UNSAT-WASTE 2023

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European Joint Programme on Radioactive Waste Management

Multiscale modelling of gas flow in Boom Clay

5th International Symposium on Unsaturated soil Mechanics and Waste Disposal
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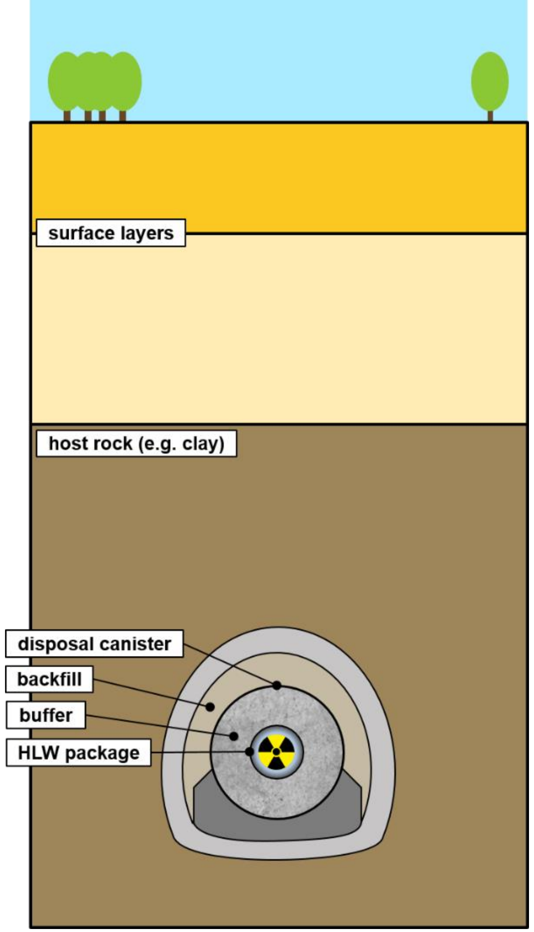
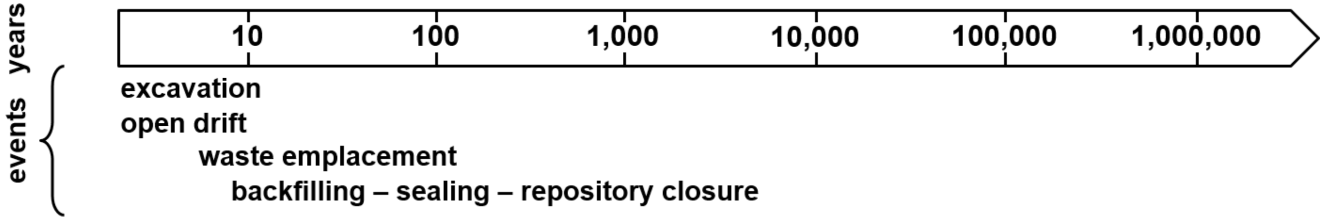
The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n° 847593.

Context

Geological disposal of radioactive wastes



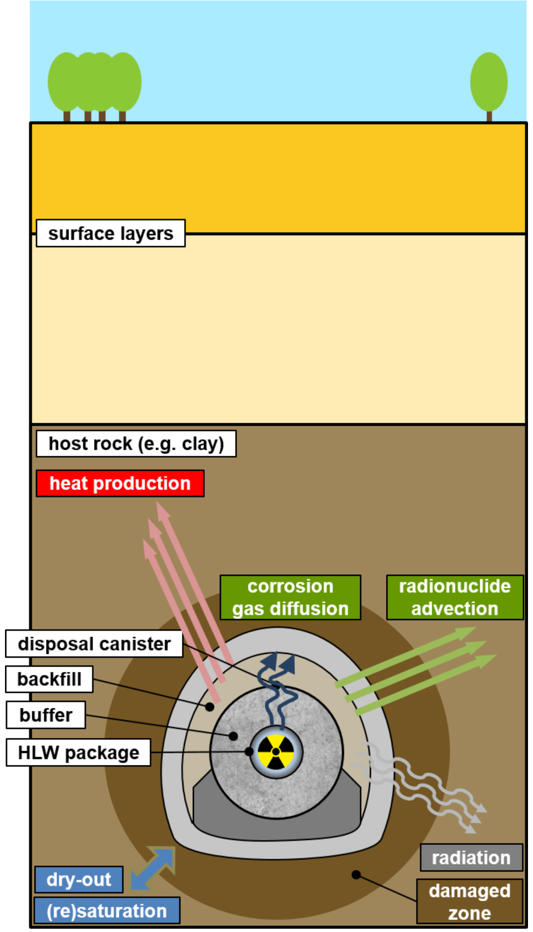
Conceptual scheme of a deep geological repository.



Context

Geological disposal of radioactive wastes

- Complex multi-physical (THMC) processes



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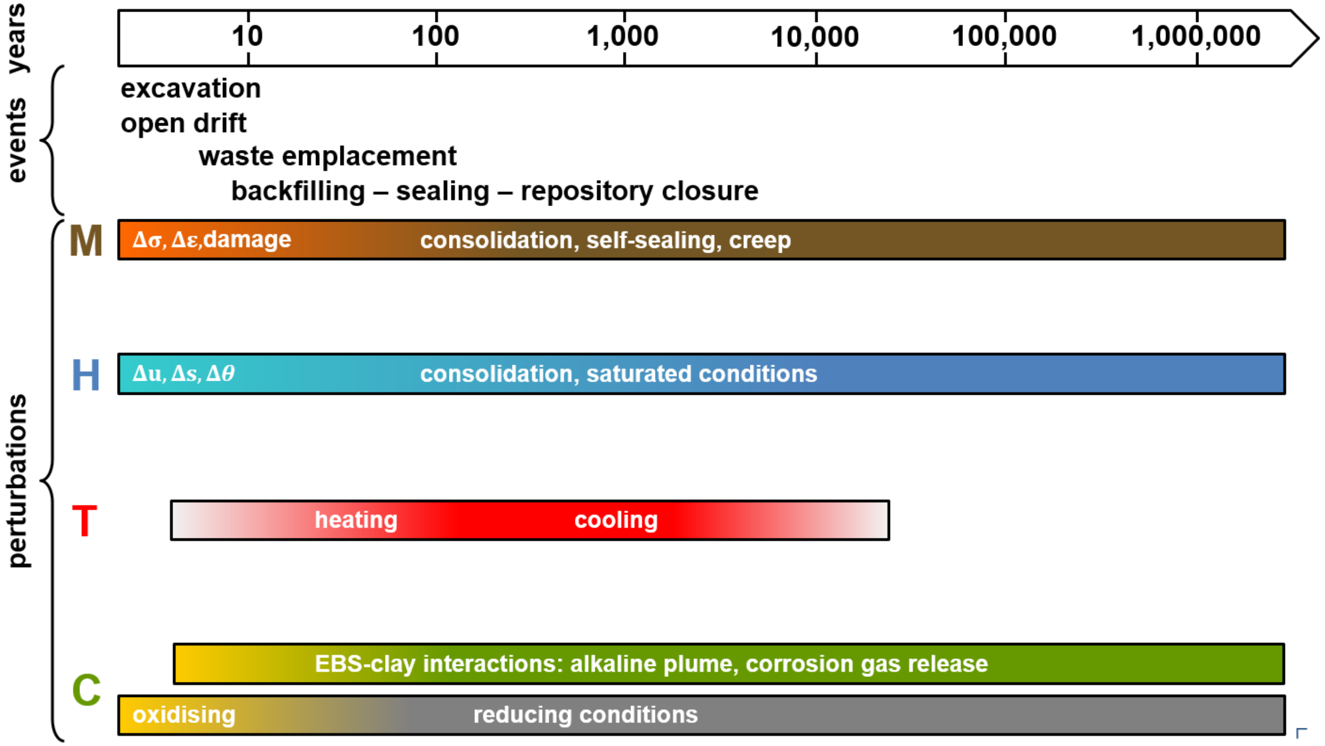
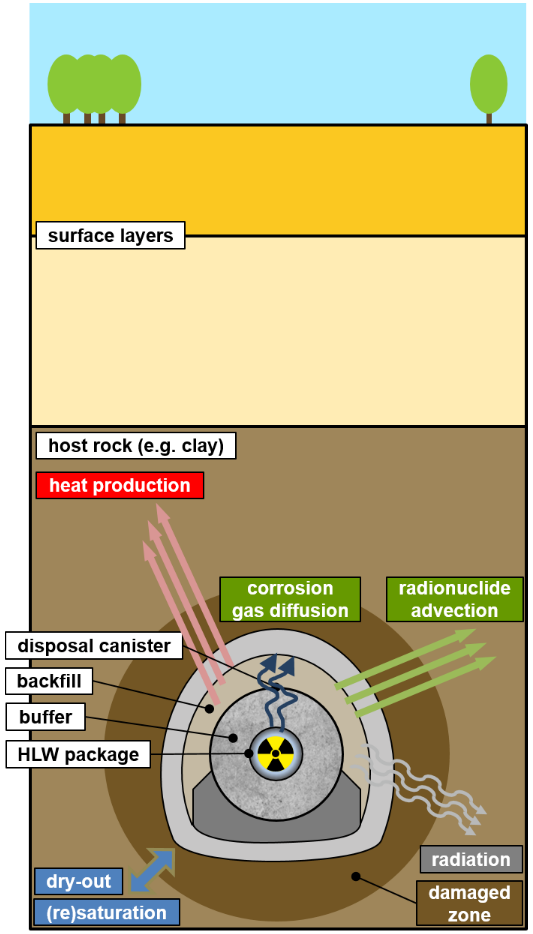


Major perturbations of the host rock over the lifetime of a geological repository, adapted from *Sillen (2012).*

Context

Geological disposal of radioactive wastes

- Complex multi-physical (THMC) processes
- Interactions between processes



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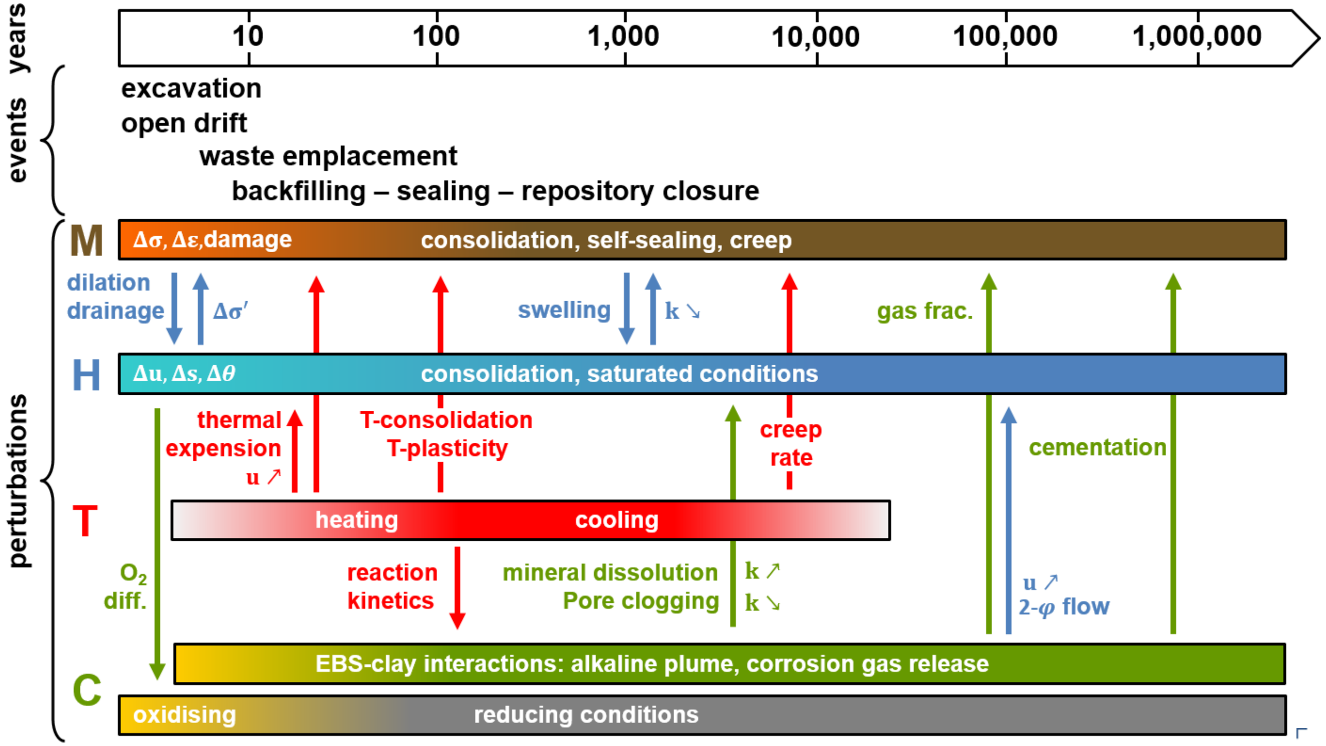

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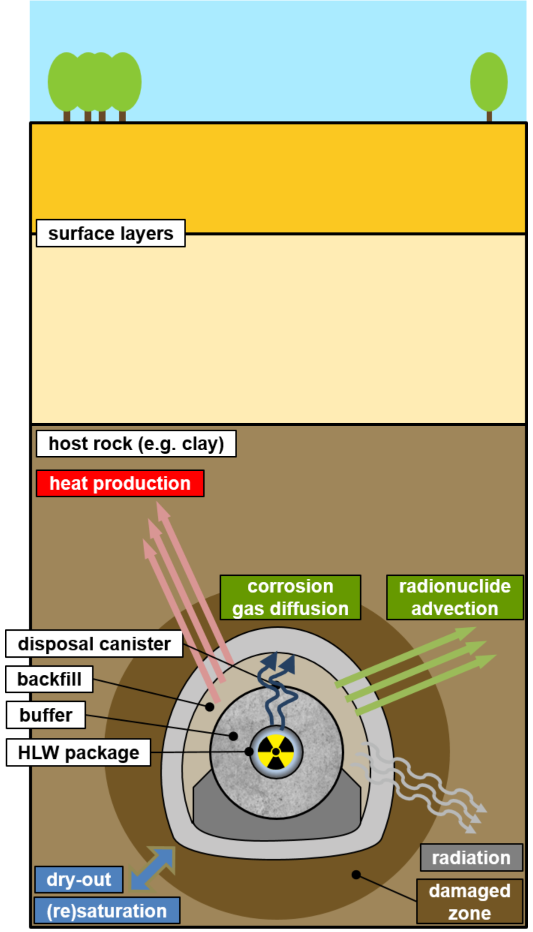

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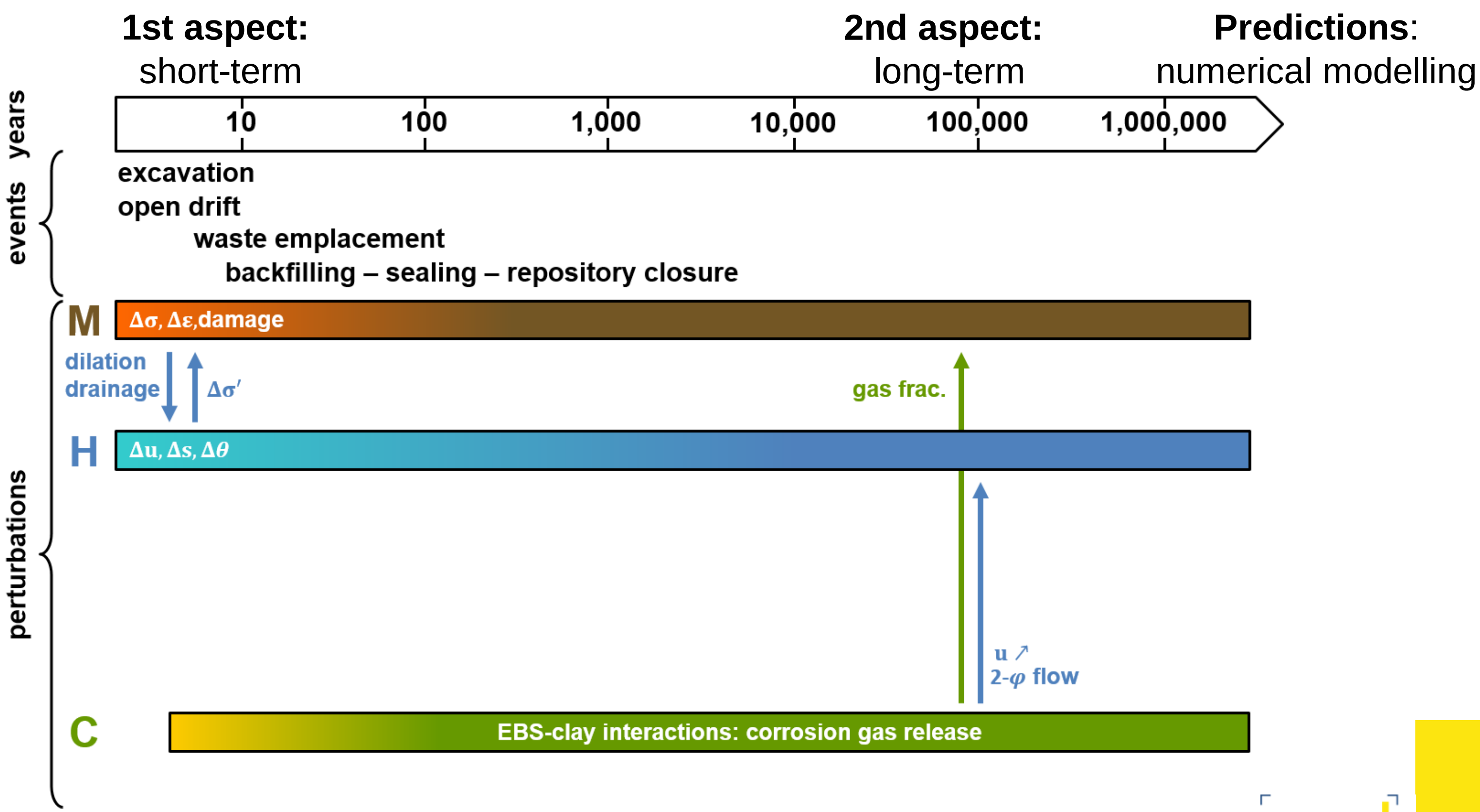

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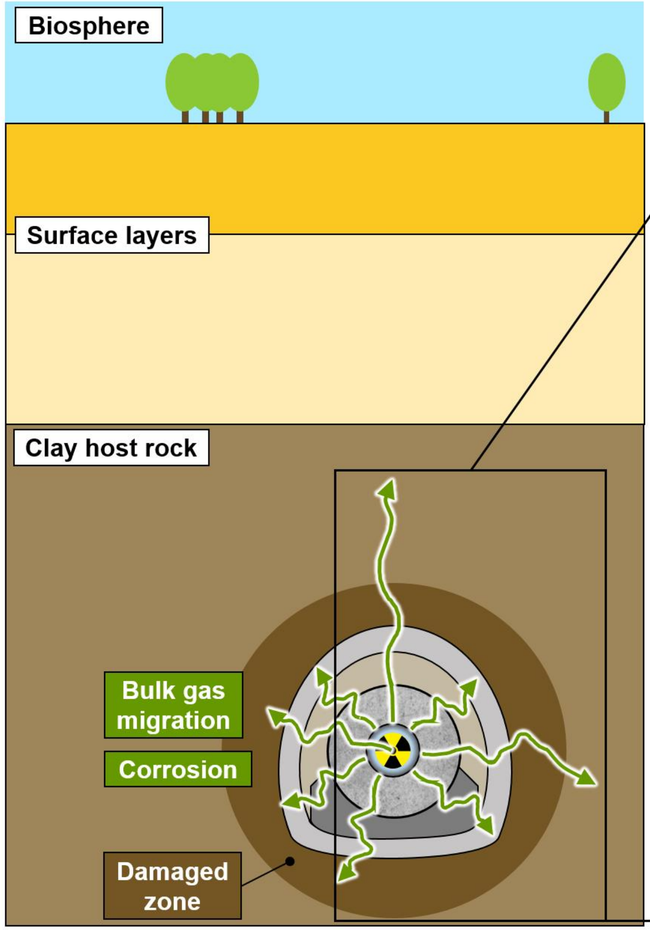
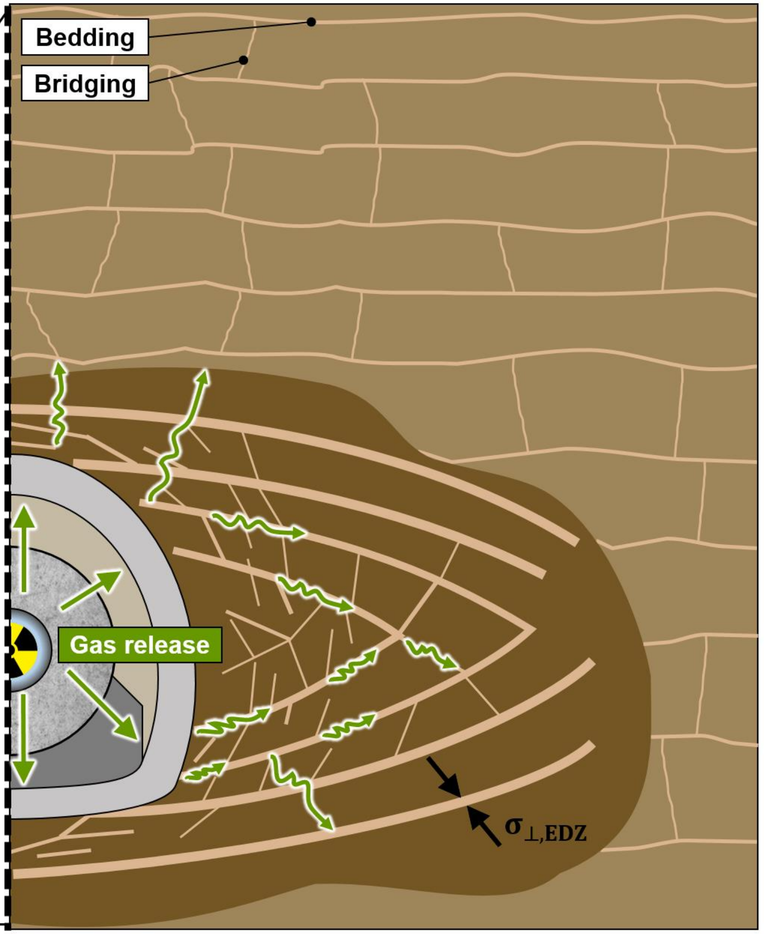
Gas migration issue



Conceptual scheme of a deep geological repository focussing on the gas generation process.



Expected gas transport modes in the EDZ and the sound rock, *from ONDRAF/NIRAS (2016).*

Excavation damaged zone (EDZ)

- Governed by the hydraulic properties modifications induced by fracturation

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Context

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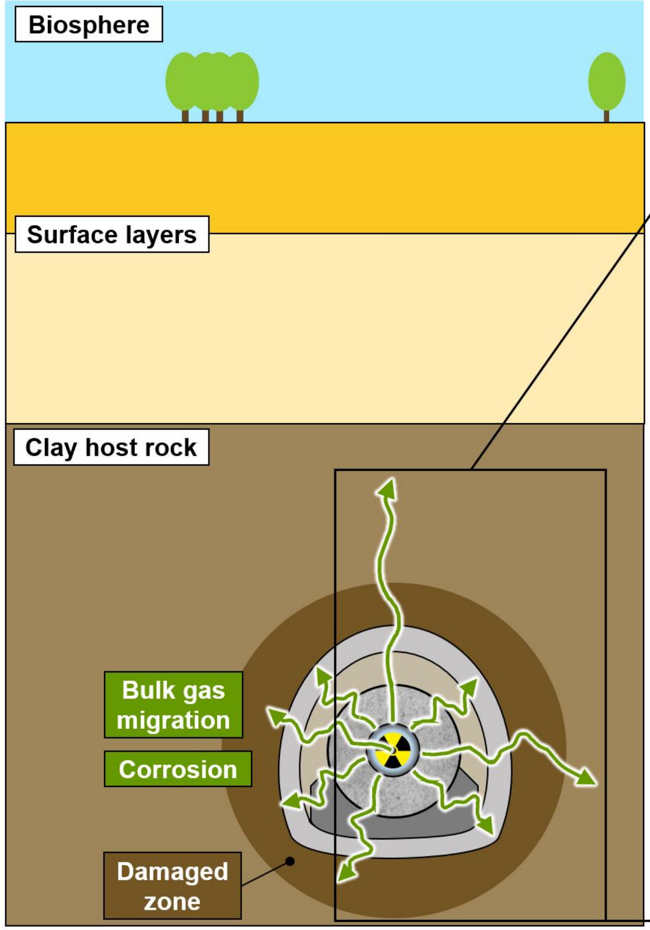

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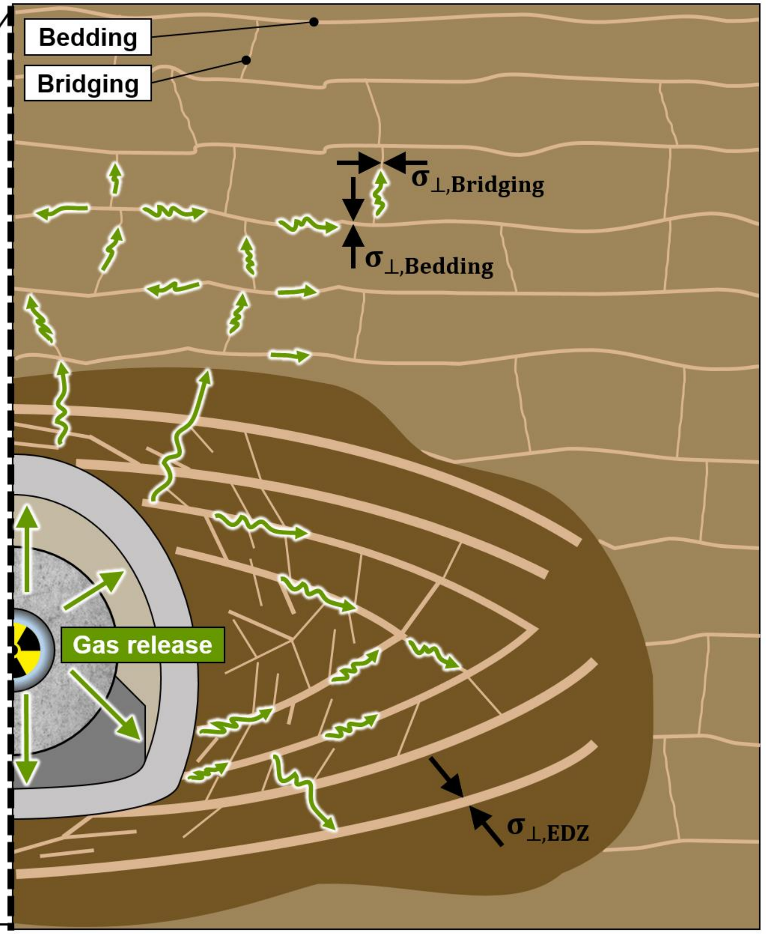

Expected gas transport modes in the EDZ and the sound rock, *from ONDRAF/NIRAS (2016).*

Sound rock layers

- Governed by the rock structure **at a micro-level**
- Multi-Scale Model

Excavation damaged zone (EDZ)

- Governed by the hydraulic properties modifications induced by fracturation

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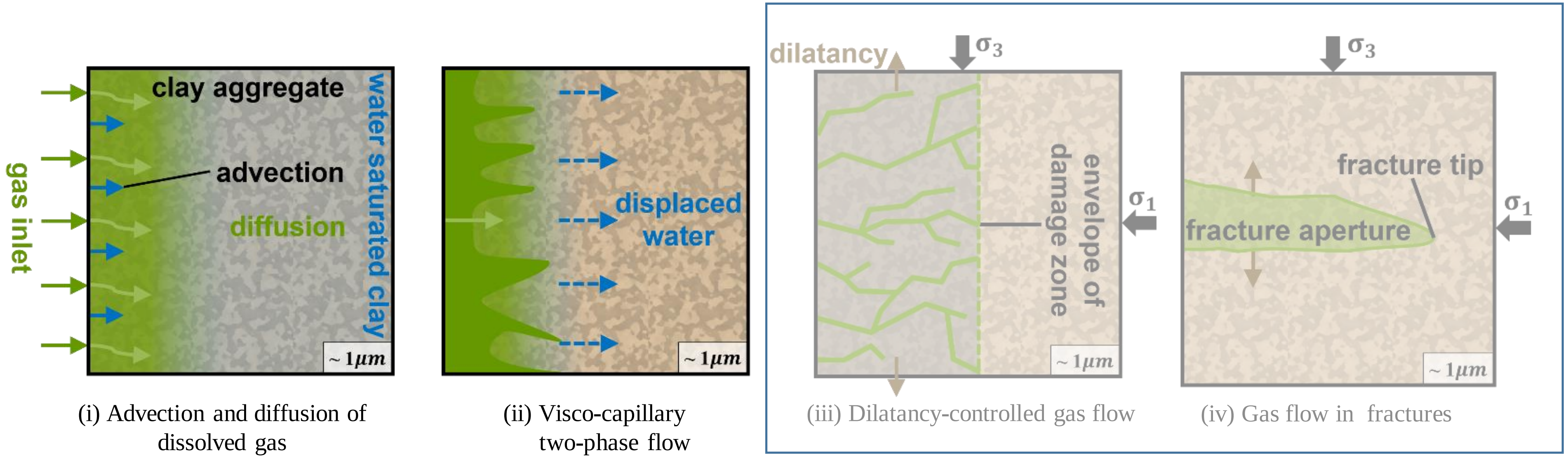
From experimental evidence to modelling

Background



(i) Advection and diffusion of dissolved gas

(ii) Visco-capillary two-phase flow

(iii) Dilatancy-controlled gas flow

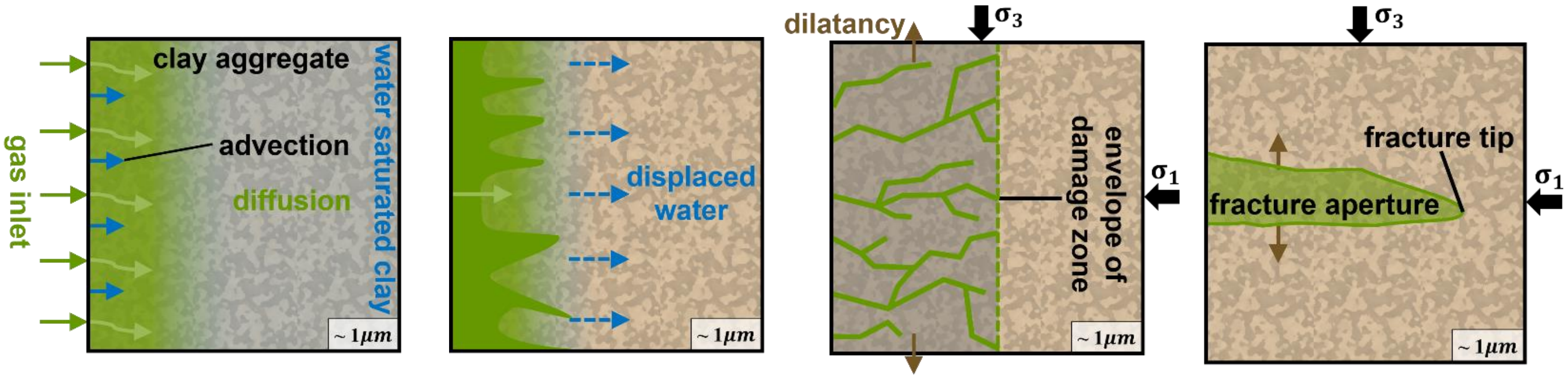
(iv) Gas flow in fractures

Phenomenological description of the gas transport processes relevant to low-permeable clayey rocks, *adapted from Marschall et al. (2005).*

Classical HM two-phase flow models

From experimental evidence to modelling

Background



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Classical HM two-phase flow models — (i), (ii)

Supported by experimental data — (iii), (iv)

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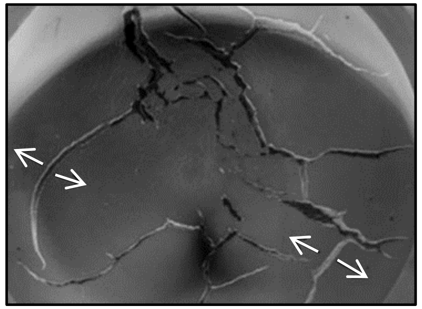
From experimental evidence to modelling

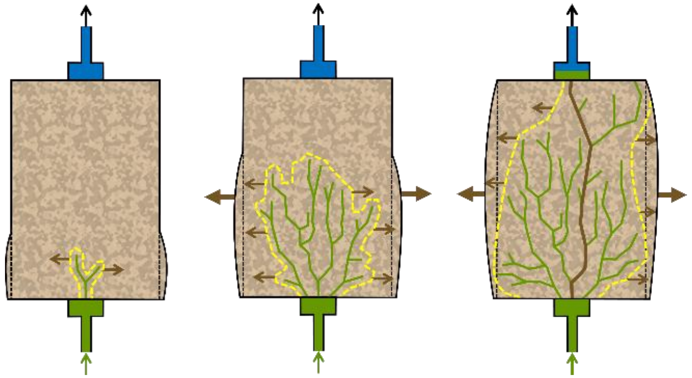
Laboratory experiments

Clay-rich material



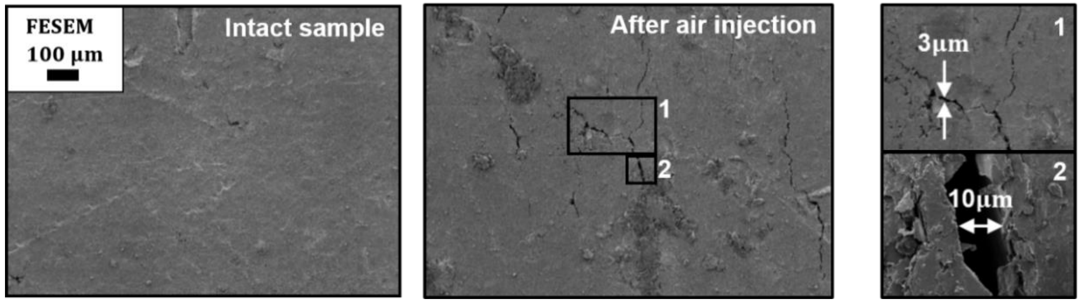
Gas-induced fracturing, *Wiseall et al. (2015)*

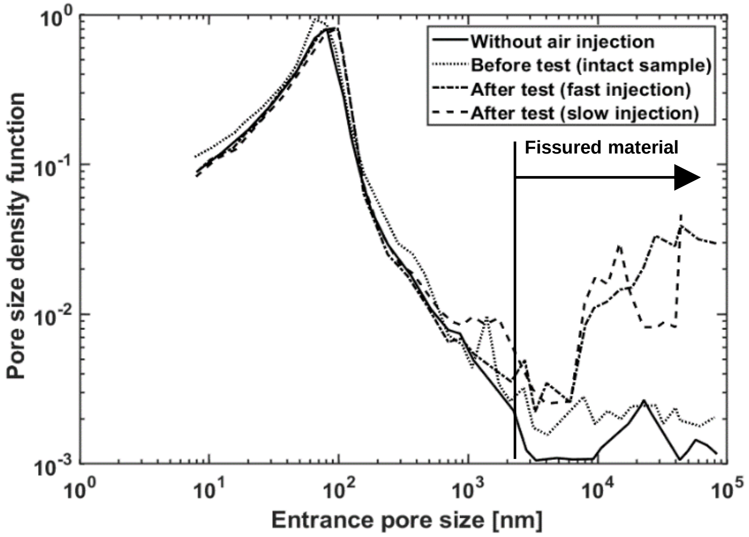
Callovo-Oxfordian claystone



Onset of gas flow, *modified after Cuss et al. (2014)*

Boom Clay

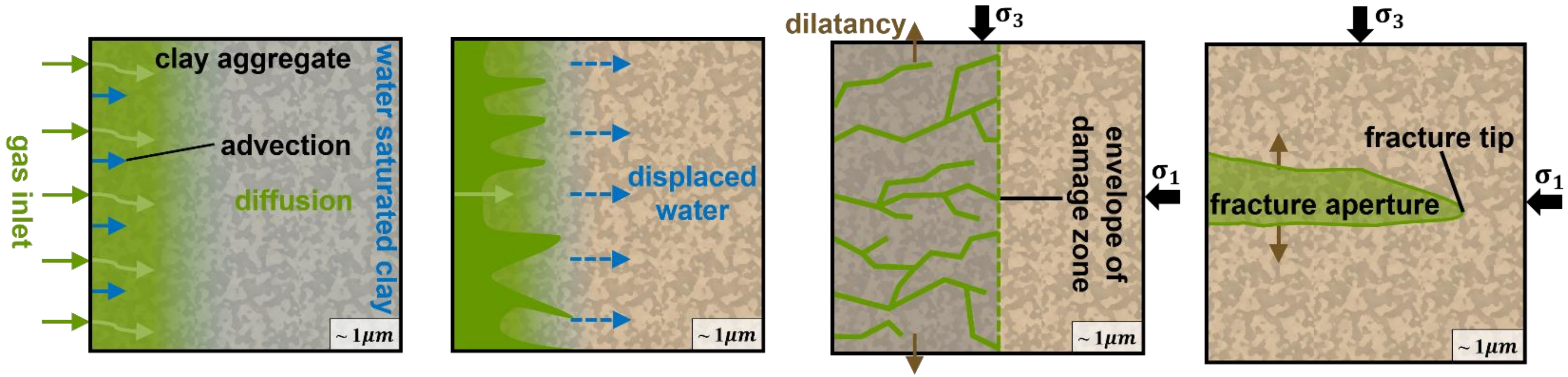




Changes in Boom Clay pore size distribution after air injection, and corresponding FESEM images with zooms on the detected fissures, *modified after Gonzalez-Blanco et al. (2022)*

From experimental evidence to modelling

Background



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Classical HM two-phase flow models

Supported by experimental data

- Natural heterogeneities represent preferred weaknesses for the process of opening discrete gas-filled pathway
- Introduce stronger coupling between gas flow and mechanical behaviour into the models.

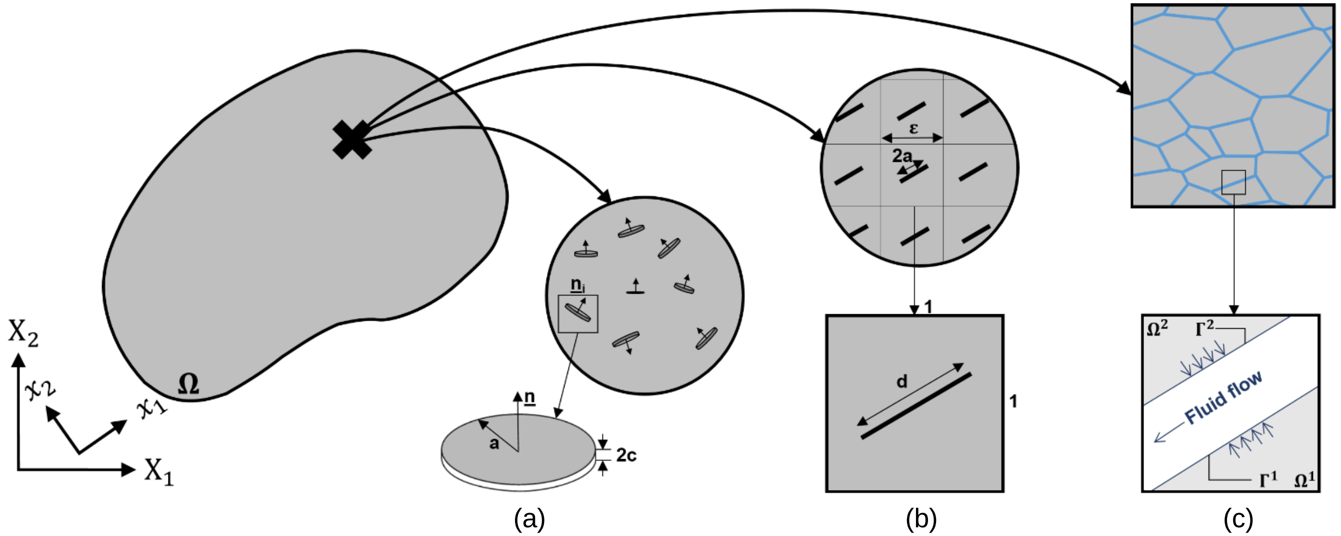
► **Advanced HM models**

From experimental evidence to modelling

Advanced HM models

Micro-macro based models

- ► Combines the benefits from large- and small-scale modelling strategies
- ► Explicit description of all the constituents on their specific length scale through a REV definition



Conceptual scheme of micro-macro based models, with microstructure definitions of a microcracked material, *after (a) Levasseur (2013), (b) François (2010), and (c) van den Eijnden (2016).*

Content

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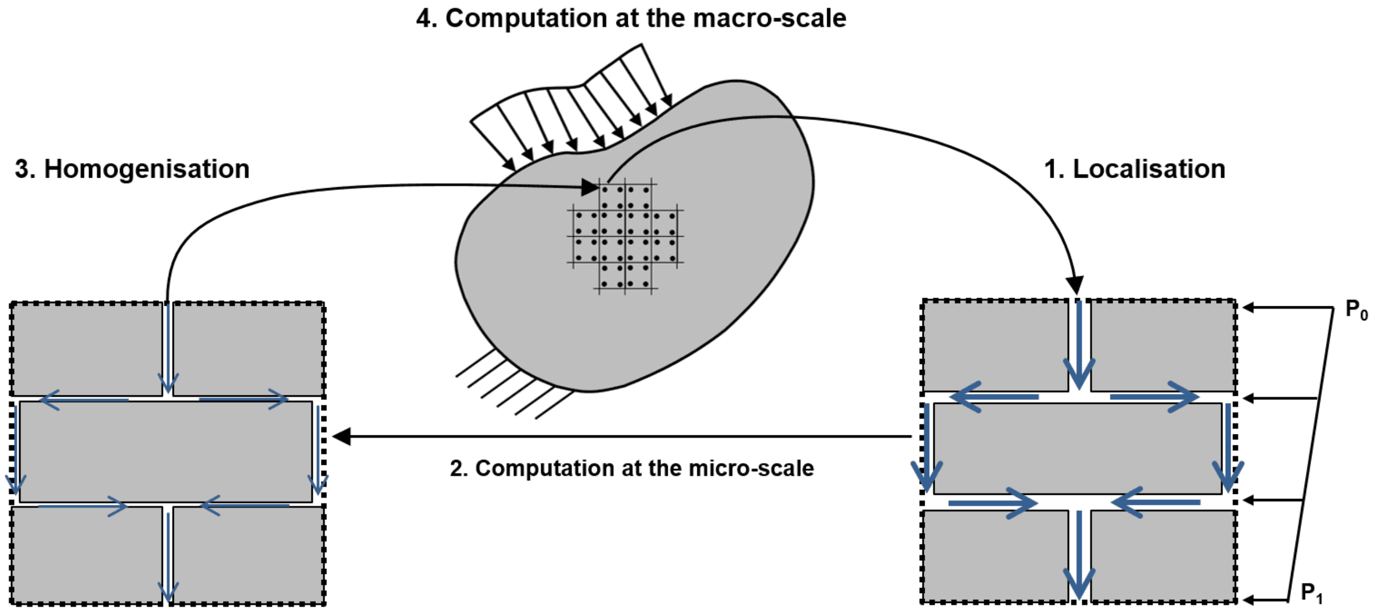
Multi-scale modelling approach

Overview

- Macro-to-micro scale transition: Localisation of the macro-scale deformations to the micro-scale
- Resolution of the boundary value problem at the micro-scale
- Micro-to-macro scale transition: Homogenisation of the micro-scale stresses to compute the macroscopic quantities
- Resolution of the boundary value problem at the macro-scale



Conceptual scheme of the iterative process for the multiscale model

Hybrid developed tool

- Complete hydraulic system implemented and solved at the micro-scale
- Mechanical effects addressed at the macro-scale and implicitly integrated at the lower scale through HM couplings

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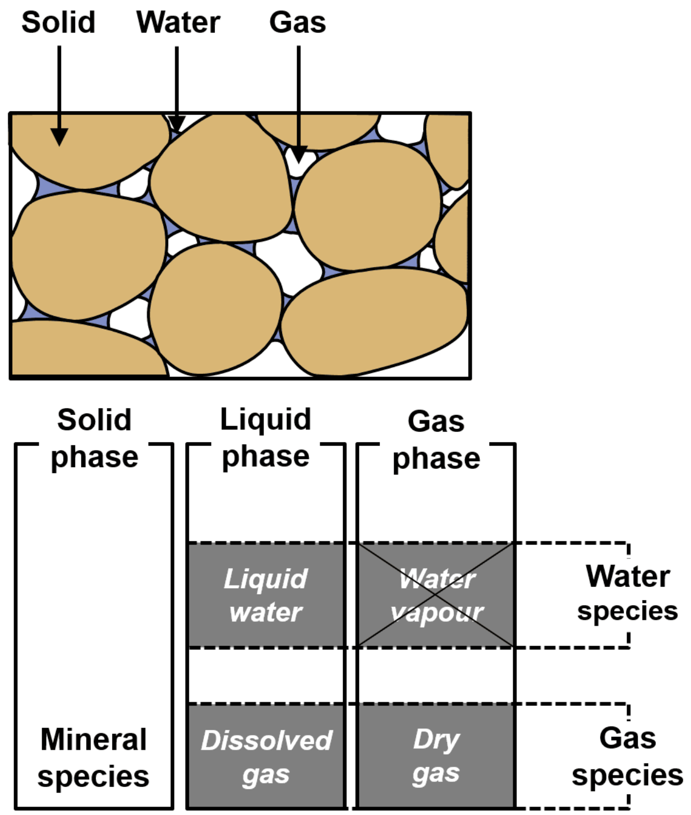
Multi-scale modelling approach

Model formulation at the macroscopic scale

Clay material treated as a porous medium



Unsaturated triphasic porous medium and definition of phases and species

Balance equations

- Momentum

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = 0$$

- Water

$$\underbrace{\dot{M}_w + \frac{\partial f_{w,i}}{\partial x_i}}_{\text{Liquid water}} - Q_w = 0$$

- Gas

$$\underbrace{\dot{M}_g + \frac{\partial f_{g,i}}{\partial x_i}}_{\text{Dry gas}} + \underbrace{\dot{M}_{dg} + \frac{\partial f_{dg,i}}{\partial x_i}}_{\text{Dissolved gas}} - Q_g = 0$$

Constitutive equations

- Total stress definition

$$\sigma_{ij} = \sigma'_{ij} + b_{ij}\left[S_{r_w} p_w^M + (1 - S_{r_w}) p_g^M\right]\delta_{ij}$$

- Variation of solid density

$$\frac{\dot{\rho}_s}{\rho_s} = \frac{(b_{ij} - \phi)(S_r^w \dot{p}_w + S_r^g \dot{p}_g) + \dot{\sigma}'}{(1 - \phi)K_s}$$

Multi-scale modelling approach

Macro-to-micro scale transition: Localisation

Decomposition of the micro-kinematics:

- Macro-pressure fields ($\square^M$) of water and gas must be identical to the micro-quantities ($\square^m$) for any point of the material

$$p_w^M(\hat{P}) = p_w^m(\hat{P}) \qquad p_g^M(\hat{P}) = p_g^m(\hat{P})$$

- For any point P close to $\hat{P}$,
  at the macroscopic scale:

$$p_w^M(P) \approx p_w^M(\hat{P}) + \frac{\partial p_w^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right) \qquad p_g^M(P) \approx p_g^M(\hat{P}) + \frac{\partial p_g^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right)$$

Higher-order terms neglected

at the microscopic scale:

$$p_w^m(P) \approx p_w^M(\hat{P}) + \frac{\partial p_w^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right) + p_w^f(\hat{P}) \qquad p_g^m(P) \approx p_g^M(\hat{P}) + \frac{\partial p_g^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right) + p_g^f(\hat{P})$$

Fluctuation fields to replace higher-order terms

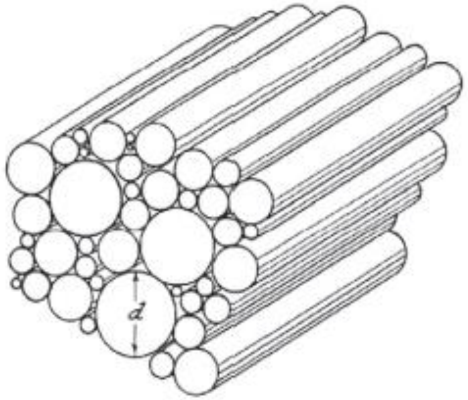
Separation of scales

- Approach restricted to situations where the variations of the macroscopic fields is large compared to the variations of micro-scale fields

$$\frac{\partial p_w^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right) + p_w^f(\hat{P}) \ll p_w^M(\hat{P})$$

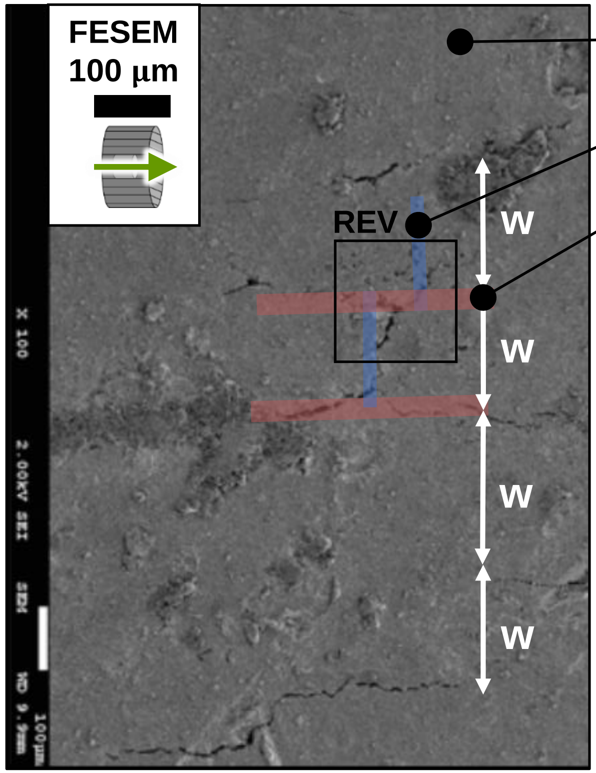
$$\frac{\partial p_g^M(\hat{P})}{\partial x_j}\left(x_j - \hat{x}_j\right) + p_g^f(\hat{P}) \ll p_g^M(\hat{P})$$

Multi-scale modelling

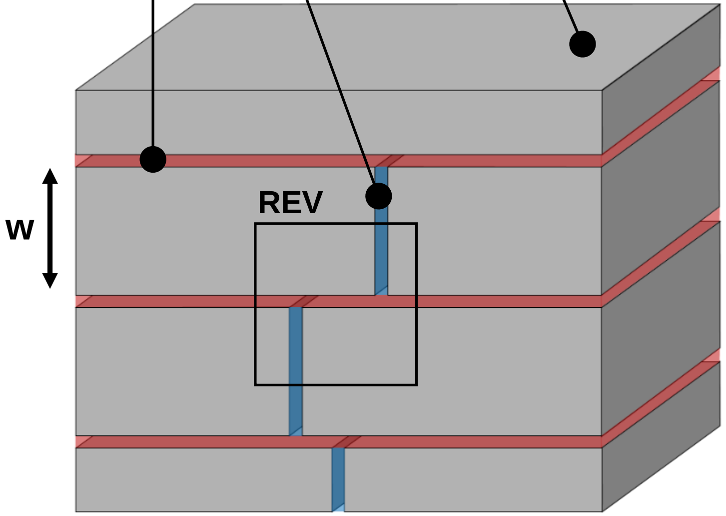


Micro-scale boundary value problem

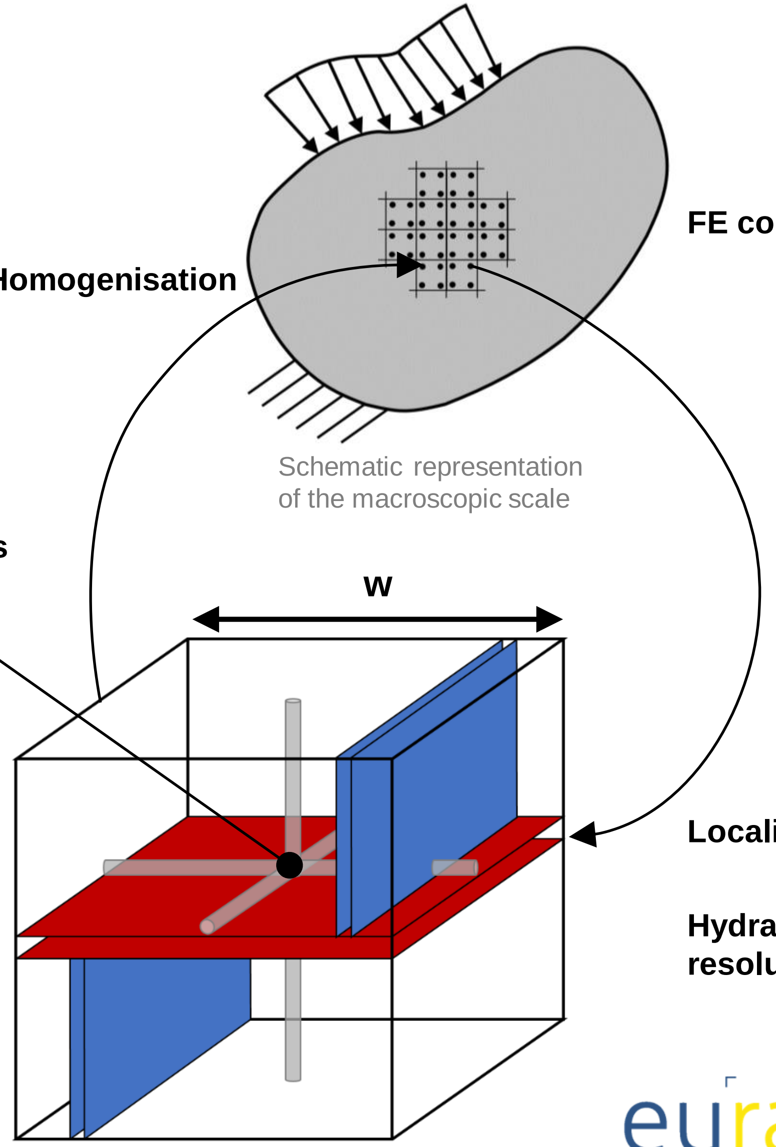
Multi-scale model supported by experimental data



Internal visualisation of a Boom Clay sample using FESEM, *from Gonzalez-Blanco (2017).*



Physical idealisation of the microstructure.



Schematic representation of the macroscopic scale

Definition of the representative element volume (REV)

Multi-scale modelling approach

Micro-scale boundary value problem

Balance equations at the micro-scale

- Gas

$$\cancel{\dot{M}_g^m} + \frac{\partial f_{g_i}^m}{\partial x_i} + \cancel{\dot{M}_{dg}^m} + \frac{\partial f_{dg_i}^m}{\partial x_i} = 0$$

- Water

$$\cancel{\dot{M}_w^m} + \frac{\partial f_{w_i}^m}{\partial x_i} = 0$$

$\dot{M}_g^m$, $\dot{M}_{dg}^m$, $\dot{M}_w^m$ Variations of fluid contents

$$f_{w_i}^m = \rho_w q_{w_i}$$

$$f_{g_i}^m = \rho_g q_{g_i}$$

$$f_{dg_i}^m = \rho_{dg} q_{w_i} + i_{dg_i}$$

Mass flows

- Mechanical effects: computed at the macro-scale and transferred to the micro-scale through HM couplings

Content

1. Context
2. From experimental evidence to modelling
3. Multi-scale modelling approach
4. Modelling gas injection experiment
5. Conclusions

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Gas injection experiment

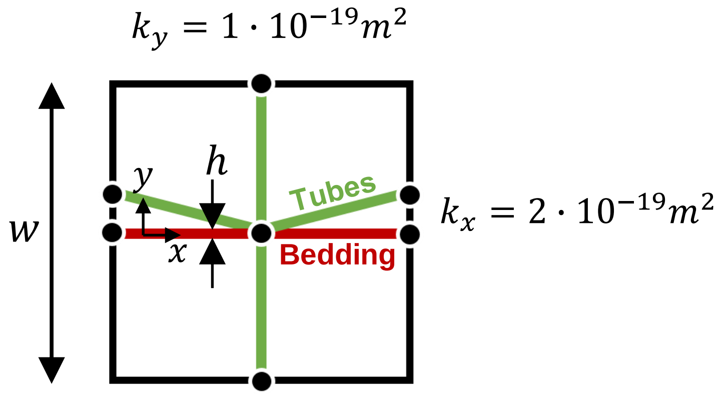
Characterisation of the microstructure parameters

► **1. Size of the REV**

Bedding plane separation
$w = 300\ \mu m$

Experimental estimations of bedding plane separation, from *Gonzalez-Blanco (2017)*

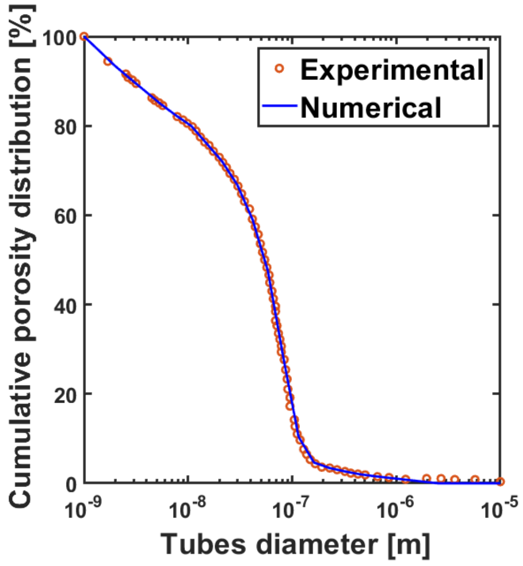
FESEM	µ-CT
150 – 270 μm	410 – 560 μm

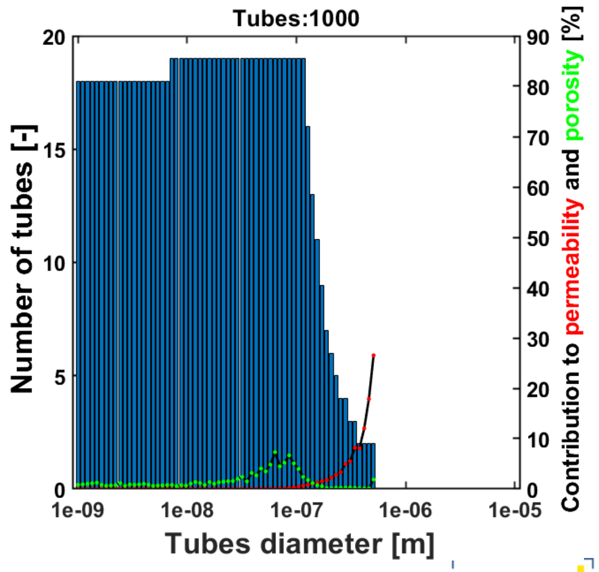


► **2. Macroporosity**

Fitting of the pore size distribution

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





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Gas injection experiment

Characterisation of the microstructure parameters

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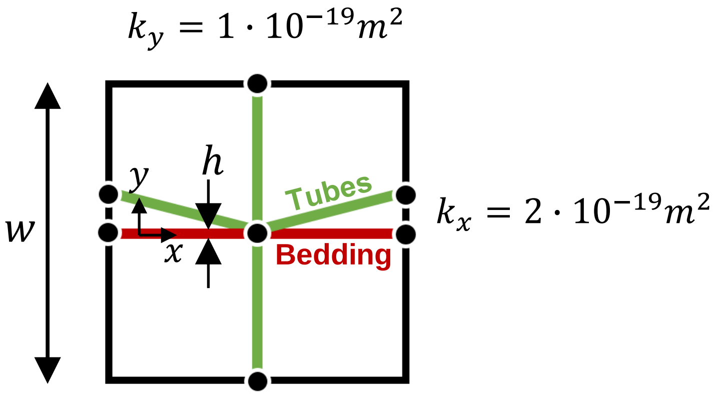

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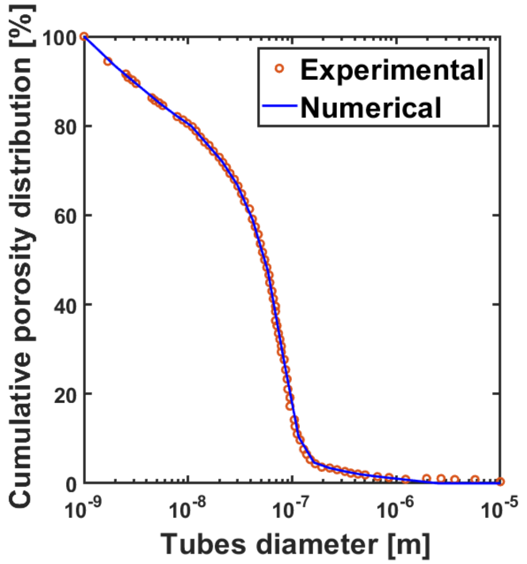
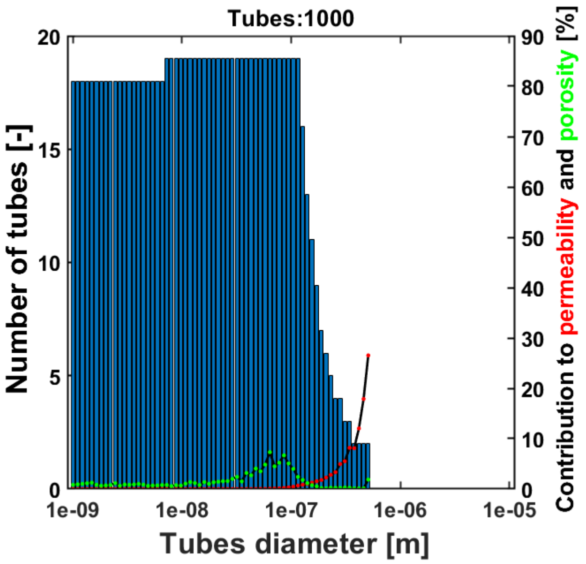




- **3. Intrinsic permeability** — Effect of large-size pores

Fracture aperture

$$k_{x,frac,0} = 10^{-19} m^2$$
$$\rightarrow h_0 = \sqrt[3]{12\, w\, k}$$

Macropores

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

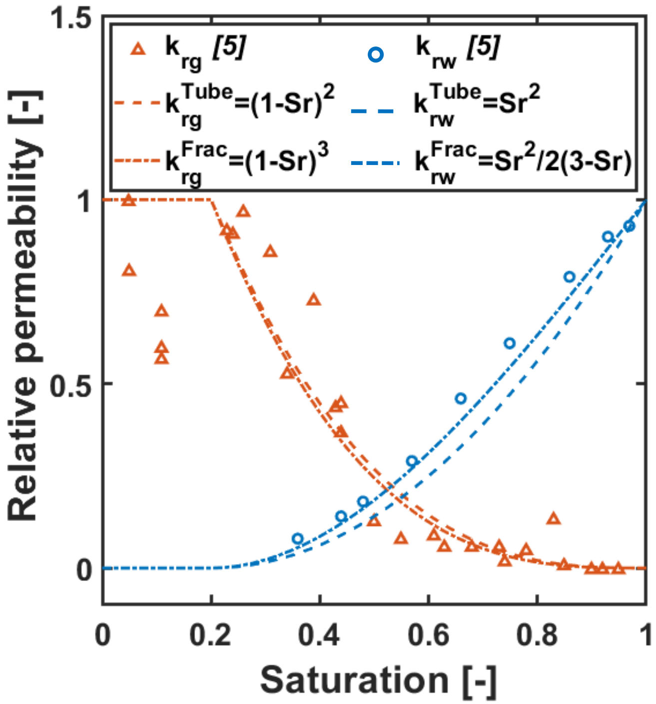
$$k_y = \frac{\pi}{8}\left(\frac{D}{2}\right)^4\left(\frac{1}{w^2}\right)$$

Gas injection experiment

Characterisation of the microstructure parameters

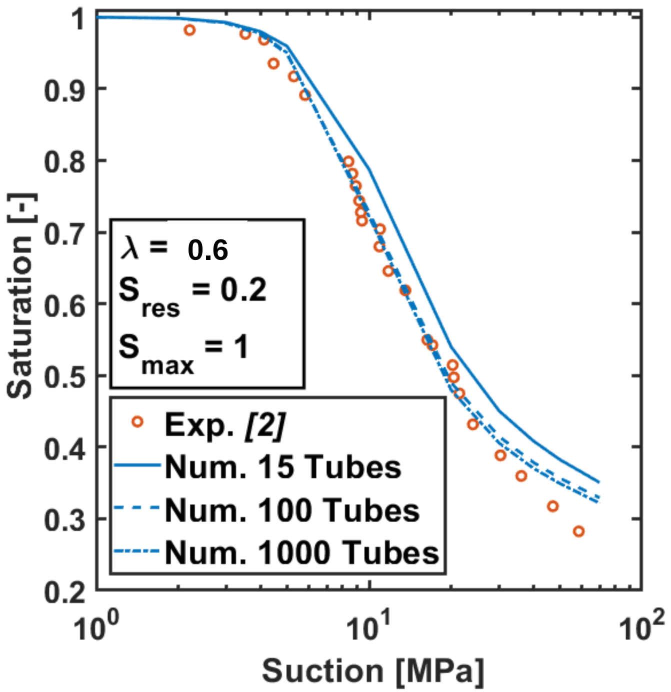
► 4. Relative permeability curves

Yuster et al. (1951)



► 5. Retention curve

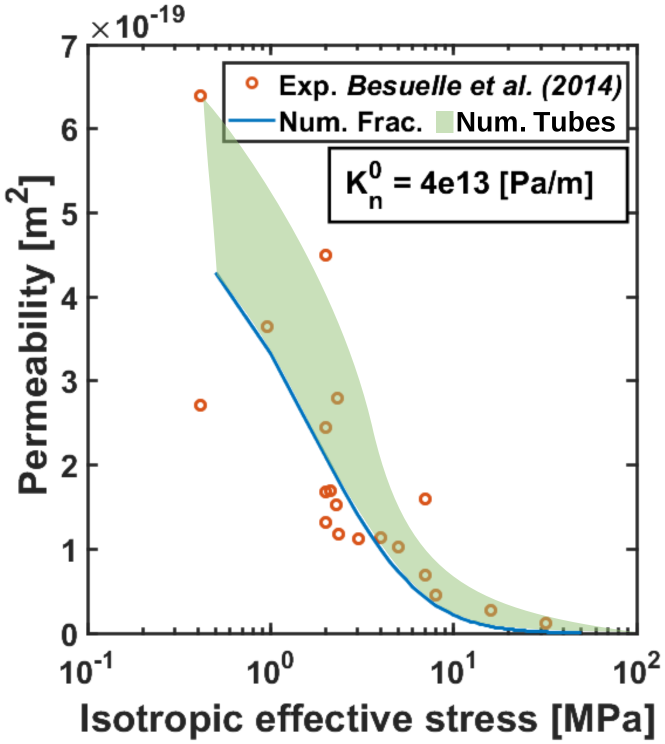
Van Genuchten (1980)



$$S_r = S_{res} + (S_{max} - S_{res})\left(1 + \left(\frac{s}{P_e}\right)^{\frac{1}{1-\lambda}}\right)^{-\lambda}$$

► 6. Normal stiffness of the fracture

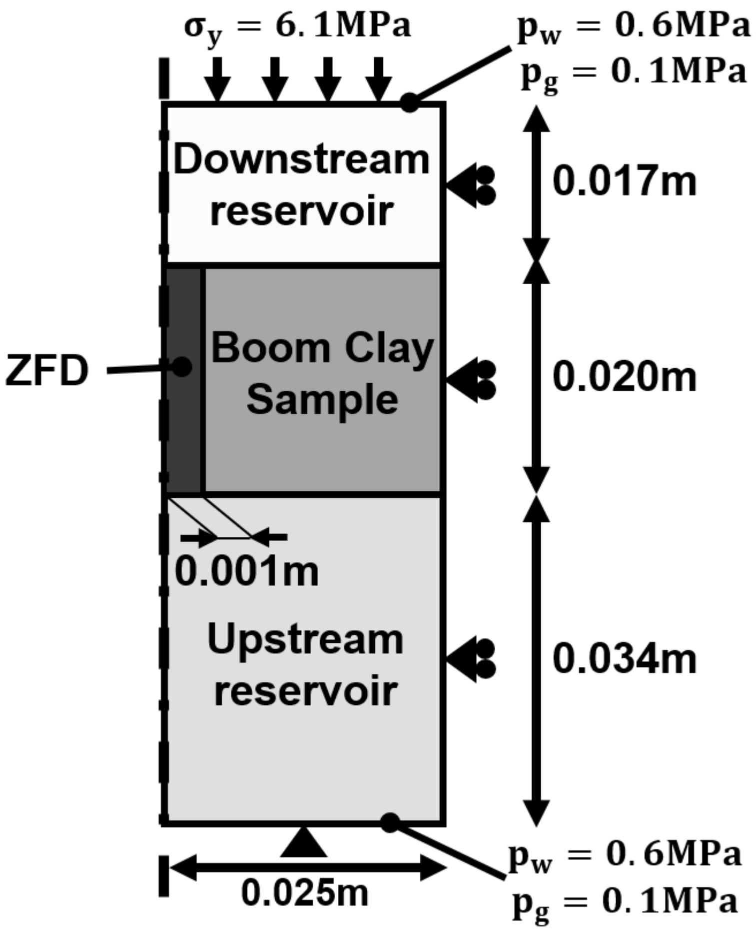
Goodman (1976)



$$\Delta\sigma' = K_n \Delta h \quad \text{with} \quad K_n = \frac{\mathbf{K_n^0}}{\left(1 + \frac{\Delta h}{h_0}\right)^2}$$

Gas injection experiment

Geometry and boundary conditions



Parameters

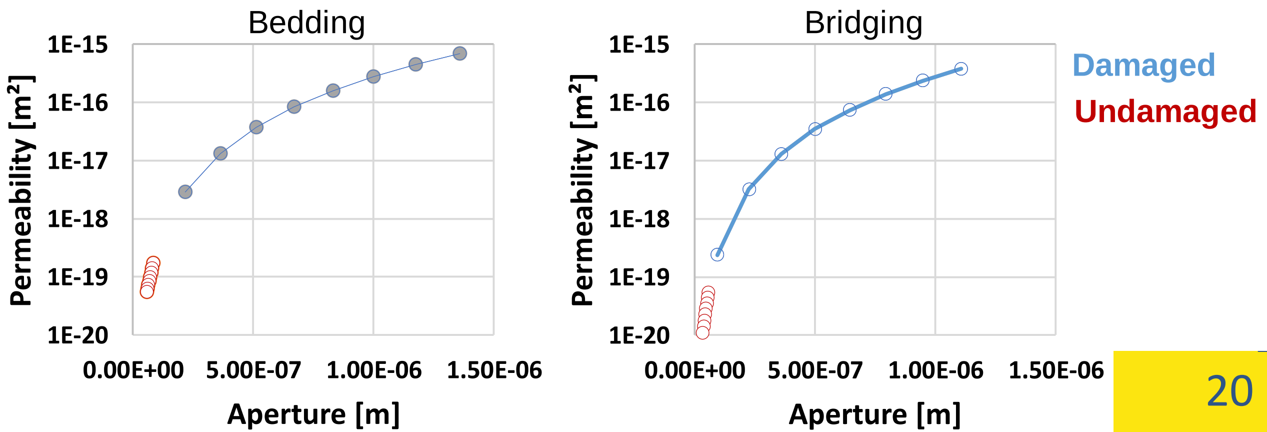
Reservoirs

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

Boom Clay matrix

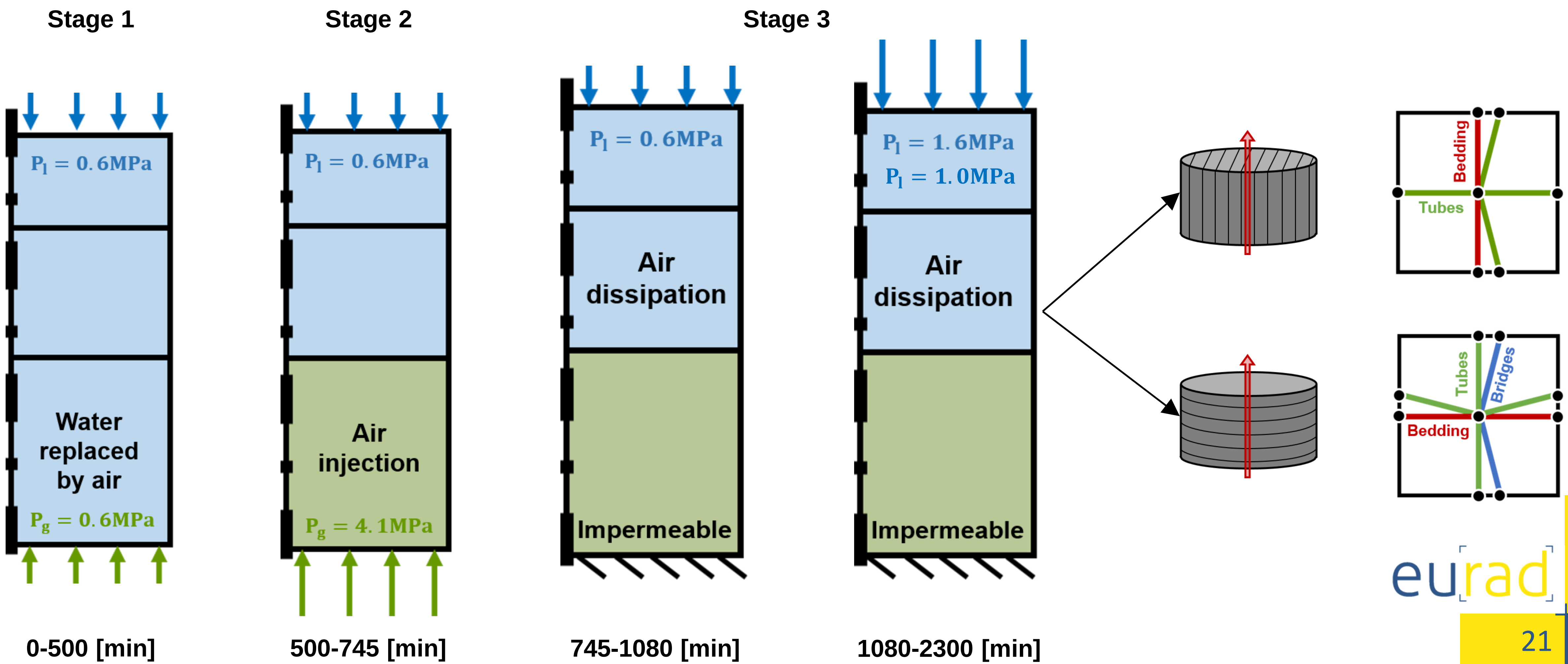
- Mechanical: $E = 200 - 400MPa$ $\nu = 0.33$
- Hydraulic:
  - Initial aperture: $0.80 - 1.27 \cdot 10^{-7} m$
  - Initial permeability: $2.0 - 4.0 \cdot 10^{-19} m^2$
  - Initial porosity: 0.363

Boom Clay Zone of Fracture Development (ZFD)



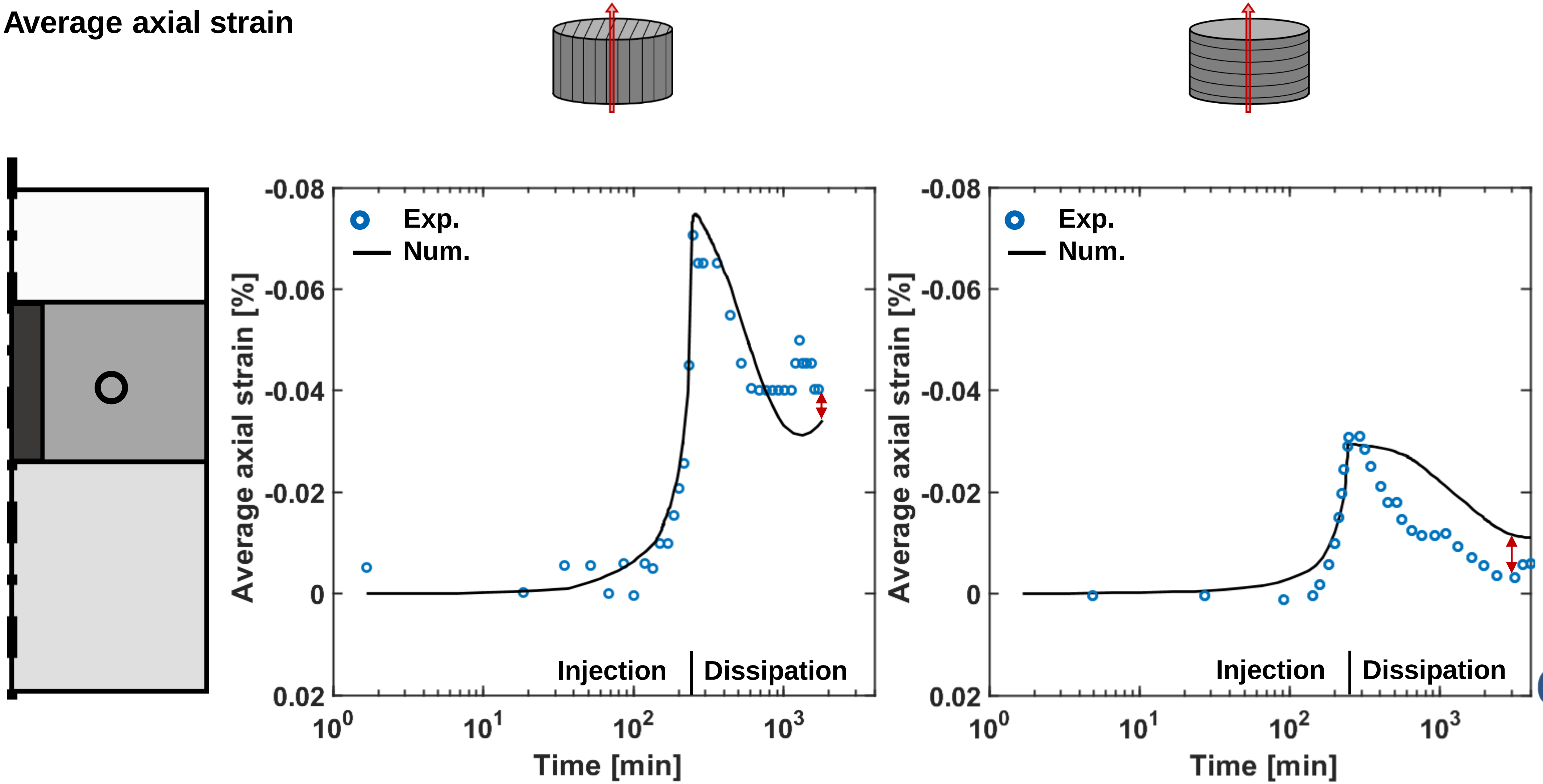
Gas injection experiment

Simulation stages



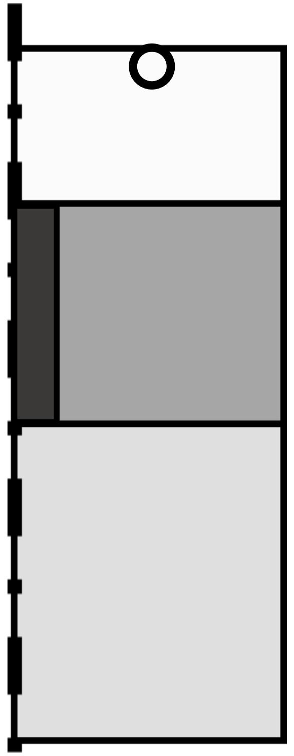
Gas injection experiment

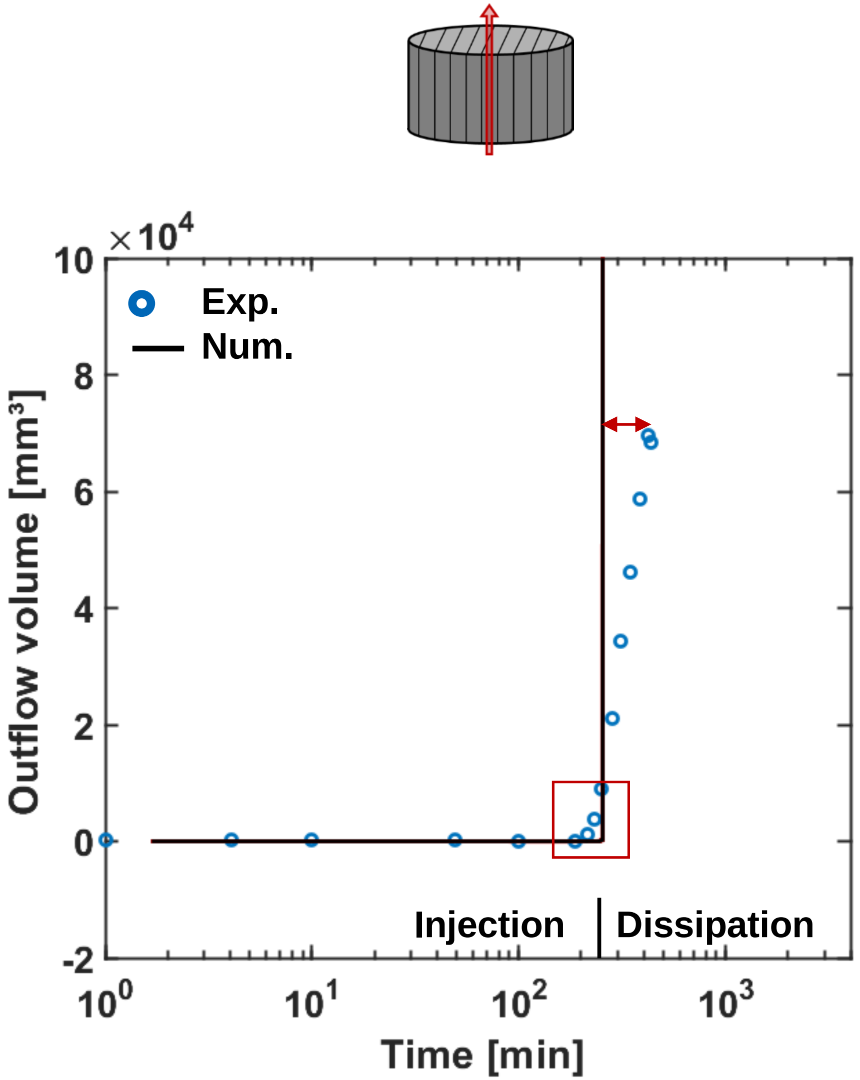
Average axial strain

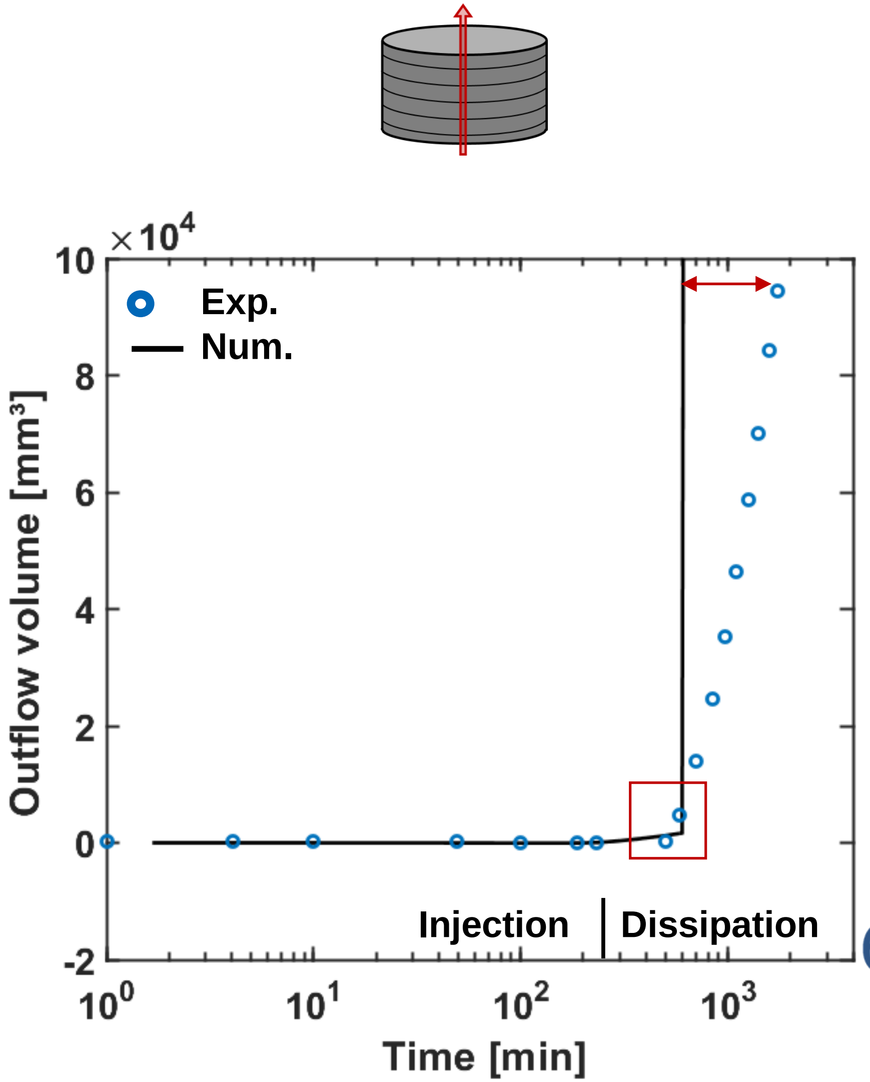


Gas injection experiment

Outflow volume

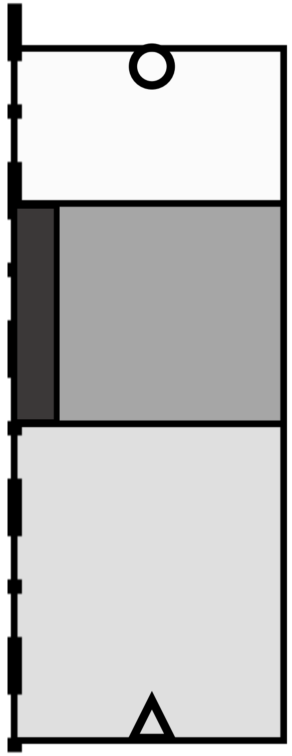


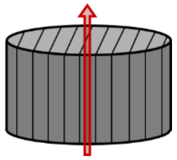


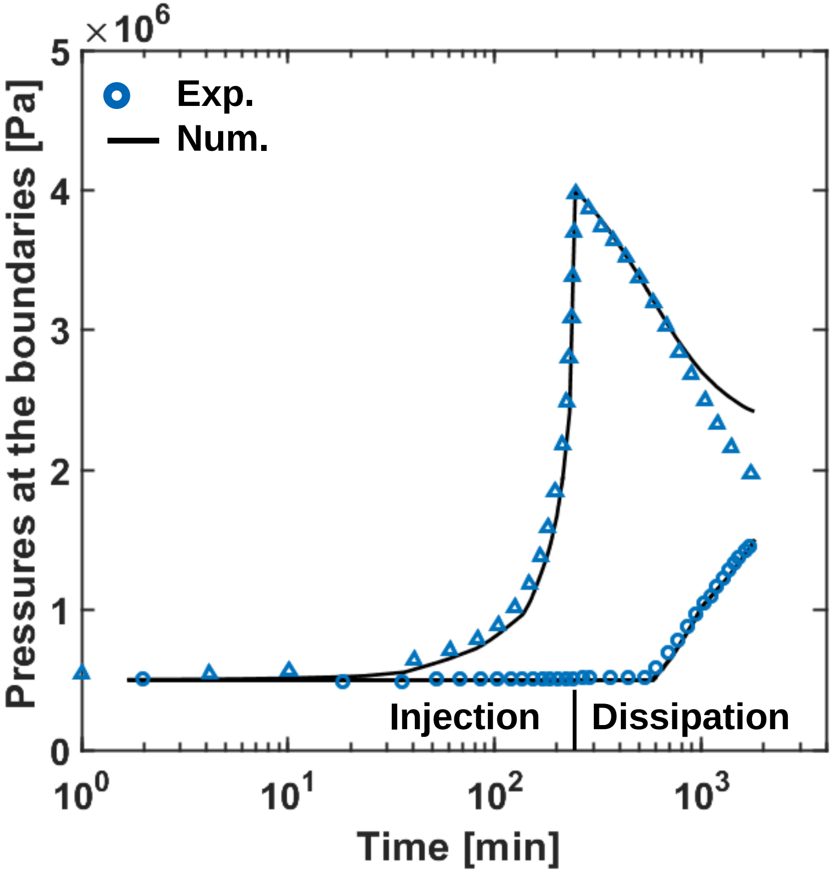


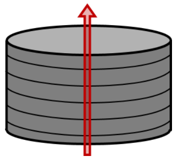
Gas injection experiment

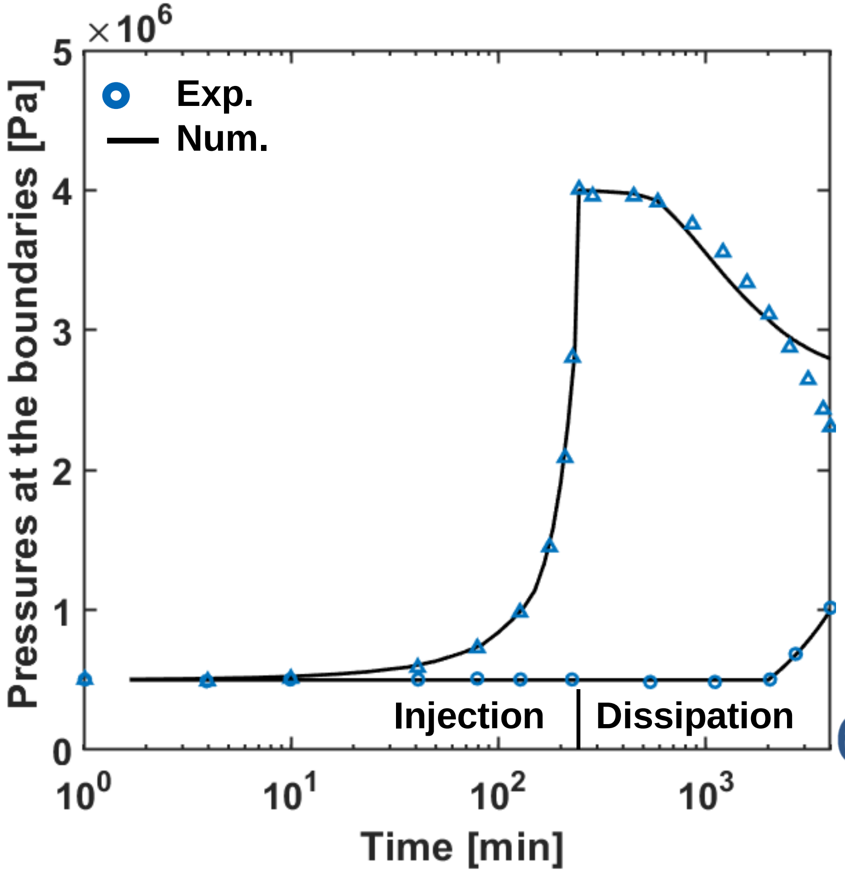
Injection and recovery pressures





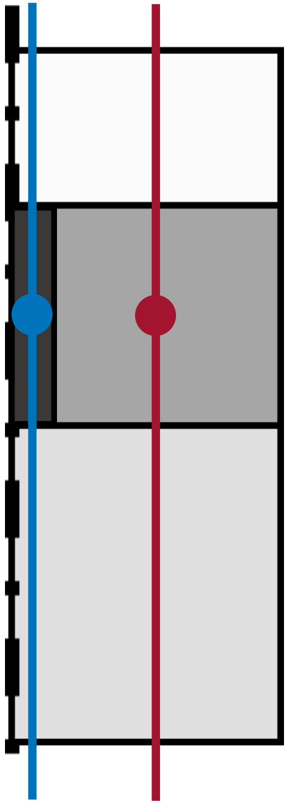


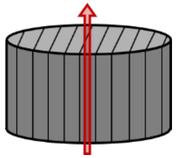


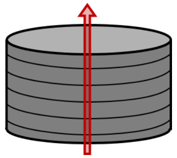


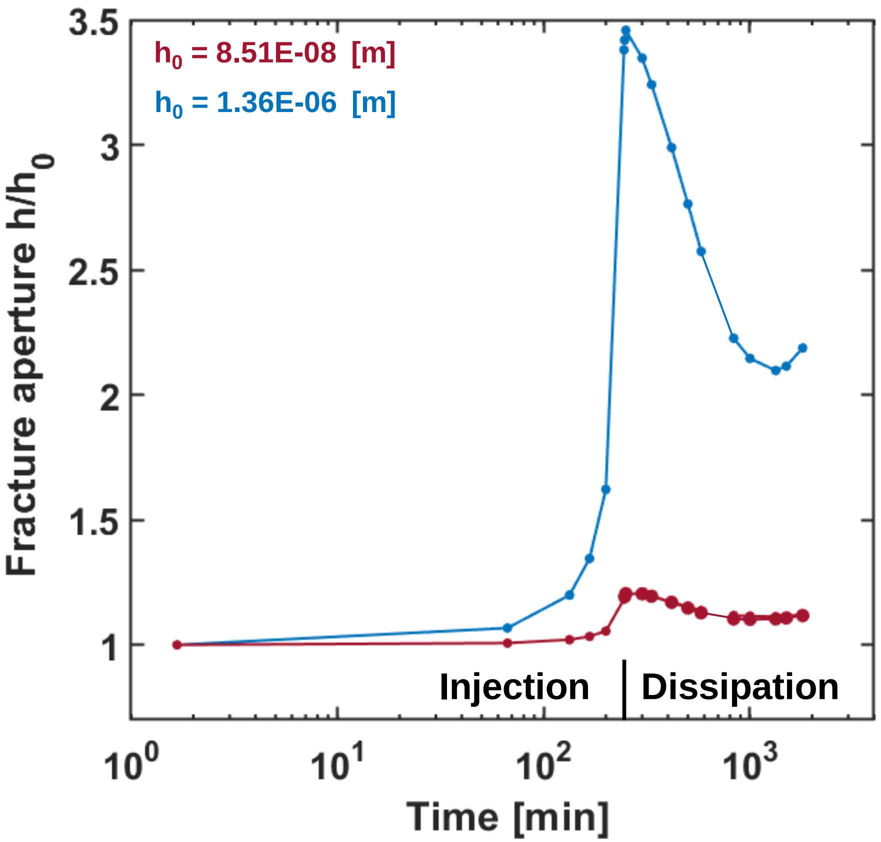
Gas injection experiment

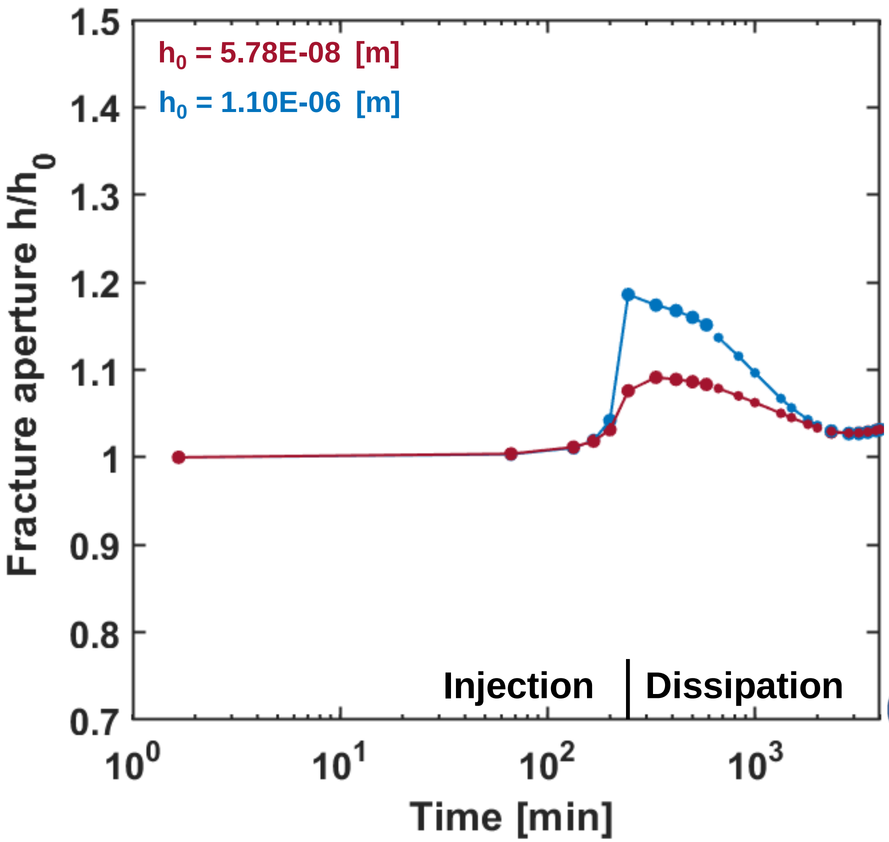
Fracture aperture



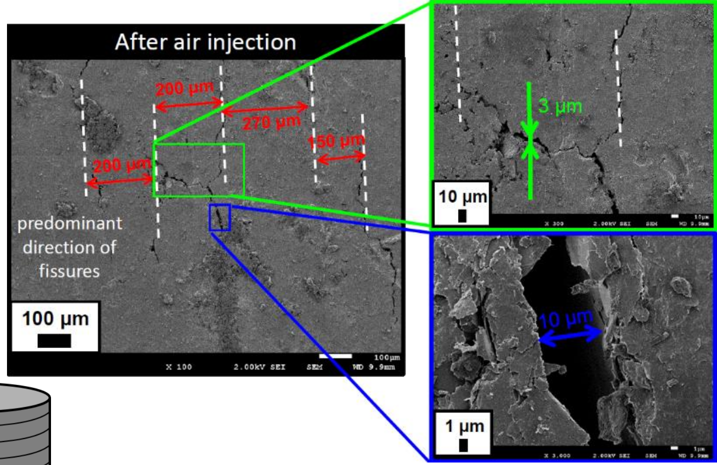








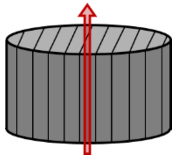
Gas injection experiment

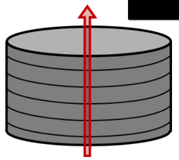


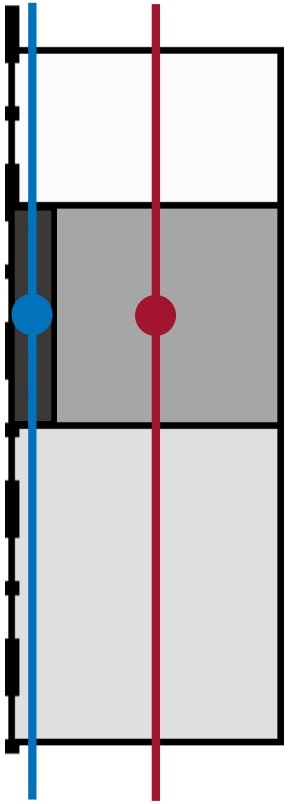
Experimental observations:
Opened fractures after injection

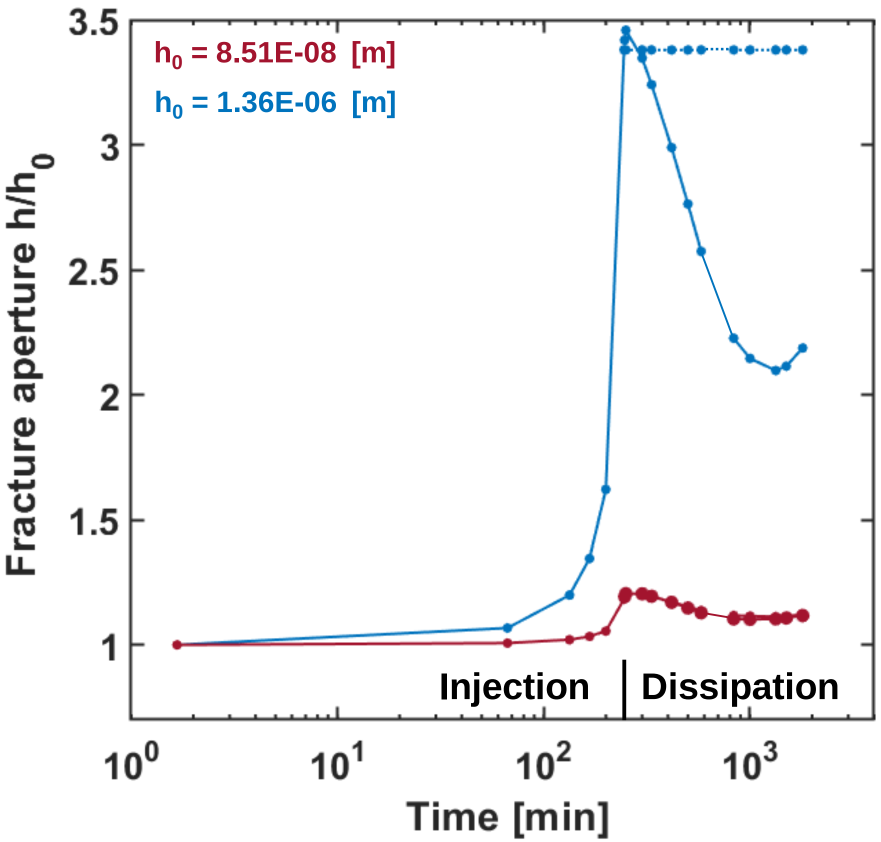
Gonzalez-Blanco & Romero (2022)

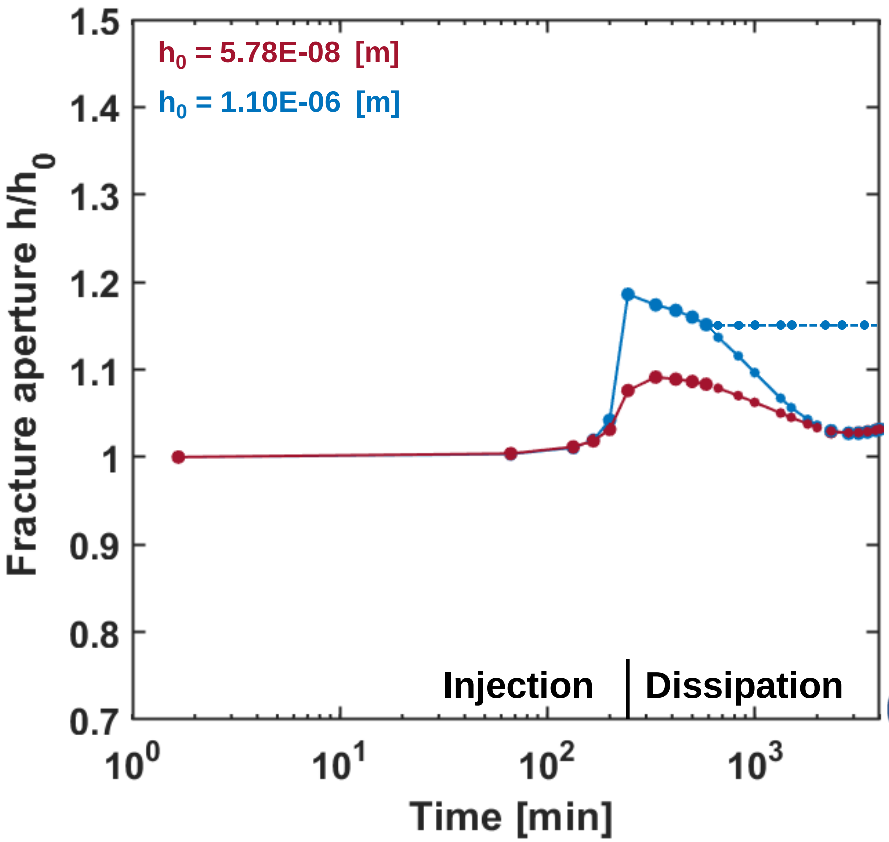
Fracture aperture











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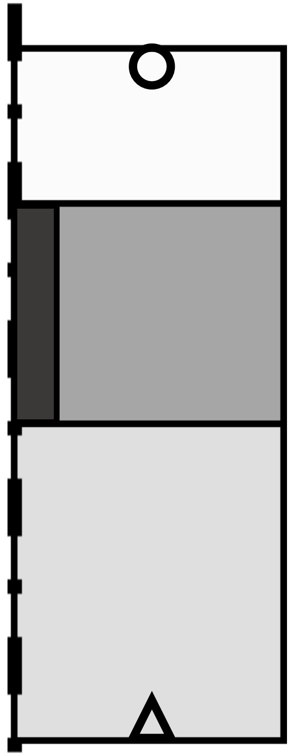
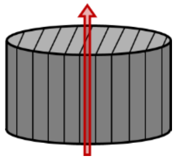
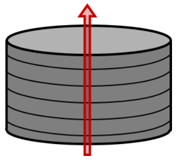
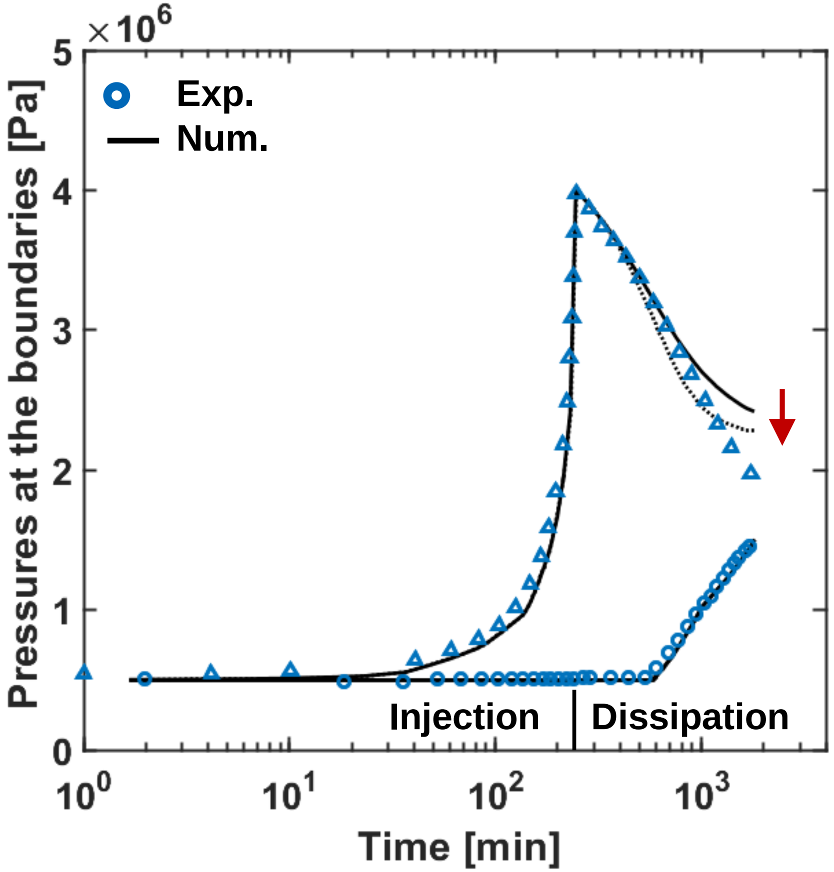
Gas injection experiment

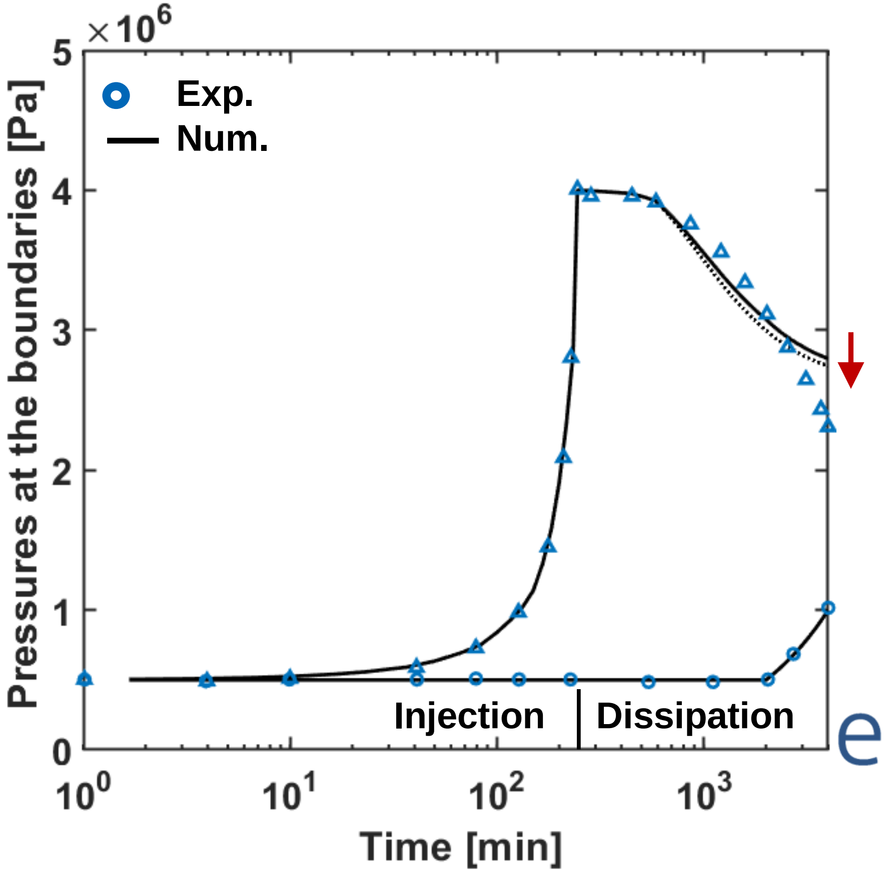
Injection and recovery pressures





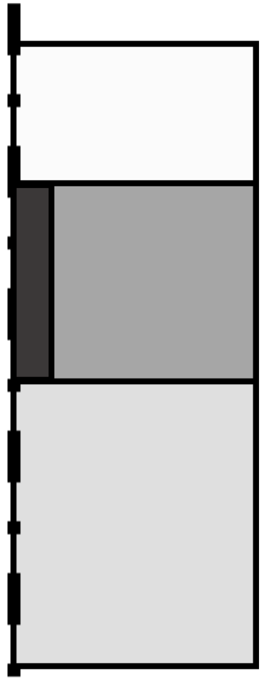


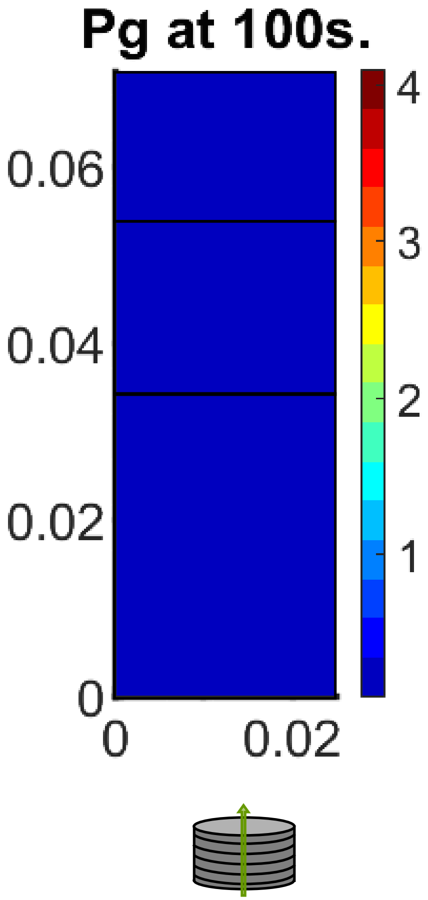


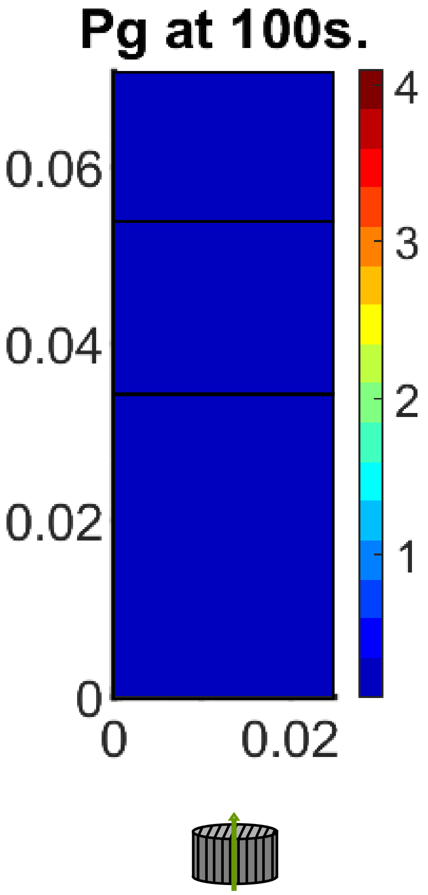


Gas injection experiment

Injection and recovery pressures

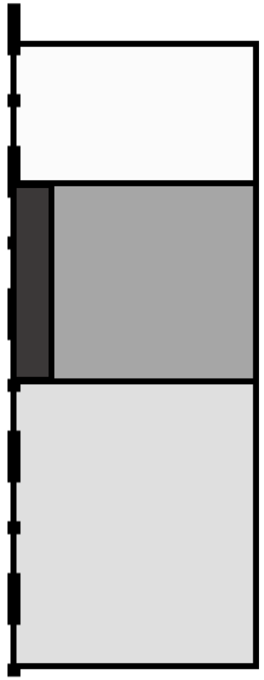


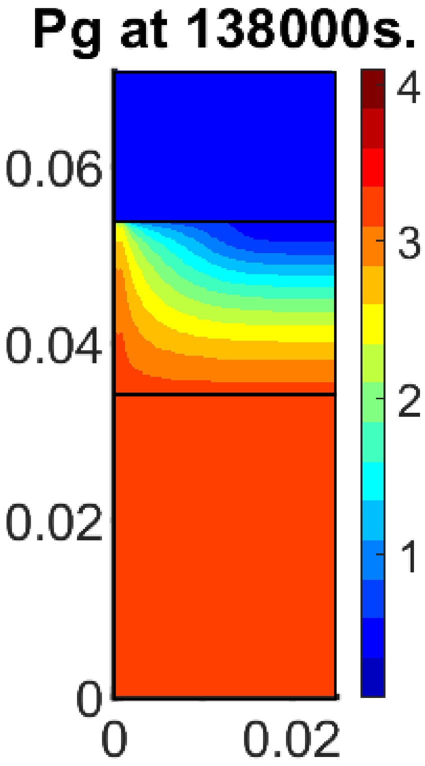


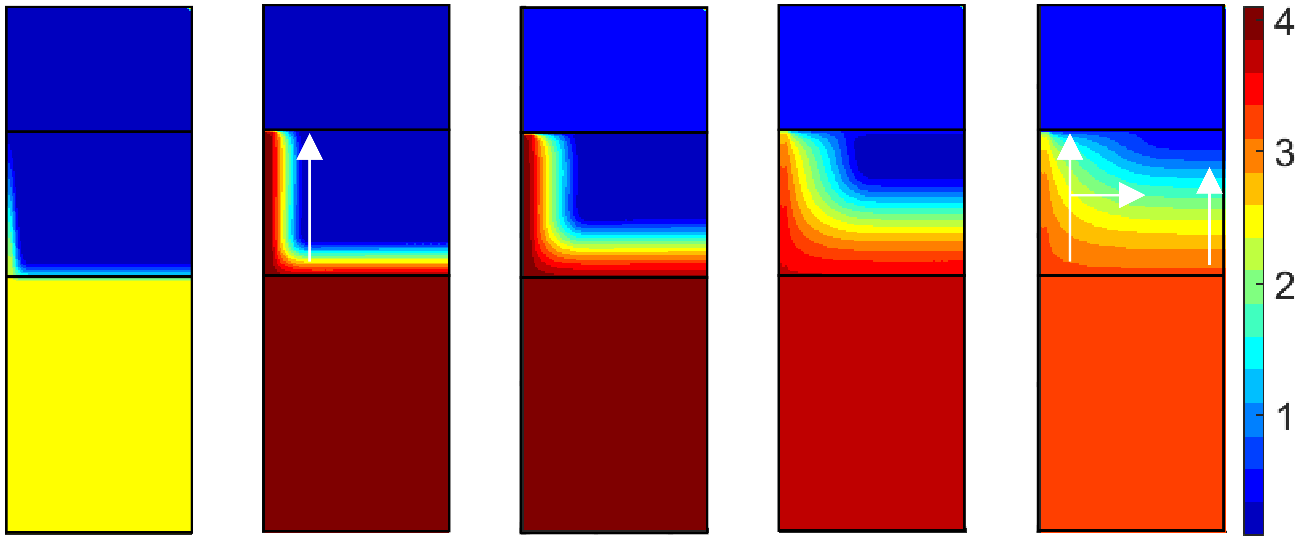


Gas injection experiment

Injection and recovery pressures



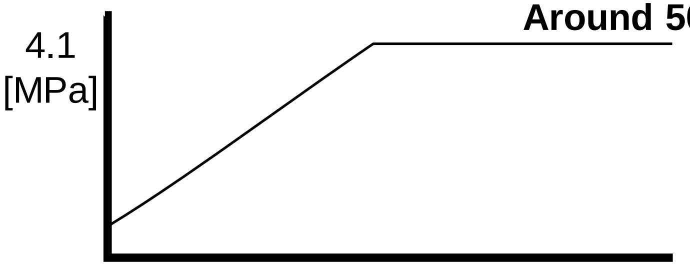




Start injection

Breakthrough
Around 50000s

Air dissipation



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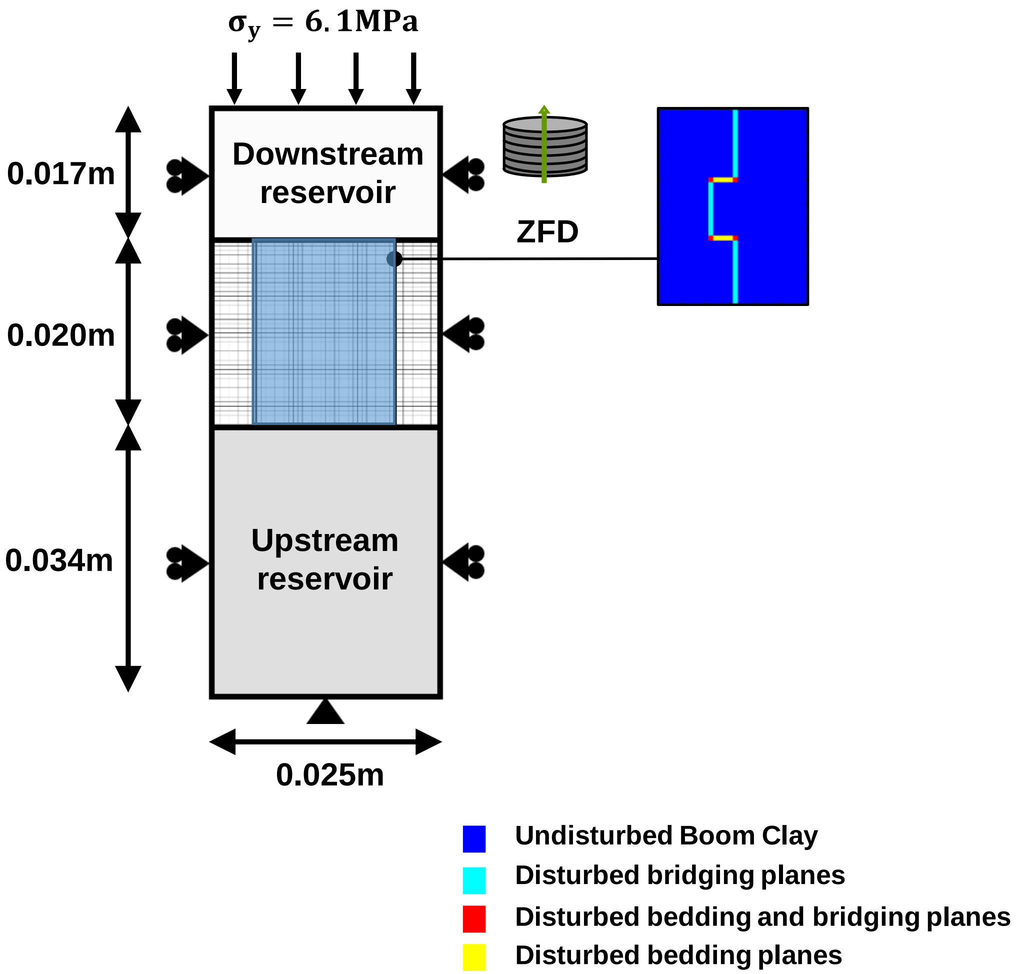
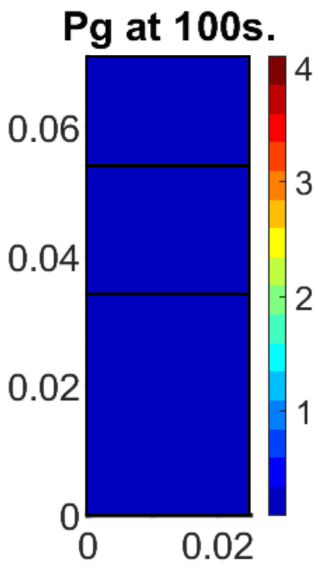
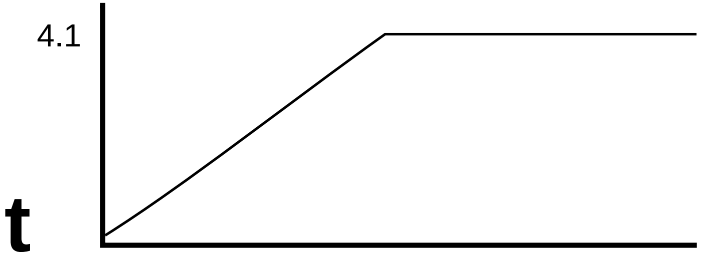
Gas injection experiment

Effect of the connectivity of the planes

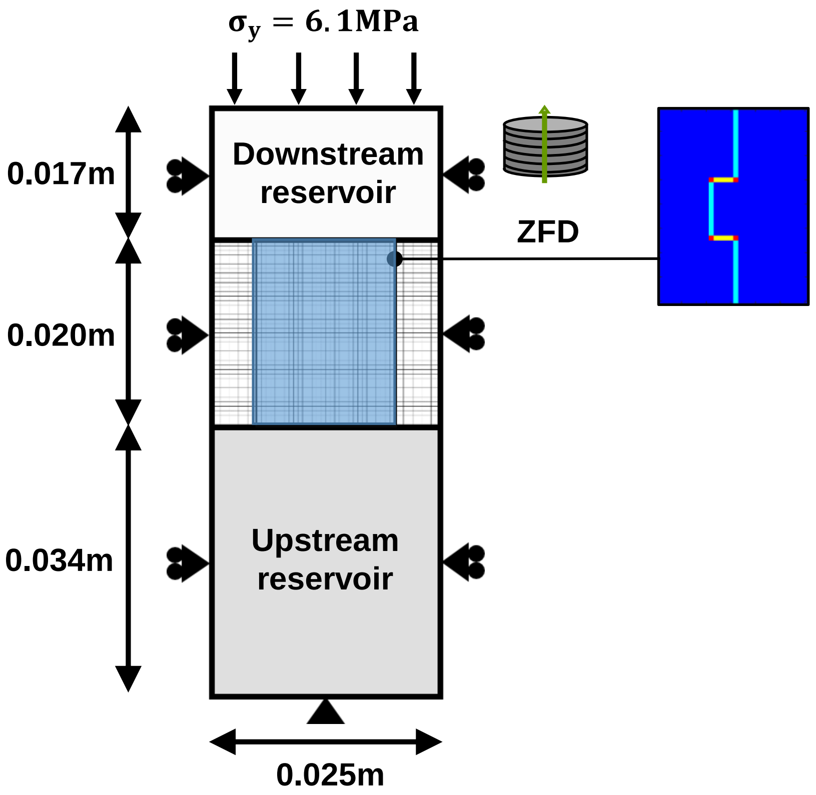


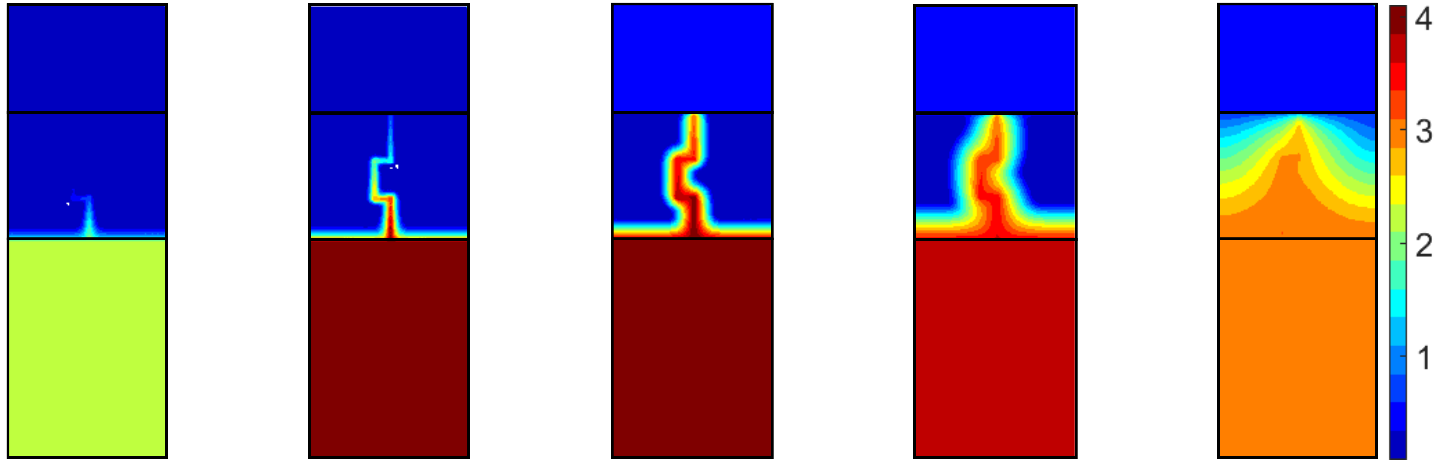


Gas injection experiment



Effect of the connectivity of the planes





Start injection

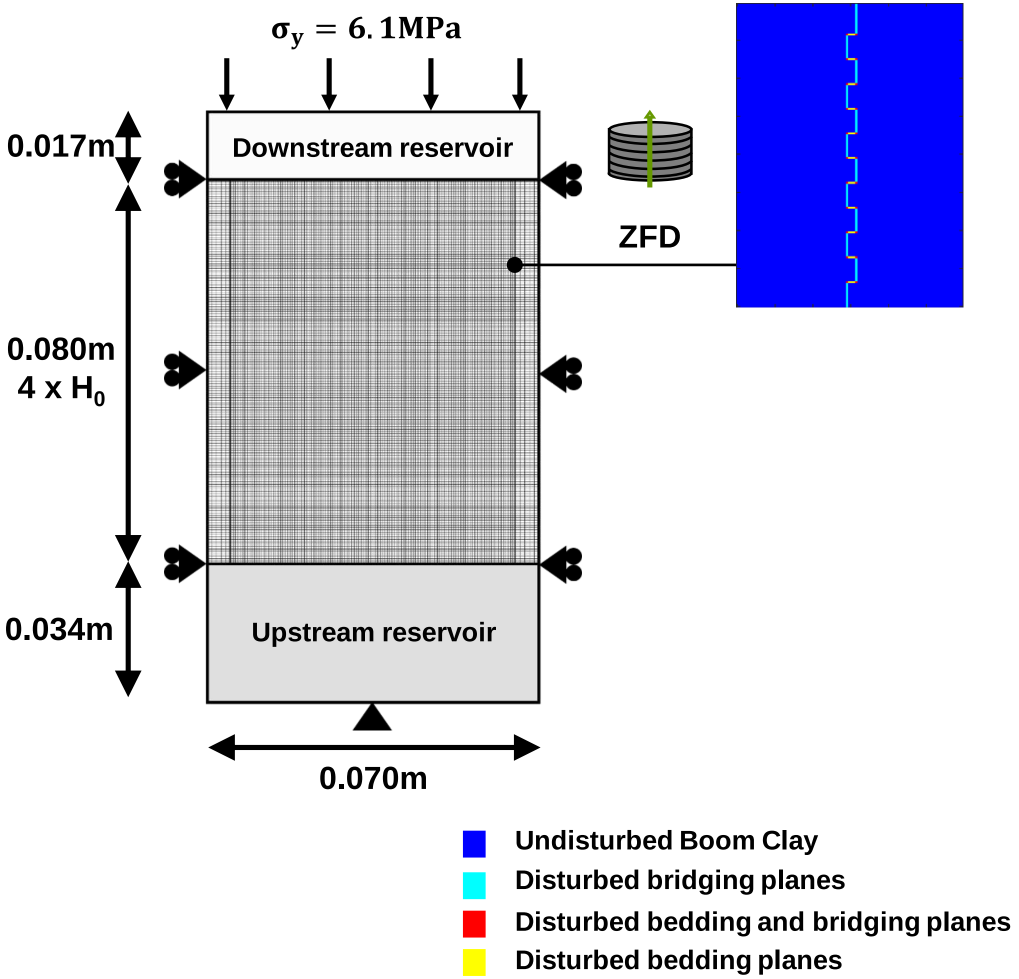
Breakthrough
Around 50000s

Air dissipation

- Undisturbed Boom Clay
- Disturbed bridging planes
- Disturbed bedding and bridging planes
- Disturbed bedding planes

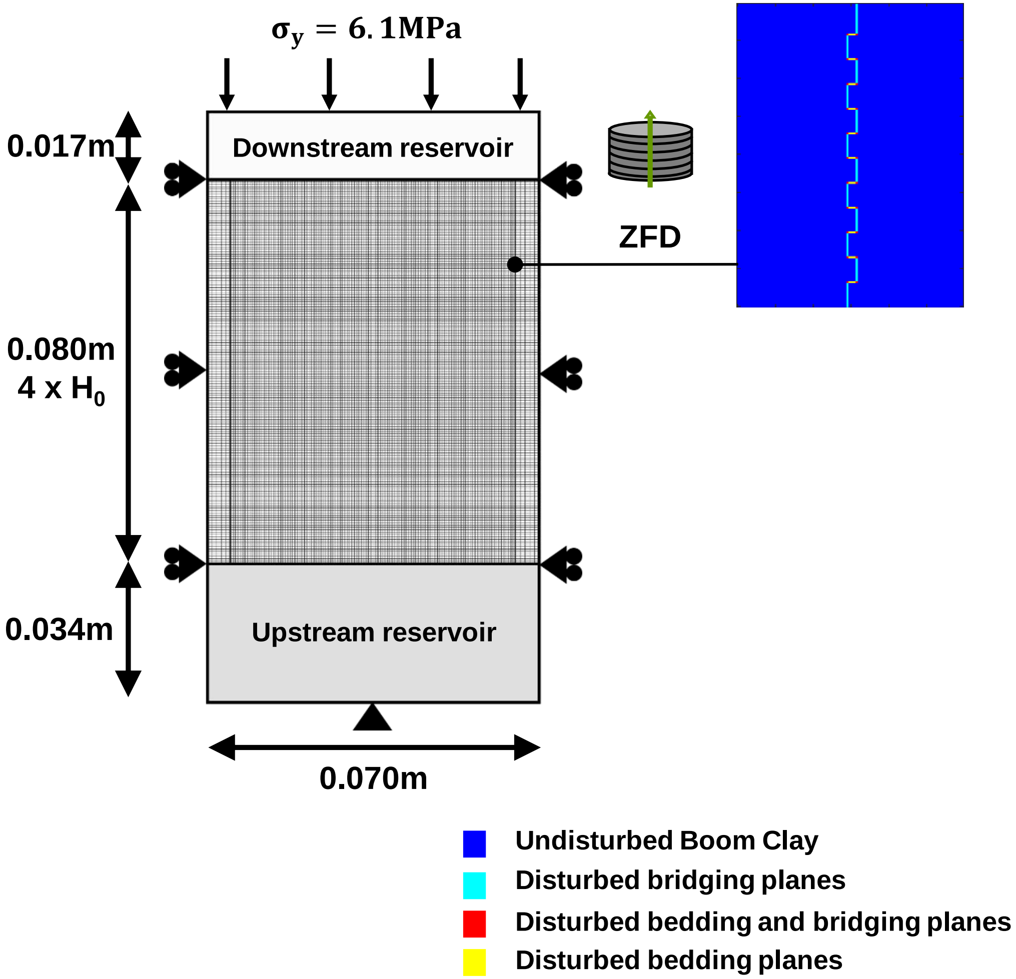
Gas injection experiment

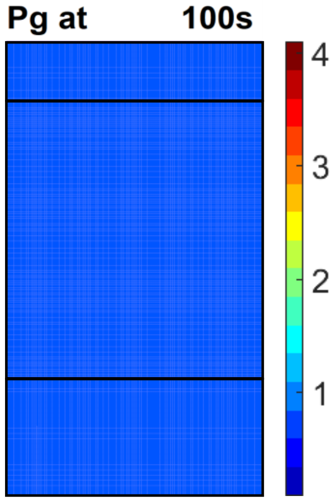
Effect of the connectivity of the planes under up-scaling



Gas injection experiment

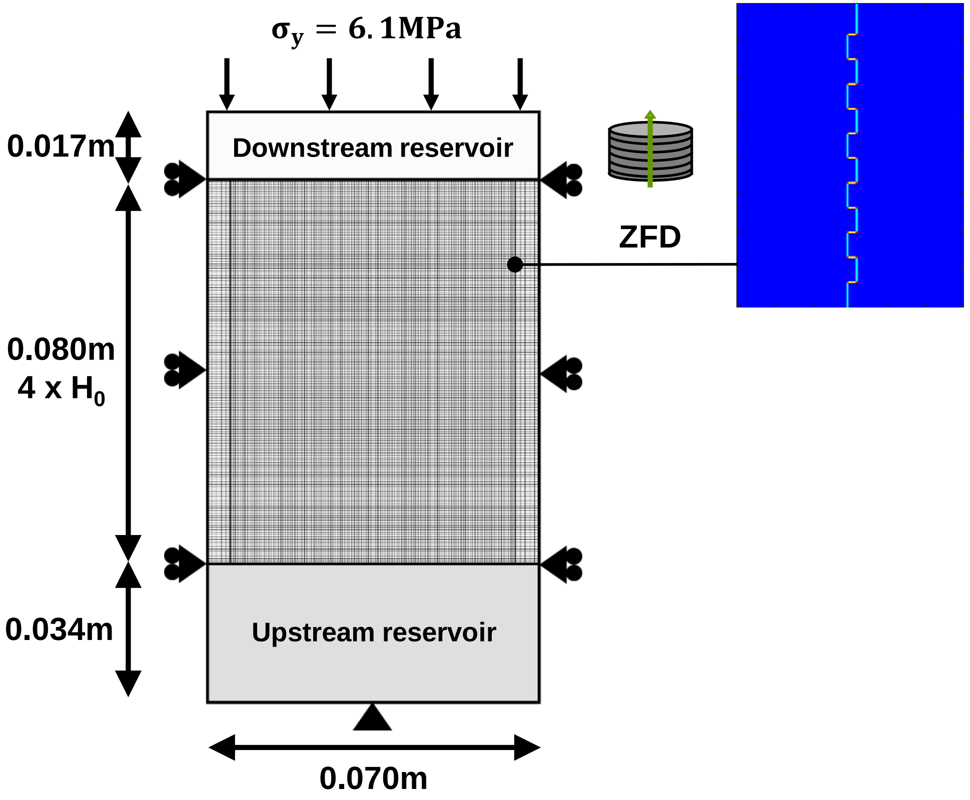
Effect of the connectivity of the planes under up-scaling



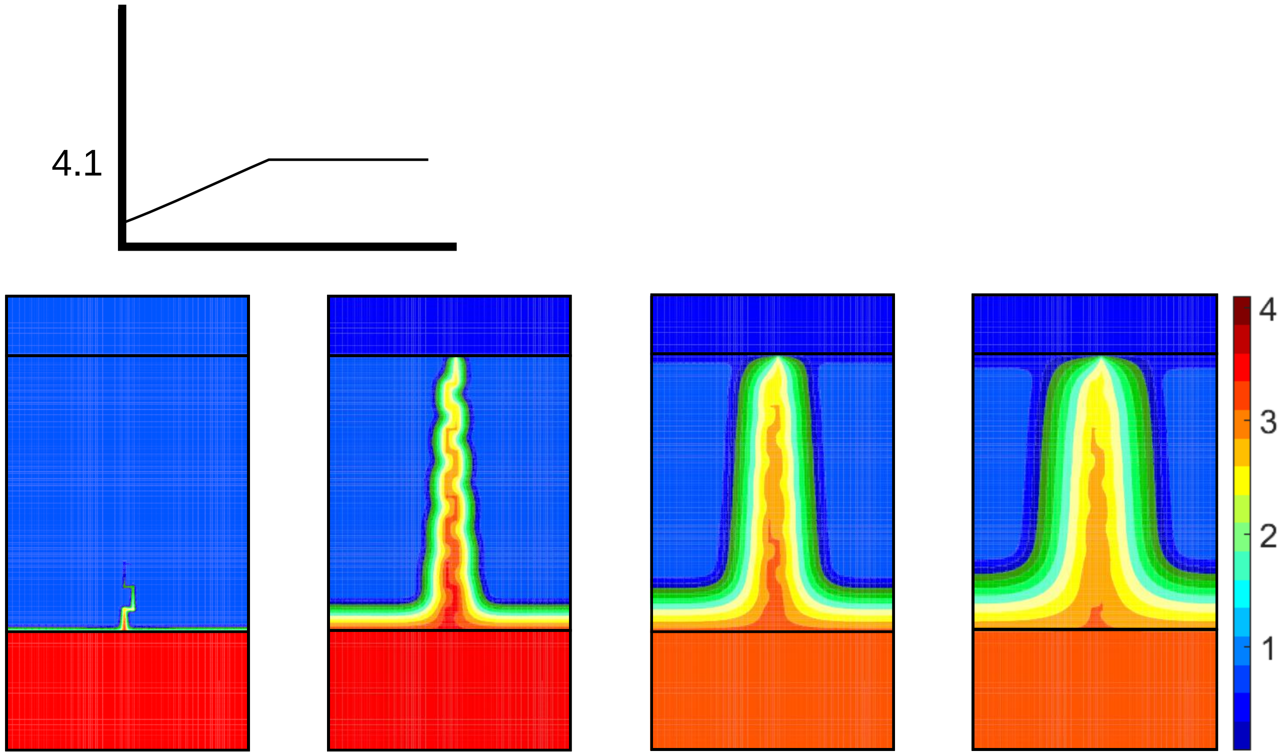


Gas injection experiment

Effect of the connectivity of the planes under up-scaling



- Undisturbed Boom Clay
- Disturbed bridging planes
- Disturbed bedding and bridging planes
- Disturbed bedding planes



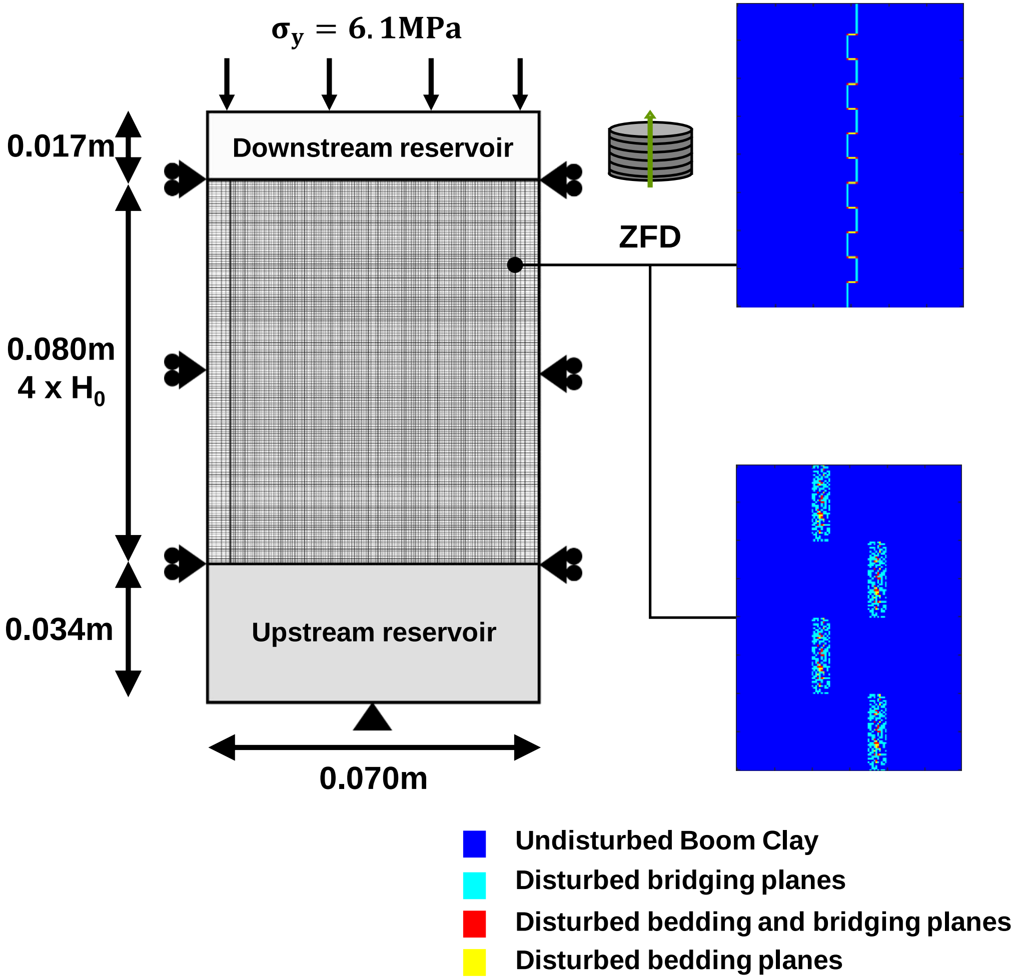
Start injection

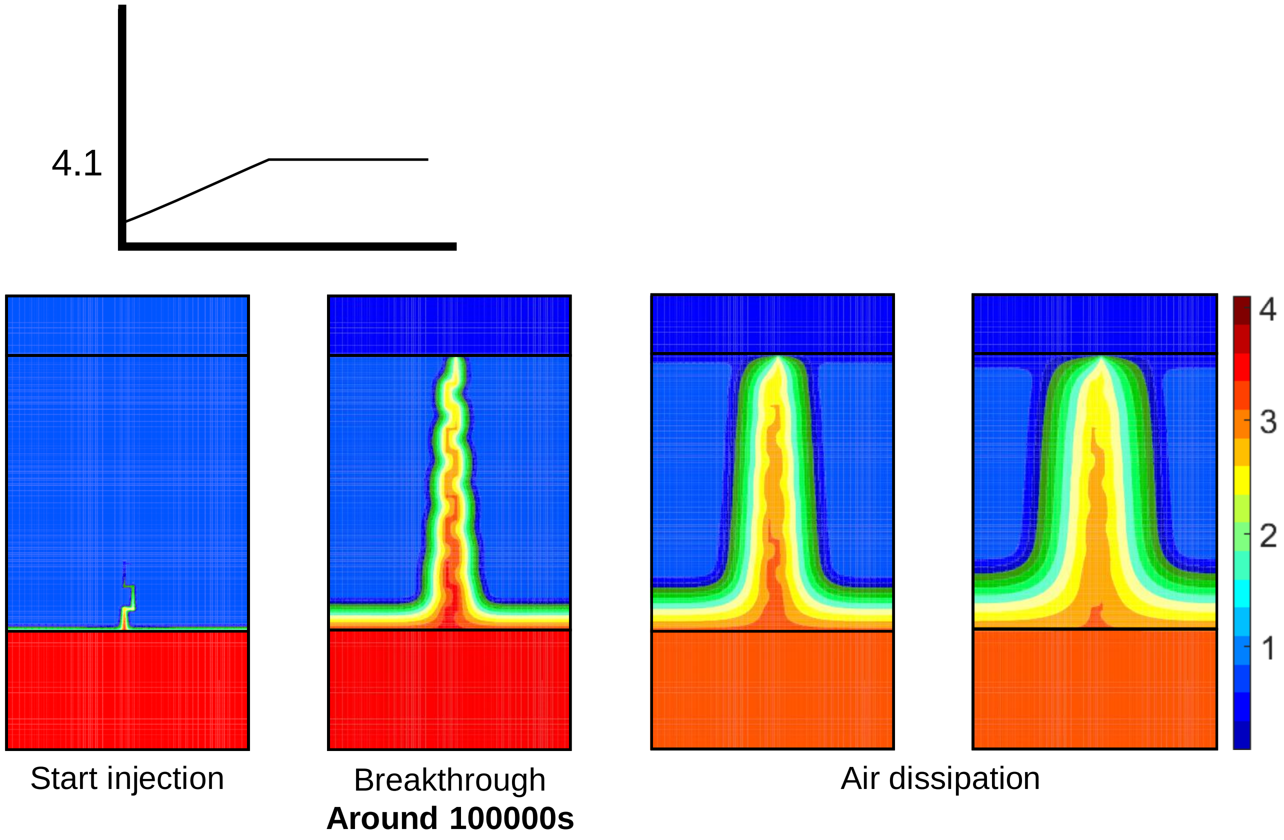
Breakthrough
Around 100000s

Air dissipation

Gas injection experiment

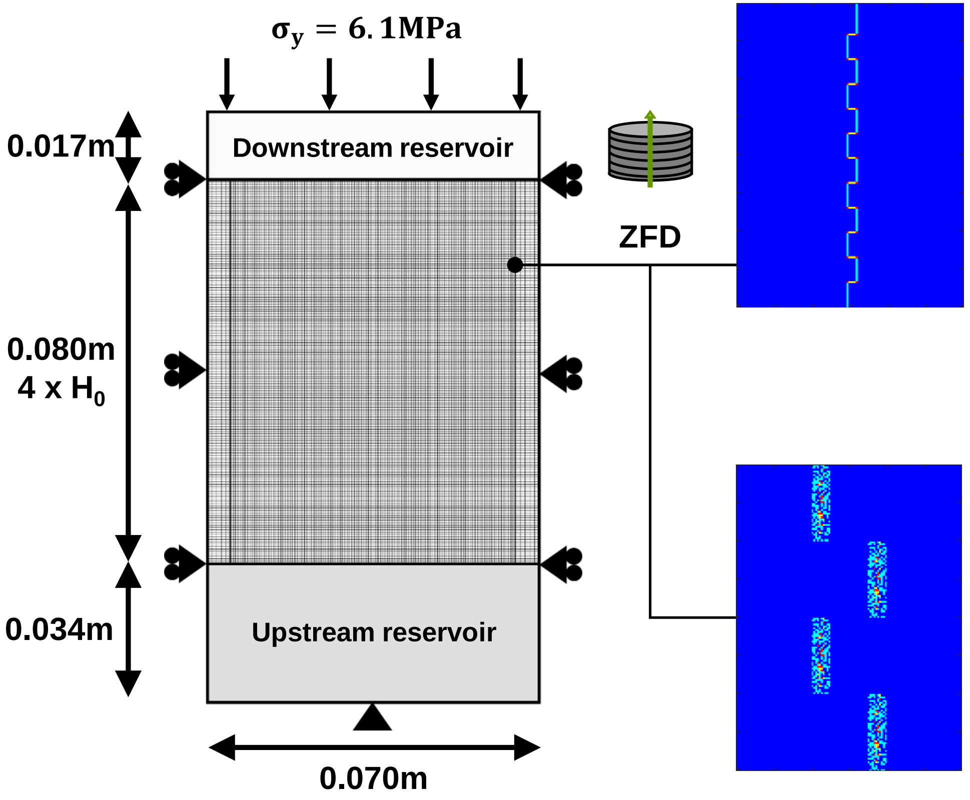
Effect of the connectivity of the planes under up-scaling



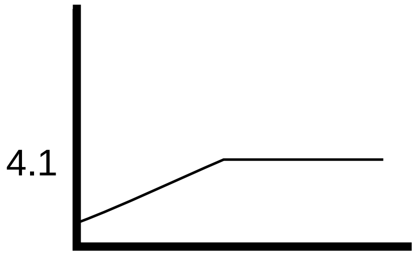


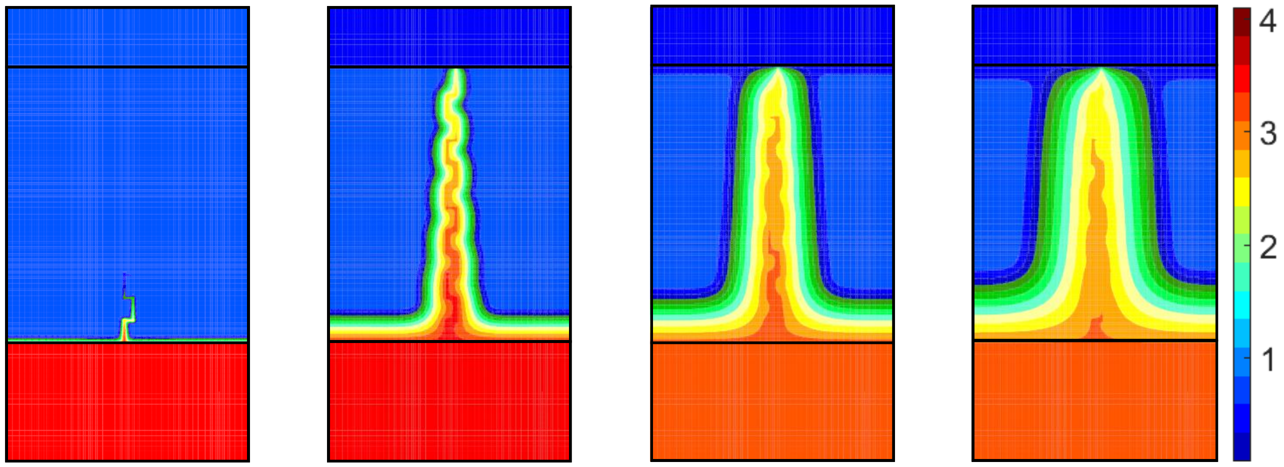
Gas injection experiment

Effect of the connectivity of the planes under up-scaling



- Undisturbed Boom Clay
- Disturbed bridging planes
- Disturbed bedding and bridging planes
- Disturbed bedding planes

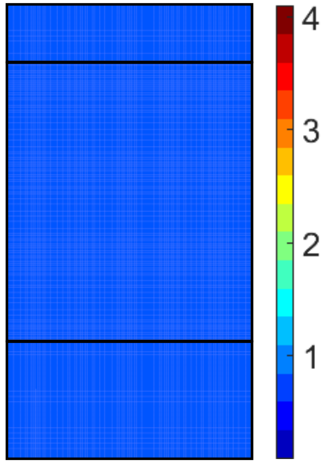




Start injection

Breakthrough
Around 100000s

Air dissipation



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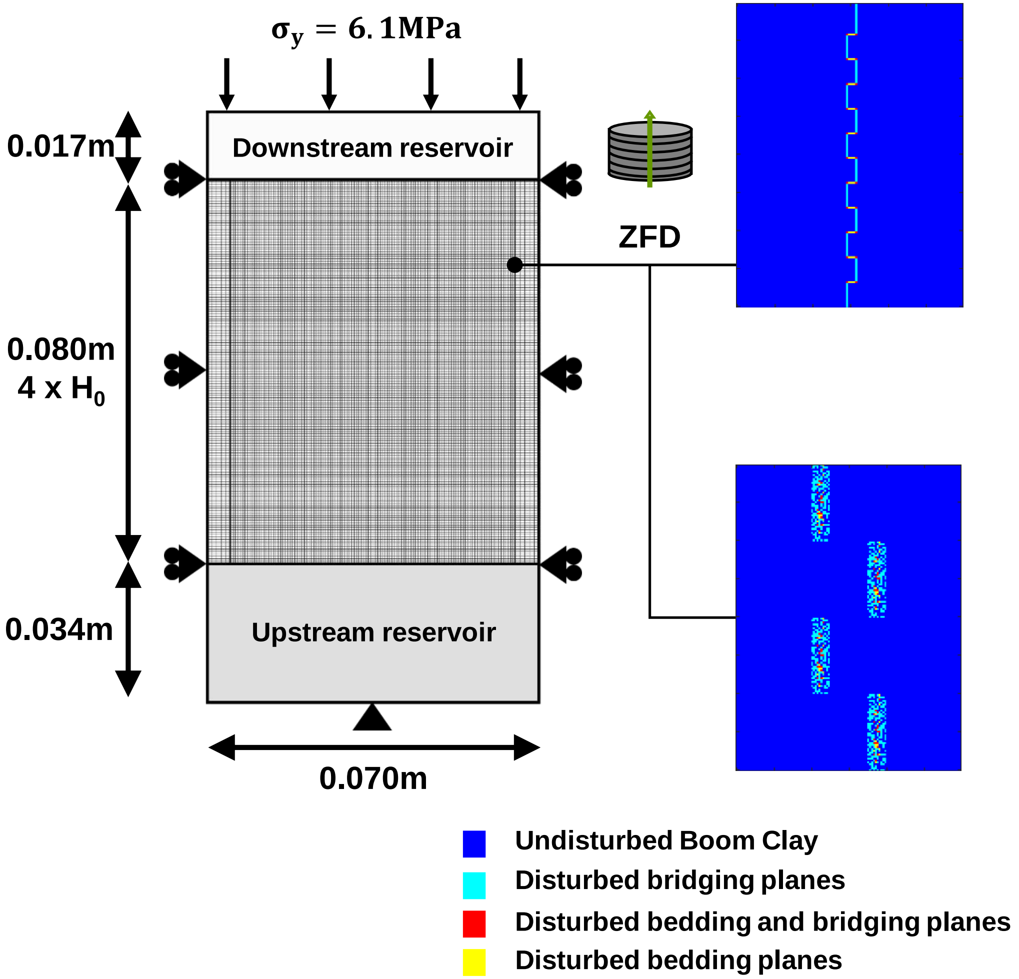
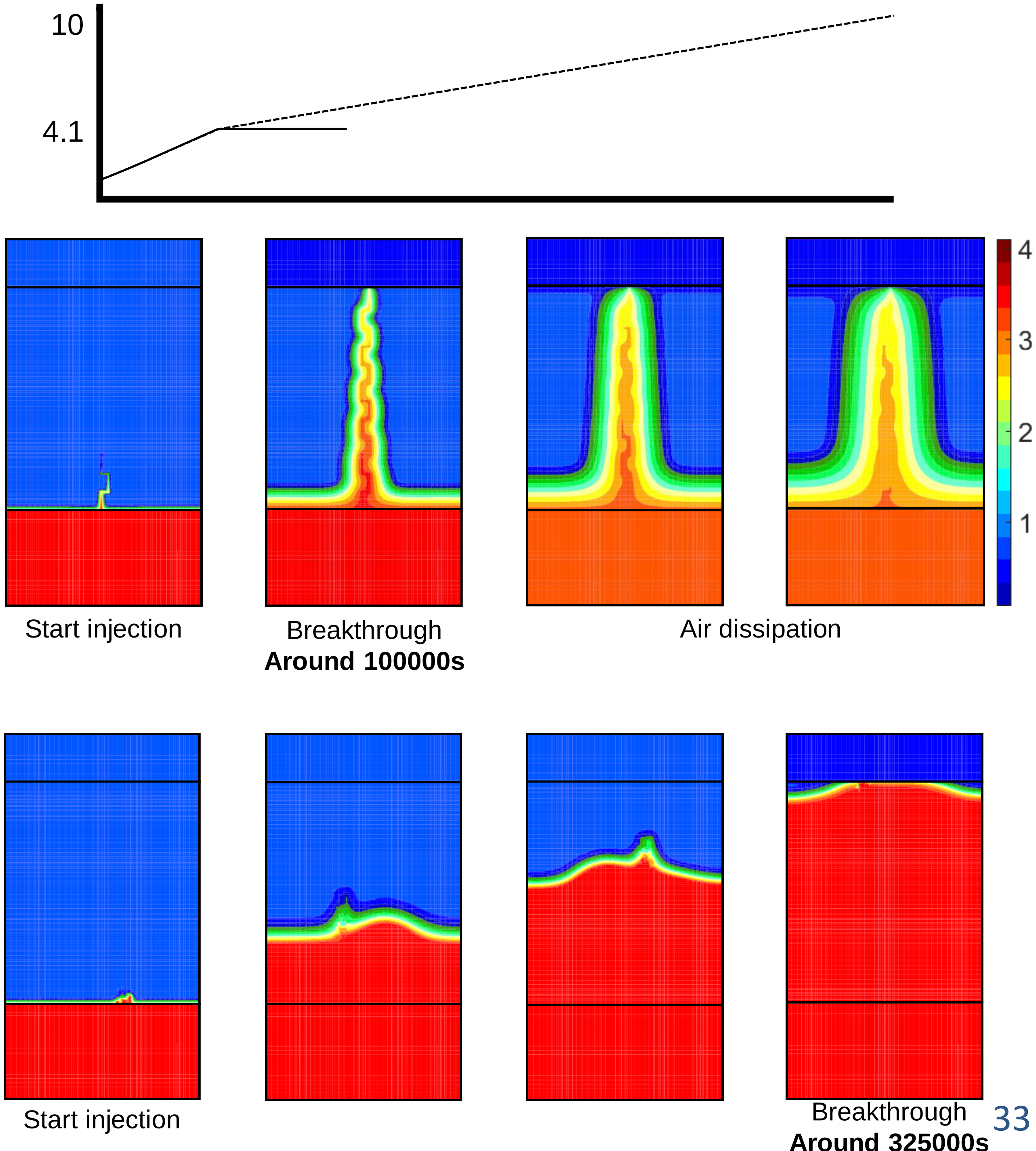
Gas injection experiment

Effect of the connectivity of the planes under up-scaling





Content

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❷ From experimental evidence to modelling

❸ Multi-scale modelling approach

❹ Modelling gas injection experiment

❺ Conclusions

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Conclusions

We **developed** a multi-scale model able to

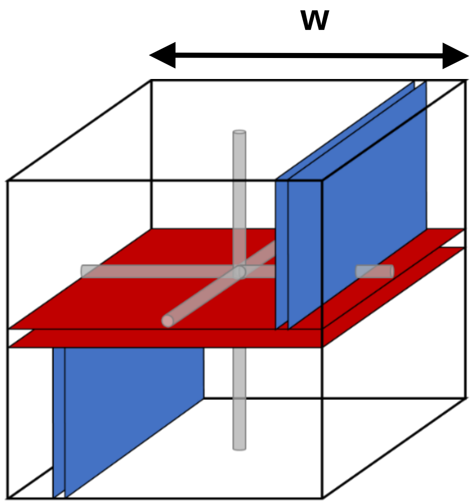
1. Simply idealise the microstructure of the rock with fractures and tubes
2. Reproduce mechanisms inherent to gas migrations in sound rock layers

We **showed** that

1. Macro-pores, bedding planes and bridging planes play different roles in gas flows
2. Preferential flow paths can be generated through fractures with weaker properties
3. Different gas mechanisms occur in the presence of weaker bridging planes

Thank you for your attention !

Multi-scale modelling approach



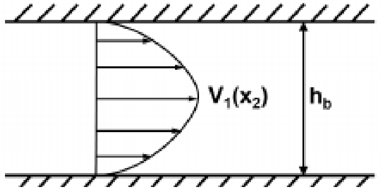
Micro-scale boundary value problem

Constitutive equations: Hydraulic problem considering a channel flow model (Navier-Stokes equations)

- Advective component:

$$q_{\alpha_i} = -\frac{k_{r\alpha}}{\mu_\alpha}\frac{1}{A}\kappa_{frac}\frac{\partial p_\alpha}{\partial x_i} = -\frac{k_{r\alpha}}{\mu_\alpha}\frac{h_b^3}{12w}\frac{\partial p_\alpha}{\partial x_i}$$

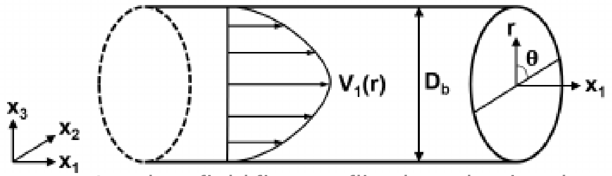
$$q_{\alpha_i} = -\frac{k_{r\alpha}}{\mu_\alpha}\frac{1}{A}\kappa_{tube}\frac{\partial p}{\partial x_i} = -\frac{k_{r\alpha}}{\mu_\alpha}\pi\frac{D^4}{128w^2}\frac{\partial p}{\partial x_i}$$



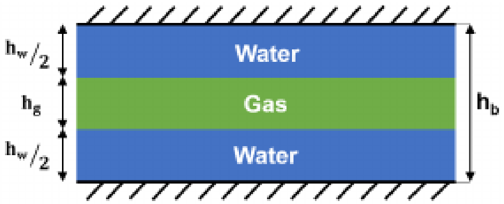
Laminar fluid flow profiles between two parallel plates

$$\kappa_{frac} = -\frac{h_b^2}{12}h_b \cdot w$$

$$\kappa_{tube} = -\pi\frac{D^4}{128}$$



Laminar fluid flow profiles in a circular pipe



Gas flow in between of water flows in a fracture space

$$k_{r_w} = \frac{S_r^2}{2}(3 - S_r)$$
$$k_{r_g} = (1 - S_r)^3$$

$$k_{r_w} = S_r^2$$
$$k_{r_g} = (1 - S_r)^2$$

Gas flow in between of water flows in a circular pipe

- Diffusive component

$$i_{dg_i} = -S_{r_w}\,\bar{\tau}\,D_{dg/w}\,\rho_w\,\frac{\partial}{\partial x_i}\left(\frac{\rho_{dg}}{\rho_w}\right)$$

Multi-scale modelling approach

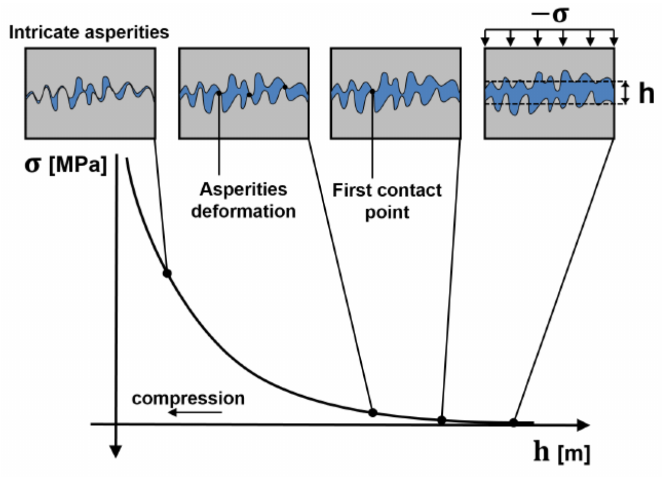
Micro-scale boundary value problem

Constitutive equations: Hydro-mechanical couplings

- Stress-dependent evolution of micro-elements aperture

$$\Delta\sigma' = K_n \Delta h \qquad\qquad \Delta\sigma' = K\,\Delta D_b$$

$$K_n = \frac{K_n^0}{\left(1+\frac{\Delta h}{h_0}\right)^2} \qquad\qquad K = \frac{2G}{D_0}$$



Constitutive law describing the normal behaviour of a rough rock joint, *Cerfontaine (2015)*

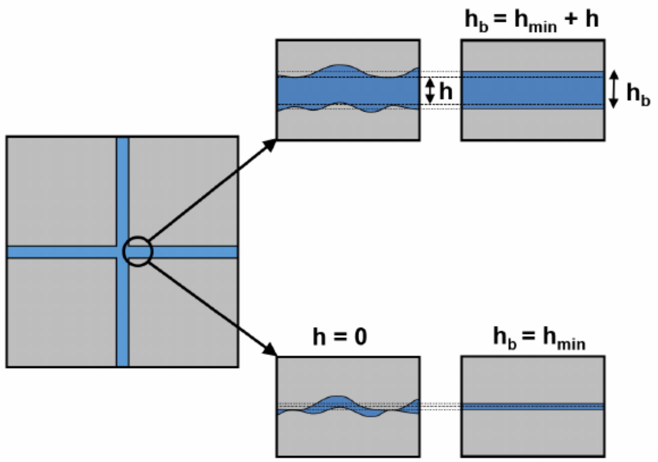
- Stress-dependent formulation of the transmissivity and the entry pressure of micro-elements

$$\kappa_{frac} = -\frac{h_b^2}{12} h_b \cdot w \qquad\qquad \kappa_{tube} = -\pi\frac{D^4}{128}$$

$$p_e = p_{e_0}\left(\frac{h_{b0}}{h_b}\right)^m \qquad\qquad p_e = p_{e_0}\left(\frac{D_{b0}}{D_b}\right)^m$$

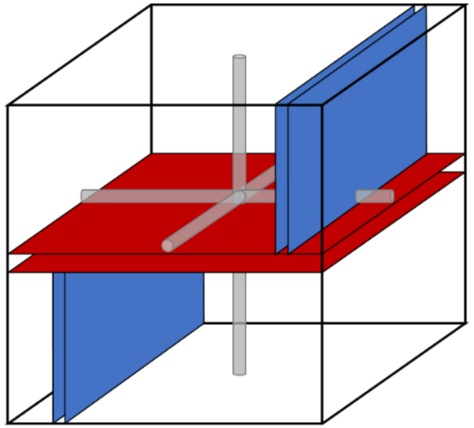
$$p_{e_0} = \frac{2\sigma_{GL}cos\theta}{h_b} \qquad\qquad p_{e_0} = \frac{2\sigma_{GL}cos\theta}{D_b/2}$$

$$h_b = h_0 + h \qquad\qquad D_b = D_0 + D$$



Definitions of the hydraulic and the mechanical aperture in reality (left) and in the modelling (right), *Marinelli (2016)*

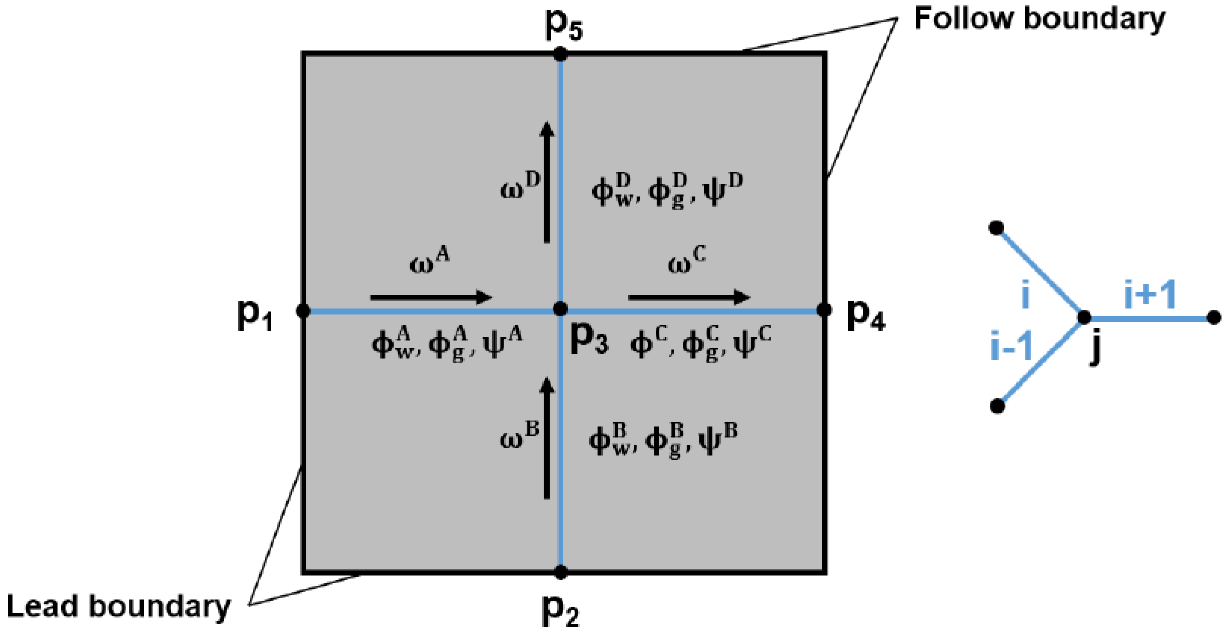
Multi-scale modelling approach



Micro-scale boundary value problem

General principles for numerical resolution of the hydraulic system

- Hydraulic network respecting these conditions:
  - Anti-symmetric boundary fluxes
  - Macroscopic pressure gradient between the boundaries
- Hydraulic problem established through mass balance on each node (j)
- Hydraulic problem solved
  - For a given configuration
  - Under steady-state conditions
  - By applying the macro-pressure to one node



Example of a channel network with the mass balance on node j

Multi-scale modelling approach

Micro-scale boundary value problem

General principles for numerical resolution of the hydraulic system

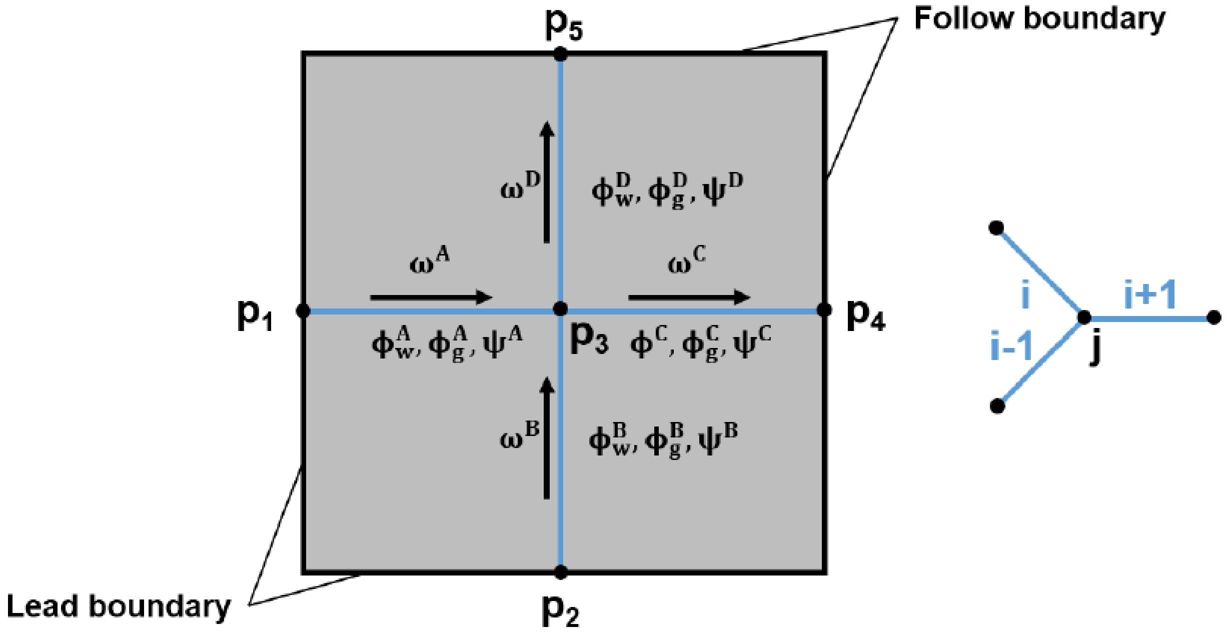
- Hydraulic network respecting these conditions:
  - Anti-symmetric boundary fluxes
  - Macroscopic pressure gradient between the boundaries

=> Channel (fracture or tube) mass fluxes of water and gas

$$\omega_w = -\underbrace{\frac{\rho_w k_{r_w}}{\mu_w}\kappa\frac{\partial p_w^m}{\partial s}}_{\text{Advection of liquid water}}$$

$$\omega_g = -\underbrace{\frac{\rho_g k_{r_g}}{\mu_g}\kappa\frac{\partial p_g^m}{\partial s}}_{\text{Advection of gaseous gas}} - \underbrace{H_g\frac{\rho_g k_{r_w}}{\mu_w}\kappa\frac{\partial p_w^m}{\partial s}}_{\text{Advection of dissolved gas}}$$

$$\underbrace{- S_{r_w}\bar{\tau}D_{dg/w}\frac{H_g}{\rho_w}\left(\frac{\rho_w\rho_{g,0}}{p_{g,0}}\frac{\partial p_g^m}{\partial s} - \frac{\rho_g\rho_{w,0}}{\chi_w}\frac{\partial p_w^m}{\partial s}\right)}_{\text{Diffusion of dissolved gas}}$$



Example of a channel network with the mass balance on node j

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Multi-scale modelling approach

Micro-scale boundary value problem

General principles for numerical resolution of the hydraulic system

- Hydraulic problem established through mass balance on each node (j)
  - Mass conservation principle, *i.e.* for each node of the network, the sum of the input flows is equal to the sum of the output flows

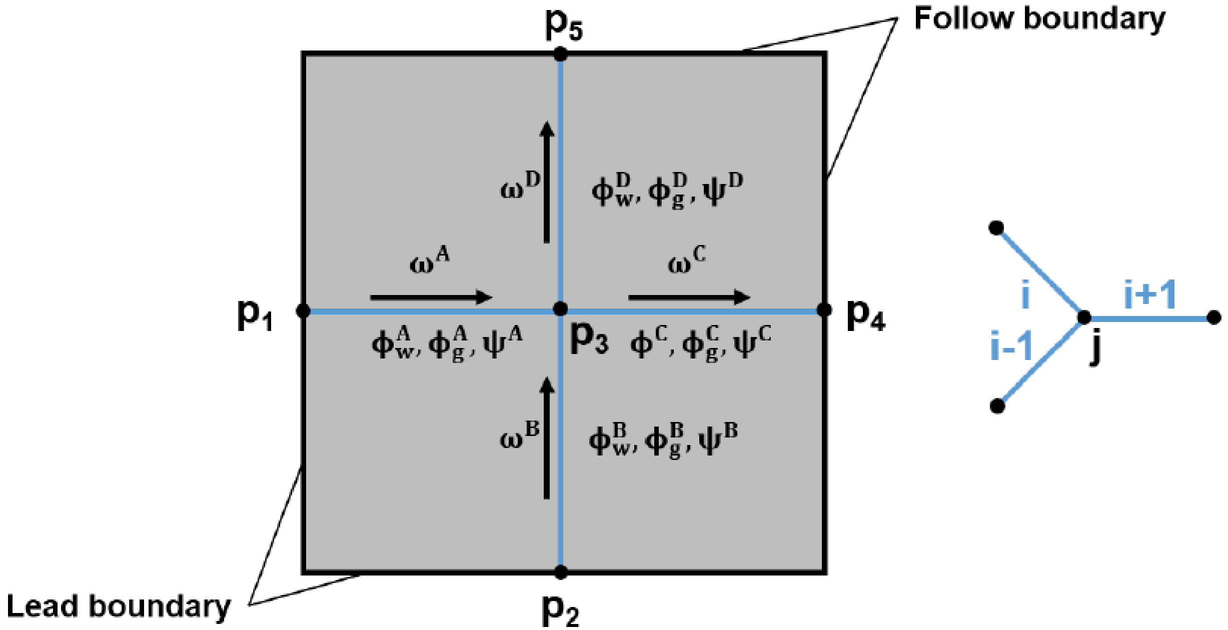
$$\frac{d\omega_\alpha^i}{ds^i} = 0 \quad \Leftrightarrow \quad \omega_\alpha^{i-1} + \omega_\alpha^i + \omega_\alpha^{i+1} = 0$$

$\alpha = w, g$ Liquid or gaseous phase

- Well-posed hydraulic system to solve

$$[G_{ww}]\{p_w^m\} = 0 \qquad [G_{gg}]\{p_g^m\} + [G_{gw}]\{p_w^m\} = 0$$

  - For a given configuration
  - Under steady-state conditions
  - By applying the macro-pressure to one node



Example of a channel network with the mass balance on node j

Multi-scale modelling approach

Micro-to-macro scale transition: Homogenisation

- Fluid fluxes

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

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

- Fluid masses: total amount of fluids inside the fractures and tubes

$$M_w^M = \frac{1}{\Omega}\int_{\Omega_w^{int}} \rho_w d\Omega$$
$$= \rho_w S_{r_w} \phi_n$$

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

eurad

Multi-scale modelling approach

Macro-scale boundary value problem

- Under matrix form:

$$\begin{bmatrix} [K^M_{ww}]_{(3\times3)} & [K^M_{wg}]_{(3\times3)} \\ [K^M_{gw}]_{(3\times3)} & [K^M_{gg}]_{(3\times3)} \end{bmatrix} \begin{Bmatrix} \begin{Bmatrix} \delta\nabla p^M_w \\ \delta p^M_w \end{Bmatrix}_{(3)} \\ \begin{Bmatrix} \delta\nabla p^M_g \\ \delta p^M_g \end{Bmatrix}_{(3)} \end{Bmatrix} = \begin{Bmatrix} \begin{Bmatrix} \delta f^M_w \\ \delta \dot{M}^M_w \end{Bmatrix}_{(3)} \\ \begin{Bmatrix} \delta f^M_g \\ \delta \dot{M}^M_g \end{Bmatrix}_{(3)} \end{Bmatrix}$$

Summarized as:

$$[A^M]_{(10\times10)} \{\delta U^M\}_{(10)} = \{\delta \Sigma^M\}_{(10)}$$