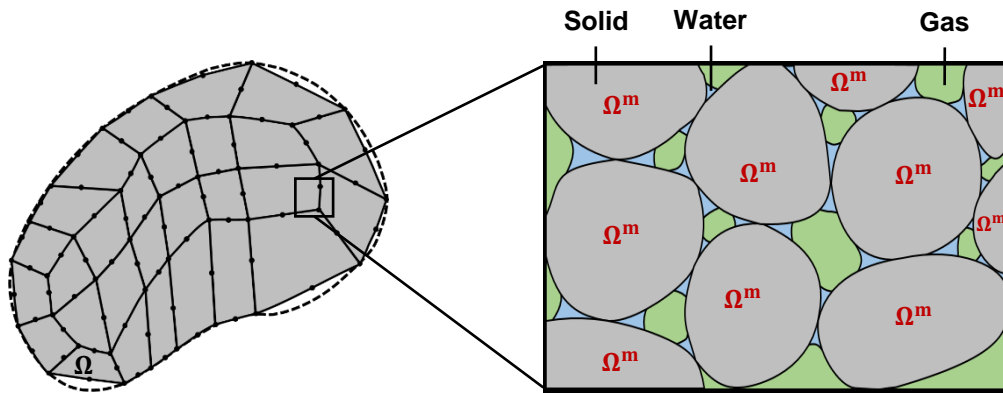
	Macro-kinematics	+	Micro-kinematics
Volume	Ω		Ω^m
Displacement	u_i		u_i^m
Deformation	$F_{ij} = \frac{\partial u_i}{\partial x_j}$		$v_{ij} = \frac{\partial u_i^m}{\partial x_j}$



Second gradient H²M model

The rock environment is modelled as

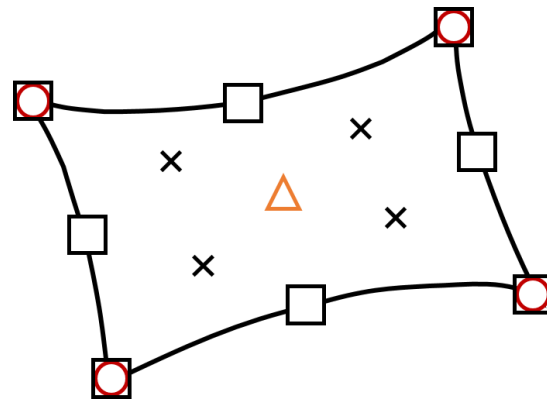
- ▶ A multiphasic porous medium
- ▶ With strain localisation in the EDZ
- ▶ Including transfer properties evolution with strain



Finite element



- Node u_i, p_w, p_g
- Node v_{ij}
- △ Node λ_{ij}
- × Integration point



Balance equations

$$\frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial^2 \Sigma_{ijk}}{\partial x_j \partial x_k} + \rho_{\text{mix}} \mathbf{g} = \mathbf{0}$$



Microstructure effects

Kinematic restriction \equiv No relative deformation of the microstructure

Field of Lagrange multipliers λ_{ij}

$$\underbrace{\frac{\partial f_{w,i}}{\partial x_i} + \frac{\partial (\rho_w \phi S_{r_w})}{\partial t}}_{\text{Liquid water}} + \underbrace{\frac{\partial f_{v,i}}{\partial x_i} + \frac{\partial (\rho_v \phi (1 - S_{r_w}))}{\partial t}}_{\text{Water vapour}} = Q_w$$

Liquid water

Water vapour

$$\underbrace{\frac{\partial f_{g,i}}{\partial x_i} + \frac{\partial (\rho_g \phi (1 - S_{r_w}))}{\partial t}}_{\text{Dry gas}} + \underbrace{\frac{\partial f_{dg,i}}{\partial x_i} + \frac{\partial (\rho_{dg} \phi S_{r_w})}{\partial t}}_{\text{Dissolved gas}} = Q_g$$

Dry gas

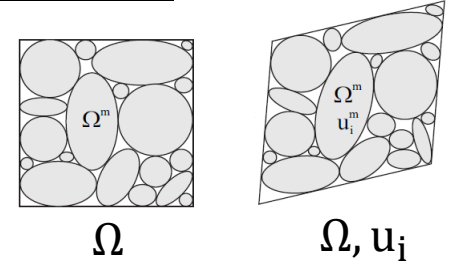
Dissolved gas

\mathring{M} : Stored fluid quantity f_i : Mass flow of fluid Q : Fluid source term

The second gradient method

- Regularisation method based on the enrichment of the continuum kinematics with the microstructure effects

	Macro-volume Ω	+	Micro-volumes Ω^m
Displacement	u_i		u_i^m
Deformation	$F_{ij} = \frac{\partial u_i}{\partial x_j}$		$v_{ij} = \frac{\partial u_i^m}{\partial x_j}$



- Principle of virtual work: the internal virtual work (*Germain, 1973*) = the external virtual work (simplified)

$$W_i^* = \int_{\Omega} \left(\sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \tau_{ij} (\mathbf{v}_{ij}^* - F_{ij}^*) + \Sigma_{ijk} h_{ijk}^* \right) d\Omega$$

$$W_e^* = \int_{\Omega} G_i u_i^* d\Omega + \int_{\partial\Omega} (t_i u_i^* + \mathbf{T}_{ij} \mathbf{v}_{ij}^*) ds$$

- The kinematical constraint $v_{ij} = F_{ij}$ implying $v_{ij} = \frac{\partial u_i}{\partial x_j}$ is added (*Chambon et al., 1998; Matsushima et al., 2002*)

$$\int_{\Omega} \left(\sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \Sigma_{ijk} \frac{\partial^2 u_i^*}{\partial x_j \partial x_k} \right) d\Omega = \int_{\Omega} G_i u_i^* d\Omega + \int_{\partial\Omega} (t_i u_i^* + \mathbf{T}_{ij} \mathbf{v}_{ij}^*) ds$$

- Finite element formulation: introduction of Lagrange multiplier fields λ_{ij}

$$\int_{\Omega} \left(\sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \Sigma_{ijk} \frac{\partial v_{ij}^*}{\partial x_k} \right) d\Omega - \int_{\Omega} \lambda_{ij} \left(\frac{\partial u_i^*}{\partial x_j} - v_{ij}^* \right) d\Omega = \int_{\Omega} G_i u_i^* d\Omega + \int_{\partial\Omega} (t_i u_i^* + \mathbf{T}_{ij} \mathbf{v}_{ij}^*) ds$$

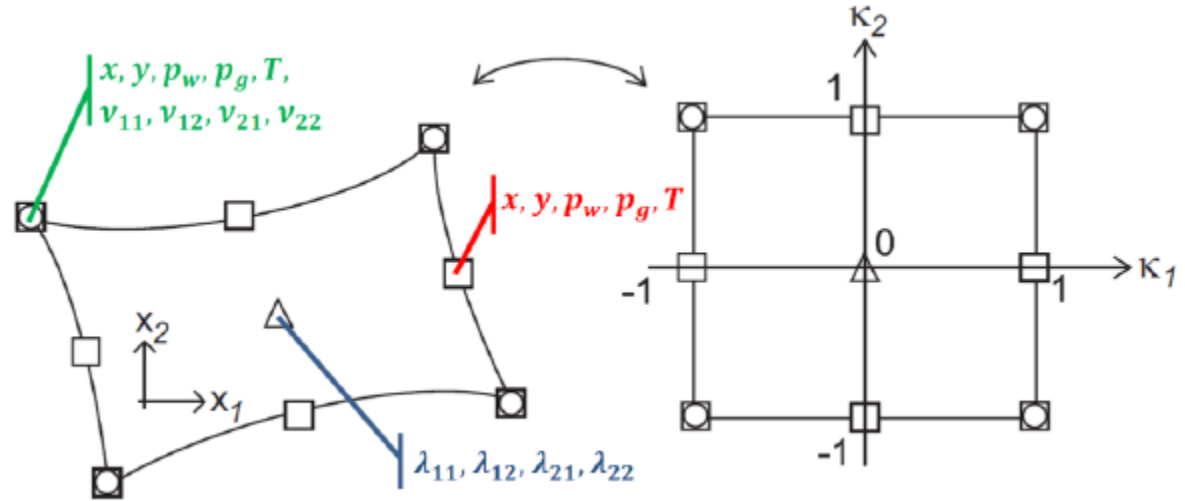
$$\int_{\Omega} \lambda_{ij}^* \left(\frac{\partial u_i}{\partial x_j} - v_{ij} \right) d\Omega = 0$$

The second gradient Finite Element

8 nodes: macro-displacements
pressure fields
temperaure

4 nodes: microkinetic gradient

1 node: Lagrange multiplier



The second gradient mechanical law

$$\tilde{\Sigma}_{ijk} = [D] \frac{\partial \dot{v}_{ij}}{\partial x_k}$$

- The double stress requires a constitutive law
- Isotropic linear relationship (*Mindlin, 1965*)
- Only one constitutive parameter D representing the microstructure (internal length scale)

$$\begin{bmatrix} \tilde{\Sigma}_{111} \\ \tilde{\Sigma}_{112} \\ \tilde{\Sigma}_{121} \\ \tilde{\Sigma}_{122} \\ \tilde{\Sigma}_{211} \\ \tilde{\Sigma}_{212} \\ \tilde{\Sigma}_{221} \\ \tilde{\Sigma}_{222} \end{bmatrix} = \begin{bmatrix} D & 0 & 0 & 0 & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\ 0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\ 0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\ 0 & 0 & 0 & D & 0 & -\frac{D}{2} & -\frac{D}{2} & 0 \\ 0 & -\frac{D}{2} & -\frac{D}{2} & 0 & D & 0 & 0 & 0 \\ \frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\ \frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\ 0 & \frac{D}{2} & \frac{D}{2} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial \dot{v}_{11}}{\partial x_1} \\ \frac{\partial \dot{v}_{11}}{\partial x_2} \\ \frac{\partial \dot{v}_{12}}{\partial x_1} \\ \frac{\partial \dot{v}_{12}}{\partial x_2} \\ \frac{\partial \dot{v}_{21}}{\partial x_1} \\ \frac{\partial \dot{v}_{21}}{\partial x_2} \\ \frac{\partial \dot{v}_{22}}{\partial x_1} \\ \frac{\partial \dot{v}_{22}}{\partial x_2} \end{bmatrix}$$

Spatial discretisation

- Linear auxiliary problem

Linearized equations in matricial form

$$\int_{\Omega^{\tau_1}} \left[U_{(x_1, x_2)}^{*, \tau_1} \right]^T [E^{\tau_1}] [dU_{(x_1, x_2)}^{\tau_1}] d\Omega^{\tau_1} = -\Delta_1^{\tau_1} - \Delta_2^{\tau_1} - \Delta_3^{\tau_1} \quad (10)$$

Local stiffness matrix $[E^{\tau_1}]$ and local out-of-balance forces $[f_{OB}^{\tau_1}]$

Global solution

- Linear auxiliary system

Assembling the elements

$$[K^{\tau_1}] [\delta U_{Node}^{\tau_1}] = -[F_{OB}^{\tau_1}] \quad (11)$$

Global stiffness matrix $[K^{\tau_1}]$ and out-of-balance forces $[F_{OB}^{\tau_1}]$

$$[K^{\tau_1}] = \begin{bmatrix} K_{MM(2 \times 2)} & K_{WM(2 \times 1)} & K_{GM(2 \times 1)} & K_{TM(2 \times 1)} & K_{vM(2 \times 1)} & K_{\lambda M(2 \times 1)} \\ K_{MW(1 \times 2)} & K_{WW(1 \times 1)} & K_{GW(1 \times 1)} & K_{TW(1 \times 1)} & K_{vW(1 \times 1)} & K_{\lambda W(1 \times 1)} \\ K_{MG(1 \times 2)} & K_{WG(1 \times 1)} & K_{GG(1 \times 1)} & K_{TG(1 \times 1)} & K_{vG(1 \times 1)} & K_{\lambda G(1 \times 1)} \\ K_{MT(1 \times 2)} & K_{WT(1 \times 1)} & K_{GT(1 \times 1)} & K_{TT(1 \times 1)} & K_{vT(1 \times 1)} & K_{\lambda T(1 \times 1)} \\ K_{Mv(1 \times 2)} & K_{Wv(1 \times 1)} & K_{Gv(1 \times 1)} & K_{Tv(1 \times 1)} & K_{vv(1 \times 1)} & K_{\lambda v(1 \times 1)} \\ K_{M\lambda(1 \times 2)} & K_{W\lambda(1 \times 1)} & K_{G\lambda(1 \times 1)} & K_{T\lambda(1 \times 1)} & K_{v\lambda(1 \times 1)} & K_{\lambda\lambda(1 \times 1)} \end{bmatrix} \quad (12)$$

- Correction of the unknowns fields

Updating current unknowns values



Get closer to well-balanced configuration

MAVL Application

Mechanical parameters

	PARAMETER	SYMBOL	VALUE	UNIT
Geomechanical	Parallel Young's modulus	E_{\parallel}	5	[GPa]
	Perpendicular Young's modulus	E_{\perp}	4	[GPa]
	Poisson's ratio	ν_{\parallel}	0.24	[-]
	Poisson's ratio	$\nu_{\parallel\perp}$	0.325	[-]
	Poisson's ratio	$\nu_{\perp\parallel}$	0.26	[-]
	Shear modulus	$G_{\parallel\perp} = G_{\perp\parallel}$	1.63	[GPa]
	Shear modulus	$G_{\parallel\parallel}$	2.016	[GPa]
	Solid grain density	ρ_s	2750	[kg/m ³]
	Initial cohesion	c_i	4.1 (0°)	[MPa]
	Cohesion parameter	A_{11}	0.117	[-]
	Cohesion parameter	b_1	14.236	[-]
	Ratio of cohesion softening	ξ_c	5	[-]
	Cohesion softening parameter	B_c	0.003	[-]
	Cohesion softening shifting	dec_c	0	[-]
	Initial compressive friction angle	$\varphi_{c,0}$	10	[°]
	Final compressive friction angle	$\varphi_{c,f}$	23	[°]
	Initial extensive friction angle	$\varphi_{e,0}$	7	[°]
	Final extensive friction angle	$\varphi_{e,f}$	23	[°]
	Friction angle hardening parameter	B_{φ}	0.001	[-]
	Friction angle hardening shifting	dec_{φ}	0	[-]
Dilatancy angles	$\psi_c = \psi_e$	0.5	[°]	
Microstructure	Second gradient elastic modulus	D	14.016	[kN]
Viscoplastic	Uniaxial compressive strength	R_c	21	[MPa]
	Internal friction coefficient	A^{vp}	2.62	[-]
	Cohesion coefficient	C^{vp}	0.03	[-]
	Viscoplastic potential parameter	β^{vp}	1.1	[-]
	Initial threshold for the VP flow	α_0^{vp}	0.142	[-]
	Reference fluidity	γ_0	700	[s ⁻¹]
	Temperature parameter	γ_1	57×10^3	[J/mol]
	Creep curve shape parameter	\mathcal{N}	5.0	[-]
VP hardening function parameter	B^{vp}	7.5×10^{-2}	[-]	

	PARAMETER	SYMBOL	VALUE	UNIT
Classic Stuffing	Elastic Young's modulus	E_{CS}	17.5	[GPa]
	Poisson's ratio	ν_{CS}	0.25	[-]
	Friction angle	φ_{CS}	30	[°]
	Cohesion	c_{CS}	2.94	[MPa]
	Density	ρ_{CS}	2300	[kg/m ³]
Compressible stuffing	Elastic Young's modulus	E_{ES}	0.1	[GPa]
	Poisson's ratio	ν_{ES}	0.0	[-]
	Density	ρ_{ES}	2300	[kg/m ³]
Arch segments	Elastic Young's modulus	E_{AS}	39	[GPa]
	Poisson's ratio	ν_{AS}	0.2	[-]
	Friction angle	φ_{AS}	38	[°]
	Cohesion	c_{AS}	14.6	[MPa]
	Density	ρ_{AS}	2650	[kg/m ³]

MAVL Application

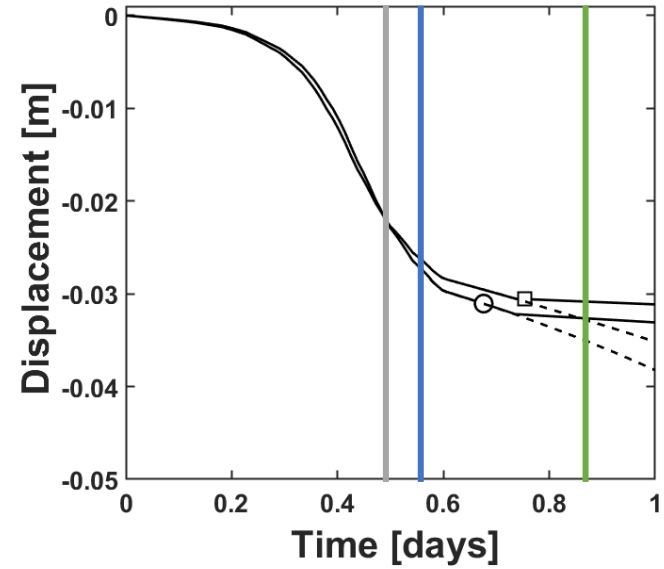
Flow parameters

	PARAMETER	SYMBOL	VALUE	UNIT
Hydraulic	Initial porosity	n	0.173	[-]
	Initial parallel intrinsic permeability	$k_{w,\parallel,0}$	4×10^{-20}	$[m^2]$
	Initial perp. intrinsic permeability	$k_{w,\perp,0}$	1.33×10^{-20}	$[m^2]$
	Water density	ρ_w	1000	$[kg/m^3]$
	H2 density	ρ_{H2}	0.0794	$[kg/m^3]$
	Water dynamic viscosity	μ_w	0.001	$[Pa.s]$
	H2 dynamic viscosity	μ_{H2}	9×10^{-6}	$[Pa.s]$
	Water compressibility	χ_w^{-1}	5×10^{-10}	$[Pa^{-1}]$
	Henry coefficient	H_{H2}	0.0193	[-]
	Air entry pressure (1 st coeff. of $S_{r,w}$)	P_r	15	$[MPa]$
	Parameter (2 nd coeff. of $S_{r,w}$)	\mathcal{G}	1.49	[-]
	Parameter (1 st coeff. of $k_{r,w}$)	\mathcal{M}	0.32886	[-]
	Parameter (1 st coeff. of $k_{r,g}$)	\mathcal{N}	3	[-]
	Max. degree of water saturation	S_{max}	1	[-]
	Residual degree of water saturation	S_{res}	0.01	[-]
	Evolution parameter	β_{perm}	10^{10}	[-]
Tortuosity	τ	0.25	[-]	

Compressible Stuffing	Initial porosity	n	0.25	[-]
	Initial parallel intrinsic permeability	$k_{w,\parallel,0}$	10^{-15}	$[m^2]$
	Initial perp. intrinsic permeability	$k_{w,\perp,0}$	10^{-15}	$[m^2]$
	Air entry pressure (1 st coeff. of $S_{r,w}$)	P_r	1	$[MPa]$
	Parameter (2 nd coeff. of $S_{r,w}$)	\mathcal{G}	1.54	[-]
	Parameter (1 st coeff. of $k_{r,w}$)	\mathcal{F}	0.3507	[-]
	Max. degree of water saturation	S_{max}	1	[-]
	Residual degree of water saturation	S_{res}	0.01	[-]
Tortuosity	τ	0.25	[-]	
Compressible Stuffing	Initial porosity	n	0.5	[-]
	Initial parallel intrinsic permeability	$k_{w,\parallel,0}$	10^{-10}	$[m^2]$
	Initial perp. intrinsic permeability	$k_{w,\perp,0}$	10^{-10}	$[m^2]$
	Air entry pressure (1 st coeff. of $S_{r,w}$)	P_r	0.2	$[MPa]$
	Parameter (2 nd coeff. of $S_{r,w}$)	\mathcal{G}	1.54	[-]
	Parameter (1 st coeff. of $k_{r,w}$)	\mathcal{F}	0.3507	[-]
	Max. degree of water saturation	S_{max}	1	[-]
	Residual degree of water saturation	S_{res}	0.01	[-]
Tortuosity	τ	0.25	[-]	
Arch Segments	Initial porosity	n	0.15	[-]
	Initial parallel intrinsic permeability	$k_{w,\parallel,0}$	10^{-18}	$[m^2]$
	Initial perp. intrinsic permeability	$k_{w,\perp,0}$	10^{-18}	$[m^2]$
	Air entry pressure (1 st coeff. of $S_{r,w}$)	P_r	5	$[MPa]$
	Parameter (2 nd coeff. of $S_{r,w}$)	\mathcal{G}	1.54	[-]
	Parameter (1 st coeff. of $k_{r,w}$)	\mathcal{F}	0.3507	[-]
	Max. degree of water saturation	S_{max}	1	[-]
Residual degree of water saturation	S_{res}	0.01	[-]	
Tortuosity	τ	0.25	[-]	

MAVL Application

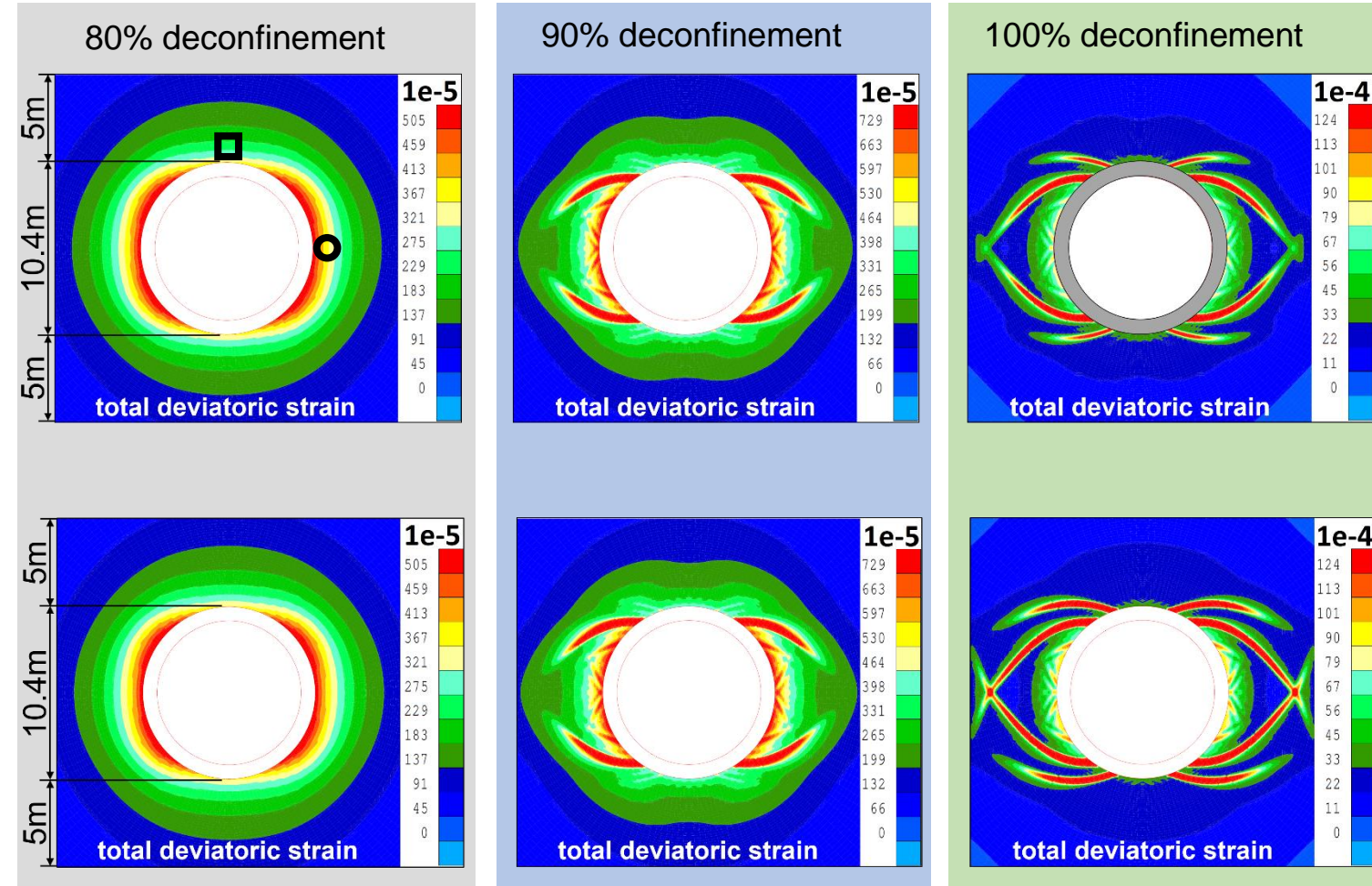
Evolution of convergence



Reference case
with transfer
properties
evolution

No support

Development of damage in the near field



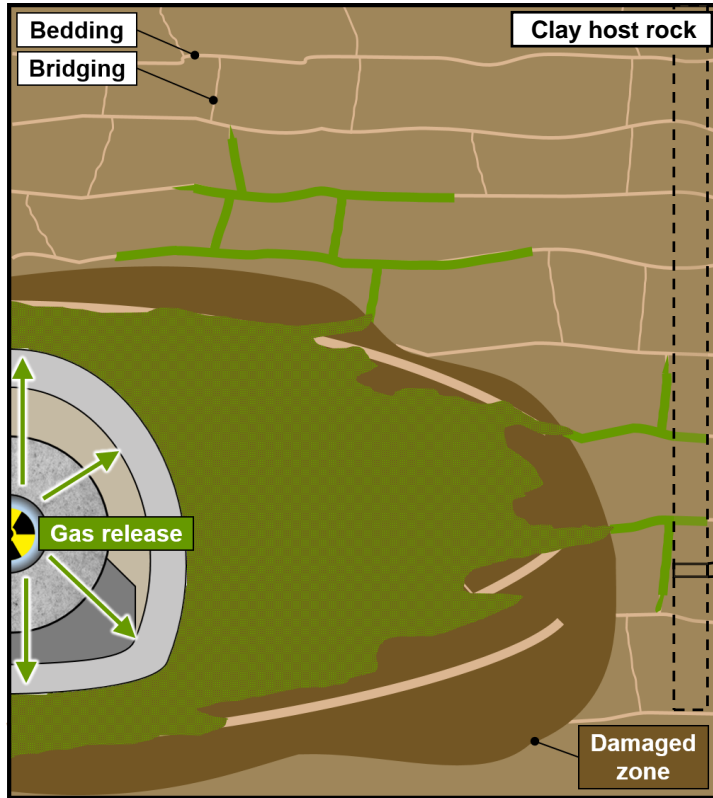
Appendices

Model 2

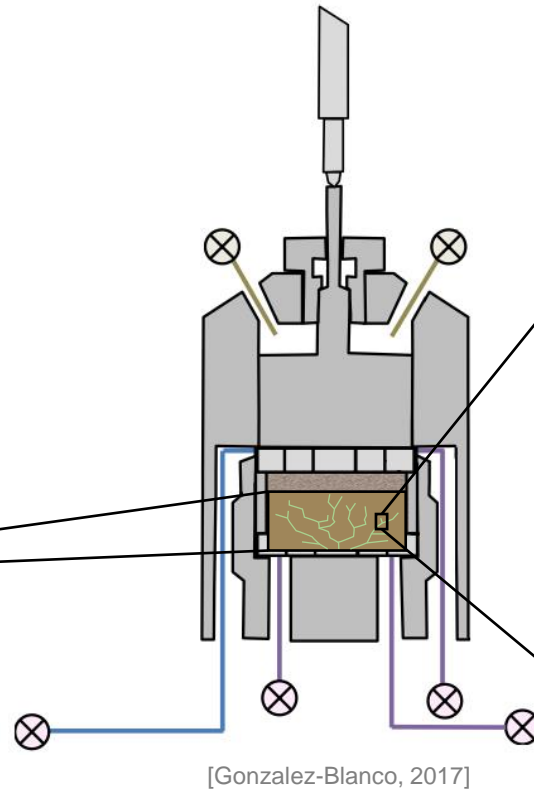
Representation of microstructure effects



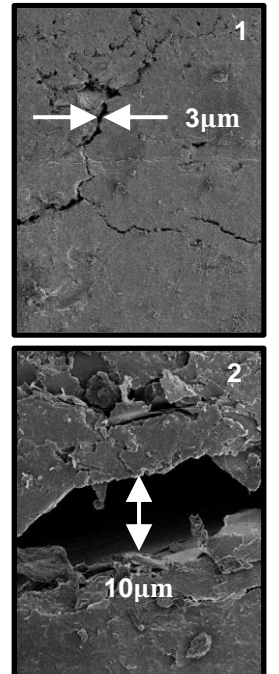
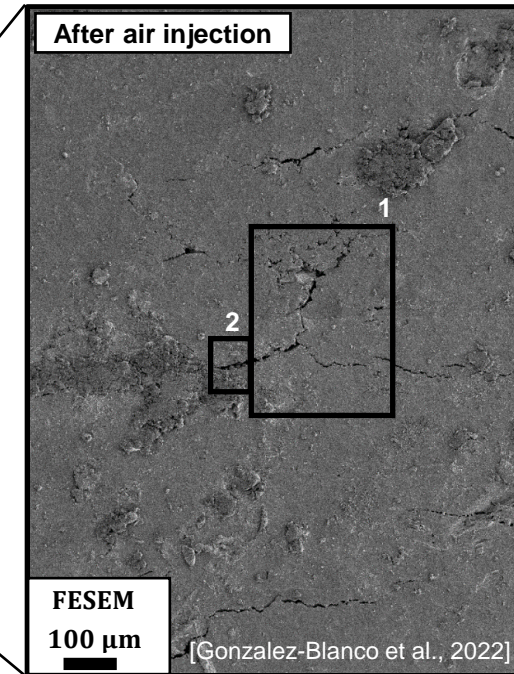
Repository scale



Laboratory scale



Process scale



Representation of microstructure effects



Large-scale models

Repository scale

- ▶ No direct representation of local phenomena
- ▶ Enriched with micro-mechanical effects, e.g. embedded fracture model

Intermediate-level multi-scale models

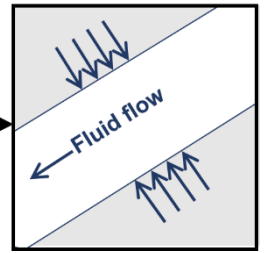
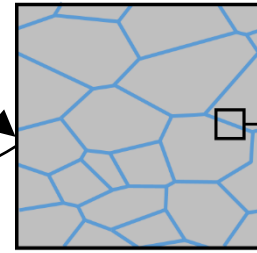
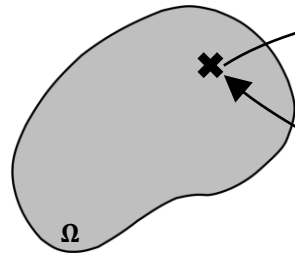
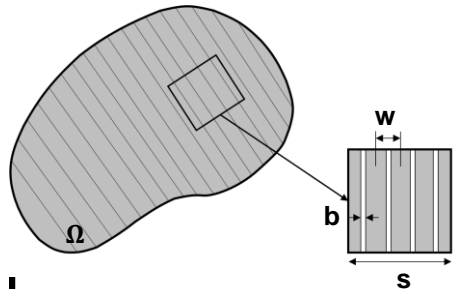
Laboratory scale

- ▶ Combination of the benefits from both scales
- ▶ Explicit description of the constituents on their specific length scale through a REV definition

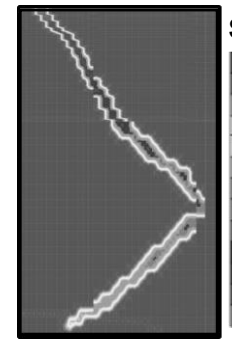
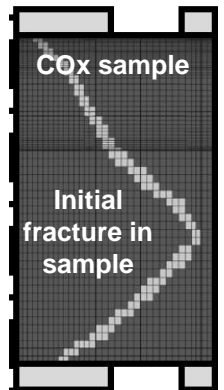
Small-scale models

Process scale

- ▶ Direct modelling of the whole microstructure
- ▶ Useful for modelling at the process scale



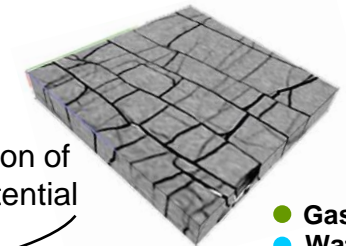
[van den Eijnden et al., 2016]



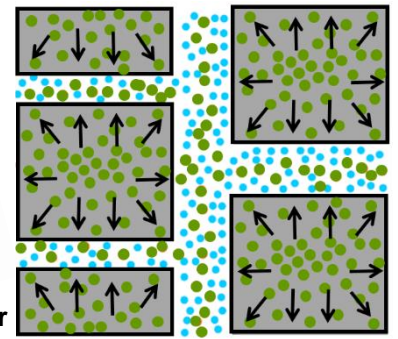
[Gerard et al., 2014]

High computational costs for upscaling

Very limited exploitation of the microstructure potential



● Gas
● Water

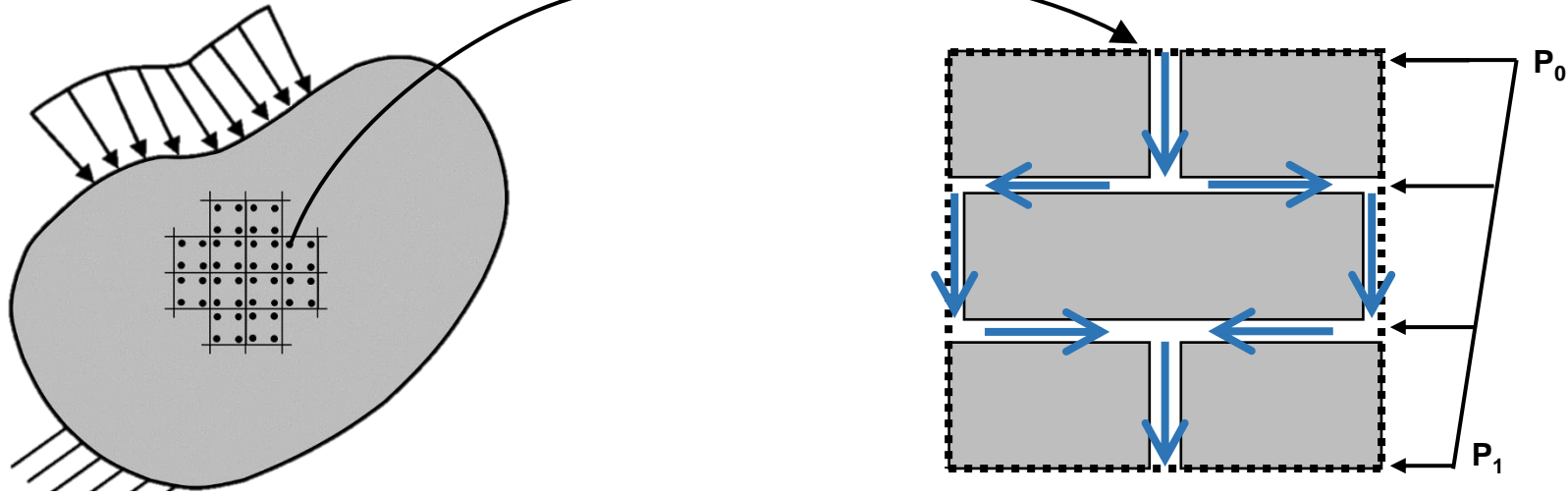


Multi-scale modelling approach

Macro-scale

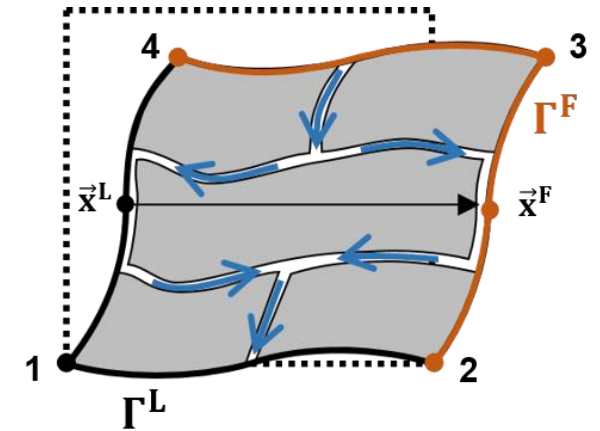
Micro-scale

1. Localisation



4 Steps

1 Localisation



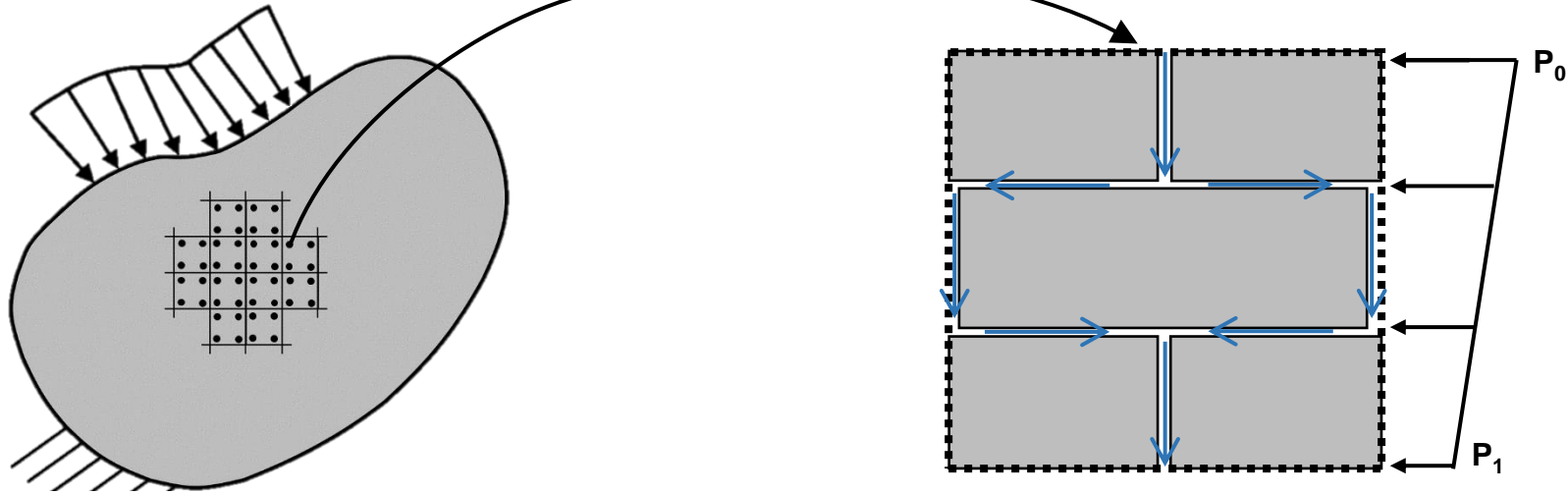
Periodic boundary conditions
Separation of scales

Multi-scale modelling approach

Macro-scale

Micro-scale

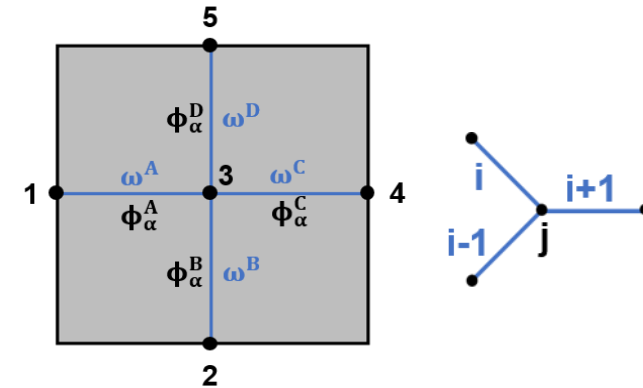
1. Localisation



2. Micro-scale computation

4 Steps

- ① Localisation
- ② Resolution of the problem at the micro-scale



Mass balance on each node:

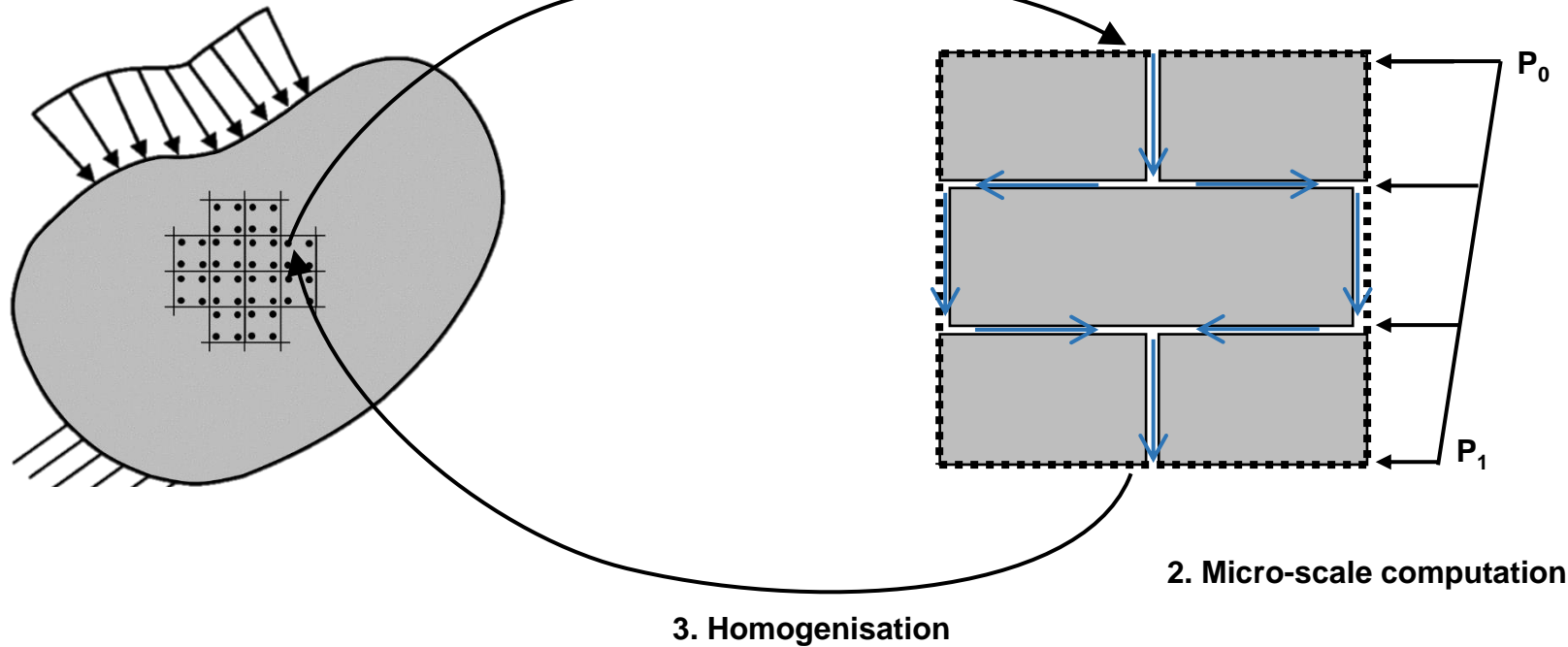
$$\omega_\alpha^{i-1} + \omega_\alpha^i + \omega_\alpha^{i+1}$$

Steady state conditions

Multi-scale modelling approach

Macro-scale

Micro-scale



4 Steps

- 1 Localisation
- 2 Resolution of the problem at the micro-scale
- 3 Homogenisation

Average micro-scale work = macro-scale work

[Hill, 1965][Mandel, 1972]

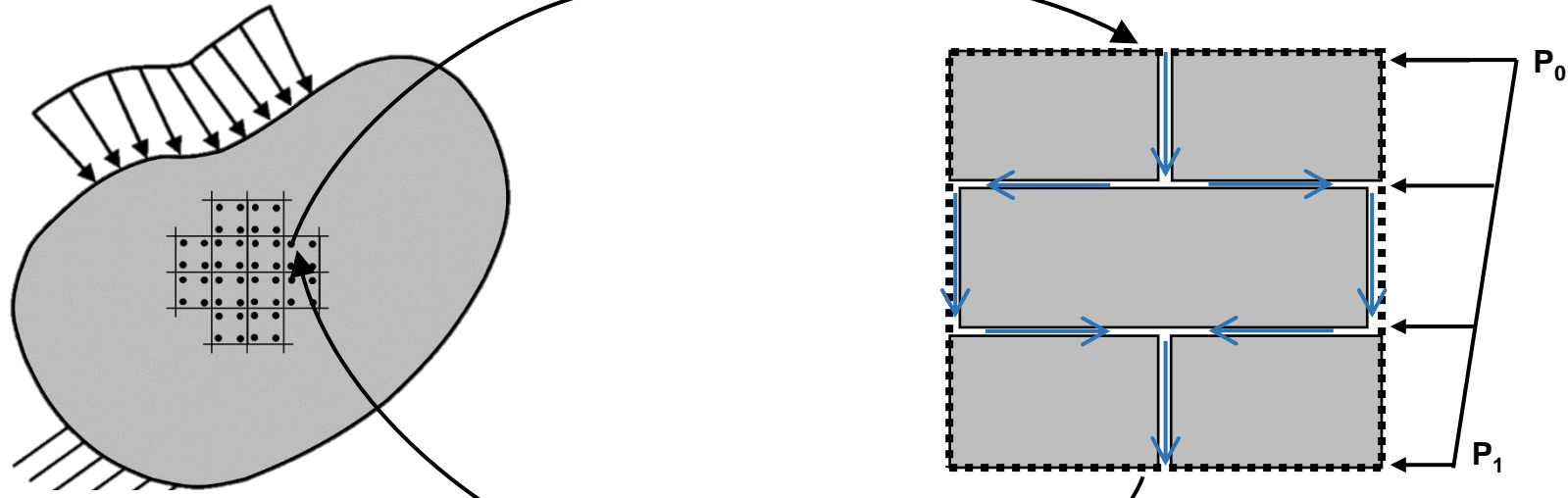
Fluxes
Fluid contents

Multi-scale modelling approach

Macro-scale

Micro-scale

1. Localisation



3. Homogenisation

2. Micro-scale computation

4. Macro-scale computation

4 Steps

- 1 Localisation
- 2 Resolution of the problem at the micro-scale
- 3 Homogenisation
- 4 Resolution of the problem at the macro-scale

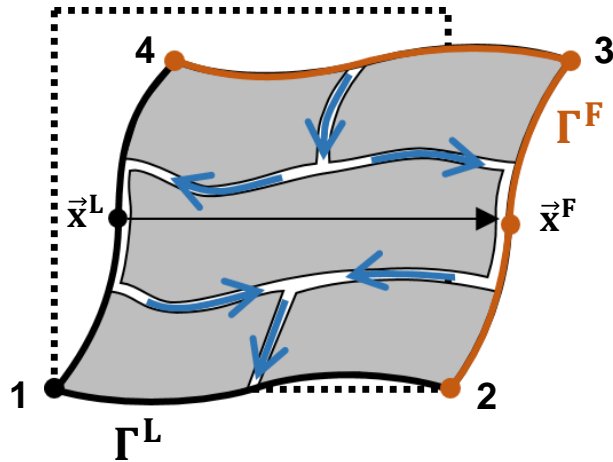
$$\begin{bmatrix} [E_{MM}^M] & [E_{MW}^M] & [E_{MG}^M] \\ [E_{WM}^M] & [E_{WW}^M] & [E_{WG}^M] \\ [E_{GM}^M] & [E_{GW}^M] & [E_{GG}^M] \end{bmatrix} \begin{Bmatrix} \{\delta \varepsilon^M\} \\ \{\delta \nabla p_w^M\} \\ \{\delta p_w^M\} \\ \{\delta \nabla p_g^M\} \\ \{\delta p_g^M\} \end{Bmatrix} = \begin{Bmatrix} \{\delta \sigma^M\} \\ \{\delta f_w^M\} \\ \{\delta M_w^M\} \\ \{\delta f_g^M\} \\ \{\delta M_g^M\} \end{Bmatrix}$$

$$[E^M]_{(10 \times 10)} \cdot \{\delta U^M\}_{10} = \{\delta \Sigma^M\}_{10}$$

- $[E^M] \equiv$ Macro-scale stiffness matrix
- $\{\delta U^M\} \equiv$ Infinitesimal variations of the macro-scale variables
- $\{\delta \Sigma^M\} \equiv$ Responses of the macro-scale variables

Multi-scale modelling approach

1 Localisation (macro- to micro-scale transition)



Periodic boundary conditions

Water pressure:

$$p_w^F = p_w^L + (\nabla p_w)^M (x_j^F - x_j^L)$$

Gas pressure:

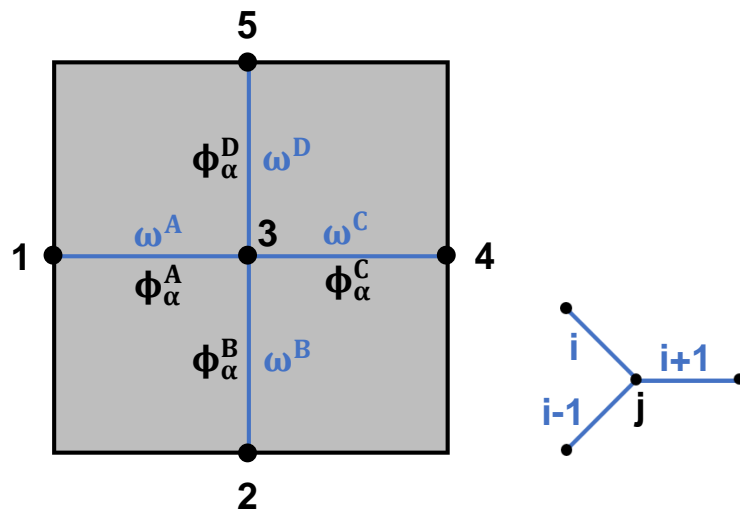
$$p_g^F = p_g^L + (\nabla p_g)^M (x_j^F - x_j^L)$$

Separation of scales:

$$l_{REV} \ll \frac{p^M [Pa]}{\nabla p^M \left[\frac{Pa}{m} \right]}$$

If important macro-solicitation, potentially not satisfied because the difference the left and right boundaries is also very important

2 Resolution of the micro-scale hydraulic network



Conditions to be respected

Anti-symmetric boundary fluxes:

$$\omega_\alpha^A = -\omega_\alpha^C$$

$$\omega_\alpha^B = -\omega_\alpha^D$$

No storage

Macroscopic pressure gradient:

$$p_4 - p_1 = (\nabla p)_x^M \Delta x$$

$$p_5 - p_2 = (\nabla p)_y^M \Delta y$$

Mass balance on each node

$$\omega_\alpha^{i-1} + \omega_\alpha^i + \omega_\alpha^{i+1}$$

In = out

$$\omega_\alpha^i = \Phi_\alpha^i (p_j - p_{j-1})$$

$$\Phi_\alpha^i \equiv \text{Flow model for the channel } i$$

Given mechanical configuration
Steady state conditions

Multi-scale modelling approach

③ Homogenisation (micro- to macro-scale transition)

Hill-Mandel macro-homogeneity condition

Average micro-scale work = macro-scale work

[Hill, 1965][Mandel, 1972]

Fluxes:
$$\mathbf{f}_{\alpha_i}^M = \frac{1}{\Omega} \int_{\Gamma} \bar{\mathbf{q}}_{\alpha}^m x_i \, d\Gamma$$

Fluid contents:
$$\mathbf{M}_w^M = \frac{1}{\Omega} \int_{\Omega_w^{int}} \rho_w \, d\Omega = \rho_w S_r \phi_n$$

$$\mathbf{M}_w^M = \mathbf{M}_g^m + \mathbf{M}_{dg}^m = \rho_g (1 - S_r) \phi_n + \rho_{dg} S_r \phi_n$$

Fluid mass storage terms:

$$\dot{\mathbf{M}}^{M,t} \approx \frac{\mathbf{M}^{M,t} - \mathbf{M}^{M,t-\Delta t}}{\Delta t}$$

④ Macro-scale computations

The macro-scale problem is solved using finite elements

under matrix form:

$$\begin{bmatrix} [\mathbf{E}_{MM}^M] & [\mathbf{E}_{MW}^M] & [\mathbf{E}_{MG}^M] \\ [\mathbf{E}_{WM}^M] & [\mathbf{E}_{WW}^M] & [\mathbf{E}_{WG}^M] \\ [\mathbf{E}_{GM}^M] & [\mathbf{E}_{GW}^M] & [\mathbf{E}_{GG}^M] \end{bmatrix} \begin{Bmatrix} \{\delta \boldsymbol{\varepsilon}^M\} \\ \{\delta \nabla \mathbf{p}_w^M\} \\ \{\delta \nabla \mathbf{p}_g^M\} \\ \{\delta \mathbf{p}_g^M\} \end{Bmatrix} = \begin{Bmatrix} \{\delta \boldsymbol{\sigma}^M\} \\ \{\delta \mathbf{f}_w^M\} \\ \{\delta \mathbf{f}_g^M\} \\ \{\delta \dot{\mathbf{M}}_g^M\} \end{Bmatrix}$$

summarised as:

$$[\mathbf{E}^M]_{(10 \times 10)} \{\delta \mathbf{U}^M\}_{10} = \{\delta \boldsymbol{\Sigma}^M\}_{10}$$

$$f_{w_i}^M \frac{\partial p_w^{*,M}}{\partial x_i} = \frac{1}{\Omega} \int_{\Omega} f_{w_i}^m \frac{\partial p_w^{*,M}}{\partial x_i} d\Omega = \frac{1}{\Omega} \int_{\Gamma} \bar{q}_w^m p_w^{*,M} d\Gamma \quad M_w^M = \frac{1}{\Omega} \int_{\Omega_w^{int}} \rho_w d\Omega = \rho_w S_r \phi_n$$

$$= \frac{1}{\Omega} \frac{\partial p_w^{*,M}}{\partial x_i} \int_{\Gamma} \bar{q}_w^m x_i d\Gamma$$

$$= \frac{1}{\Omega} \int_{\Gamma} \bar{q}_w^m x_i d\Gamma$$

$$f_{g_i}^M + f_{dg_i}^M = \frac{1}{\Omega} \int_{\Gamma} \bar{q}_g^m x_i d\Gamma$$

$$M_g^M = M_g^m + M_{dg}^m = \frac{1}{\Omega} \left(\int_{\Omega_g^{int}} \rho_g d\Omega + \int_{\Omega_w^{int}} \rho_{dg} d\Omega \right) = \rho_g (1 - S_{rw}) \phi_n + \rho_{dg} S_{rw} \phi_n$$

Steady state

Perturbation: Numerically compute the derivative terms in the rigidity matrix

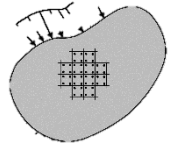
$[\mathbf{E}^M] \equiv$ Macro-scale stiffness matrix

$\{\delta \mathbf{U}^M\} \equiv$ Infinitesimal variations of the macro-scale variables

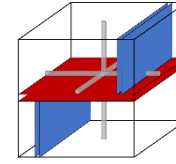
$\{\delta \boldsymbol{\Sigma}^M\} \equiv$ Responses of the macro-scales variables

Hydro-mechanical multi-scale model

Macro-scale



Micro-scale (REV)



Mechanical model

- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

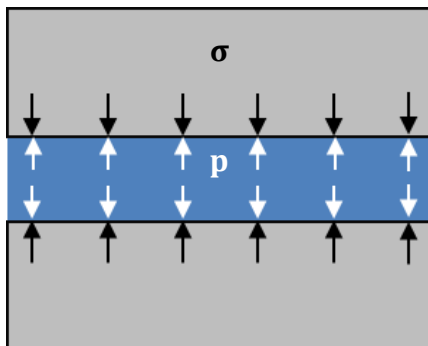
$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

Hydro-mechanical couplings

- ▶ Effective stress definition

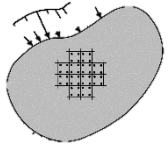
[Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$



Hydro-mechanical multi-scale model

Macro-scale



Mechanical model

- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

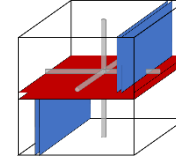
Hydro-mechanical couplings

- ▶ Effective stress definition

[Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$

Micro-scale (REV)



Hydraulic model

- ▶ Permeability

$$\mathbf{k}_{\text{frac}} = \frac{h_b^2 h_b}{12 w}$$

Navier-Stokes equations

Planes

between two parallel plates

Tubes

$$\mathbf{k}_{\text{tube}} = \pi \frac{D_b^4}{128 w^2}$$

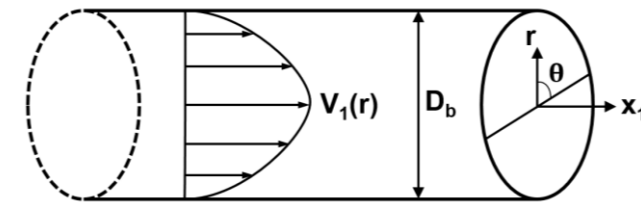
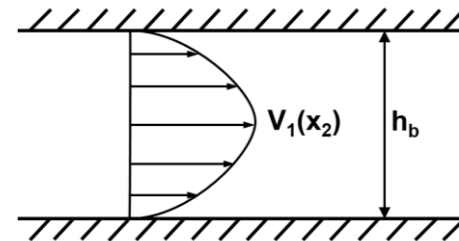
in a cylinder

Non-slip boundary conditions

Laminar flow

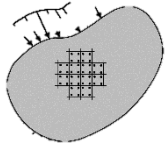
Steady state conditions

No body force



Hydro-mechanical multi-scale model

Macro-scale



Mechanical model

- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

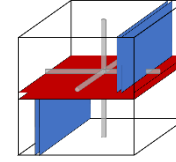
$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

Hydro-mechanical couplings

- ▶ Effective stress definition
[Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$

Micro-scale (REV)



Hydraulic model

- ▶ Permeability
- ▶ Multi-phase flow
[Yuster et al., 1951]

Planes

$$k_{\text{frac}} = \frac{h_b^2 h_b}{12 w}$$

$$k_{\text{rw}} = \frac{S_r^{*2}}{2} (3 - S_r^*)$$

$$k_{\text{rg}} = (1 - S_r^*)^3$$

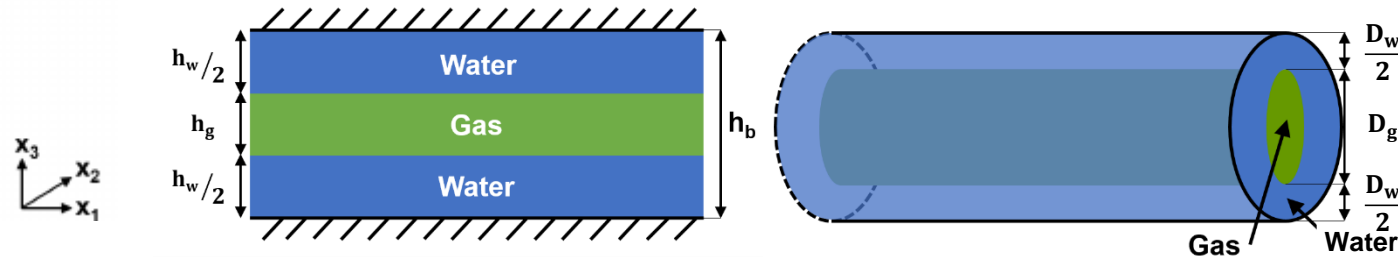
Tubes

$$k_{\text{tube}} = \pi \frac{D_b^4}{128 w^2}$$

$$k_{\text{rw}} = S_r^{*2}$$

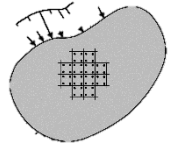
$$k_{\text{rg}} = (1 - S_r^*)^2$$

Integrating Navier-Stokes in each stratum considering that the fluids are flowing simultaneously



Hydro-mechanical multi-scale model

Macro-scale



Mechanical model

- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

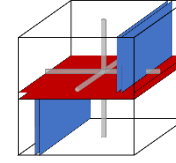
$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

Hydro-mechanical couplings

- ▶ Effective stress definition [Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$

Micro-scale (REV)



Hydraulic model

- ▶ Permeability
- ▶ Multi-phase flow [Yuster et al., 1951]

- ▶ Retention curve [van Genuchten., 1980]

Planes

$$k_{\text{frac}} = \frac{h_b^2 h_b}{12 w}$$

$$k_{\text{rw}} = \frac{S_r^{*2}}{2} (3 - S_r^*)$$

$$k_{\text{rg}} = (1 - S_r^*)^3$$

Tubes

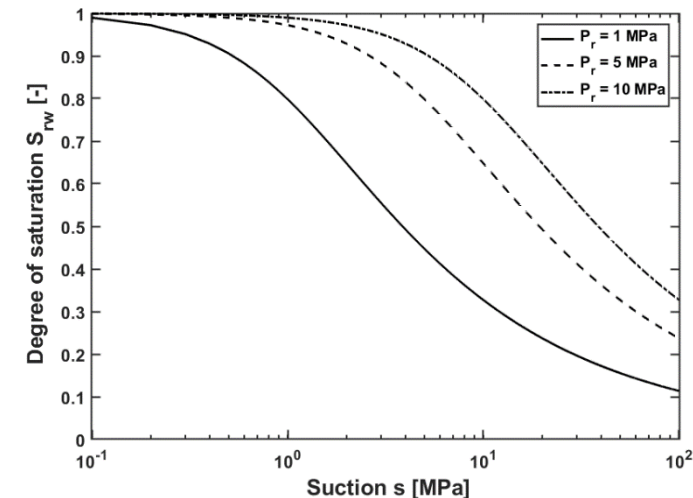
$$k_{\text{tube}} = \pi \frac{D_b^4}{128 w^2}$$

$$k_{\text{rw}} = S_r^{*2}$$

$$k_{\text{rg}} = (1 - S_r^*)^2$$

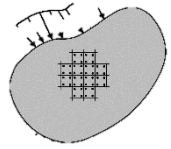
$$S_{\text{rw}} = S_{\text{r,res}} + (S_{\text{max}} - S_{\text{r,res}}) \left(1 + \left(\frac{p_c}{P_r} \right)^{\mathcal{N}} \right)^{\frac{1}{\mathcal{N}-1}}$$

$$P_{r,0} = \frac{2\sigma \cos \theta}{h_b} \quad P_{r,0} = \frac{2\sigma \cos \theta}{D_b/2}$$



Hydro-mechanical multi-scale model

Macro-scale



Mechanical model

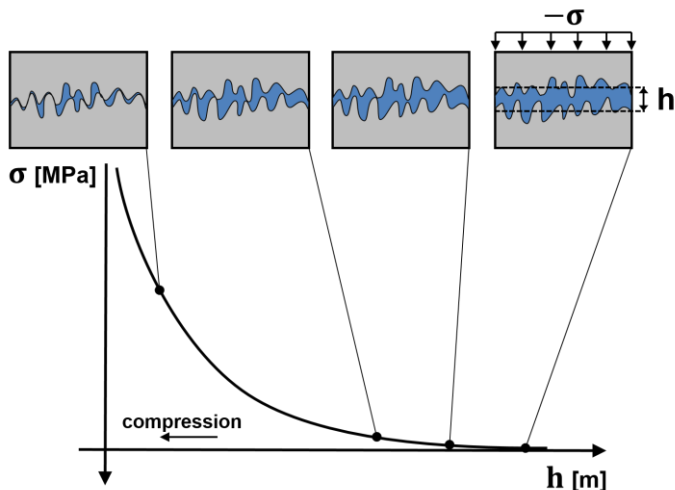
- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

Hydro-mechanical couplings

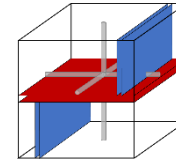
- ▶ Effective stress definition [Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$



Modified after [Cerfontaine et al., 2015]

Micro-scale (REV)



Hydraulic model

- ▶ Permeability
- ▶ Multi-phase flow [Yuster et al., 1951]

- ▶ Retention curve [van Genuchten., 1980]

Hydro-mechanical couplings

- ▶ Mechanical aperture [Goodman., 1976]

Planes

$$k_{\text{frac}} = \frac{h_b^2 h_b}{12 w}$$

$$k_{\text{rw}} = \frac{S_r^{*2}}{2} (3 - S_r^*)$$

$$k_{\text{rg}} = (1 - S_r^*)^3$$

$$S_{\text{rw}} = S_{\text{r,res}} + (S_{\text{max}} - S_{\text{r,res}}) \left(1 + \left(\frac{p_c}{P_r} \right)^{\mathcal{N}} \right)^{\frac{1}{\mathcal{N}} - 1}$$

$$P_{\text{r},0} = \frac{2\sigma \cos \theta}{h_b}$$

Tubes

$$k_{\text{tube}} = \pi \frac{D_b^4}{128 w^2}$$

$$k_{\text{rw}} = S_r^{*2}$$

$$k_{\text{rg}} = (1 - S_r^*)^2$$

$$P_{\text{r},0} = \frac{2\sigma \cos \theta}{D_b/2}$$

$$h_{\text{b}(x)} = \frac{\dot{\sigma}'_{(xx)}}{K_{\text{n}(x)}}$$

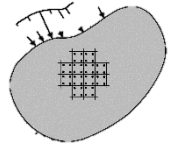
$$K_{\text{n}} = \frac{K_{\text{n}}^0}{\left(1 - \frac{h_0 - h}{h_0} \right)^2}$$

$$\dot{D}_{\text{b}(x)} = \frac{\dot{\sigma}'_{(xx)}}{K_{(x)}}$$

$$K = \frac{2G}{D_0}$$

Hydro-mechanical multi-scale model

Macro-scale



Mechanical model

- ▶ Isotropic elastic law
- ▶ Elasto-plastic law

$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}) = f(\mathbf{E}, \mathbf{v}, \mathbf{c}, \boldsymbol{\varphi})$$

Hydro-mechanical couplings

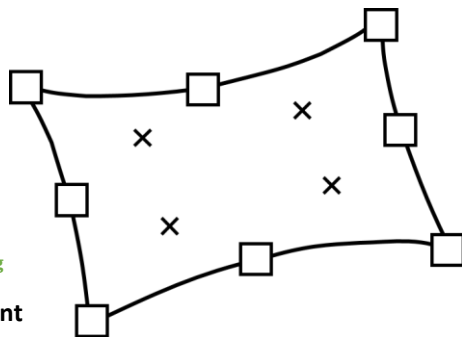
- ▶ Effective stress definition
[Bishop, 1959]

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \mathbf{p} \quad \mathbf{p} = \mathbf{S}_r \cdot \mathbf{p}_w + (\mathbf{1} - \mathbf{S}_r) \cdot \mathbf{p}_g$$

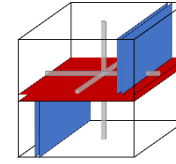
Model implemented in the FE code LAGAMINE



- Node $\mathbf{u}_i, \mathbf{p}_w, \mathbf{p}_g$
- × Integration point



Micro-scale (REV)



Hydraulic model

- ▶ Permeability
- ▶ Multi-phase flow
[Yuster et al., 1951]

- ▶ Retention curve
[van Genuchten., 1980]

Planes

$$\mathbf{k}_{\text{frac}} = \frac{h_b^2 h_b}{12 w}$$

$$\mathbf{k}_{\text{rw}} = \frac{S_r^{*2}}{2} (3 - S_r^*)$$

$$\mathbf{k}_{\text{rg}} = (1 - S_r^*)^3$$

$$S_{\text{rw}} = S_{\text{r,res}} + (S_{\text{max}} - S_{\text{r,res}}) \left(1 + \left(\frac{p_c}{P_r} \right)^{\mathcal{N}} \right)^{\frac{1}{\mathcal{N}} - 1}$$

$$P_{\text{r},0} = \frac{2\sigma \cos \theta}{h_b}$$

Tubes

$$\mathbf{k}_{\text{tube}} = \pi \frac{D_b^4}{128 w^2}$$

$$\mathbf{k}_{\text{rw}} = S_r^{*2}$$

$$\mathbf{k}_{\text{rg}} = (1 - S_r^*)^2$$

$$P_{\text{r},0} = \frac{2\sigma \cos \theta}{D_b/2}$$

Hydro-mechanical couplings

- ▶ Mechanical aperture
[Goodman., 1976]

$$h_{\text{b}(x)} = \frac{\dot{\boldsymbol{\sigma}}'_{(xx)}}{\mathbf{K}_{\text{n}(x)}}$$

$$\mathbf{K}_{\text{n}} = \frac{K_{\text{n}}^0}{\left(1 - \frac{h_0 - h}{h_0} \right)^2}$$

→ Permeability (implicit)

→ Entry pressure (implicit) $P_r = P_{\text{r},0} \left(\frac{h_{\text{b}0}}{h_b} \right)^m$

$$\mathbf{D}_{\text{b}(x)} = \frac{\dot{\boldsymbol{\sigma}}'_{(xx)}}{\mathbf{K}_{(x)}}$$

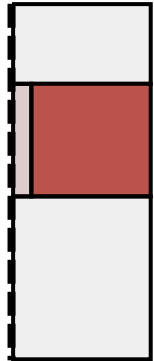
$$\mathbf{K} = \frac{2G}{D_0}$$

$$P_r = P_{\text{r},0} \left(\frac{D_{\text{b}0}}{D_b} \right)^m$$

Applications

Gas injection experiment (lab scale, BC)

Characterisation of the sample



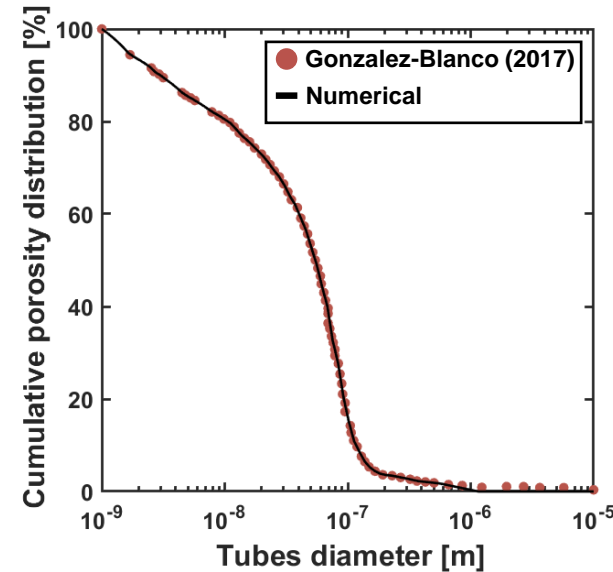
1. Size of the REV

Bedding plane separation
 $w = 300 \mu\text{m}$

2. Macro-porosity

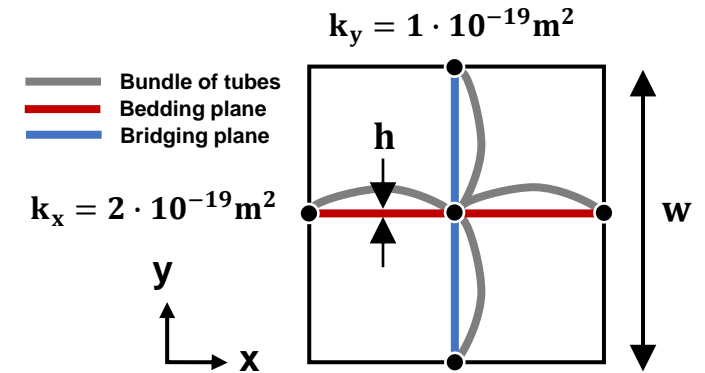
Fitting of the pore size distribution

Effect of small-size pores
(Tortuosity = Calibration factor)



[Gonzalez-Blanco, 2017]

FESEM	μ -CT
150 – 270 μm	410 – 560 μm



3. Global permeability

Effect of large-size pores

Fracture aperture

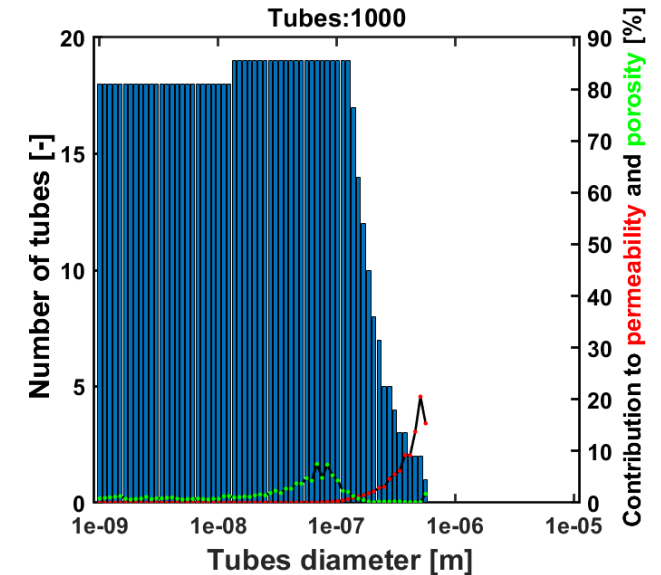
$$k_{x, \text{frac}, 0} = 10^{-19} \text{m}^2$$

$$\rightarrow h_{b,0} = \sqrt[3]{12 w k}$$

Macro-pores

$$k_x = \frac{\pi}{8} \left(\frac{D_b}{2} \right)^4 \left(\frac{1}{w^2} \right) + \frac{k_{x, \text{frac}}}{12} \left(\frac{h}{w} \right)^2$$

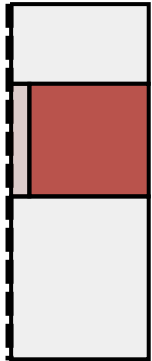
$$k_y = \frac{\pi}{8} \left(\frac{D_b}{2} \right)^4 \left(\frac{1}{w^2} \right)$$



Applications

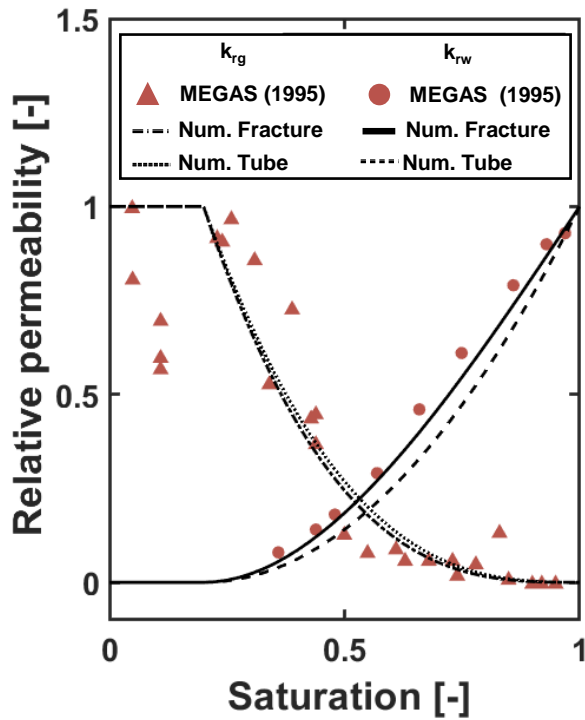
Gas injection experiment (lab scale, BC)

Characterisation of the sample



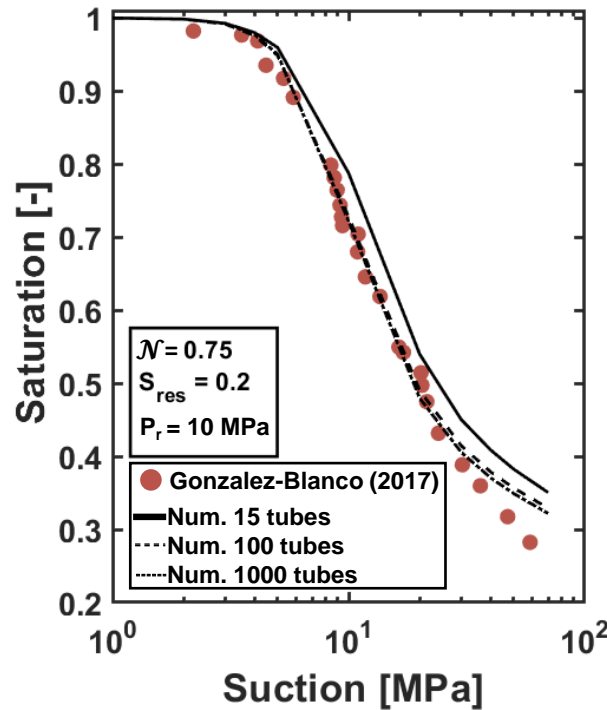
4. Relative permeability curves

[Yuster et al., 1951]



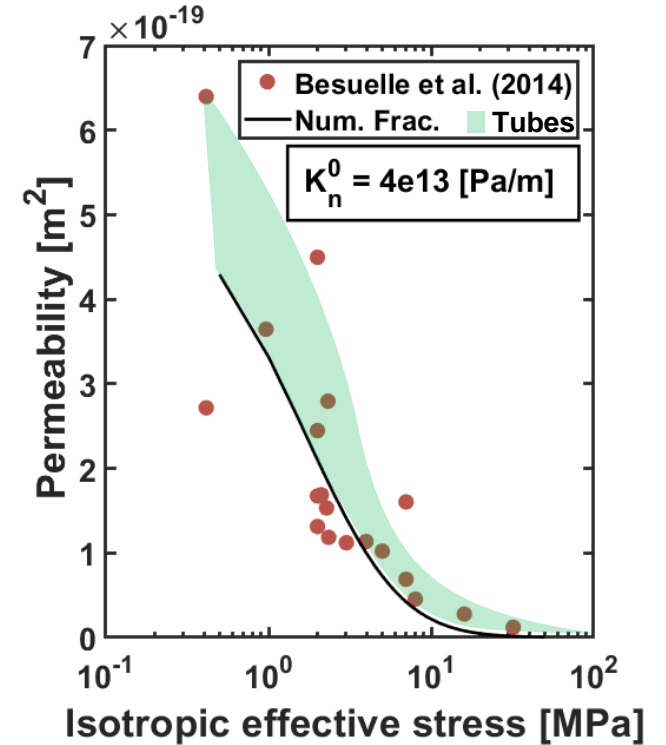
5. Retention curve

[van Genuchten, 1980]



6. Normal stiffness of the fracture

[Goodman, 1976]



Planes

$$k_{rw} = \frac{S_r^{*2}}{2} (3 - S_r^*)$$

$$k_{rg} = (1 - S_r^*)^3$$

Tubes

$$k_{rw} = S_r^{*2}$$

$$k_{rg} = (1 - S_r^*)^2$$

$$S_{rw} = S_{r,res} + (S_{max} - S_{r,res}) \left(1 + \left(\frac{p_c}{P_r} \right)^N \right)^{\frac{1}{N}-1}$$

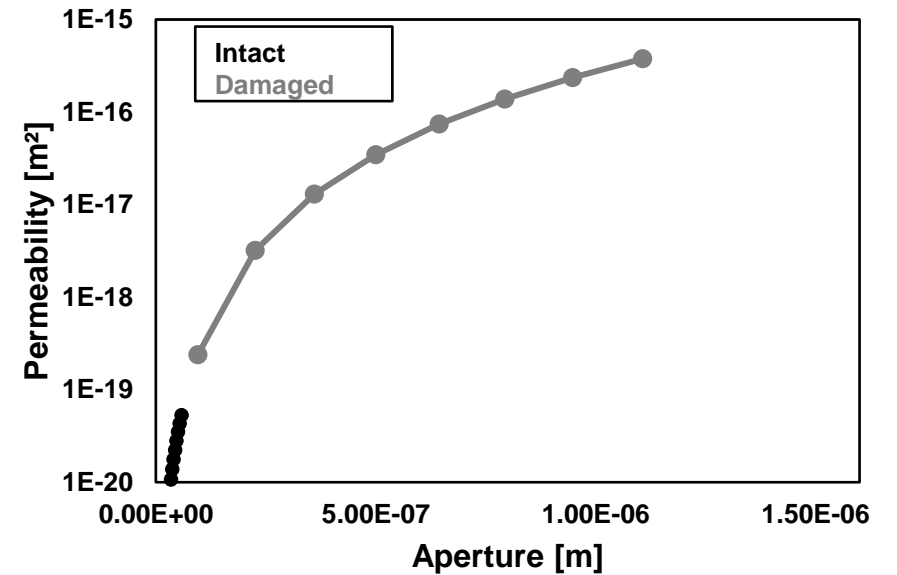
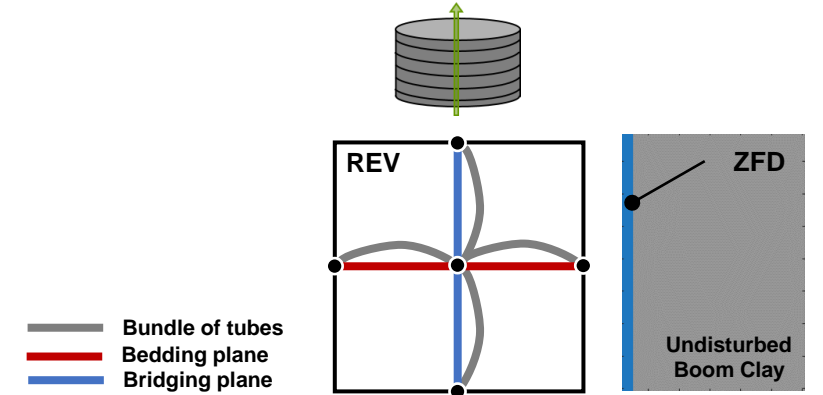
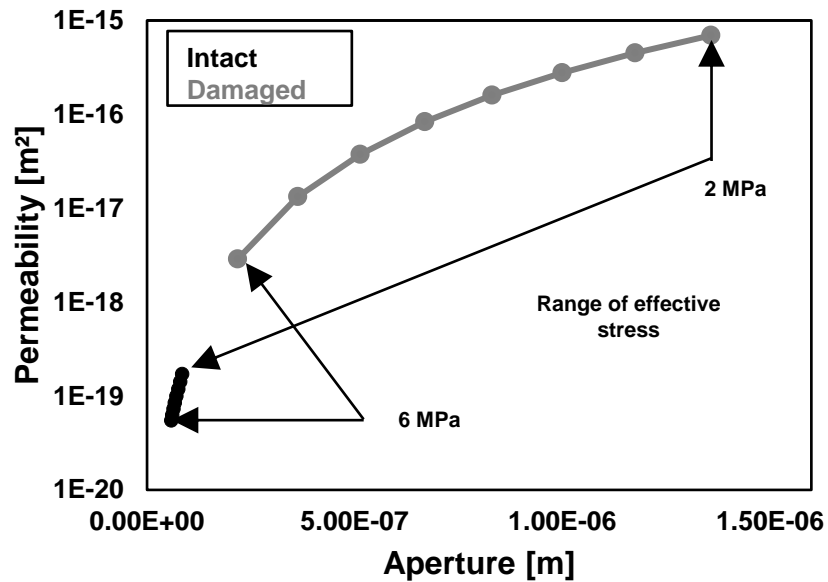
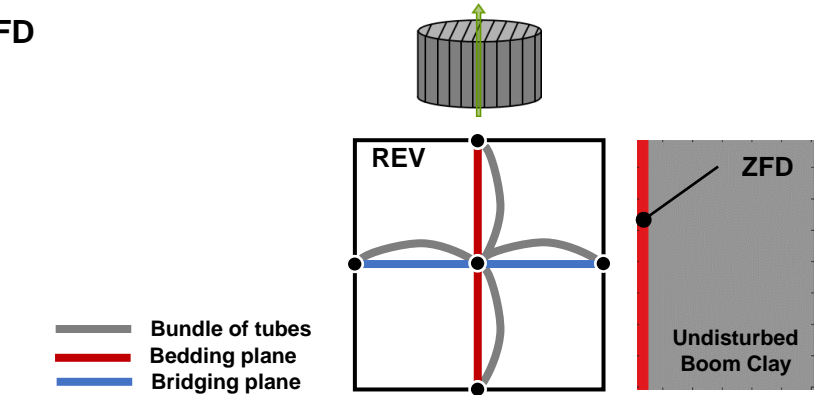
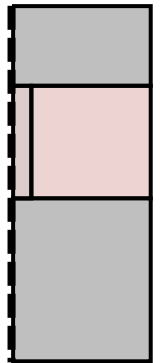
$$h_{b(x)} = \frac{\sigma_{(xx)}}{K_n(x)}$$

$$K_n = \frac{K_n^0}{\left(1 - \frac{h_0 - h}{h_0} \right)^2}$$

Applications

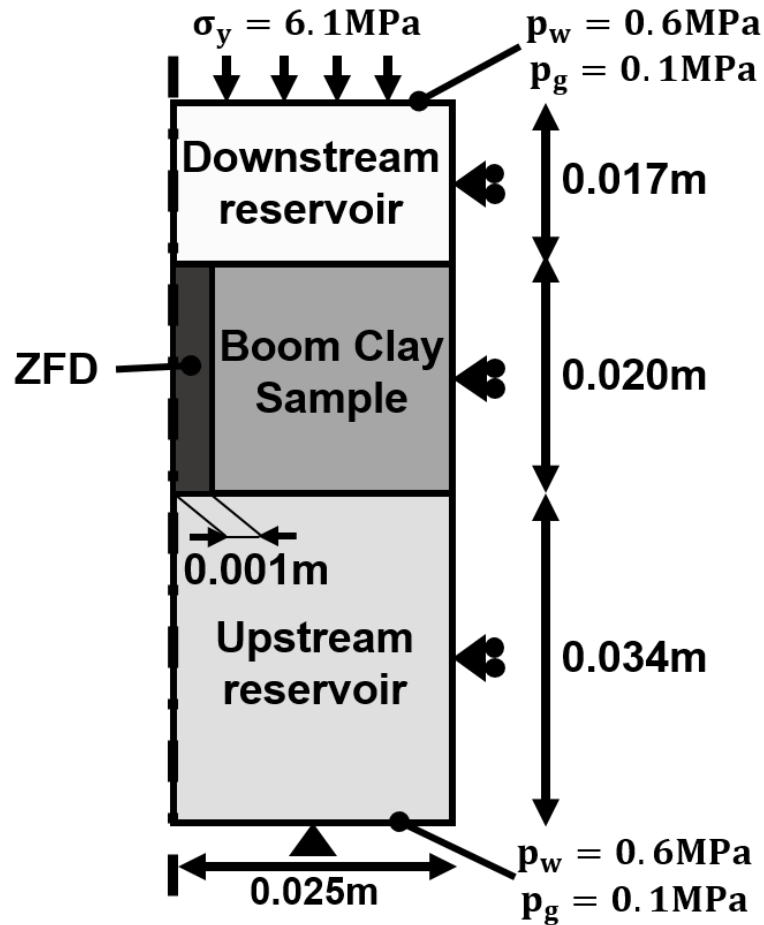
Gas injection experiment (lab scale, BC)

Characterisation of the ZFD



Multi-scale application

Geometry and boundary conditions



Parameters

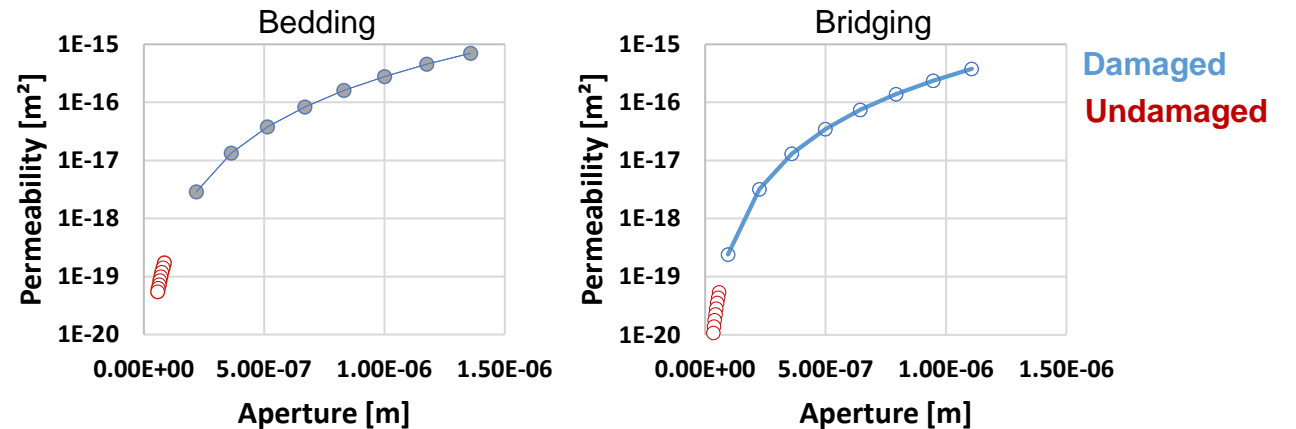
Reservoirs

- Stiff elements: $E = 10000\text{MPa}$ $\nu = 0.3$
- Highly conductive: $n = 0.5$ $k = 10^{-10}\text{m}^2$
- Flat retention curve: $P_{\text{entry}} = 0.01\text{MPa}$

Boom Clay matrix

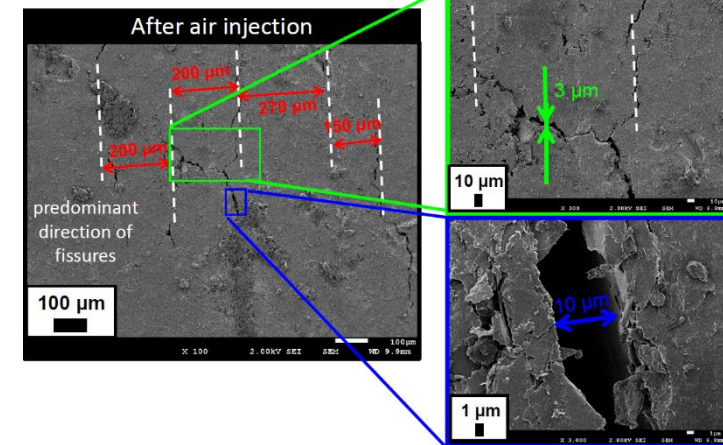
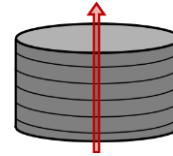
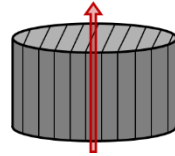
- Mechanical: $E = 200 - 400\text{MPa}$ $\nu = 0.33$
- Hydraulic:
 - Initial aperture: $0.80 - 1.27 \cdot 10^{-7}\text{m}$
 - Initial permeability: $2.0 - 4.0 \cdot 10^{-19}\text{m}^2$
 - Initial porosity: 0.363

Boom Clay Zone of Fracture Development (ZFD)



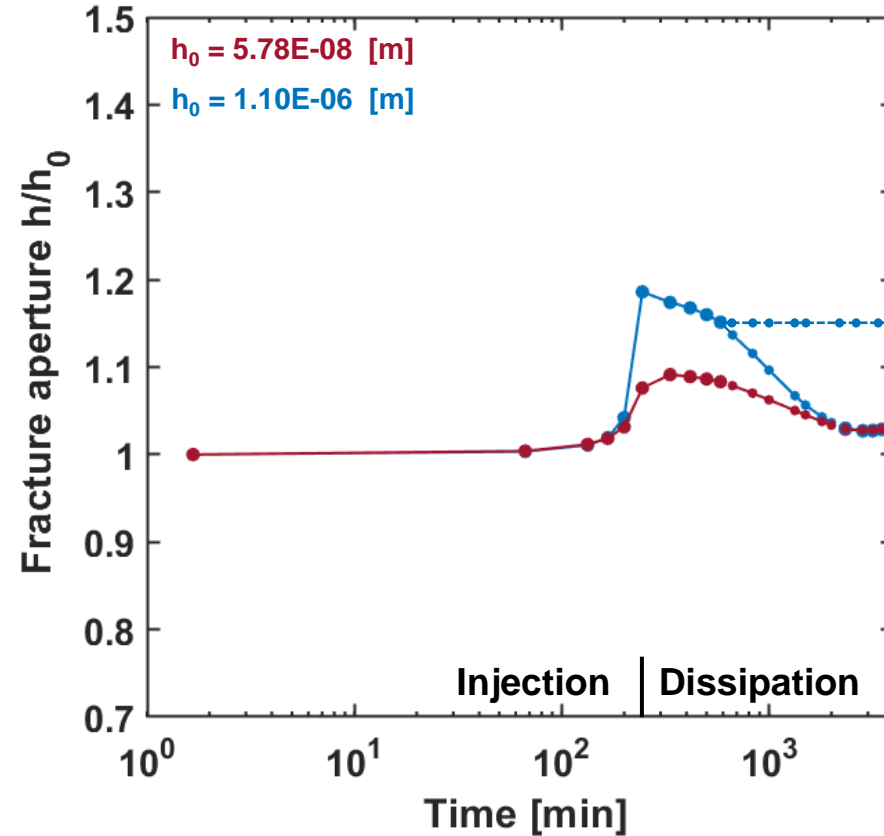
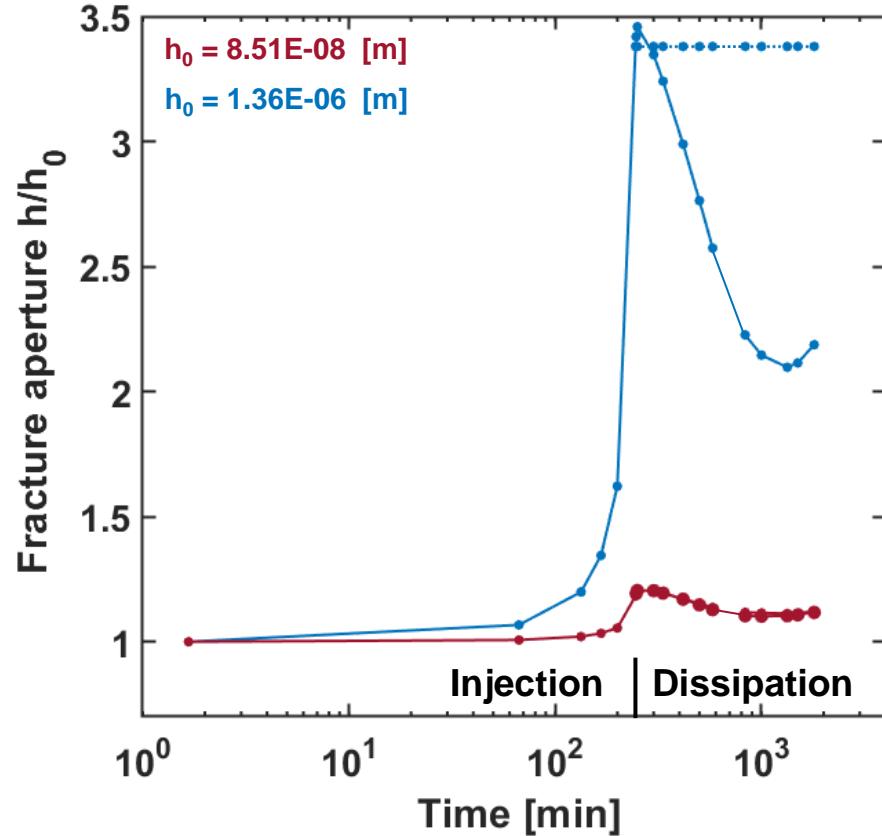
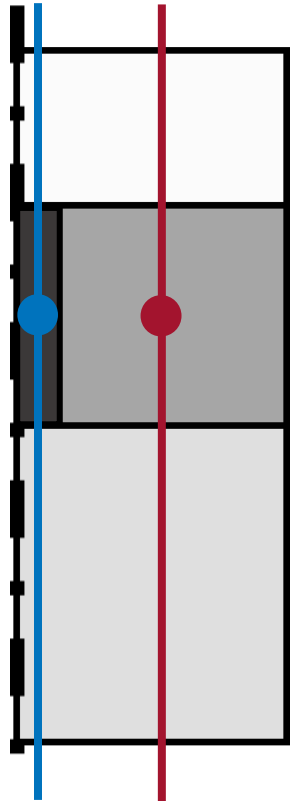
Multi-scale application

Fracture aperture



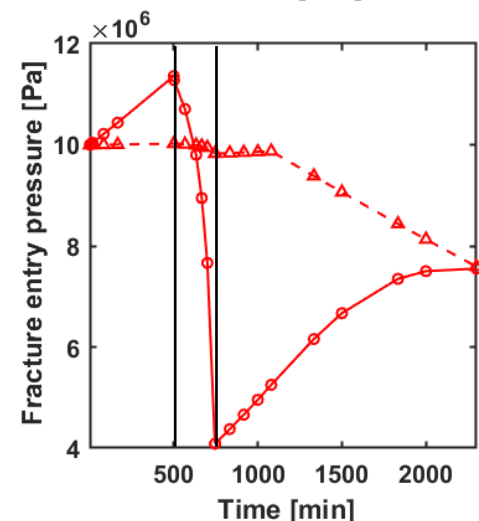
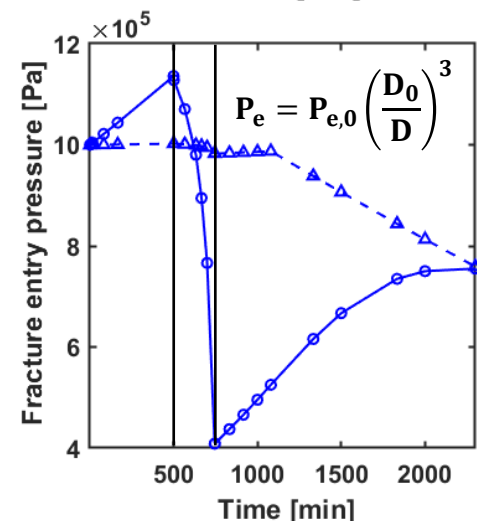
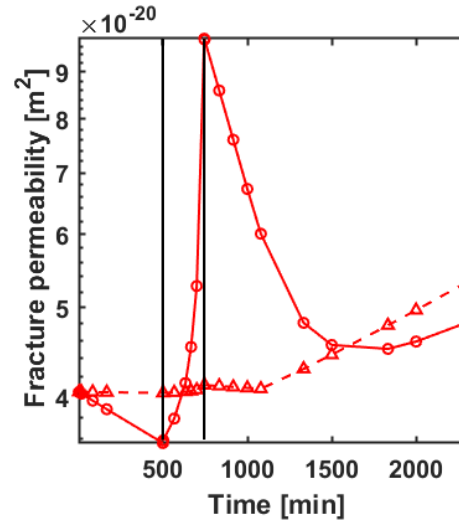
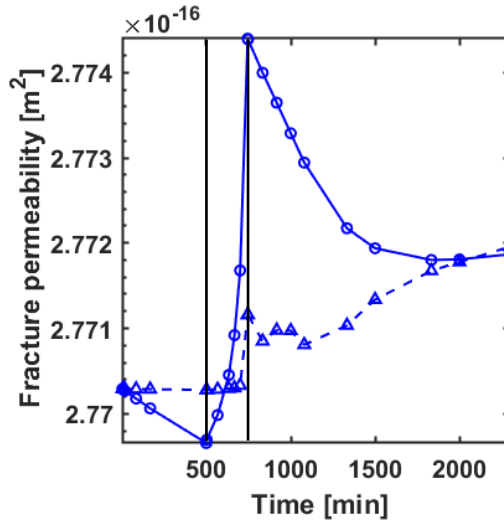
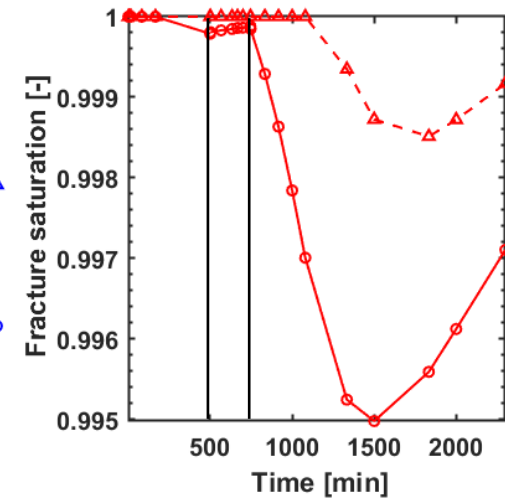
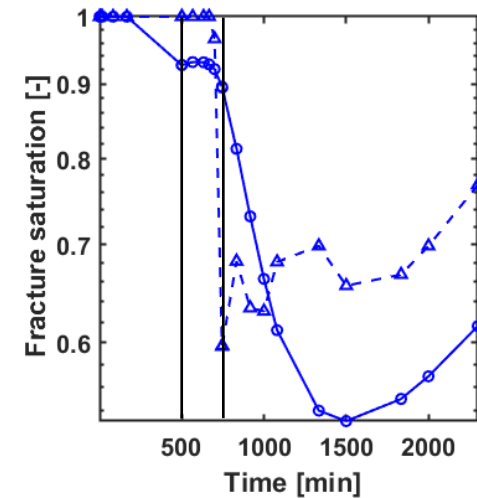
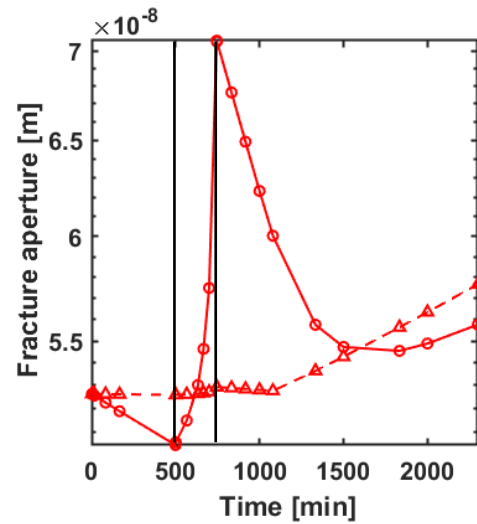
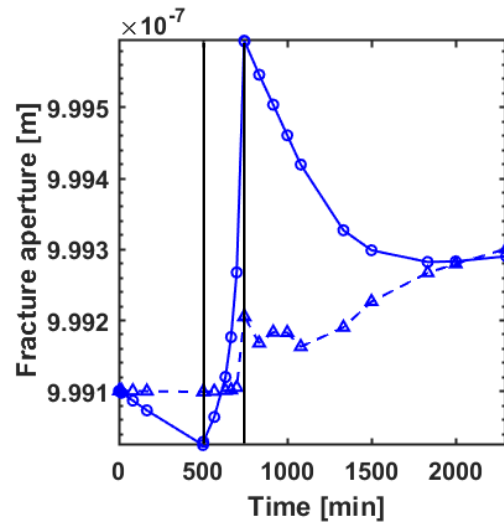
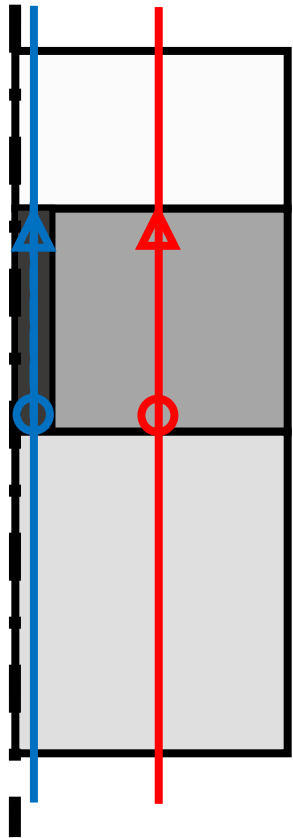
Experimental observations: Opened fractures after injection

Gonzalez-Blanco & Romero (2022)



Multi-scale application

Fracture aperture



Original contributions

Second gradient H²M model

[Corman et al., 2022]

- A new degree of freedom for **gas**
- A **biphasic fluid transfer model** into the second gradient framework.
- **HM couplings** between the transfer properties and the deformations
- **Small-scale** and **large-scale applications** to assess the impact of the HM couplings inherent to the EDZ on gas flows

Integration of the models

- **3D modelling**
- **Stochastic approach**
- **Predictability**

Multi-scale HM model

[Corman et al. 2024] (under review)

- **Microstructure** (tube and fracture), and related parameters for clay rocks
- **HM couplings** between the transfer properties (micro-scale) and the stress state (macro-scale)
- Mechanism of **diffusion of dissolved gas** within the liquid phase
- **Lab-scale** gas injection tests and of **up-scaled configurations**, to assess the potential development of gas preferential pathways

Perspectives

- Improve the fracture modelling
 - Integrate other types of fractures
 - Investigate the onset of strain localisation
- Improve the coupled processes modelling
 - Thermal effects
 - Self-sealing capacity
- Improve the coupled processes modelling
 - Macroscopic fractures
 - Self-sealing capacity
- Improve the integration of heterogeneity and variability