



***ALERT Geomaterials***  
**Alliance of Laboratories in Europe for Education, Research and Technology**  
<http://alertgeomaterials.eu>

**eurad**  
European Joint Programme  
on Radioactive Waste Management

*Multiphysics and multiscale coupled processes  
in geomaterials.*

*Focus on thermal effects and gas transfer  
impact on the behaviour of geomaterials.*

S. Levasseur, A-C Dieudonné, Frédéric Collin



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



WELCOME

## What about ALERT Geomaterials ?

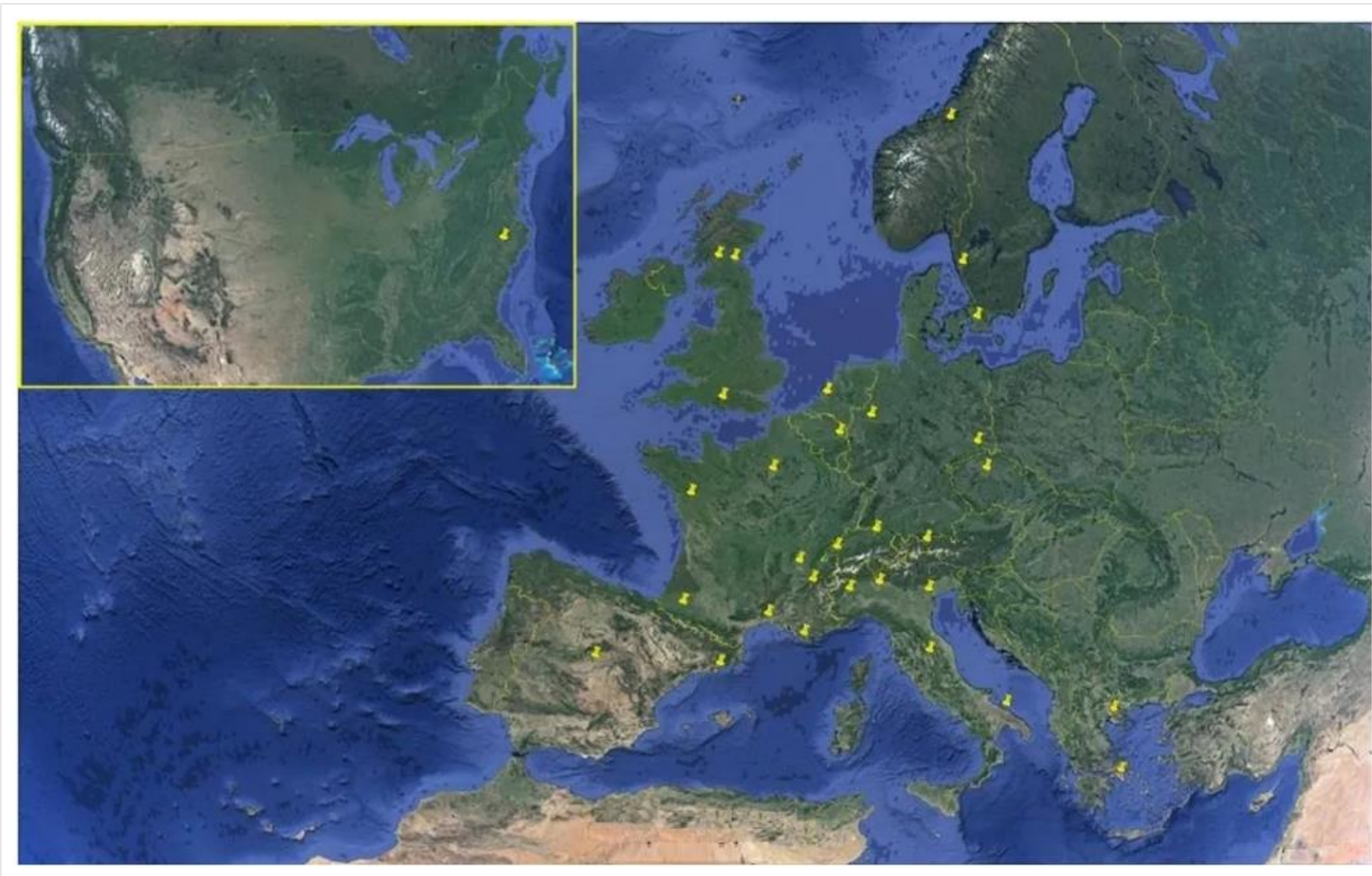
The Alliance of Laboratories in Europe for Education, Research and Technology (ALERT) “Geomaterials” has been **created in 1989** by ***Roberto Nova, Manuel Pastor, Ian Smith, Peter Vermeer, Olek Zienkiewicz and Félix Darve*** as a pioneering (at that time!) effort to develop a **European School of Thinking in the field of the Mechanics of Geomaterials**. The generic name “**Geomaterials**” is viewed as gathering together **materials, whose mechanical behaviour depends on the pressure level**, which can be dilatant under shearing and which are multiphase because of their porous structure. So, **the “geomaterials” label brings together mainly soils, rocks and concrete**. It has been obvious from the very beginning that there is a crucial need for a joint Graduate School in order to build firmly this European scientific group in the Mechanics of Geomaterials, in **close link with the doctoral students**.





WELCOME

**Who are ALERT Geomaterials members? 38 Universities or organizations**





**WELCOME**

## **What are the activities of ALERT Geomaterials members?**

ALERT Workshop

ALERT Doctoral school

Every year in end September in Aussois (France)







WELCOME

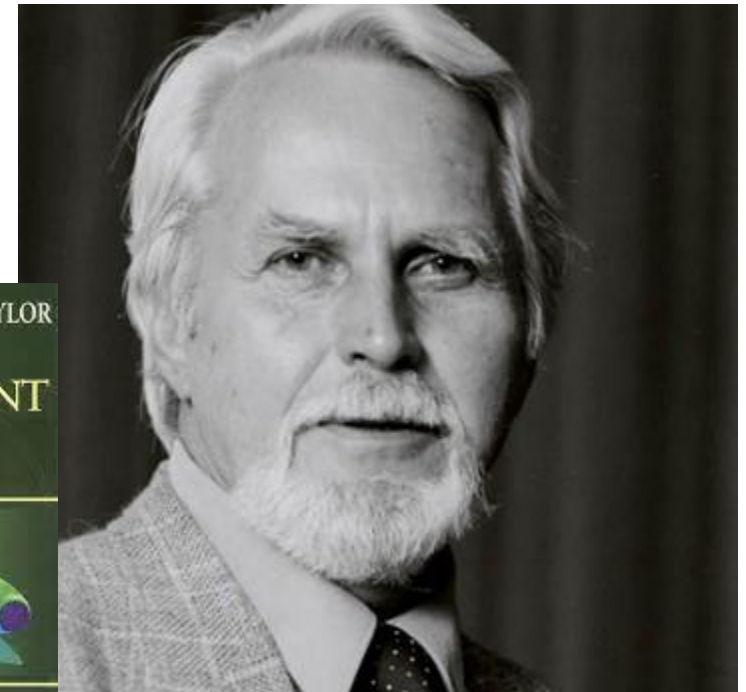
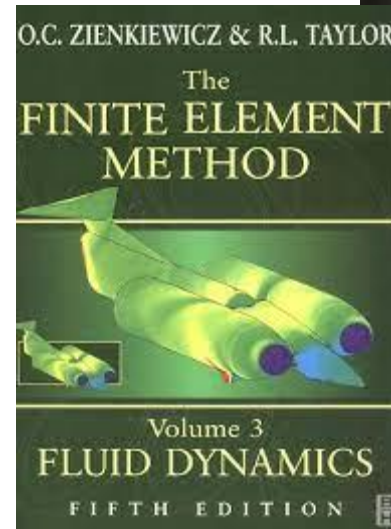
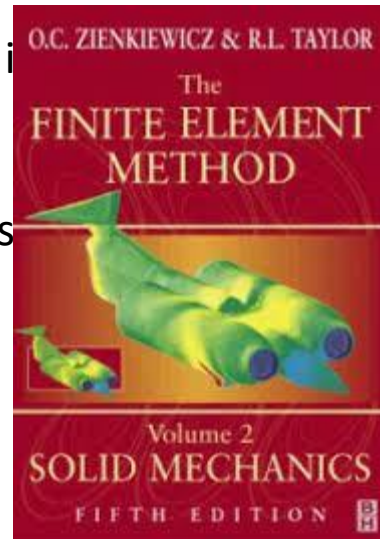
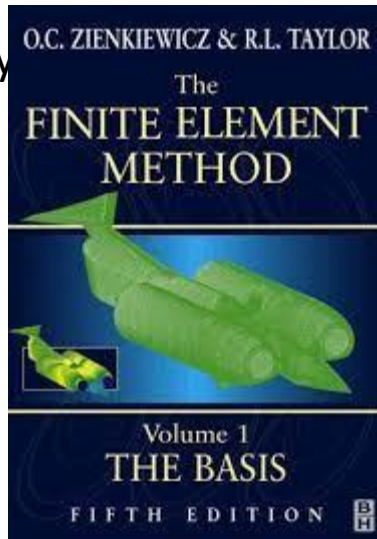
## What are the activities of ALERT Geomaterials members?

ALERT Workshop

ALERT Doctoral school

Every year

ALERT



Olek Zienkiewicz (1921-2009)



eurad



WELCOME

## What about EURAD (Grant agreement ID: 847593) ?

The European Joint Programme on Radioactive Waste Management (EURAD/2019-2024) is a project that will **help the EU member states implement Directive 2011/70/Euratom (Waste Directive)** by working with their national programmes. It will also coordinate action on joint targets among all related organisations involved at European level, whether in research or technical support. Building on the EC JOPRAD project, the EURAD project will help member states obtain the know-how required to **implement safe and long-term management of radioactive waste**. EURAD will also provide management knowledge to operate disposal facilities, and help transfer that knowledge between countries and organisations.

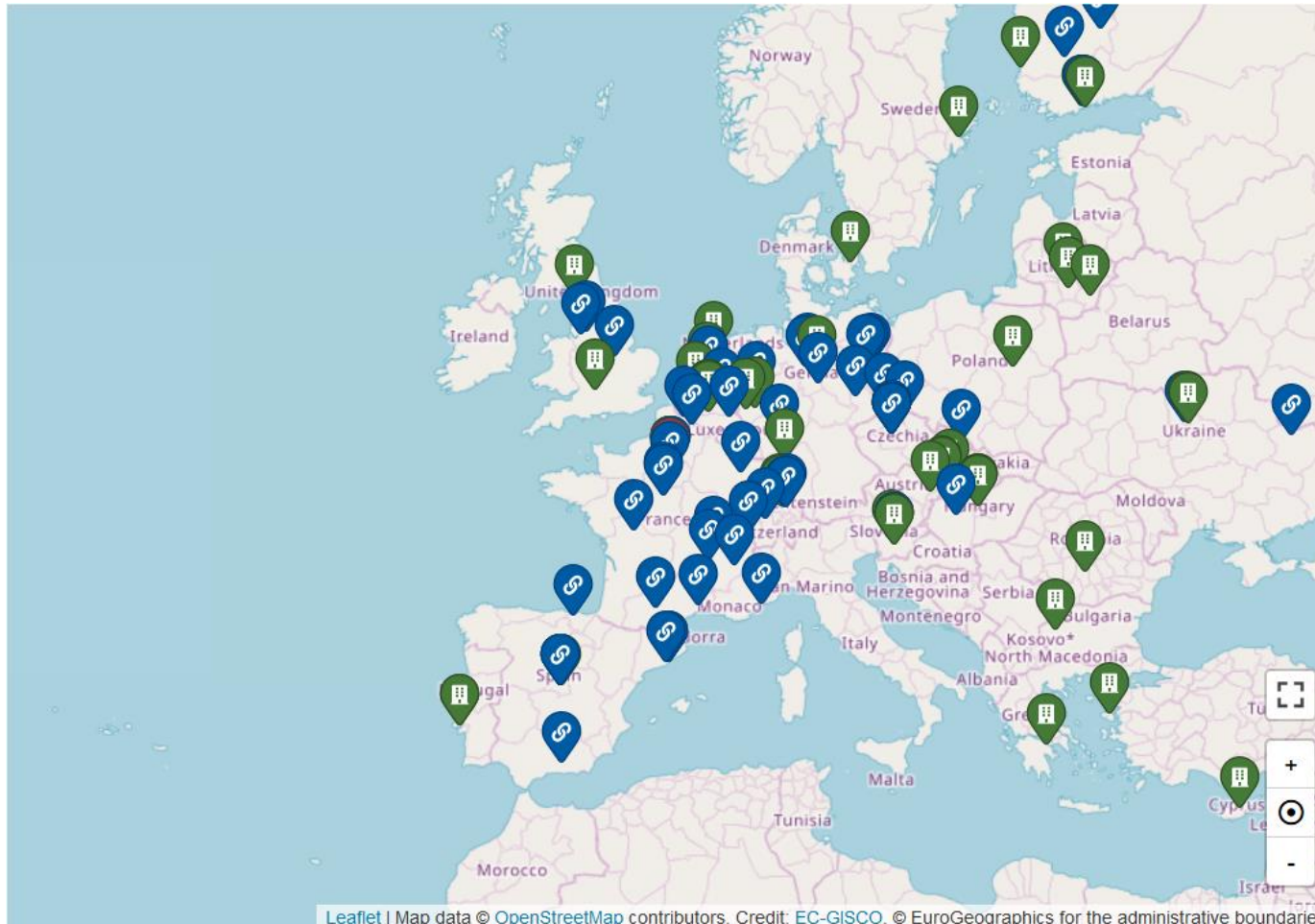


eurad



WELCOME

## Who are EURAD participants?





**WELCOME**

## **What are the activities of EURAD?**

### ***EURAD - GAS WP***

Mechanistic understanding of gas transport in clay materials (GAS)

The main objectives of this WP are:

To improve the mechanistic understanding of gas transport processes in natural and engineered clay materials, their couplings with the mechanical behaviour and their impact on the properties of these materials;

To evaluate the gas transport regimes that can be active at the scale of a geological disposal system and their potential impact on barrier integrity and repository performance.







**WELCOME**

## **What are the activities of EURAD?**

### ***EURAD - HITEC WP***

The overall objective is to evaluate whether an increase of temperature is feasible and safe by applying existing and within the work package produced novel knowledge about the behaviour of clay materials at elevated temperatures:

- to improve understanding of the THM behaviour of clay rock and engineered clay material (buffer) under high temperature and provide suitable THM models both for clay rock and buffer,
- to better assess effect of overpressures build up induced by the heat produced from the radioactive waste on the THM behaviour and properties of the clay host rock, and
- to identify processes at high temperature and the impact of high temperature on the THM properties of the buffer material.





**WELCOME**

## What will you do during this school?

Monday 28 August	
9.00 – 12.30	Basics of thermo-hydro-mechanical processes in geomaterials F. Collin, ULiège
13.30 – 17.00	Basics of experimental testing of geomaterials Alessio Ferrari, EPFL
Tuesday 29 August	
9.00 – 12.30	Constitutive modelling of thermo-hydro-mechanical processes in geomaterials Jean-Michel Pereira, ENPC
13.30 – 17.00	Development, validation and maintenance of numerical codes Olaf Kolditz, UFZ
19.30	Banquet at the city center





WELCOME

**What will you do during this school?**



Banquet at Selys Vander Valk Restaurant close to the city center





WELCOME

## What will you do during this school?

Wednesday 30 August	
9.00 – 12.30	PhD day: poster sessions and pitches
13.30 – 17.00	Advanced multiphysics experimental testing and imaging of geomaterials Laura Gonzalez-Blanco (UPC), Dragan Grigc (U Lorraine), Jiri Svoboda (CTU), Andrew Wiseall (BGS)
Thursday 31 August	
9.00 – 12.30	Advanced multiphysics modelling of geomaterials: multiscale approaches and heterogeneities Pierre Bésuelle (UGA), Frédéric Collin (ULiège), Anne-Catherine Dieudonné (TU Delft), Sebastià Olivella (UPC)
13.30 – 17.00	<i>In situ</i> THM and gas experiments Arnaud Dizier (Euridice), Emiliano Stopelli (TBC), Carlos Plua (ANDRA), Maria Victoria Villar (CIEMAT)







WELCOME

## What will you do during this school?

Friday 1 September	
Departure to Mol at 8.00	
9.30 – 12.00	Group 1 visits Tabloo expositions Group 2 visits EURIDICE_HADES underground research laboratory
12.15 – 13.15	Sandwich lunch
13.15 – 15.30	Group 2 visits Tabloo expositions Group 1 visits EURIDICE_HADES underground research laboratory
Return from Mol at 15.45	





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*Multiphysics and multiscale coupled processes in geomaterials.*

*Focus on thermal effects and gas transfer impact on the behaviour of geomaterials.*

## Basics of thermo-hydro-mechanical processes in geomaterials



Frédéric COLLIN

University of Liège – UEE Research Unit



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



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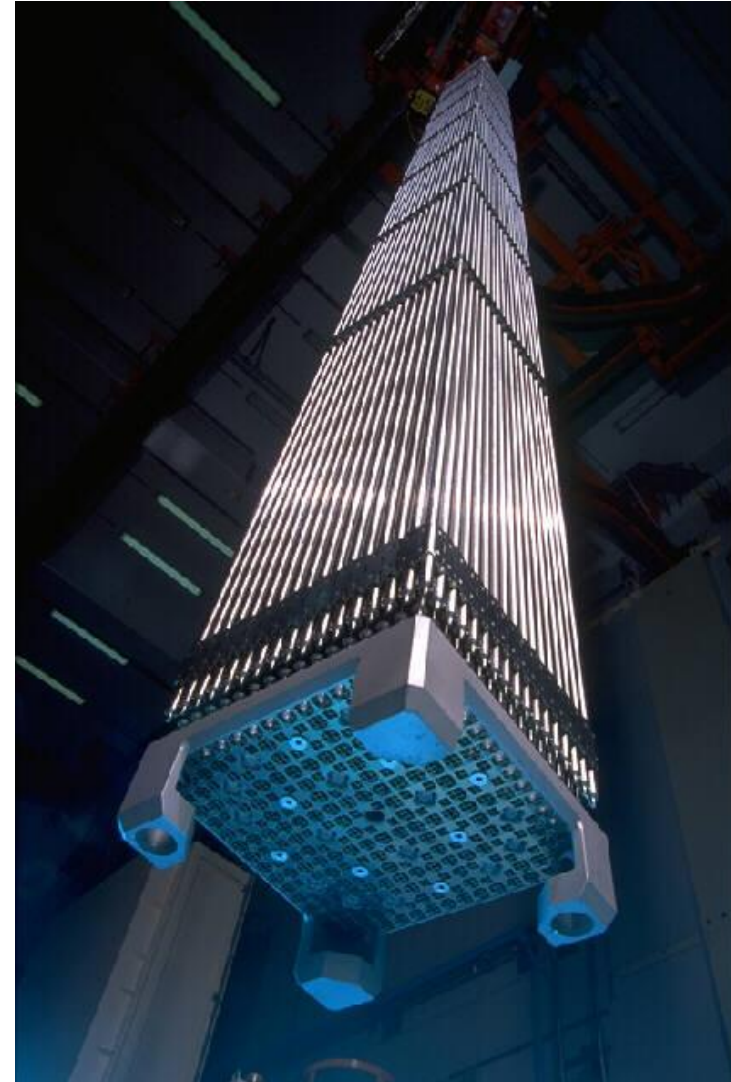
1. WELCOME
2. INTRODUCTION
3. THERMO-HYDRAULIC PROCESSES (saturated conditions)
4. UNSATURATED FLOW PROCESSES
5. THMG PROCESSES



## INTRODUCTION

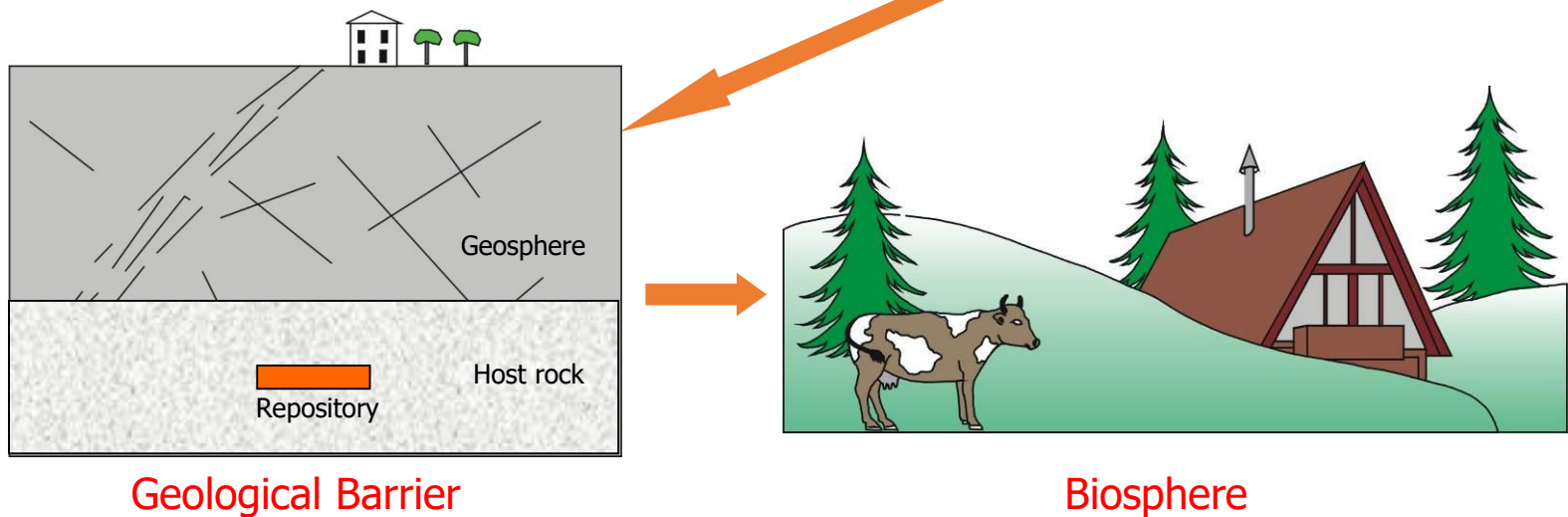
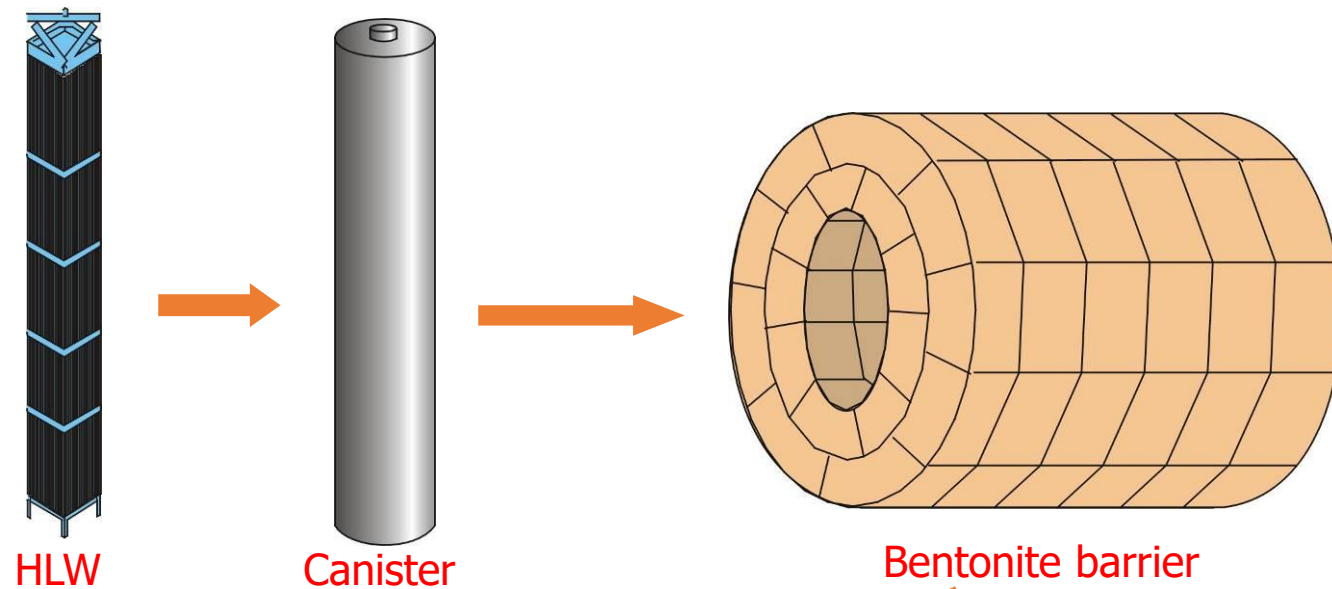
### Nuclear electricity production :

- + Low CO<sub>2</sub> emission
- Noxious ionizing radiations
- Radioactive waste production





# INTRODUCTION



# INTRODUCTION



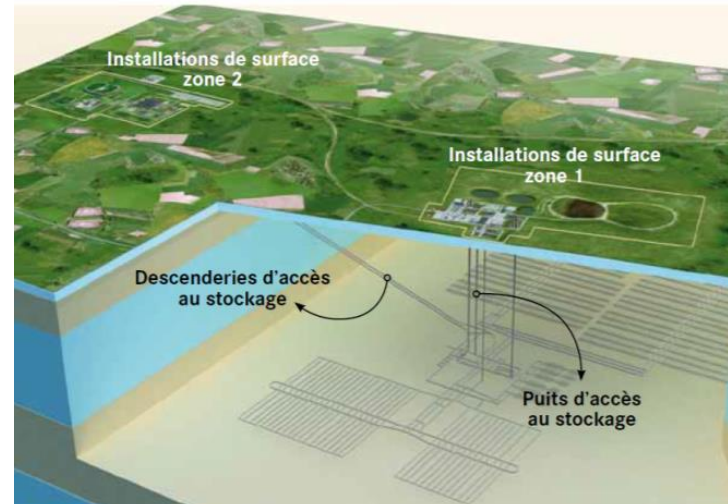
Intermediate  
(long-lived)  
&  
high activity  
wastes



**Deep geological disposal**

Repository in deep geological media with good confining properties

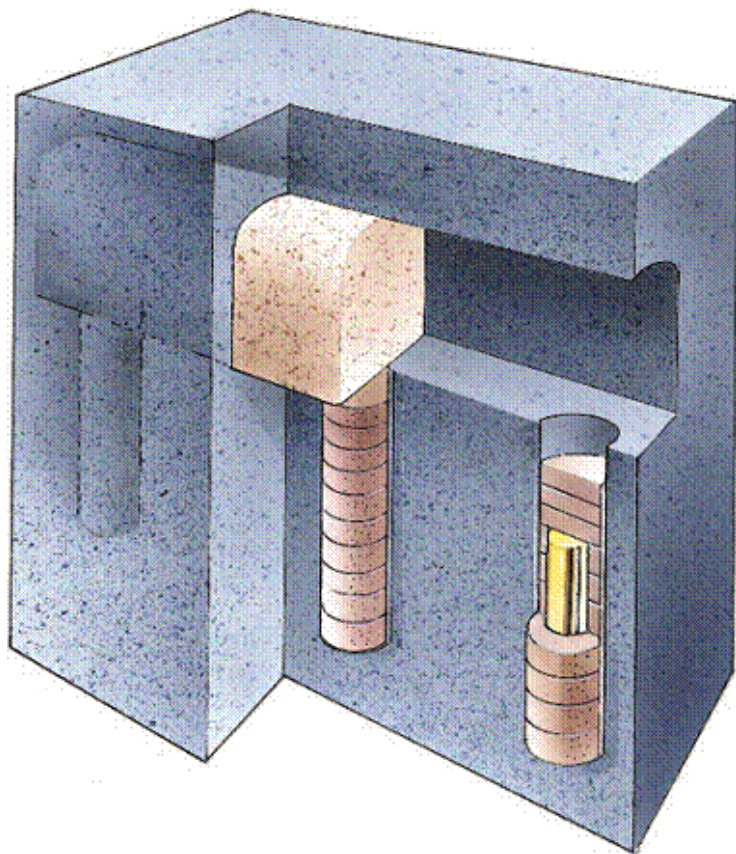
(Low permeability  
 $K < 10^{-12}$  m/s)



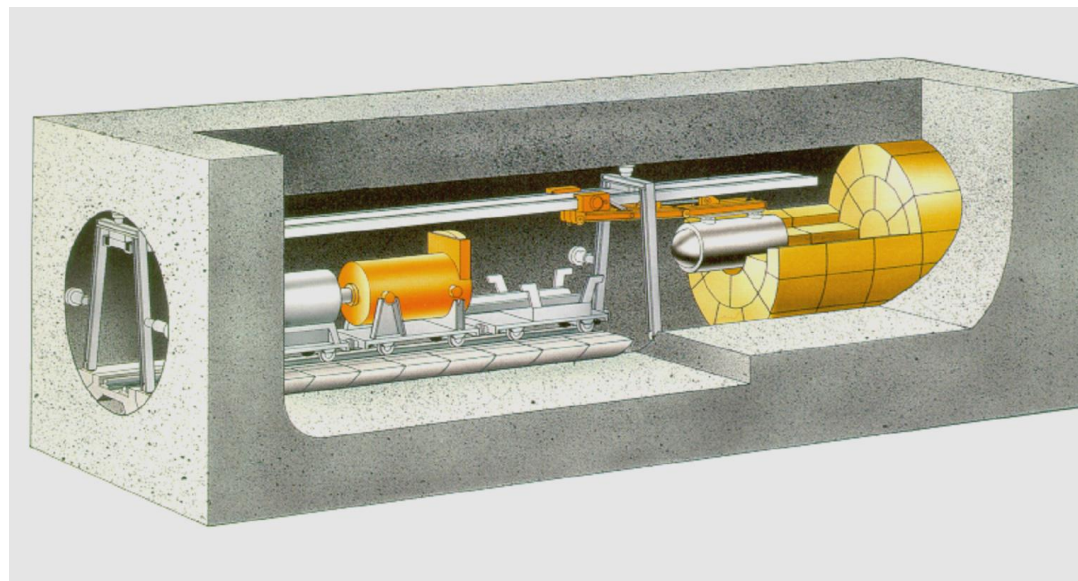
Disposal facility of Cigéo project in France  
(Labalette et al., 2013)



# INTRODUCTION



Disposal in vertical shaft



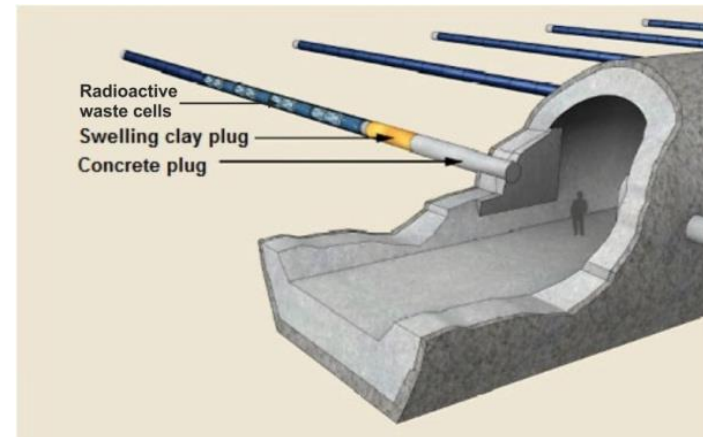
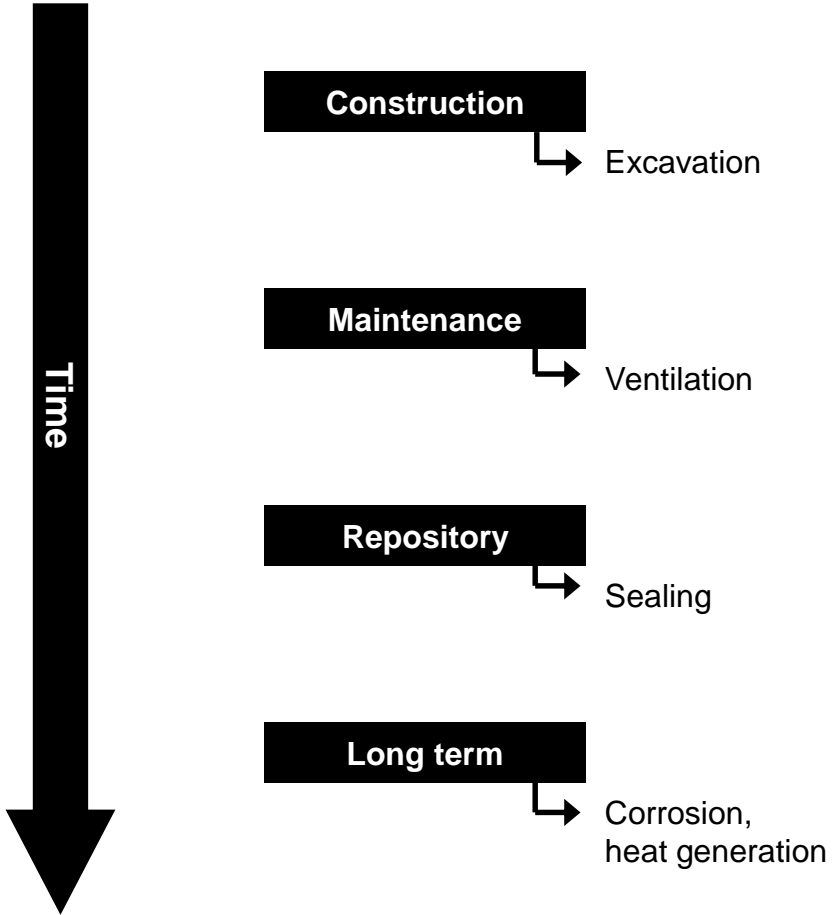
Disposal in horizontal gallery





# INTRODUCTION

## Repository phases

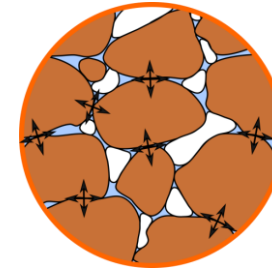
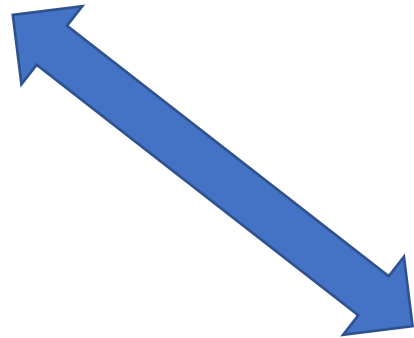
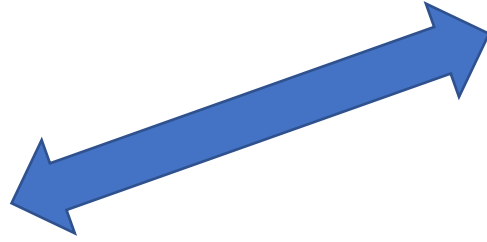


Type C wastes (Andra, 2005)

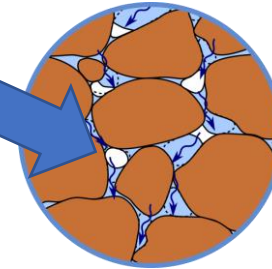




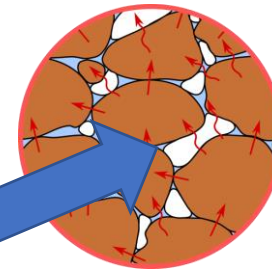
# INTRODUCTION



Mechanics



Water and gas flows



Heat transfer



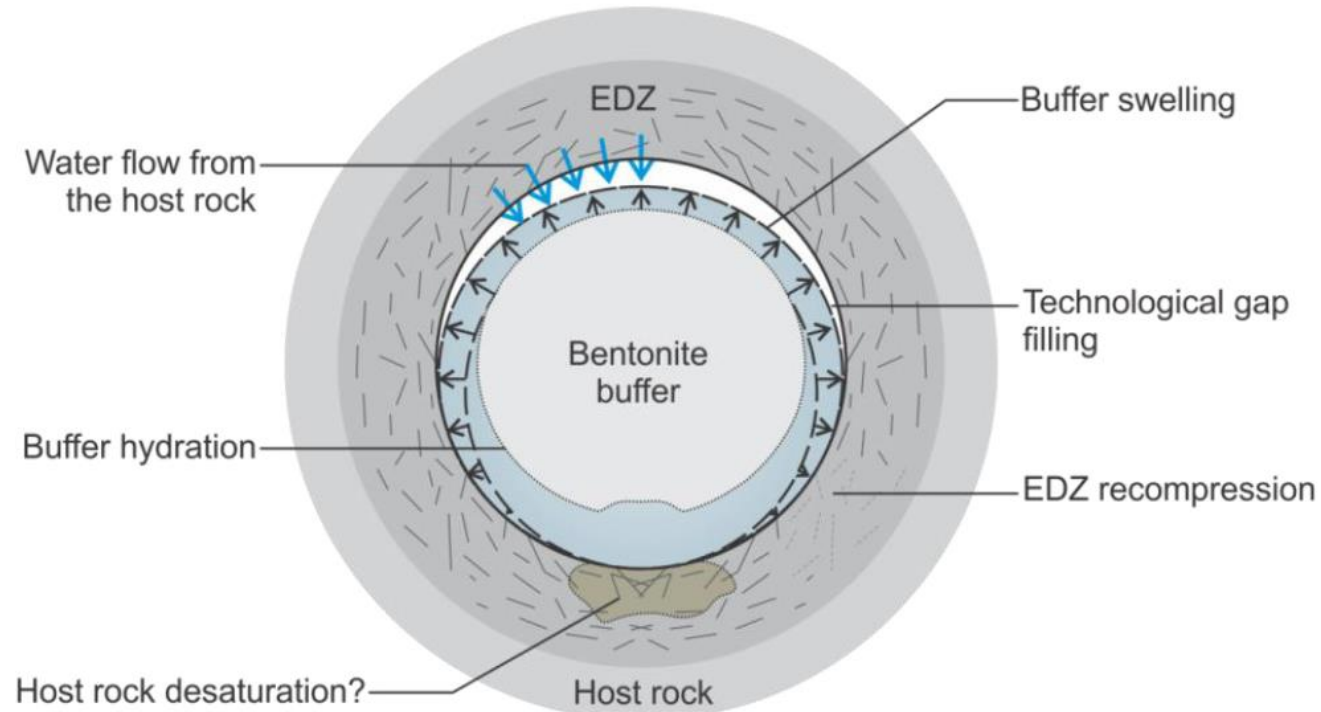
no reaction

In the following, we will not address the bio-chemo processes although there are of importance.



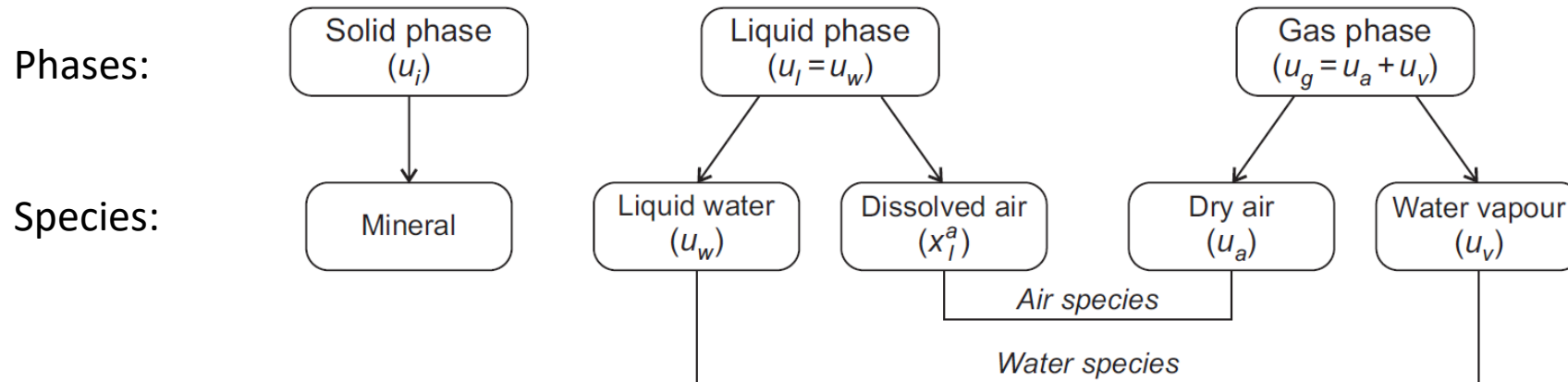
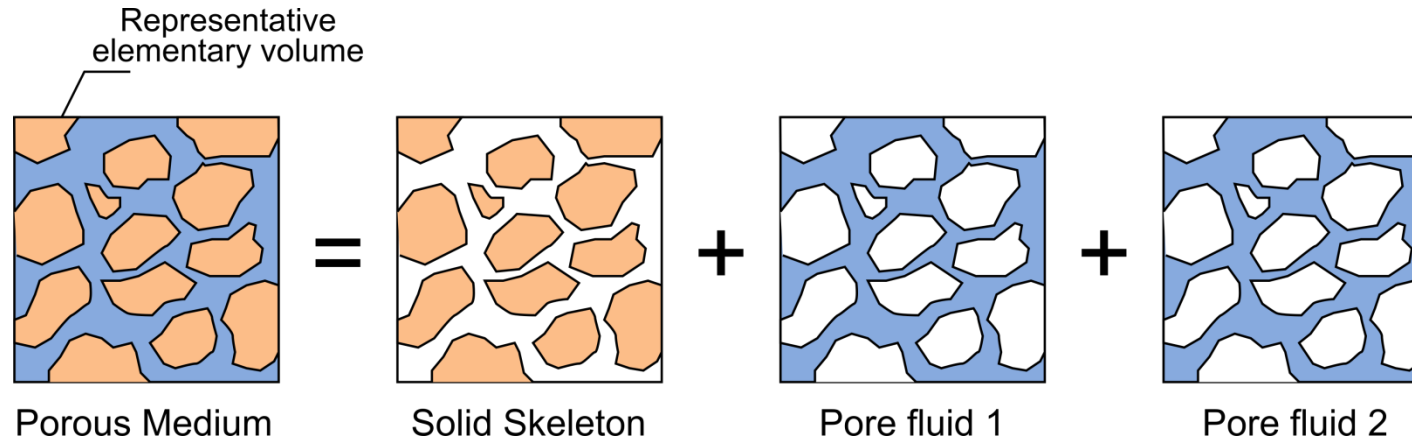
# INTRODUCTION

The material involved in the processes are Saturated/Unsaturated porous media



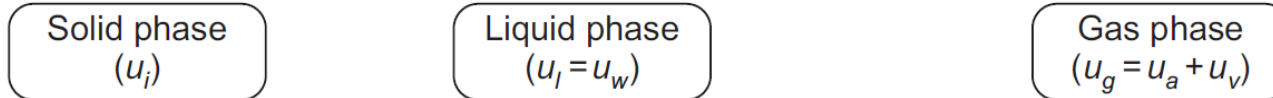
# INTRODUCTION

The material involved in the processes are Saturated/Unsaturated porous media



# INTRODUCTION

The material involved in the processes are Saturated/Unsaturated porous media



Volume fraction:

$$1 - \phi$$

$$S_r \cdot \phi$$

$$(1 - S_r) \cdot \phi$$

Porosity:

$$\phi = \frac{\Omega_v}{\Omega} = \frac{\Omega_l + \Omega_g}{\Omega}$$

Saturation:

$$S_r = \frac{\Omega_l}{\Omega_v}$$

$\Omega_v$  Porous volume

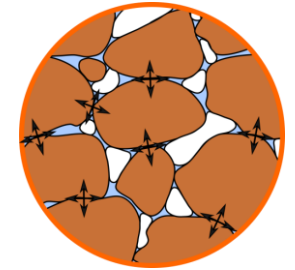
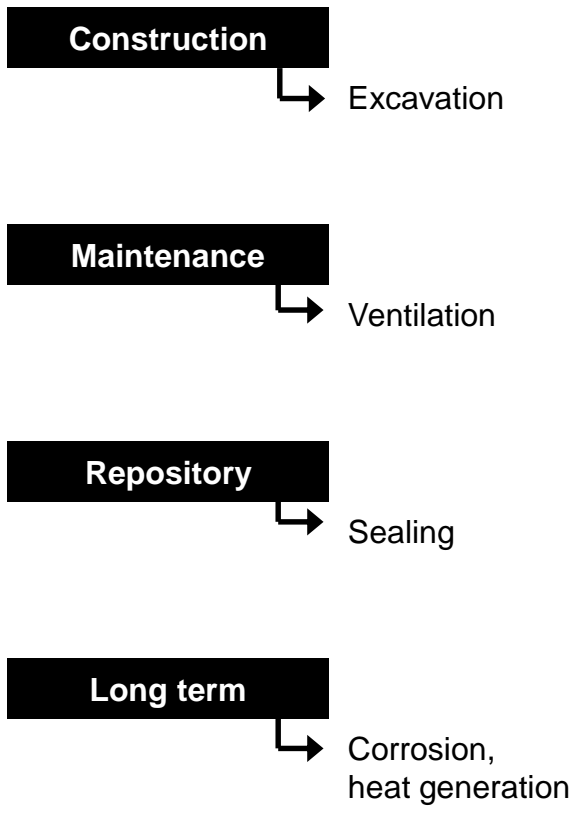
$\Omega_l$  Liquid phase volume

$\Omega_g$  Gas phase volume

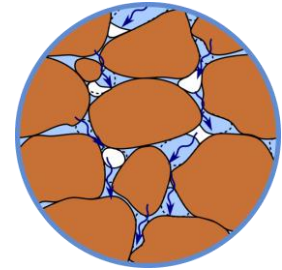


# INTRODUCTION

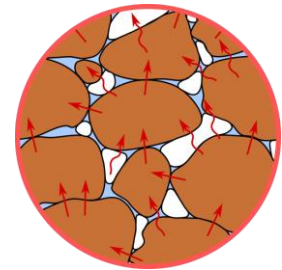
## Repository phases



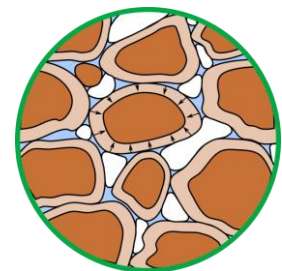
Mechanics



Water and gas flows



Heat transfer



Bio-chemo reaction





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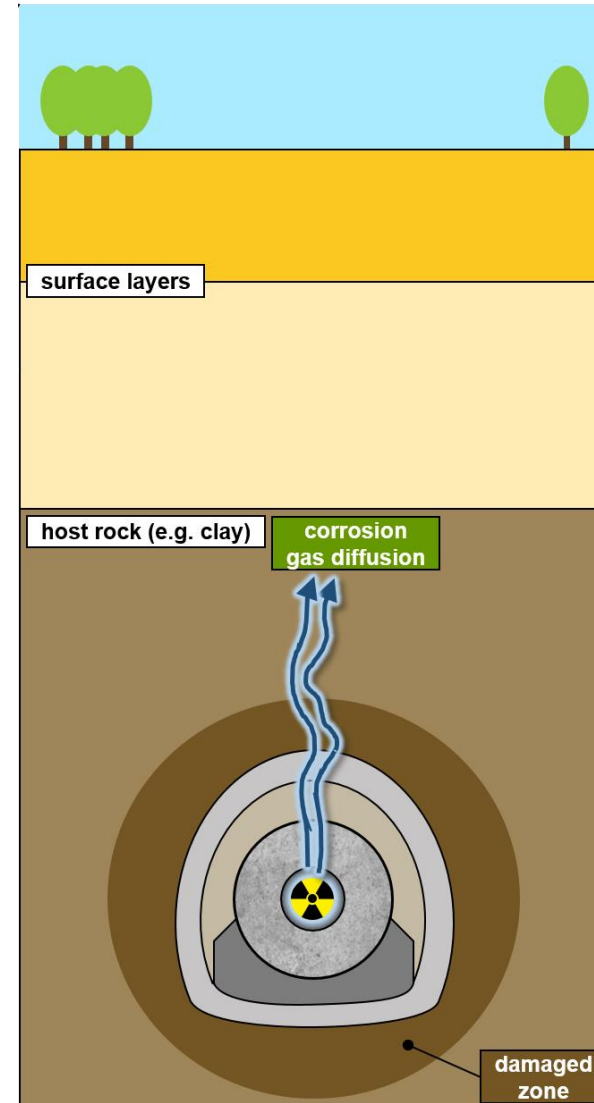


## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

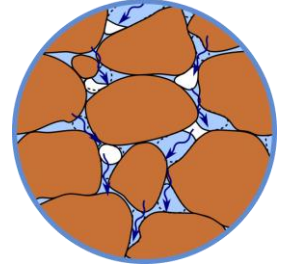
In the sound host rock, the medium remains saturated (most of the time) and the three main processes are heat transfer, liquid transport and mechanical behaviour.

We will focus first on the coupled thermo-hydraulic processes:

- Physical phenomena
- Constitutive equations
- Balance equations



## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



**Advection flow of the liquid phase: Darcy's law**

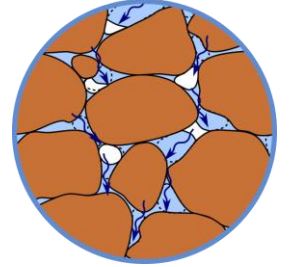
$$\underline{q}_l = - \frac{\underline{K}_{int}^{sat}}{\mu_w} \left[ \underline{\text{grad}}(p_w) + g \rho_w \underline{\text{grad}}(z) \right]$$

where

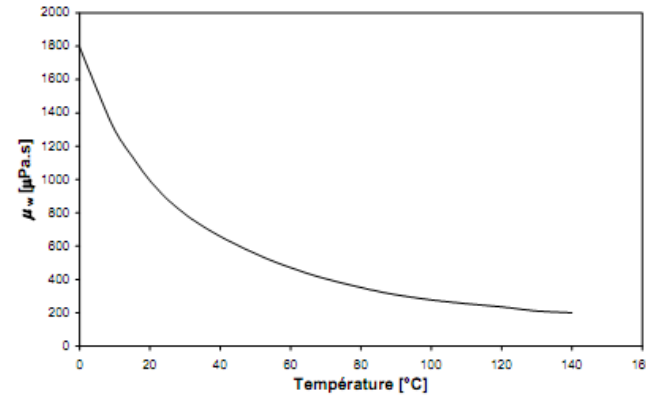
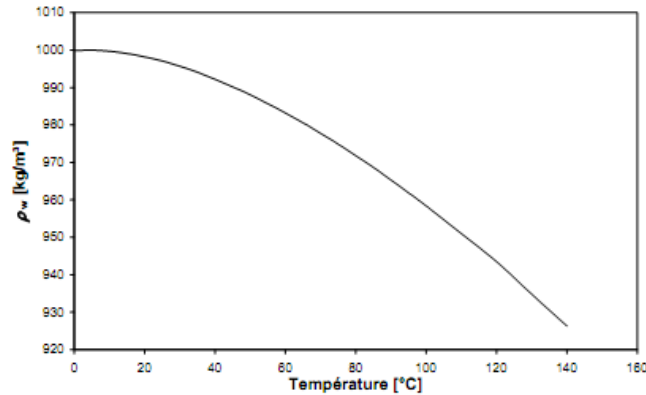
- $\underline{K}_{int}^{sat}$  [m<sup>2</sup>] is the intrinsic permeability
- $\mu_w$  [Pa.s] is the water dynamic viscosity
- $p_w$  [Pa] is the pore water pressure
- $\rho_w$  [kg/m<sup>3</sup>] is the liquid water density



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



## Water properties



The water dynamic viscosity  $\mu_w$  [Pa.s] and the liquid water density  $\rho_w$  [kg/m<sup>3</sup>] (related to the thermal dilation coefficient) are a function of the temperature.

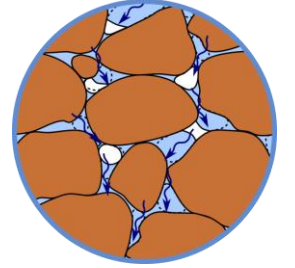
$$\alpha_w = 1/\rho_w \frac{\partial \rho_w}{\partial T}$$

$$\alpha_w [10^{-4} 1/^\circ\text{C}] = 4\text{E-}06 T^3 - 0,001 T^2 + 0,1404T - 0,3795 \text{ [Kell,1975]}$$

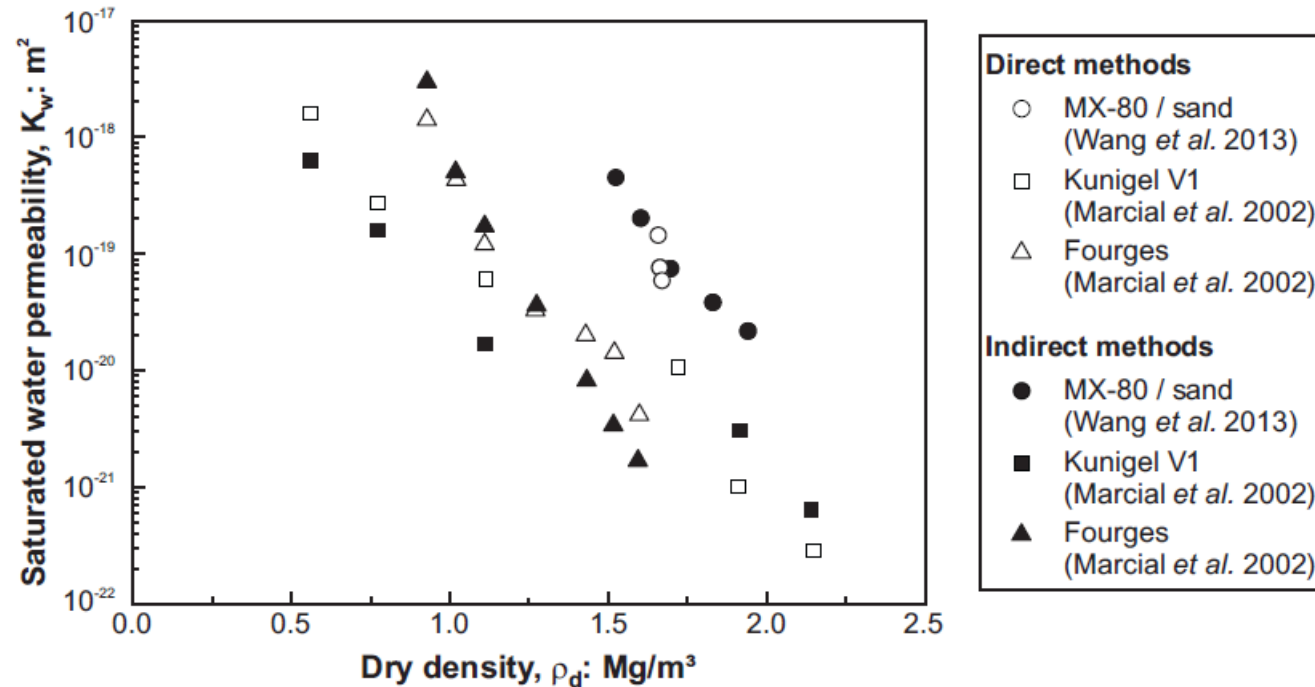
$$\mu = e^{A + \frac{B}{c+T}} \text{ [Rumble, 2019]}$$



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



## Water properties



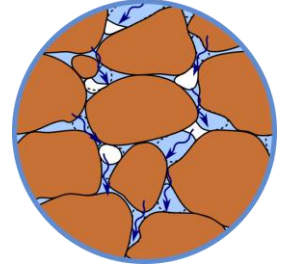
The intrinsic permeability [m<sup>2</sup>] depends on the density.

Kozeny-Carman law:

$$K_w = K_{w0} \frac{\phi^N}{(1 - \phi)^M} \frac{(1 - \phi_0)^M}{\phi_0^N}$$



## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



Storage of the liquid phase per unit volume:

$$S_w = \rho_w \cdot n$$

The influence of the temperature on the density explains the thermal pressurization mechanism in undrained conditions:

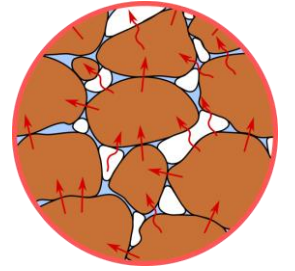
$$dp = \Pi d\sigma + \Lambda dT \quad [\text{Minh. 2020}]$$

Isotropic case

$$\left\{ \begin{array}{l} \Pi = \frac{-\frac{b}{K}}{\frac{b^2}{K} + \frac{b-\phi}{K_s} + \frac{\phi}{K_w}} \\ \Lambda = \frac{3\phi(\alpha_l - \alpha)}{\frac{b^2}{K} + \frac{b-\phi}{K_s} + \frac{\phi}{K_w}} \end{array} \right.$$



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



## Modes of heat transfer

- *Conduction*

Heat transfer by direct contact of particles

- *Advection*

Heat transfer by mass movement

The term convection is used when the mass movement is driven by buoyancy (density differences) caused by the thermal field

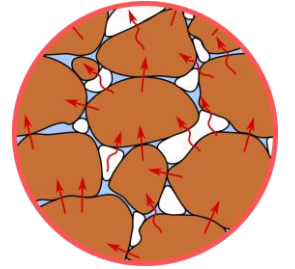
- *Radiation*

Heat transfer by electromagnetic waves





## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



### Modes of heat transfer

- *Conduction : Fourier's law*

$$i_{cond} = -\Gamma_m \cdot \underline{grad}(T)$$

$\Gamma_m$  is the thermal conductivity of the medium. It depends on the thermal conductivity of its constituents (solid and liquid phase).

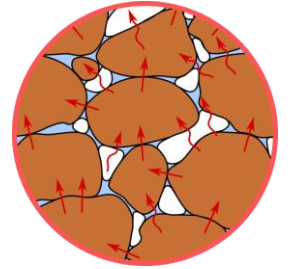
Serial constituents (S + L):  $1/\Gamma_m = 1/\Gamma_s(1 - n) + 1/\Gamma_w n$

Constituents in parallel (S+L):  $\Gamma_m = \Gamma_s(1 - n) + \Gamma_w n$

Geometric mean (S+L):  $\Gamma_m = \Gamma_s^{(1-n)} + \Gamma_w^n$



## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



### Modes of heat transfer

- *Internal energy per unit volume*

$$\rho_m c_{p,m} (T - T_0)$$

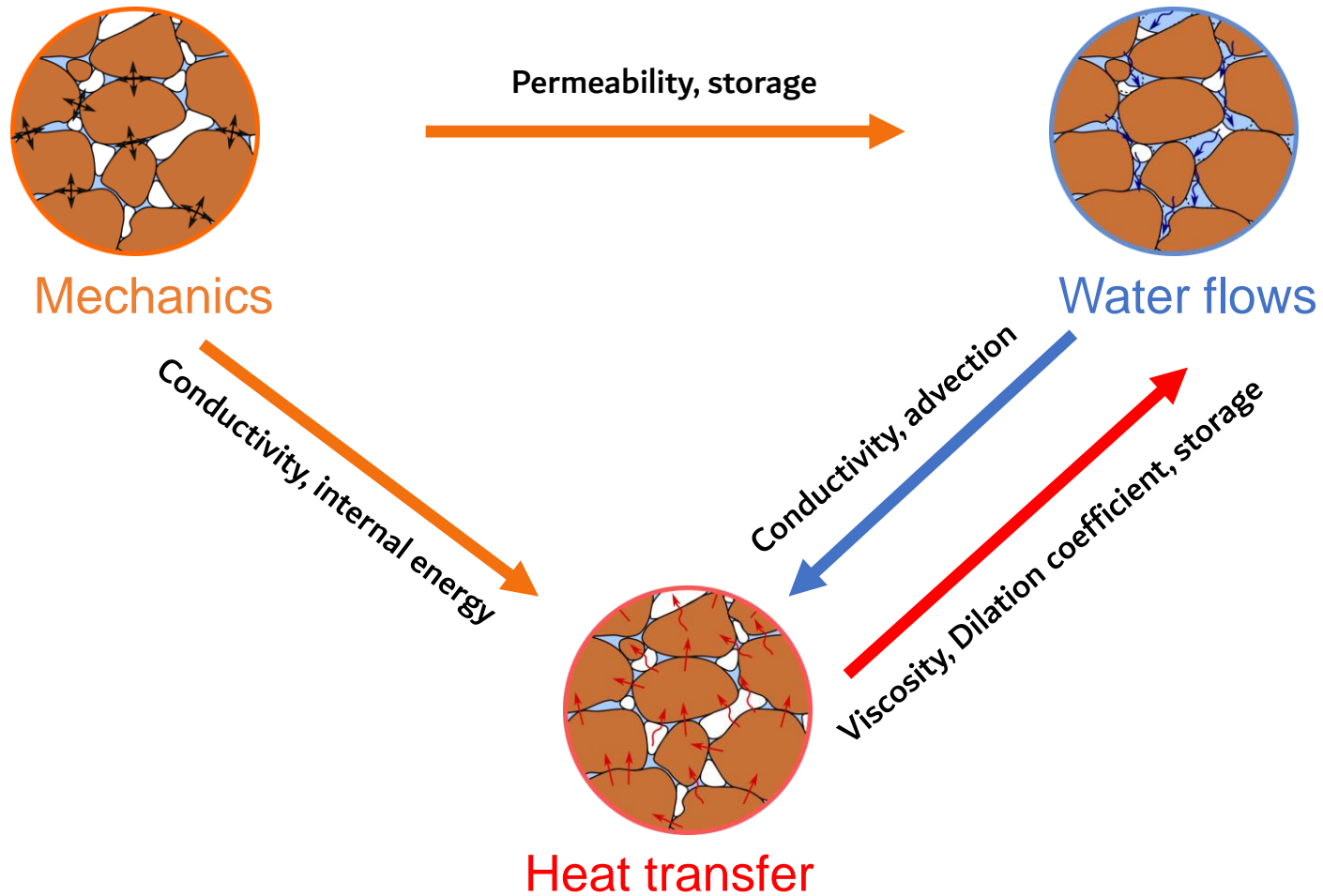
where  $\rho_m$  is the density of the medium,  $c_{p,m}$  is the heat capacity of the medium (under constant pressure).

In order to evidence the influence of each constituent, an additive formulation is also used:

$$\rho_s c_{p,s} (1 - n) (T - T_0) + \rho_w c_{p,w} n (T - T_0)$$



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)



## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

### Balance equations

- Water mass balance

$$\frac{\partial}{\partial t} (\rho_w n) + \operatorname{div}(\underline{f}_w) - Q_w = 0 \quad \underline{f}_w = \rho_w \underline{q}_l$$

- Internal energy balance

$$\frac{\partial S_T}{\partial t} + \operatorname{div}(\underline{V}_T) - Q_T = 0$$

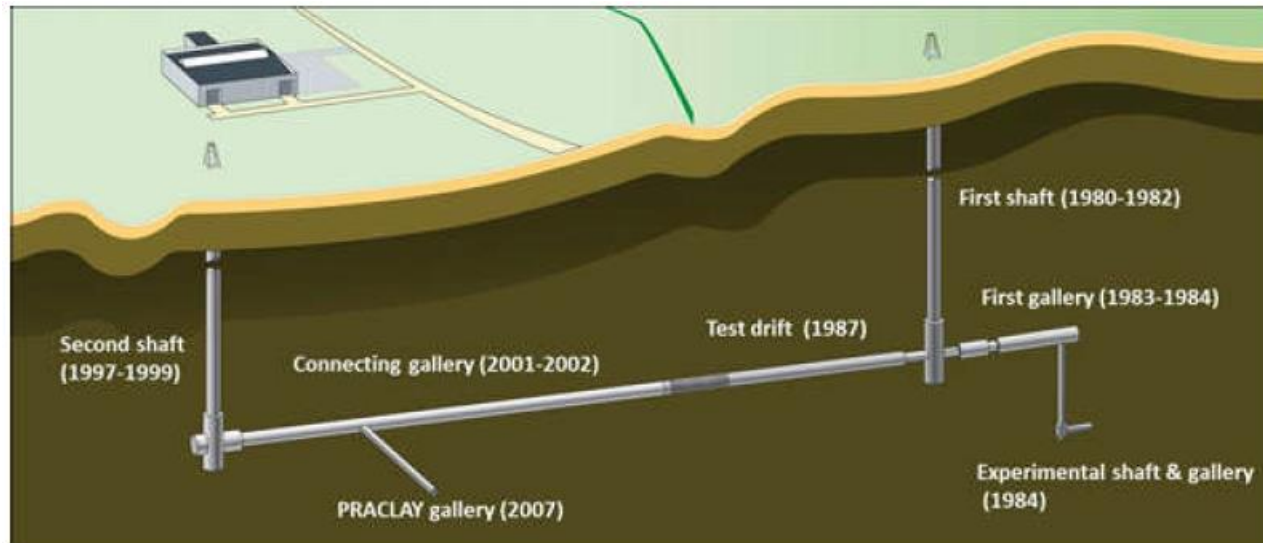
$$S_T = n \rho_w c_{pw} (T - T_0) + (1 - n) \rho_s c_{ps} (T - T_0)$$

$$\underline{V}_T = -\Gamma \nabla T + c_{pw} \rho_w \underline{q}_l (T - T_0)$$

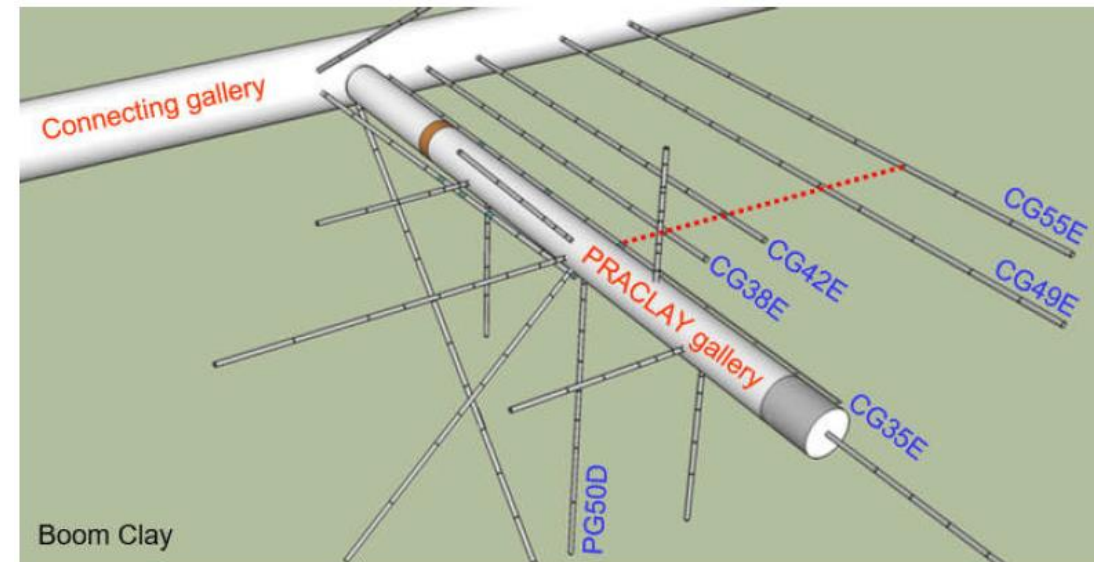


# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

## Praclay heater test in Mol



Layout of the underground laboratory at Mol, Belgium (EURIDICE website, 2018)

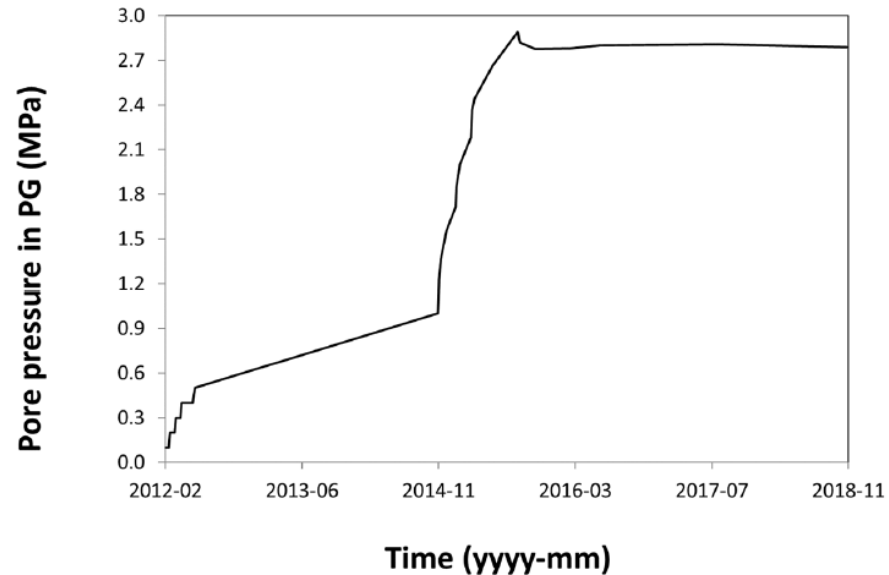
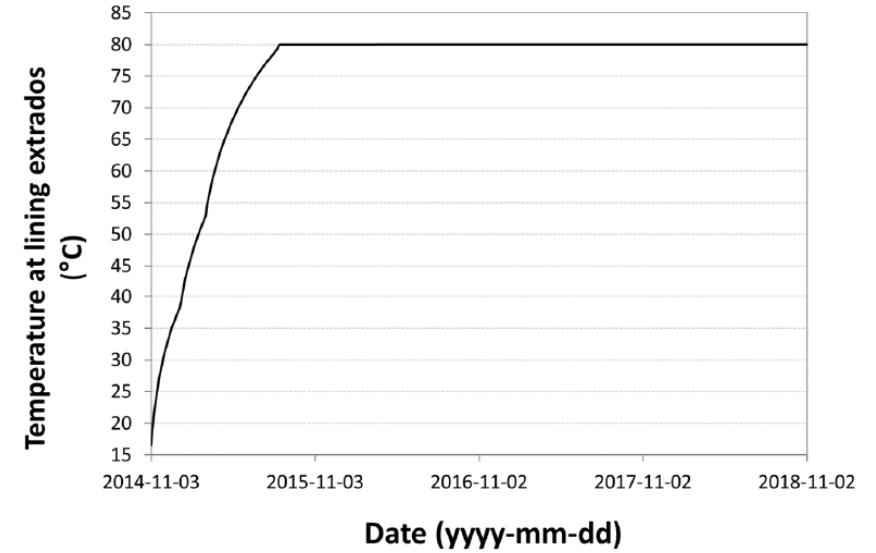
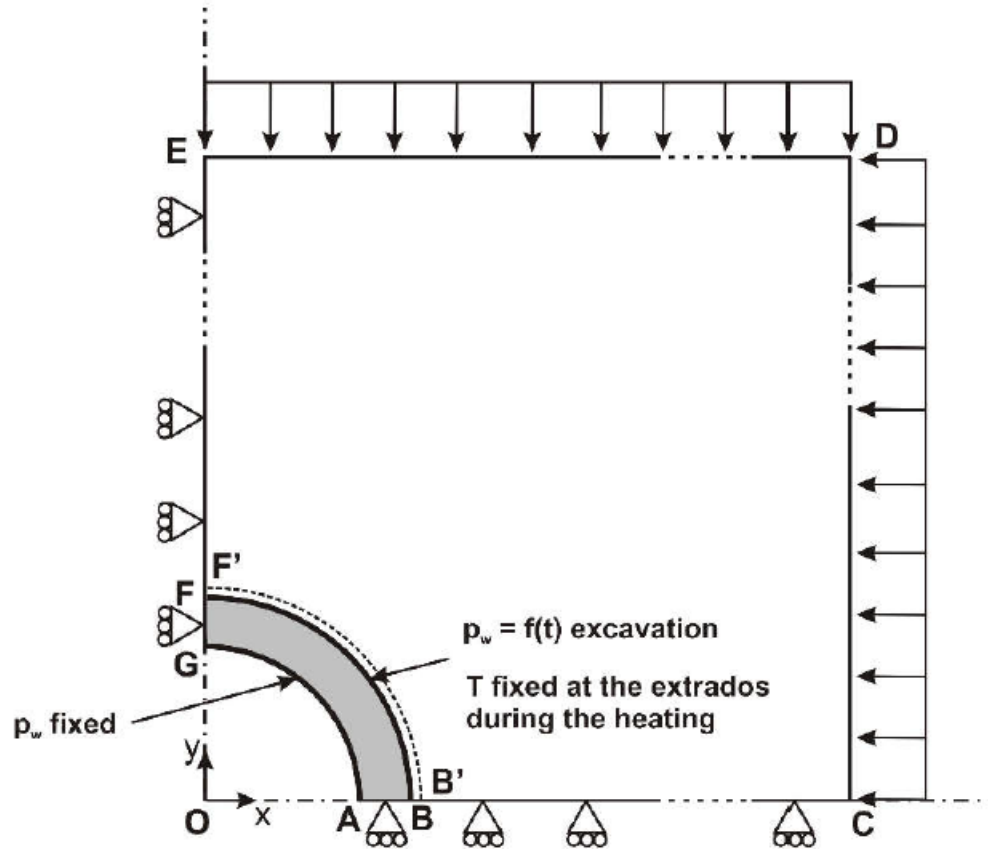


Layout of the monitoring boreholes around the PRACLAY gallery



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

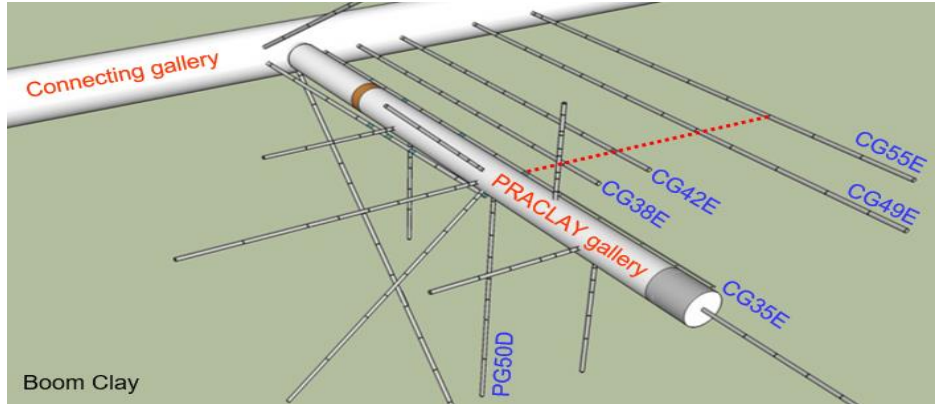
Benchmark exercise (EURAD-HITEC WP – Task 2.3)





# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

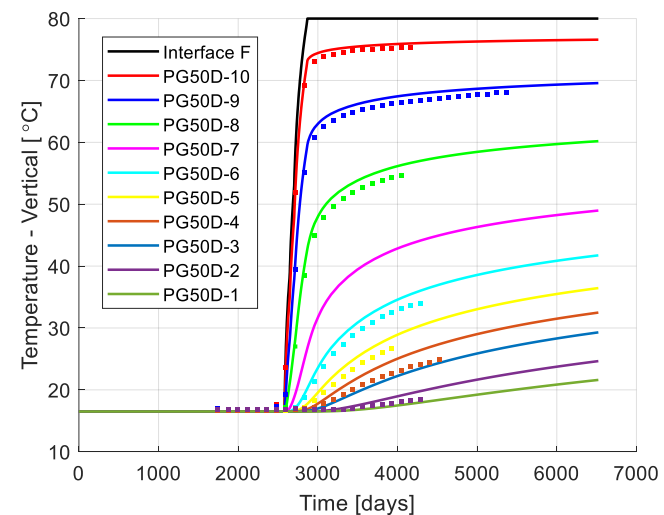
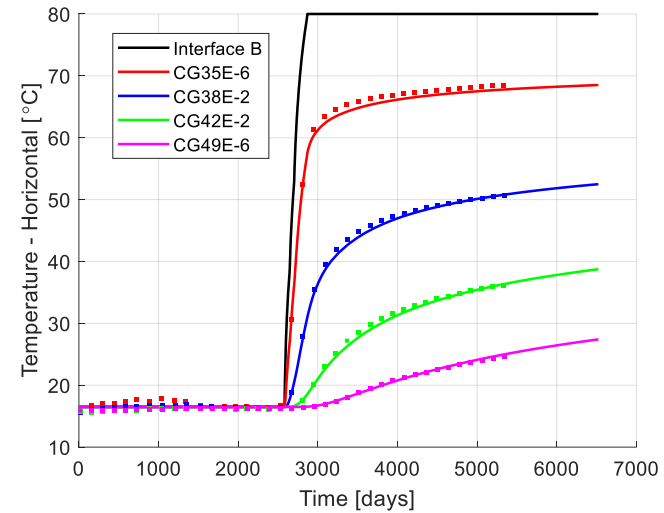
Monitoring boreholes around the PRACLAY gallery



Main physical, thermo-hydraulic parameters for the Boom Clay

Material parameters		Boom Clay
Solid phase density [kg/m <sup>3</sup> ]	$\rho_s$	2639
Porosity [-]	$n$	0.39
Vertical intrinsic permeability [m <sup>2</sup> ]	$k_v$	$2E^{-19}$
Horizontal intrinsic permeability [m <sup>2</sup> ]	$k_h$	$4E^{-19}$
Vertical thermal conductivity [W/mK]	$\lambda_v$	1.31
Horizontal thermal conductivity [W/mK]	$\lambda_h$	1.65
Linear thermal expansion coefficient [°C <sup>-1</sup> ]	$\alpha_s$	$1E^{-5}$
Solid phase specific heat [J/(kg.K)]	$C_p$	769
Young's modulus parallel to bedding [MPa]	$E_{  }$	400
Young's modulus normal to bedding [MPa]	$E_{\perp}$	200
Poisson's ratio parallel to bedding [-]	$\nu_{    }$	0.25
Poisson's ratio normal to bedding [-]	$\nu_{  \perp}$	0.25
Shear modulus normal to bedding [MPa]	$G_{\perp}$	80

Evolution of temperature



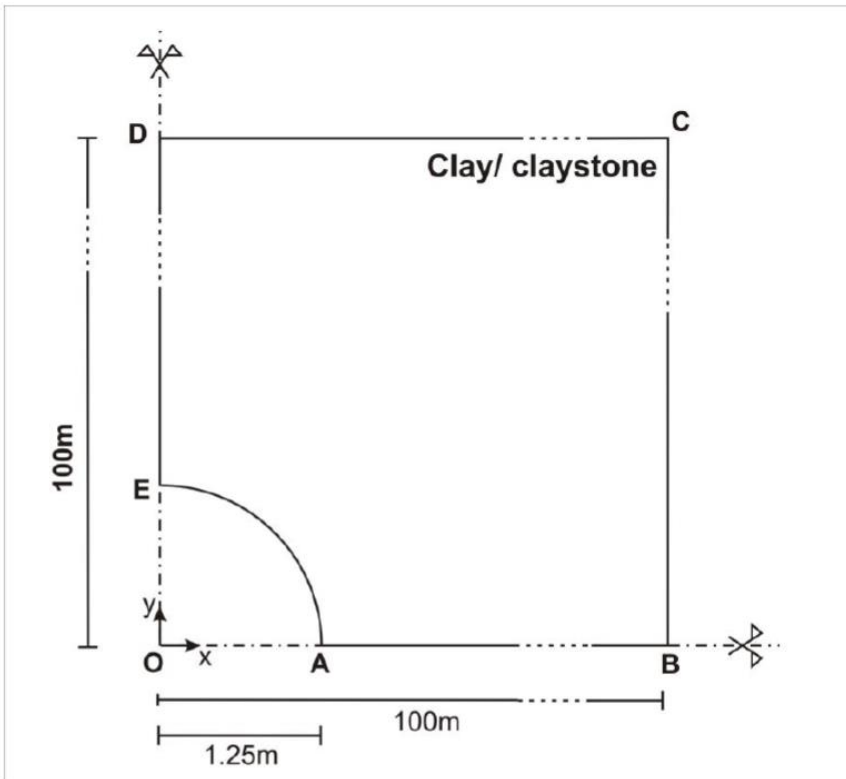
## Conclusions:

- Anisotropy of the thermal conductivity
- Negligible influence of the water advection



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

## Benchmark exercise: Near field case (EURAD-HITEC WP – Task 2.3)

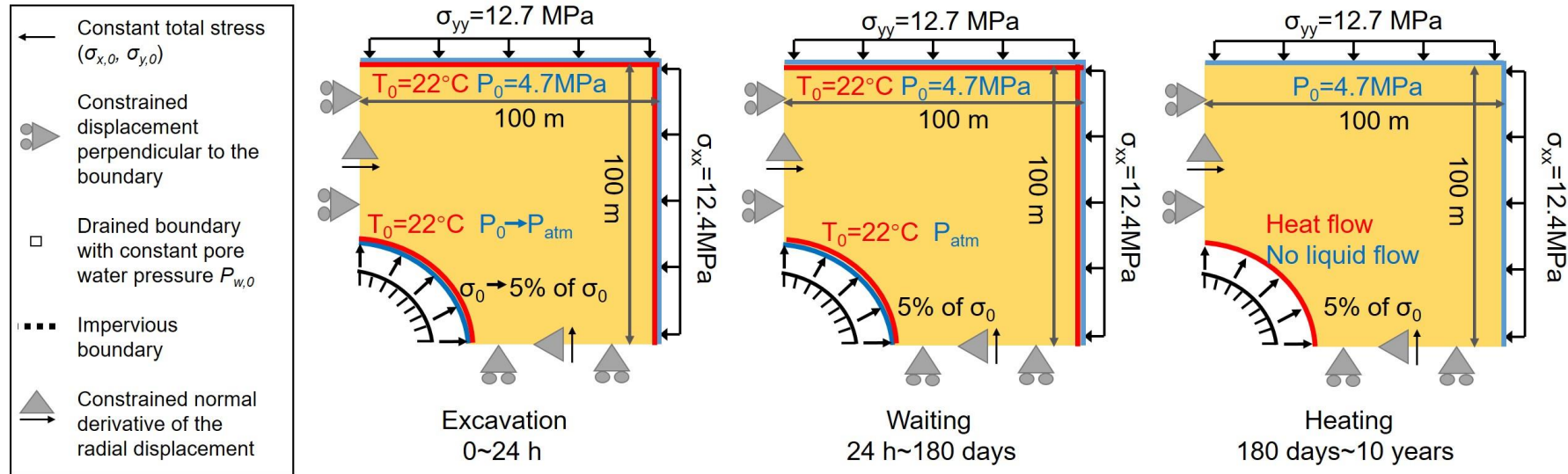


		<b>Boom Clay</b>	<b>COx</b>	<b>OPA</b>
Solid phase density [kg/m <sup>3</sup> ]	$\rho_s$	2639	2690	2340
Bulk density [kg/m <sup>3</sup> ]	$\rho'$	2000	2450	2030
Porosity	$n$	0.39	0.18	0.13
Isotropic intrinsic permeability [m <sup>2</sup> ]	$K$	$2.83E^{-19}$	$2.3E^{-20}$	$3.0E^{-20}$
Isotropic Young's modulus [MPa]	$E$	300	7000	6000
Poisson's ratio [-]	$\nu$	0.125	0.3	0.3
Isotropic thermal conductivity [W/m/K]	$\lambda$	1.47	1.67	1.85
Linear thermal expansion coefficient [°C <sup>-1</sup> ]	$\alpha_s$	$1E^{-5}$	$1.25E^{-5}$	$1.7E^{-5}$
Solid phase specific heat [J/kg/K]	$c_p$	769	978	995



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

## Benchmark exercise: Near field case (EURAD-HITEC WP – Task 2.3)



Period	Mechanical conditions	Hydraulic conditions	Thermal conditions
$T_0 - T_0 + 24$ hours : excavation	Stress reduction to 5% of the initial in-situ stress	Pore pressure reduced to $P_{atm}$ (0.1 MPa)	No flow at the borehole wall
$T_0 + 24$ hours - $T_0 + 6$ months : waiting	As above	PP = $P_{atm}$	As above
$T_0 + 6$ months - $T_0 + 10$ years : heating	As above	No flow	Thermal flow outside the lining (200 W/m)



## THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

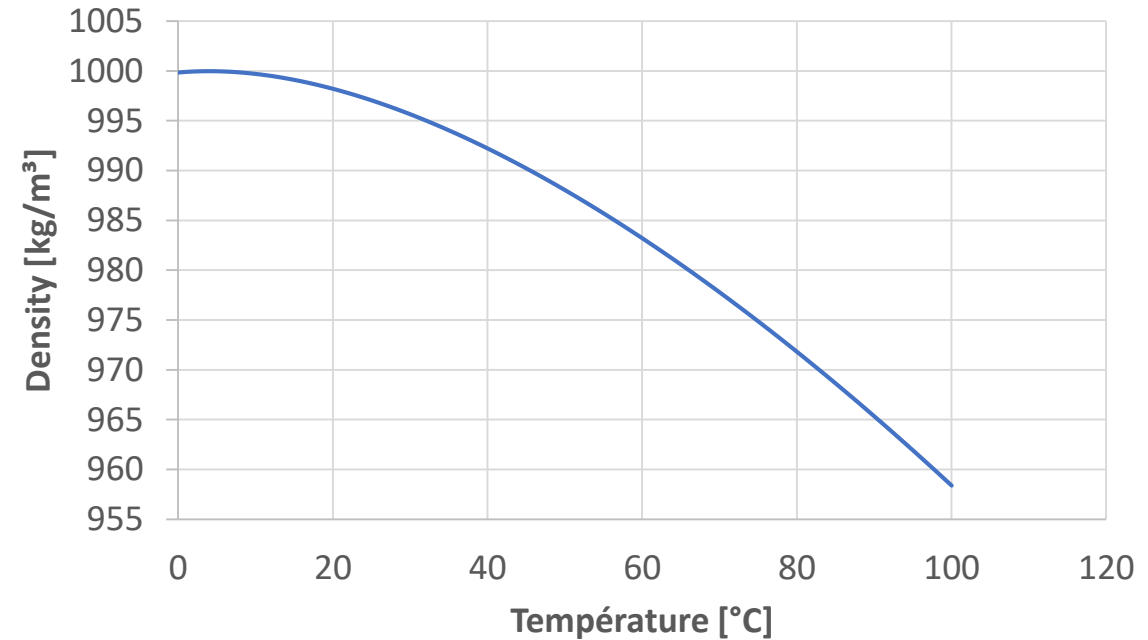
From experimental values of the density (Kell, 1975), the dilation coefficient is computed as:

$$\alpha_w = 1/\rho_w \frac{\partial \rho_w}{\partial T}$$

$$\alpha_w [10^{-4} 1/^\circ\text{C}] = 4\text{E-}06 T^3 - 0,001 T^2 + 0,1404T - 0,3795 \quad [\text{Kell}, 1975]$$

$$\mu = e^{A + \frac{B}{c+T}} \quad [\text{Rumble}, 2019]$$

Temperature evolution of water density (Kell, 1975)



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

## CO<sub>x</sub> in isotropic elasticity

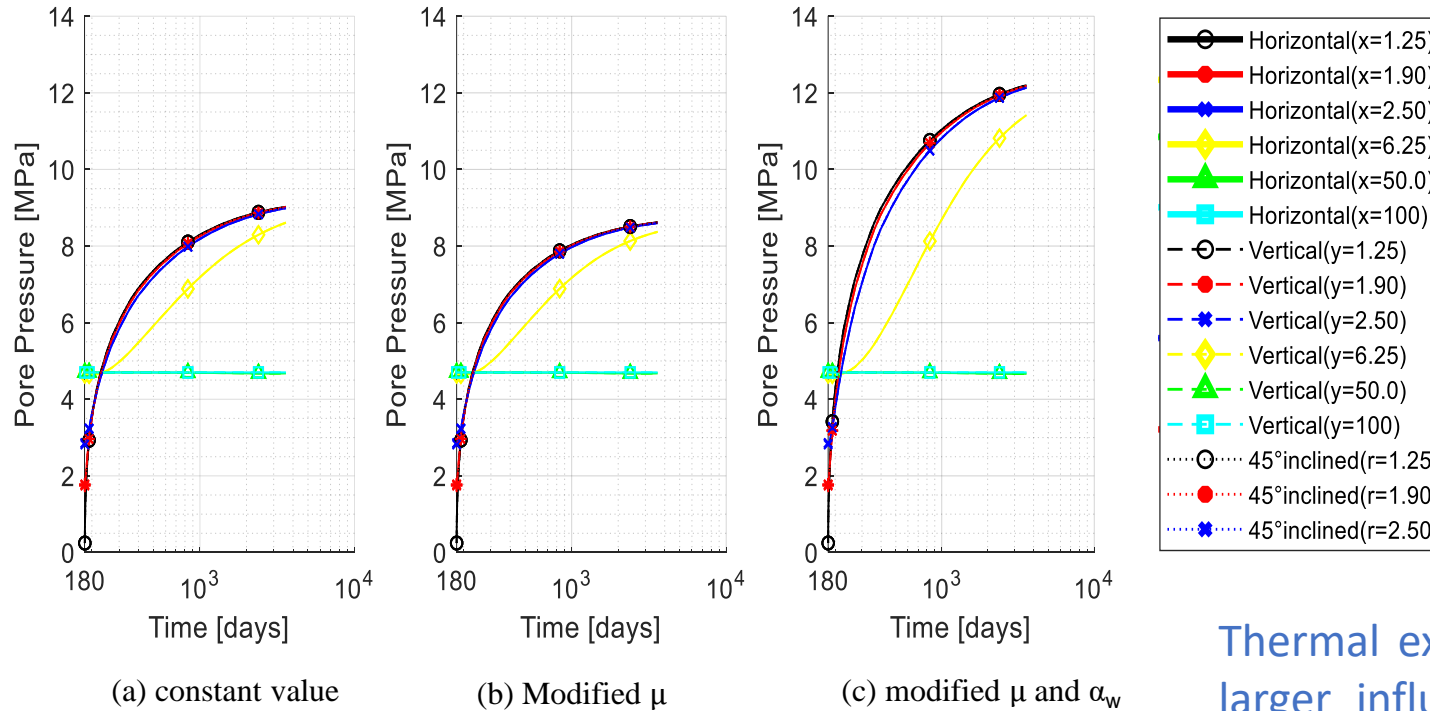


Figure: Pore pressure at heating

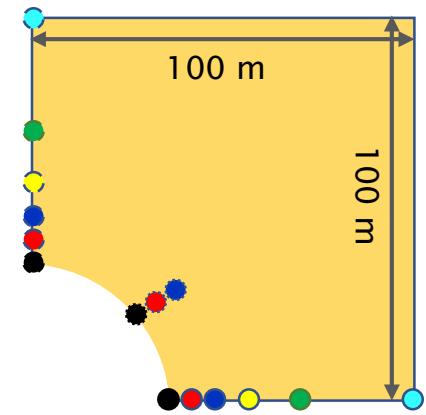


Figure: Schematic distribution of the output nodes

Thermal expansion coefficient of water has larger influence on the evolution of pore pressure, displacement, etc. than its viscosity.





# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

Boom clay in isotropic elasticity

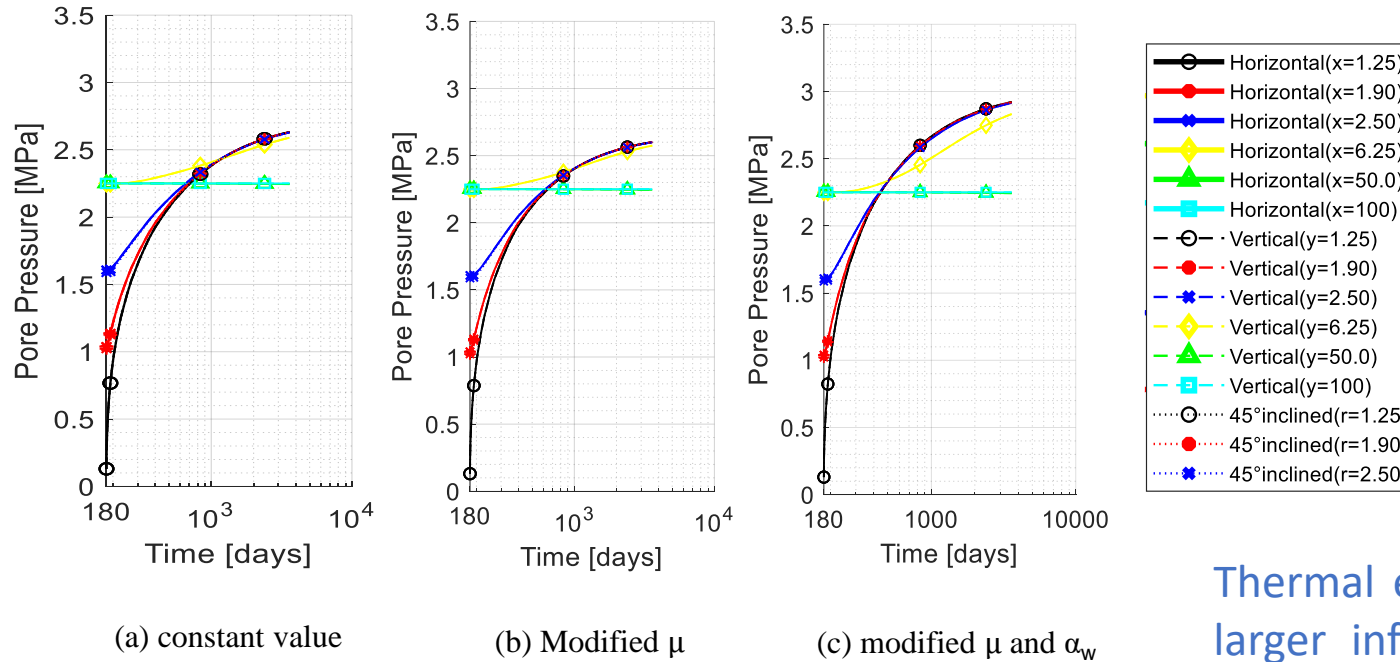


Figure: Pore pressure at heating

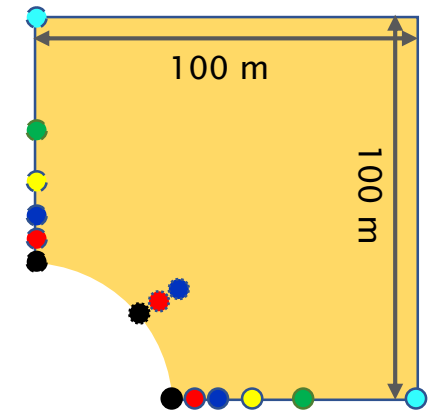


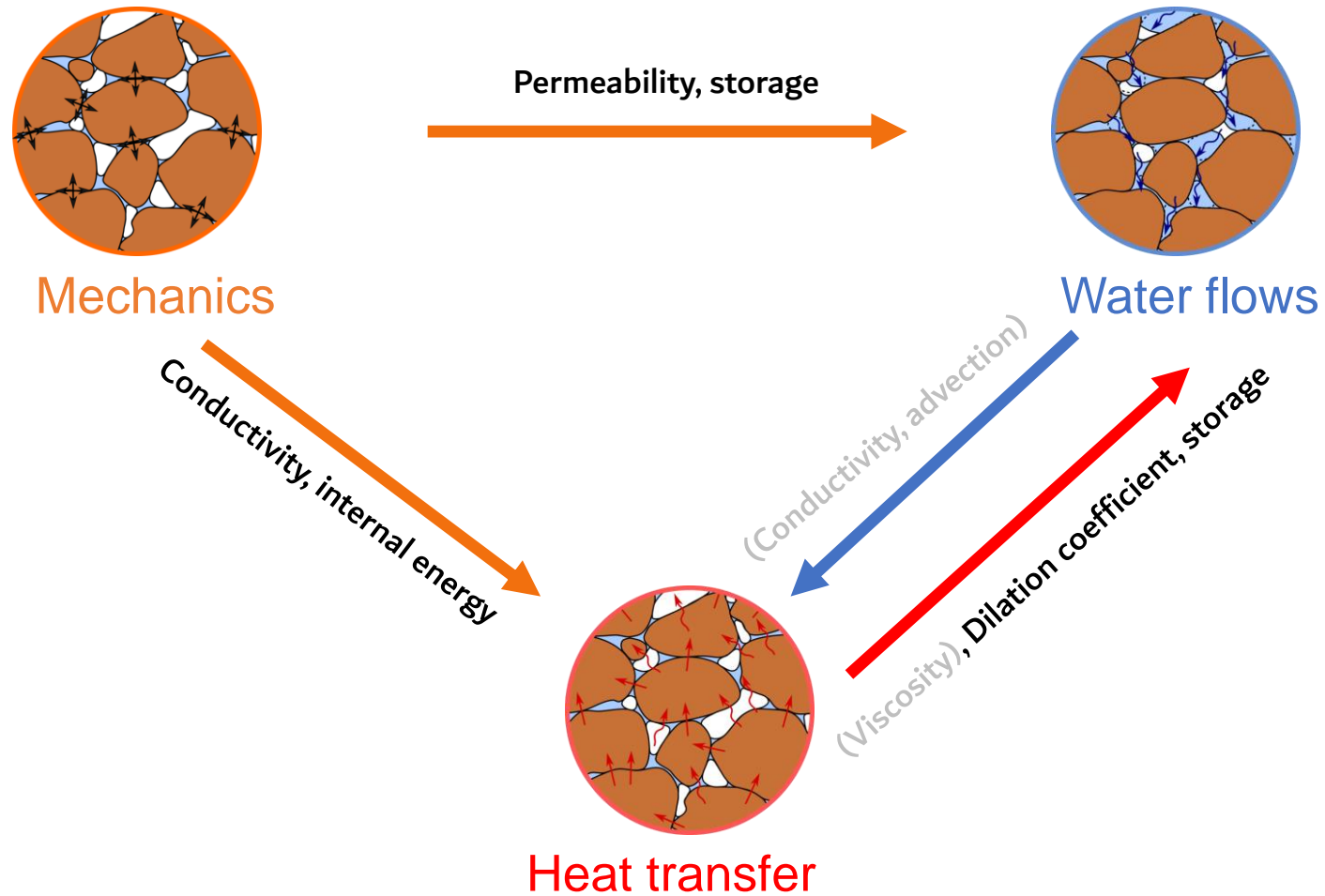
Figure: Schematic distribution of the output nodes

Thermal expansion coefficient of water has larger influence on the evolution of pore pressure, displacement, etc. than its viscosity.



# THERMO-HYDRAULIC PROCESSES (SATURATED CONDITIONS)

**Conclusion :**





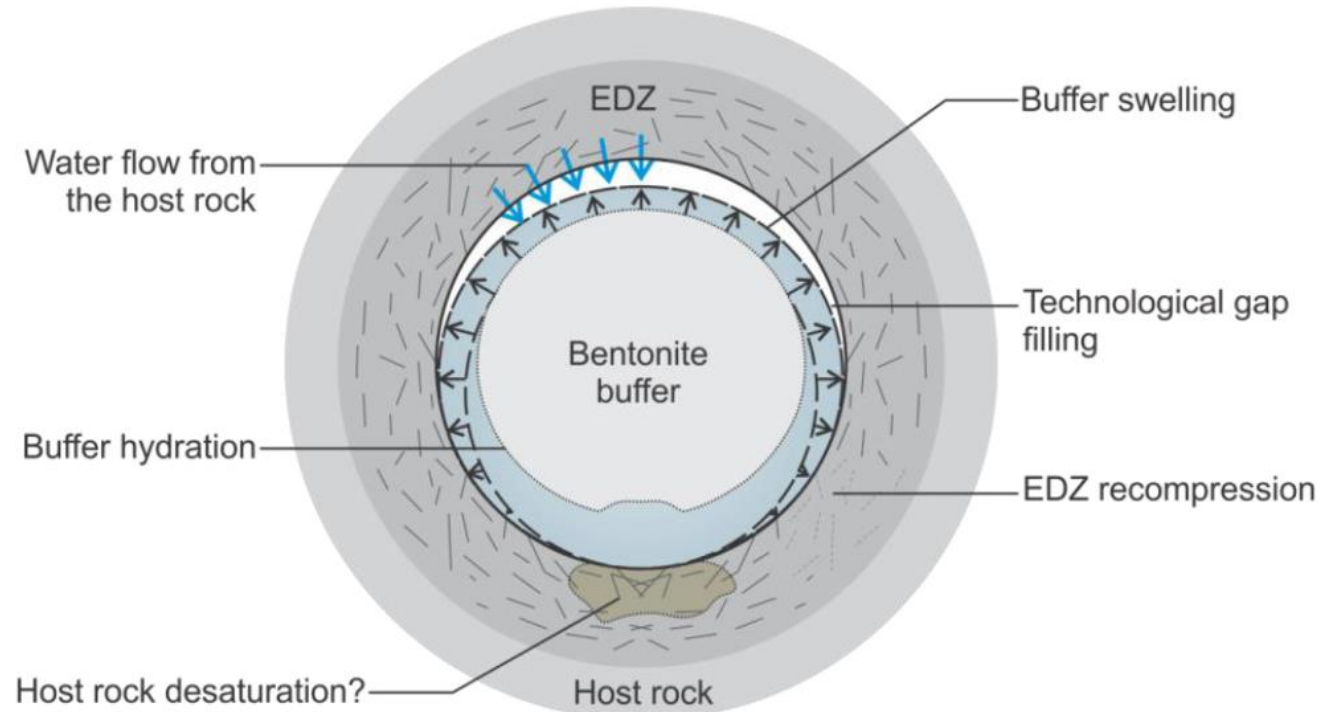
## TABLE OF CONTENT

1. WELCOME
2. INTRODUCTION
3. THERMO-HYDRAULIC PROCESSES (saturated conditions)
- 4. UNSATURATED FLOW PROCESSES**
5. THMG PROCESSES



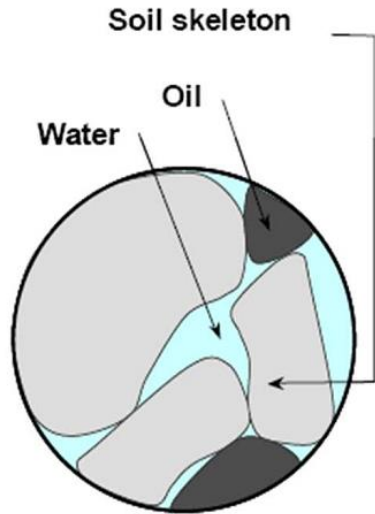
# UNSATURATED FLOW PROCESSES

The material involved in the processes are Saturated/Unsaturated porous media



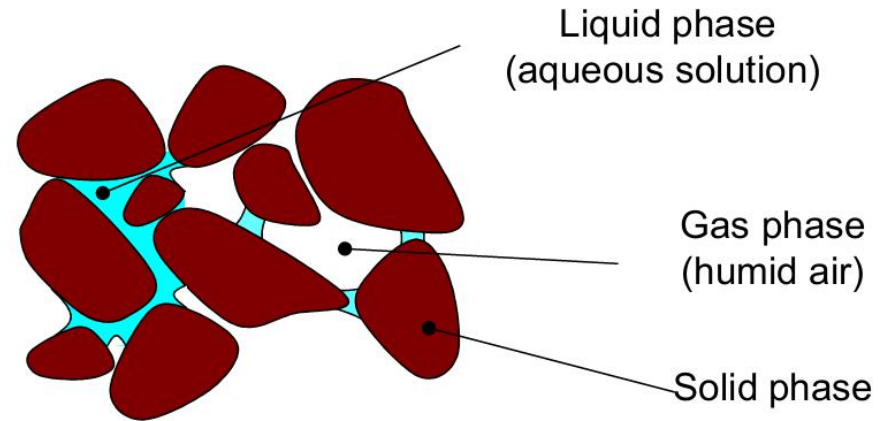
# UNSATURATED FLOW PROCESSES

## Granular materials

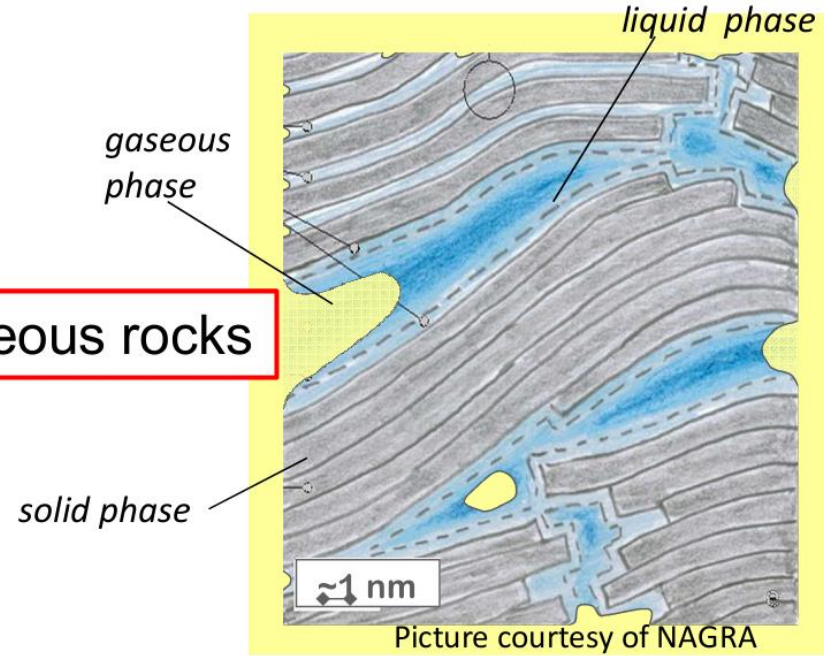


(Hydrocarbon-polluted soils, petroleum extraction)

(Priol et al. 2004)



## Argillaceous rocks





## UNSATURATED FLOW PROCESSES

### WATER POTENTIAL AND CONCEPT OF SUCTION

The total potential of water  $\psi$  is defined as the amount of work (per unit mass of pure Water) required to transport reversibly and isothermally an infinitesimal quantity of water from a reservoir of pure water at a specified elevation and atmospheric pressure to the point under consideration (Aitchison, 1965).

The total potential is often expressed as the sum of four contributions, such that:

$$\psi = \psi_g + \psi_p + \psi_m + \psi_o$$

where  $\psi_g$  is the gravitational potential,  $\psi_p$  the external pressure potential,  $\psi_m$  the matric potential and  $\psi_o$  the osmotic potential. The sum of the matric and osmotic potentials is referred to as the internal potential.





# UNSATURATED FLOW PROCESSES

## WATER POTENTIAL AND CONCEPT OF SUCTION

In soil mechanics, the concept of suction is often used as an alternative to the internal potential. The gravitational and external pressure potentials are indeed not relevant for constitutive modelling of the soil (Gens, 2010). The suction is an energy per unit volume (instead of per unit mass) and is expressed in terms of pressure. The total suction  $s_t$  is defined as:

$$s_t = s + \pi_{osm}$$

$$s = -\rho_w \psi_m$$

$$\pi_{osm} = -\rho_w \psi_o$$

where  $s$  is the matric suction and  $\pi_{osm}$  is the osmotic suction. The matric suction is associated to the interactions between liquid and solid, while the osmotic suction is related to differences in water chemistry.

*The total suction is directly related to relative humidity.*





## UNSATURATED FLOW PROCESSES

### WATER POTENTIAL AND CONCEPT OF SUCTION

The matric suction  $s$  contains two distinct contributions, namely the capillary suction and the adsorption suction (Baker & Frydman, 2009; Frydman, 2012; Blatz et al., 2009; Lu & Likos, 2004).

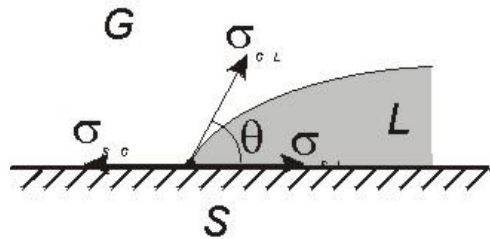
The capillary suction is associated to capillary phenomena, while the adsorption suction results from electrochemical interactions between the water and the clay minerals.



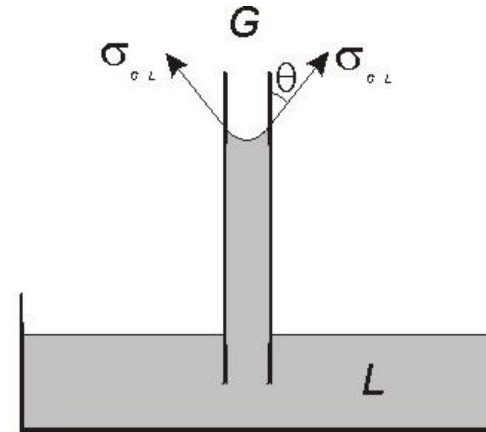
# UNSATURATED FLOW PROCESSES

## CAPILLARY SUCTION

The surface tension is able to maintain different pressure of liquid and gas in the interface.

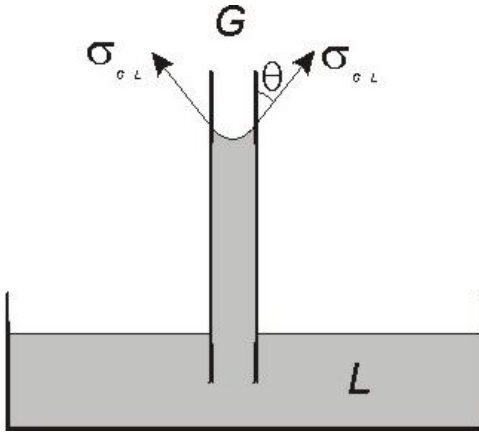


The height of capillary rise depends on the surface tension between the two phases



# UNSATURATED FLOW PROCESSES

## CAPILLARY SUCTION: Laplace's law



Force equilibrium

$$\pi \cdot r_c^2 \cdot h \cdot \gamma_w = 2\pi \cdot r_c \cdot \sigma_{GL} \cos \theta$$

$$h = \frac{2 \cdot \sigma_{GL} \cos \theta}{r_c \cdot \gamma_w}$$

$\theta$  : contact angle

$\sigma_{GL}$  : Surface tension between phases G and L

$r_c$  : capillary tube radius

$$s = p_g - p_w = \gamma_w \cdot h = \frac{2 \cdot \sigma_{GL} \cos \theta}{r_c}$$

If  $\theta < 90^\circ$ , the liquid enters the cavities in the solid surface and the liquid is said to wet the surface

If  $\theta < 90^\circ$ , the air pressure is partly sustained by the meniscus. The water pressure is lower than the air pressure.



# UNSATURATED FLOW PROCESSES

## CAPILLARY SUCTION: Laplace's law

$$\theta = 0^\circ$$

$$\sigma_{GL} = 0.073 \text{ N/m (20}^\circ\text{C)}$$

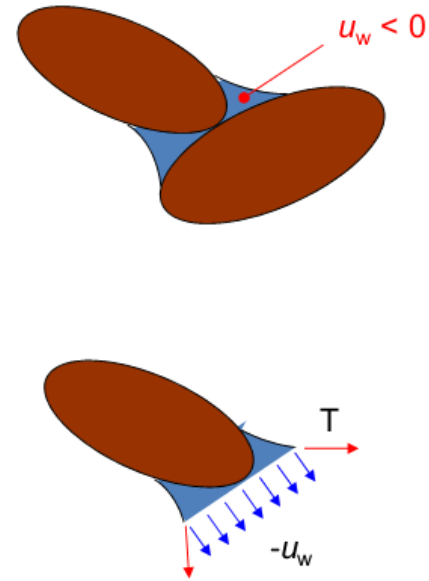
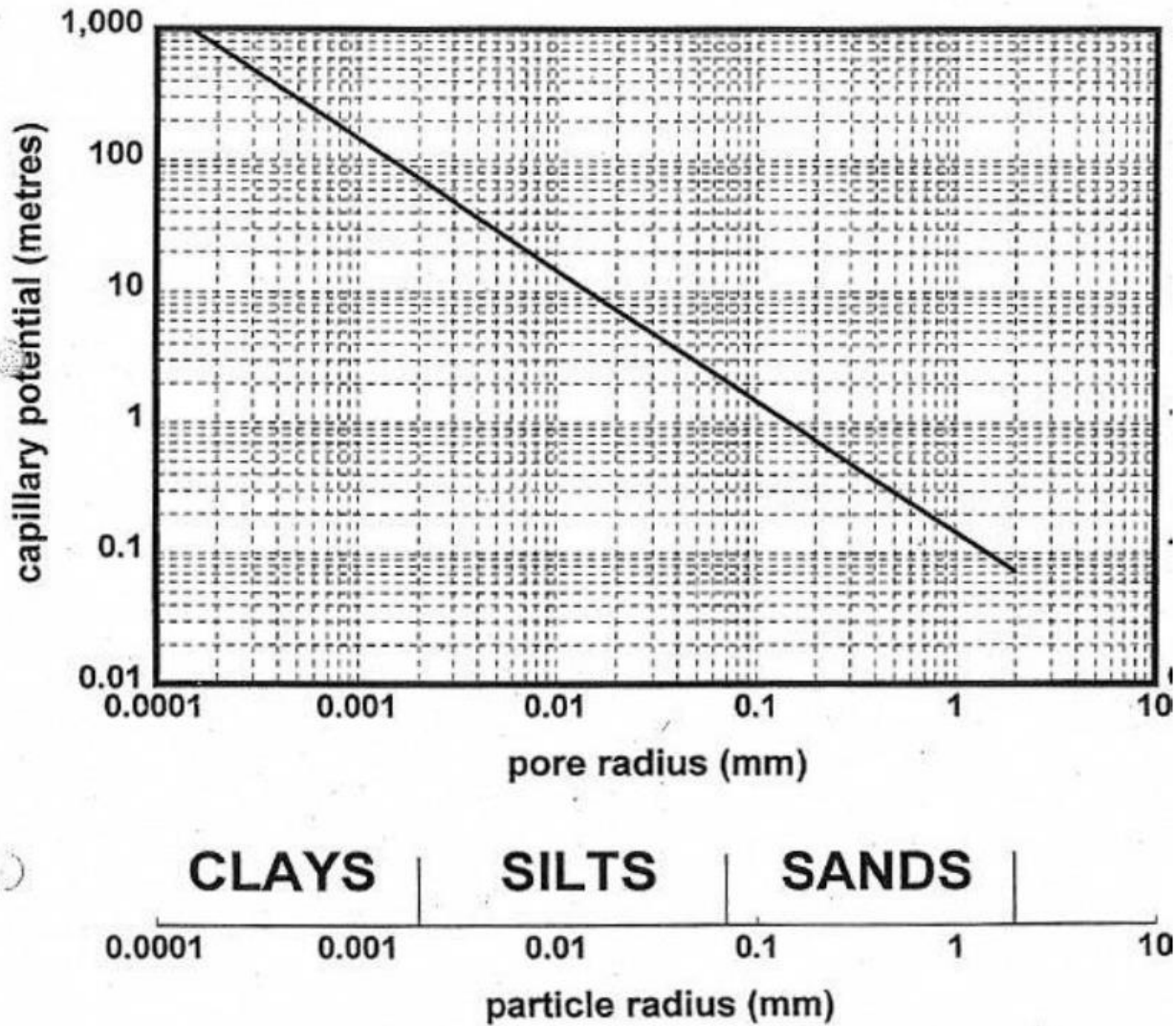
$$p_g = 100 \text{ kPa (absolute pressure)}$$

r (mm)	1	0.01	0.001	$10^{-4}$
s (kPa)	0.146	14.6	146	1460
$p_w$ (kPa)	99.854	85.4	-46	-1360



# UNSATURATED FLOW PROCESSES

## CAPILLARY SUCTION: Laplace's law



The contact angle of water with the particle surface is less than  $90^\circ$

The meniscus is concave toward the air side and pore water pressure is **negative**

Particles are stuck together by surface tension and negative pressure

(Ferrari, 2020)





## UNSATURATED FLOW PROCESSES

### CAPILLARY SUCTION: Laplace's law

The capillary suction is defined as the gas pressure in excess of the water pressure

$$s = p_g - p_w$$

This definition corresponds to the capillary suction, and not to the matric suction (see Baker & Frydman, 2009, for a discussion). However, essentially for historical reasons, it is used to express quantitatively the degree of attachment of the liquid phase onto the solid phase, regardless the attraction mechanism.

Therefore, the suction as defined by this Equation reflects interactions between water and solid and should be differentiated from capillary phenomena (Gens, 2010).

Very large negative 'water pressures' are just an expression of the potential. They do not correspond to the usual bulk thermodynamic pressures.

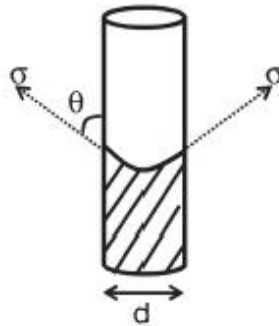
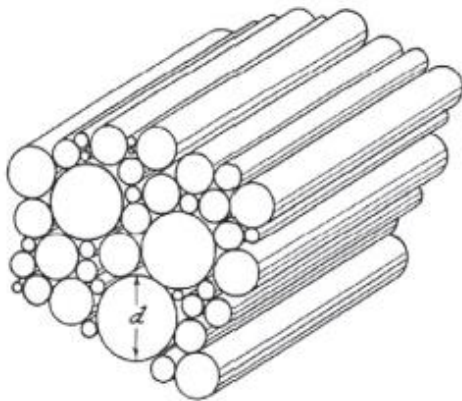
*"suction must be considered merely as a convenient index of the affinity of soil for free water"*  
(Blight, 1965)



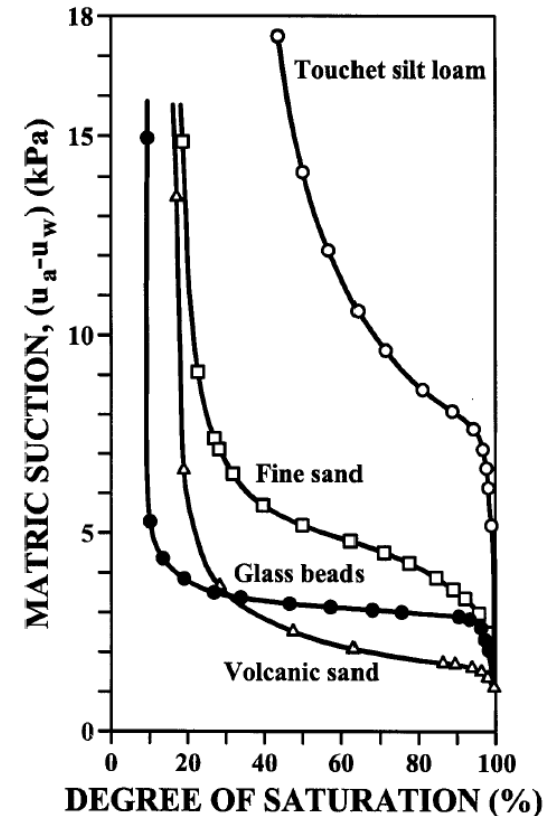
# UNSATURATED FLOW PROCESSES

## Retention properties

The water retention curve is defined as the relationship between the amount of water stored in a porous medium and suction. The amount of water stored may be expressed in terms of water content, water ratio or degree of saturation. Yet, the degree of saturation, which provides normalisation of the volume fractions of the liquid and gas phases, is directly involved in the mass balance equations



Bundle of capillary tubes model. After [Gates et al., 1950] and [Chen et al., 2013].

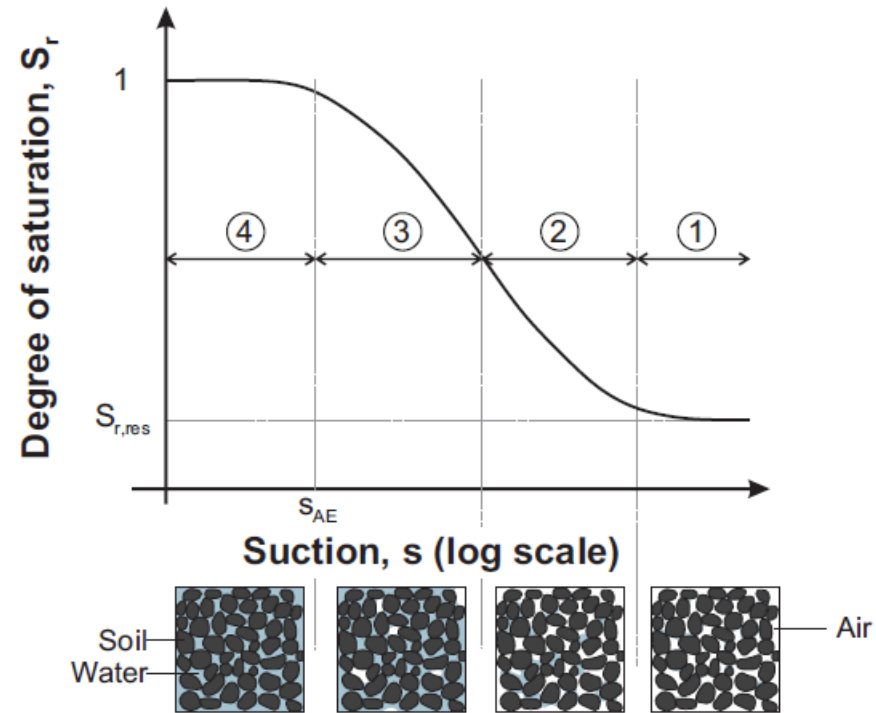


Retention curve [Brooks and Corey, 1964]



# UNSATURATED FLOW PROCESSES

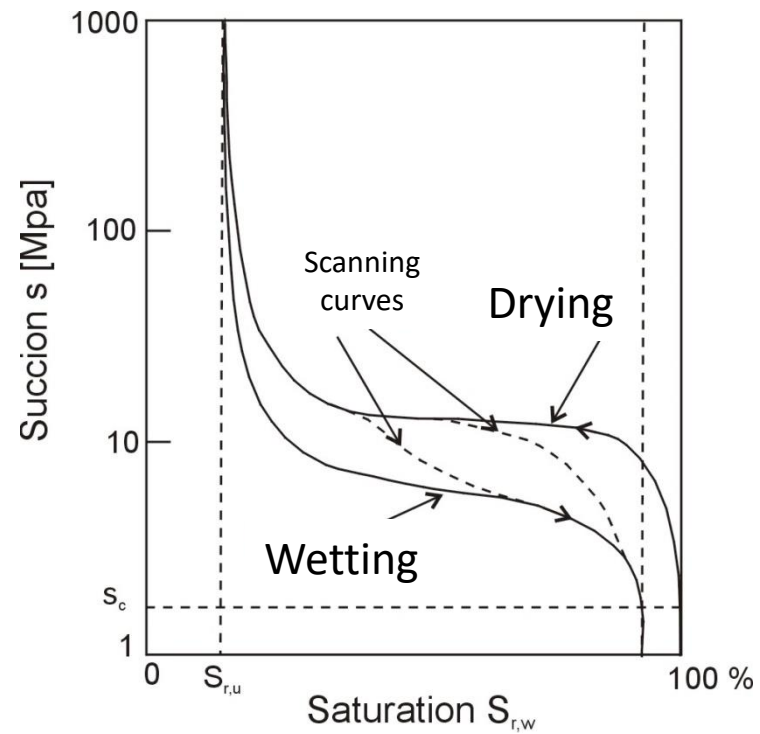
## Retention properties



Water retention curve and schematic stages of saturation in porous media (modified after Nuth & Laloui, 2008a)

# UNSATURATED FLOW PROCESSES

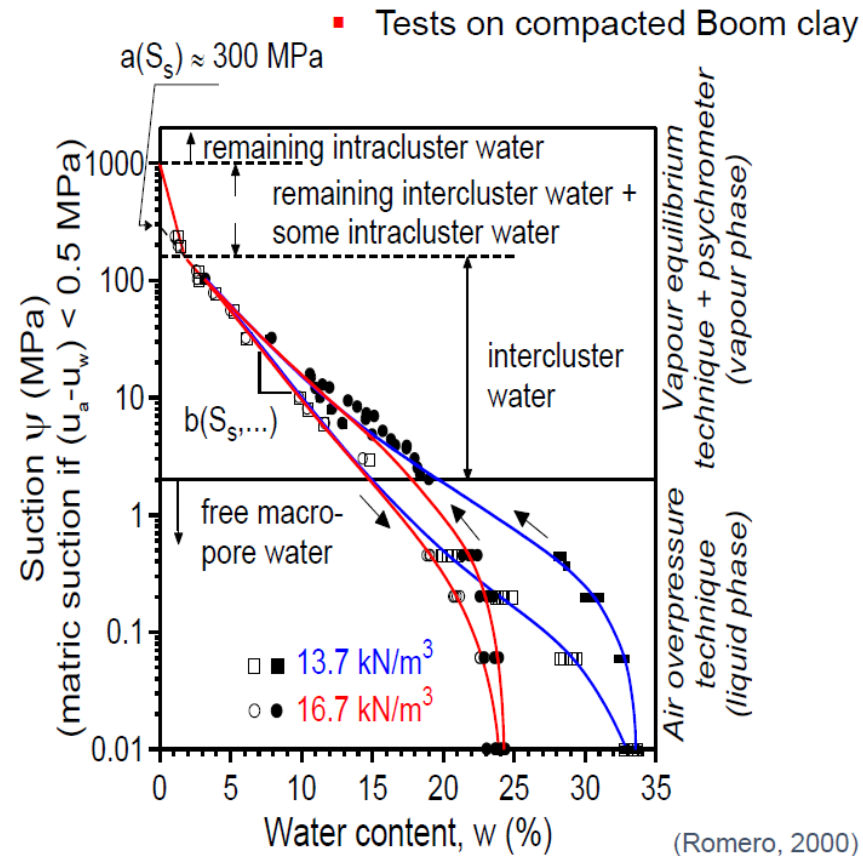
## Retention properties: hysteresis



Retention curves

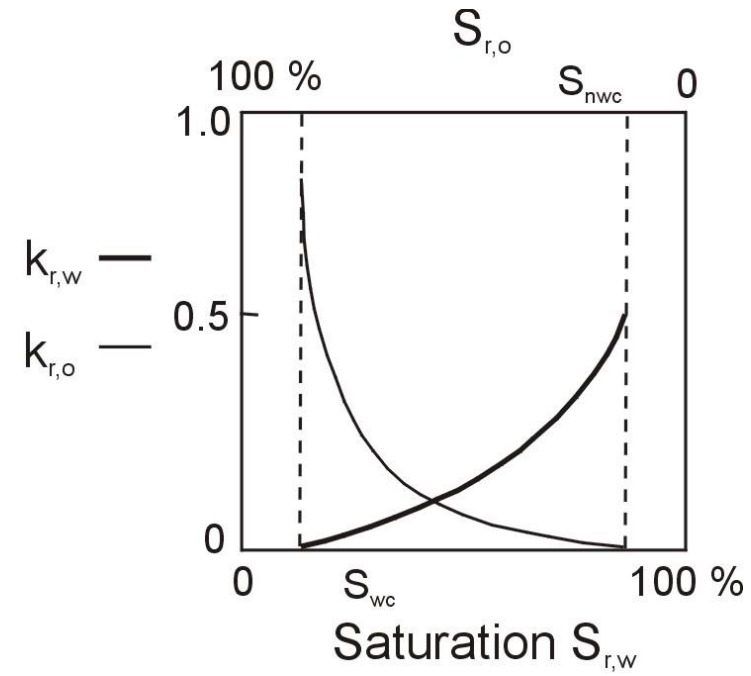
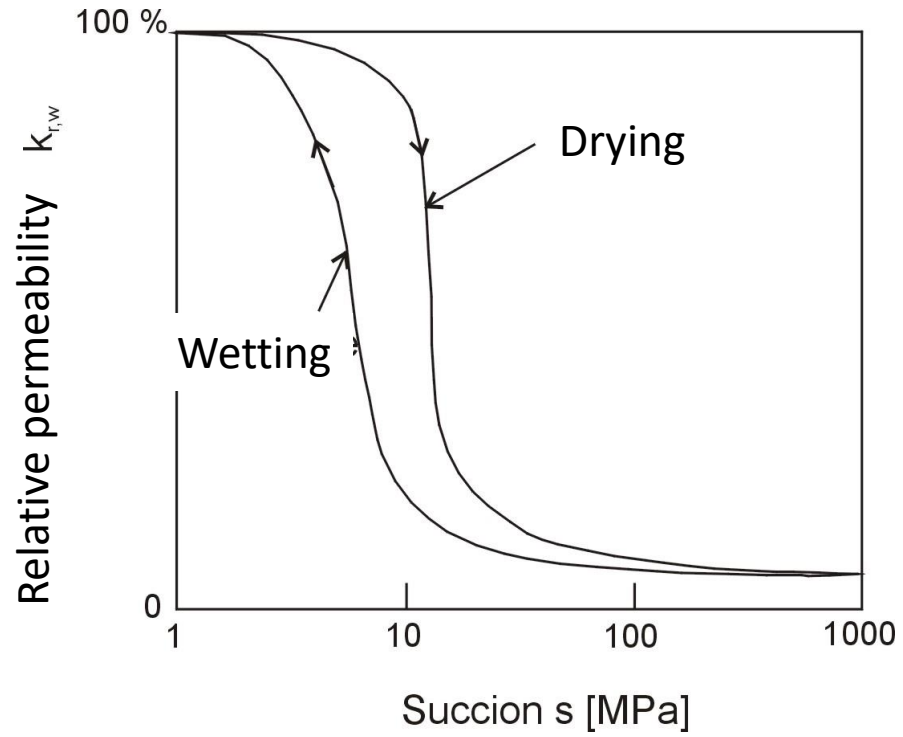
# UNSATURATED FLOW PROCESSES

## Retention properties: influence of the dry density



# UNSATURATED FLOW PROCESSES

## Transfer properties



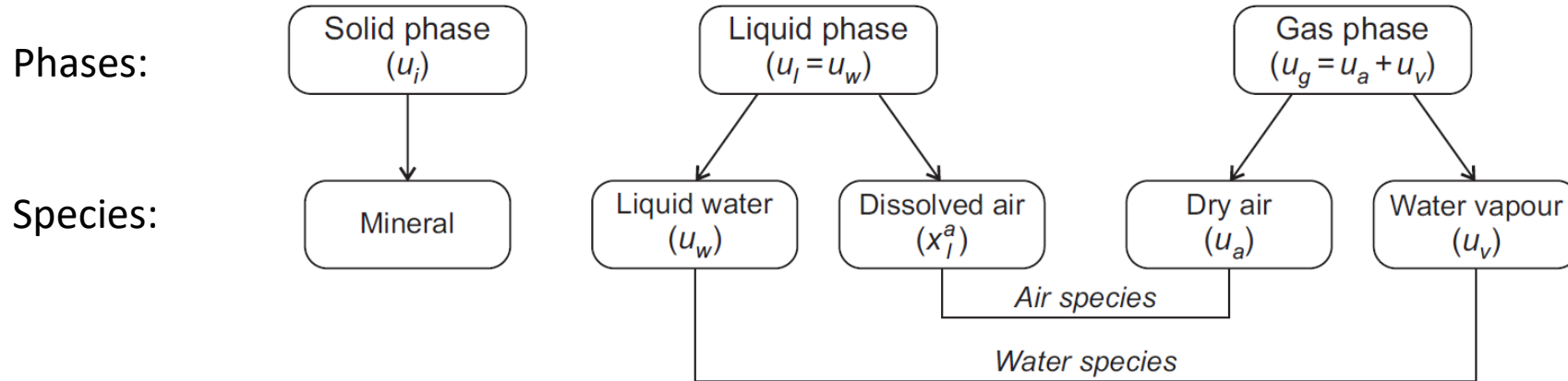
Permeability





# UNSATURATED FLOW PROCESSES

## Equilibrium restrictions

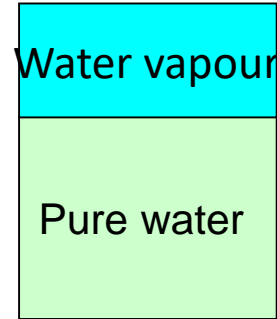
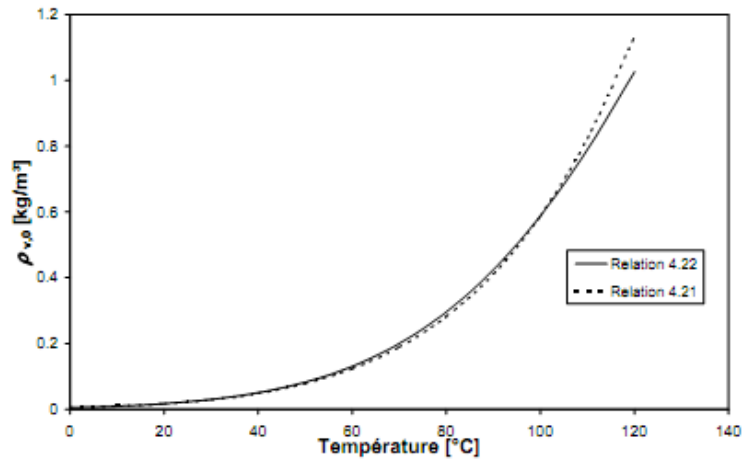
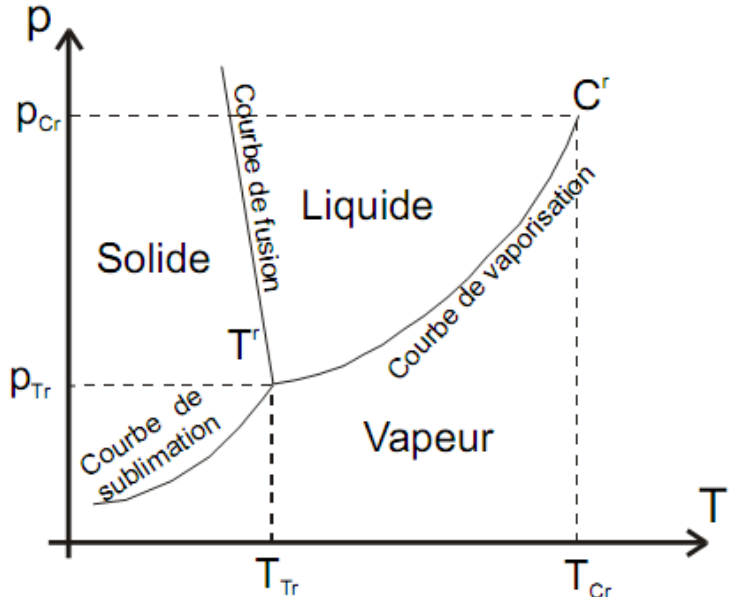


Equilibrium restrictions relate dependent variables with the kinematics variables. They are obtained assuming thermodynamic equilibrium between the different phases of the species. This hypothesis is justified by the fast kinetics of the dissolution processes compared to the transport phenomena.



# UNSATURATED FLOW PROCESSES

Equilibrium restrictions: Kelvin's law



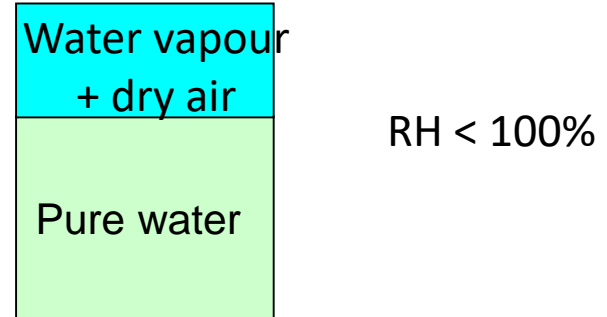
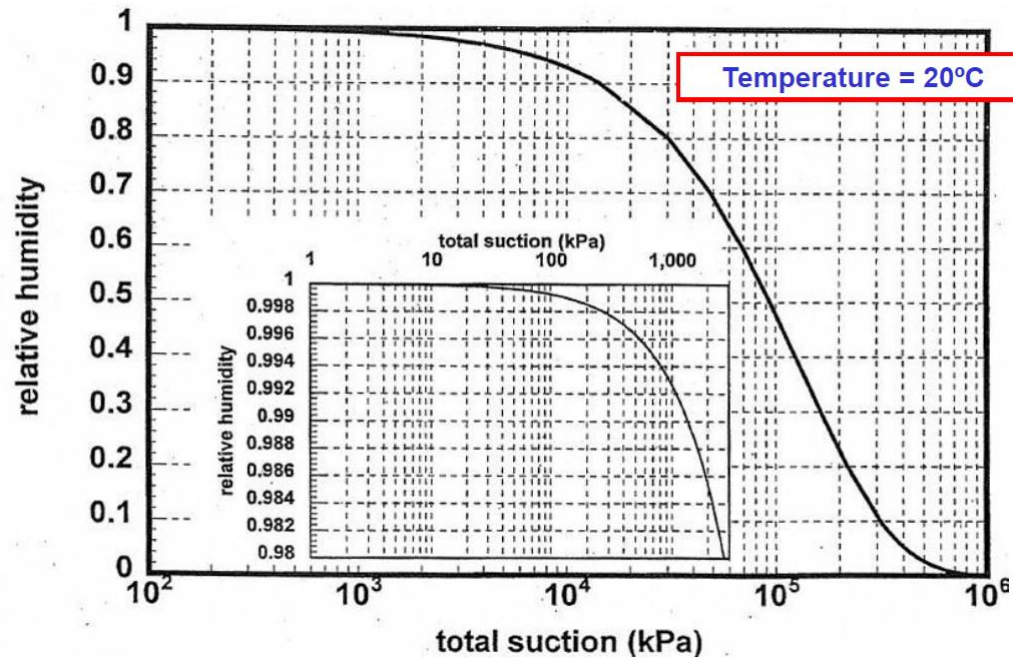
RH = 100%

$$\frac{1}{\rho_{H_2O,0}^g} = 194.4 \exp(-0.06374(T - 273) + 0.1634 \cdot 10^{-3} (T - 273)^2)$$

$$p_{H_2O,0}^g = \frac{\rho_{H_2O,0}^g}{M_{H_2O}} RT$$

# UNSATURATED FLOW PROCESSES

## Equilibrium restrictions: Kelvin's law



Kelvin's law: 
$$\rho_{H_2O}^g = \rho_{H_2O,0}^g \cdot \exp\left(\frac{(p_w - p_g)M_{H_2O}}{\rho_w RT}\right)$$

$$RH = \frac{p_{H_2O}^g}{p_{H_2O,0}^g} = \frac{\rho_{H_2O}^g}{\rho_{H_2O,0}^g}$$





## UNSATURATED FLOW PROCESSES

### Equilibrium restrictions: Henry's law

Henry's law expresses the equilibrium between dissolved air in the liquid phase and dry air in the gas phase. Under constant temperature, the amount of dissolved air is proportional to the air partial pressure

$$p_a = K_{al} x_{al}$$

where  $K_a$  is a constant. This law may be written in terms of densities, so that

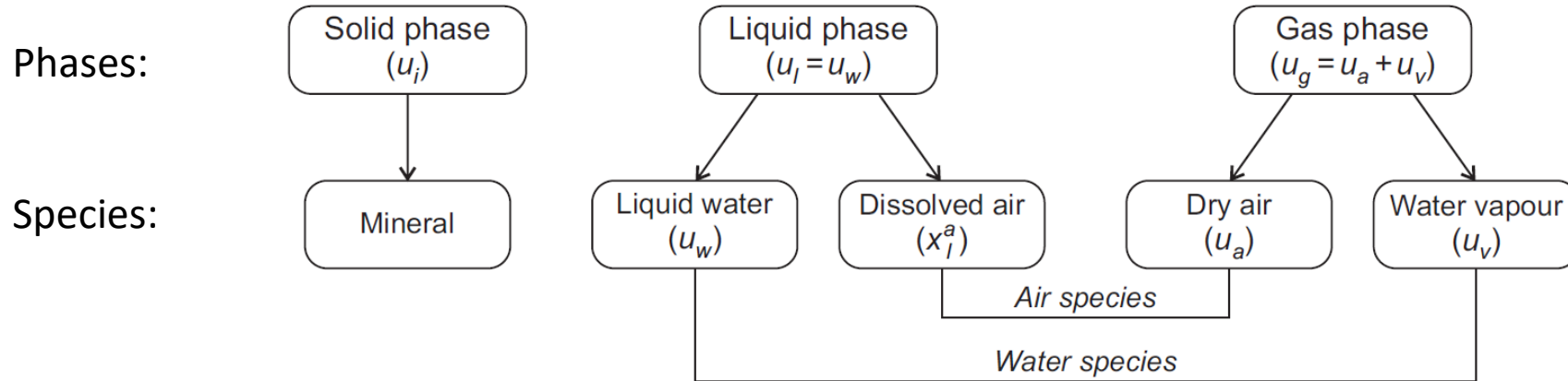
$$\rho_{da} = H_a \rho_a$$

where  $H_a$  is called the Henry's constant and is equal to 0.0234 for air.



# UNSATURATED FLOW PROCESSES

## Balance equations



The compositional approach (Panday & Corapcioglu, 1989; Olivella et al., 1994; Collin, 2003) is adopted to establish the mass balance equations. It consists of balancing species rather than phases. This approach has the advantage that phase exchange terms cancel out, which is particularly useful when equilibrium is assumed.



# UNSATURATED FLOW PROCESSES

## Water Mass Balance

$$\frac{\partial}{\partial t} (\rho_w n S_{rw}) + \text{div}(\underline{f}_w) + \frac{\partial}{\partial t} (\rho_v n S_{rg}) + \text{div}(\underline{f}_v) - Q_w = 0$$

Liquid water,  $S_{rw}$  water saturation degree

Water vapour,  $S_{rg} = 1 - S_{rw}$  gas saturation degree

Source term

## Gas Mass Balance

$$\frac{\partial}{\partial t} (\rho_{d,a} n S_{rw}) + \text{div}(\underline{f}_{d,a}) + \frac{\partial}{\partial t} (\rho_a n S_{rg}) + \text{div}(\underline{f}_a) - Q_a = 0$$

Dissolved air,  $S_{rw}$  water saturation degree

Dry air,  $S_{rg} = 1 - S_{rw}$  gas saturation degree

Source term





## UNSATURATED FLOW PROCESSES

### Fluid transfer equations

In both liquid and gas phases, water and air fluxes are a combination of advective and non-advective fluxes. Advective fluxes are associated to the phase movements, while non-advective fluxes are associated to the motion of species within phases. The mass fluxes of liquid water, water vapour, dry gas and dissolved gas are given respectively by

$$\underline{f}_{(H_2O)_l} = \rho_w \cdot \underline{q}_l$$

$$\underline{f}_{(H_2O)_g} = \rho_{H_2O}^g \cdot \underline{q}_g + \underline{i}_{(H_2O)_g}$$

$$\underline{f}_{(Air)_g} = \rho_{Air}^g \cdot \underline{q}_g + \underline{i}_{(Air)_g}$$

$$\underline{f}_{(Air)_d} = \rho_{Air}^g \cdot H_{Air} \cdot \underline{q}_l + \underline{i}_{(Air)_d}$$



## UNSATURATED FLOW PROCESSES

### Fluid transfer equations: advective fluxes

Advective fluxes of both liquid and gas phases are described by the generalized Darcy's law for partially saturated porous media.

$$\underline{q}_l = - \frac{\underline{K}_{int}^{sat} \cdot k_{rw}}{\mu_w} \left[ \underline{\text{grad}}(p_w) + g \rho_w \underline{\text{grad}}(z) \right]$$

where

- $\underline{K}_{int}^{sat}$  [m<sup>2</sup>] is the intrinsic permeability
- $k_{rw}$  [-] is the water relative permeability function
- $\mu_w$  [Pa.s] is the water dynamic viscosity
- $p_w$  [Pa] is the pore water pressure
- $\rho_w$  [kg/m<sup>3</sup>] is the liquid water density

## UNSATURATED FLOW PROCESSES

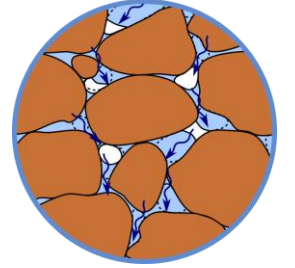
### Transfer properties

The intrinsic permeability [ $\text{m}^2$ ] depends on the density.

Kozeni-Carman law: 
$$K_w = K_{w0} \frac{\phi^N}{(1 - \phi)^M} \frac{(1 - \phi_0)^M}{\phi_0^N}$$

The intrinsic permeability depends on the pore size (and the interconnectivity of the pores)

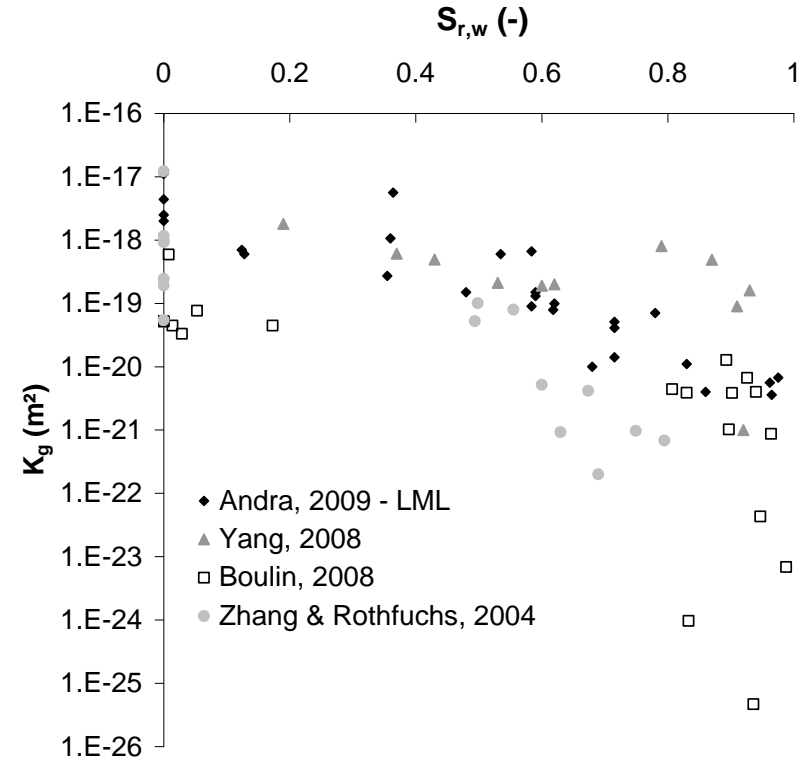
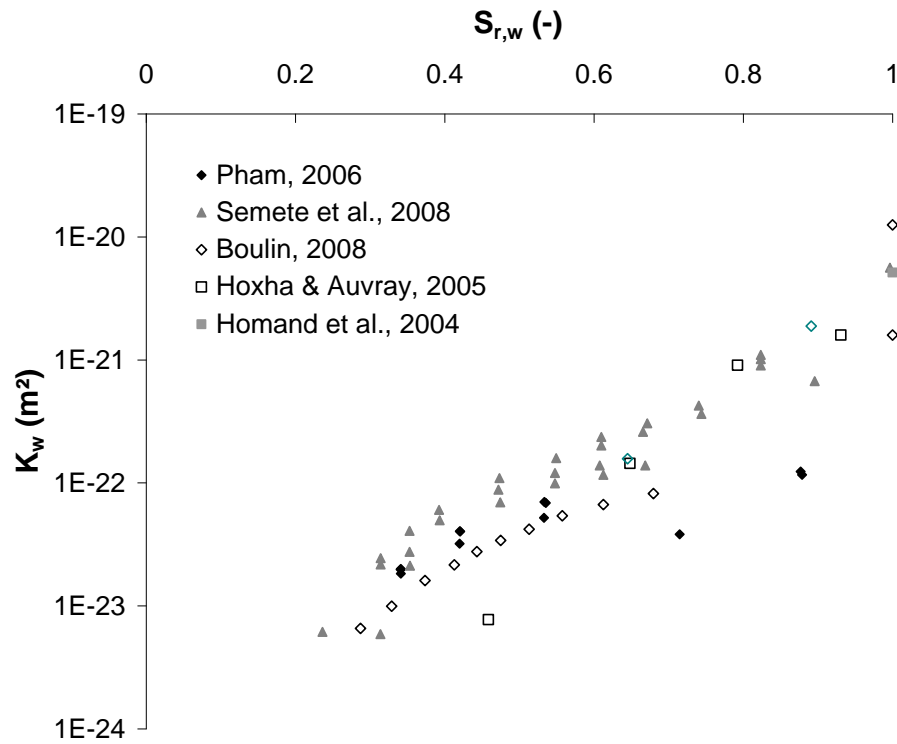
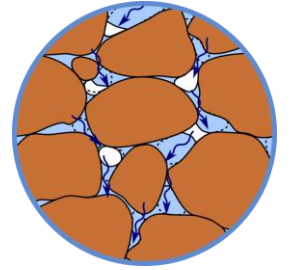
The pore size of expansive clays may change very significantly due to hydration (even during constant volume conditions)



# UNSATURATED FLOW PROCESSES

## Transfer properties

The intrinsic permeability [ $m^2$ ] to gas and liquid are not the same !



## UNSATURATED FLOW PROCESSES

### Fluid transfer equations: advective fluxes

Advective fluxes of both liquid and gas phases are described by the generalized Darcy's law for partially saturated porous media.

$$\underline{q}_g = - \frac{\underline{K}_{int}^{sat} \cdot k_{rg}}{\mu_g} \left[ \underline{\text{grad}}(p_g) + g \rho_g \underline{\text{grad}}(z) \right]$$

where

- $\underline{K}_{int}^{sat}$  [m<sup>2</sup>] is the intrinsic permeability
- $k_{rg}$  [-] is the gas relative permeability function
- $\mu_g$  [Pa.s] is the gas dynamic viscosity
- $p_g$  [Pa] is the pore gas pressure
- $\rho_g$  [kg/m<sup>3</sup>] is the gas density



## UNSATURATED FLOW PROCESSES

### Fluid transfer equations: non-advective fluxes

The diffusive fluxes are governed by Fick's law. According to Fick's law, the diffusive flux is proportional to the gradient of mass fraction of species, the proportionality coefficient being the hydrodynamic dispersion coefficient. The diffusive fluxes of water vapour and dissolved air read

*Diffusion within the gaseous phase*

$$\underline{i}_v = -n S_{rg} \tau D_{v/a} \rho_g \underline{\text{grad}} (\rho_v / \rho_g) = -\underline{i}_a$$

- $D_{v/a}$  [m<sup>2</sup>/s] is the diffusion coefficient of water vapour in dry air
- $\tau$  [-] is the tortuosity

$$D_{v/a} = D_0 \frac{p_0}{p_g} \left( \frac{T}{T_0} \right)^{1,75} \text{ with } p_0=101 \text{ kPa, } D_0= 2.42 \cdot 10^{-5} \text{ m}^2/\text{s and } T_0=303^\circ\text{K}$$



## UNSATURATED FLOW PROCESSES

### Fluid transfer equations: non-advective fluxes

The diffusive fluxes are governed by Fick's law. According to Fick's law, the diffusive flux is proportional to the gradient of mass fraction of species, the proportionality coefficient being the hydrodynamic dispersion coefficient. The diffusive fluxes of water vapour and dissolved air read

*Diffusion within the liquid phase*

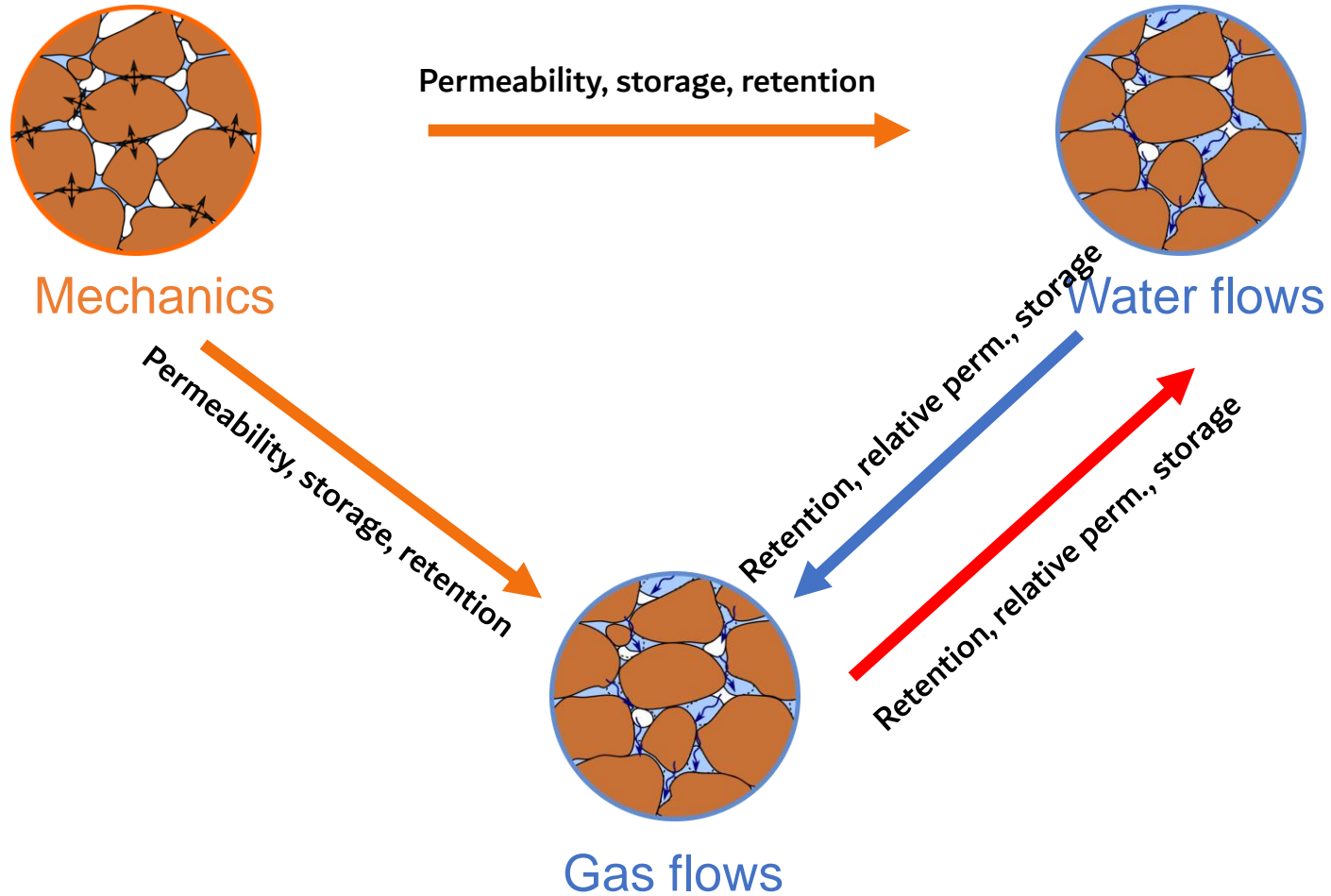
$$\underline{i}_{d,a} = -n S_{rw} \tau D_{d-a/w} \rho_w \underline{\text{grad}} (\rho_{d,a} / \rho_w)$$

- $D_{d-a/w}$  [m<sup>2</sup>/s] is the diffusion coefficient of dissolved air in water





# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

## Balance equations

- Water mass balance

$$\frac{\partial}{\partial t} (\rho_w n S_{rw}) + \text{div} (\underline{f}_w) + \frac{\partial}{\partial t} (\rho_v n S_{rg}) + \text{div} (\rho_v \underline{q}_g + \underline{i}_v) - Q_w = 0$$

- Gas mass balance

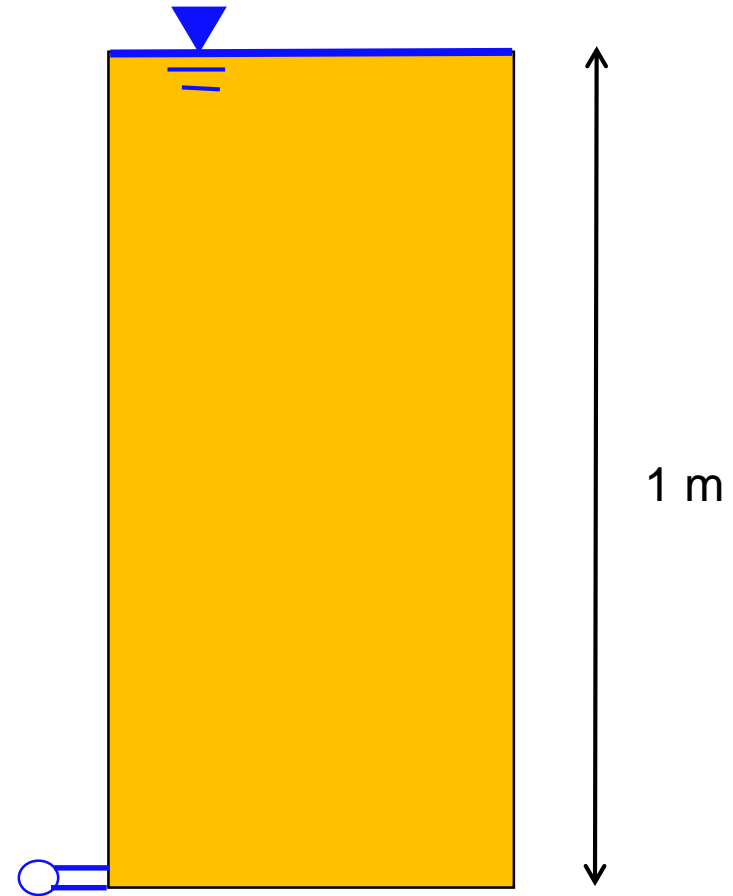
$$\frac{\partial}{\partial t} (\rho_{d,a} n S_{rw}) + \text{div} (\rho_{d,a} \underline{q}_l + \underline{i}_{d,a}) + \frac{\partial}{\partial t} (\rho_a n S_{rg}) + \text{div} (\rho_a \underline{q}_g + \underline{i}_a) - Q_a = 0$$



## UNSATURATED FLOW PROCESSES

Liakopoulos (1965) experiment on a column of del Monte sand

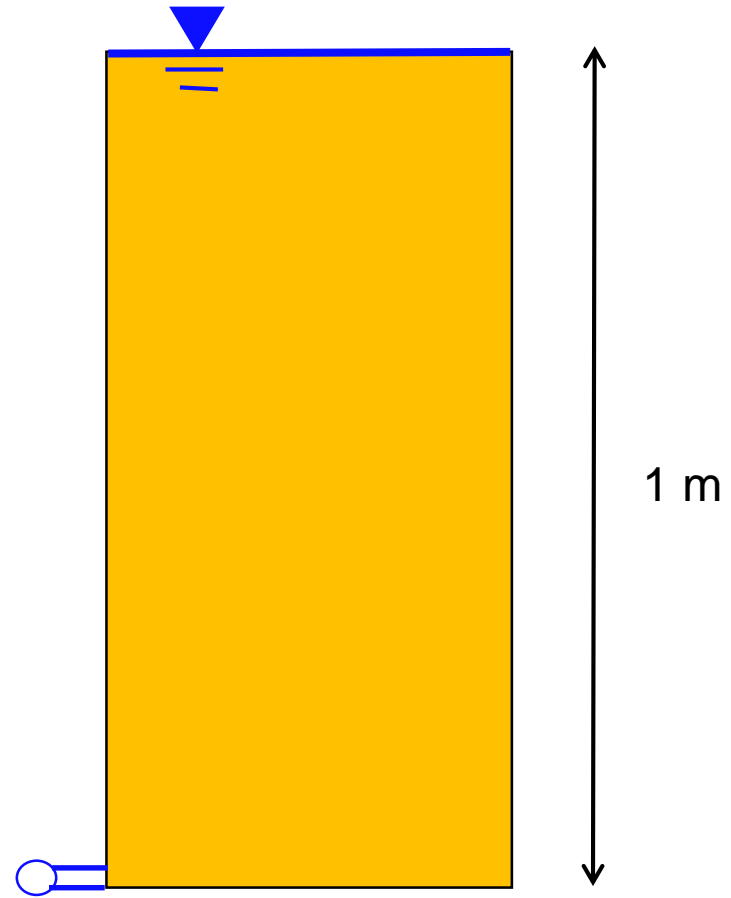
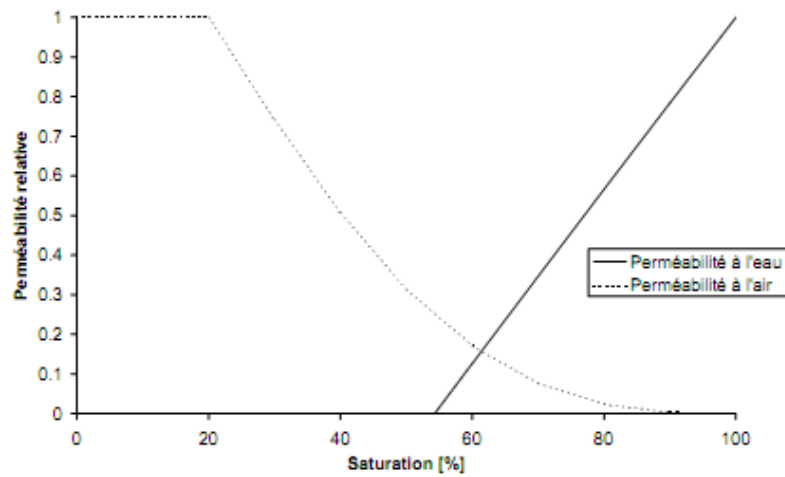
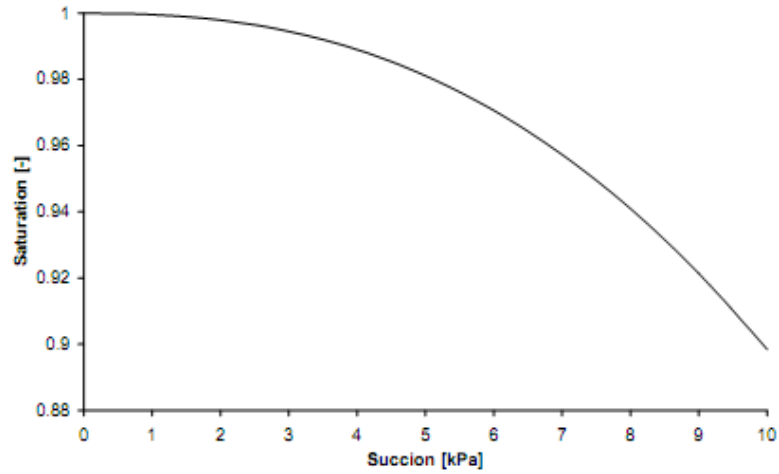
Benchmark exercise\*



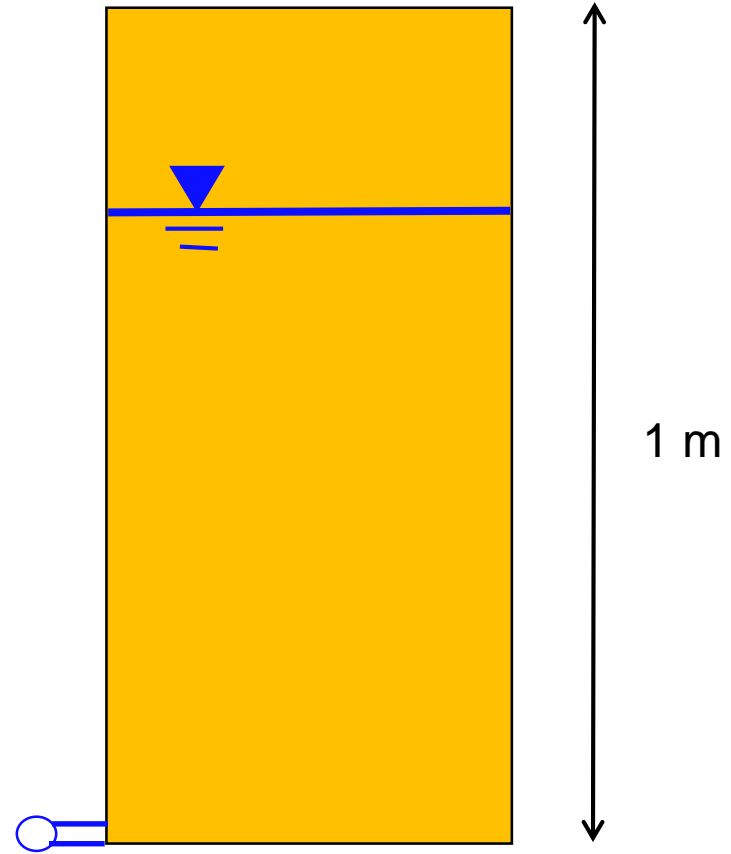
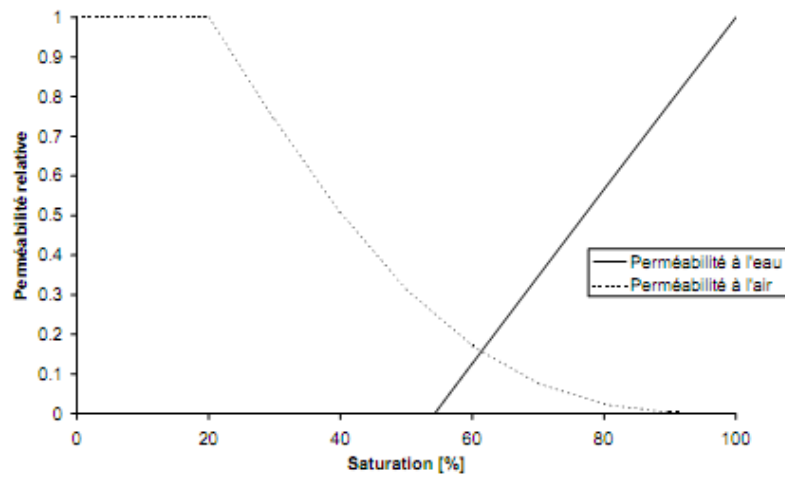
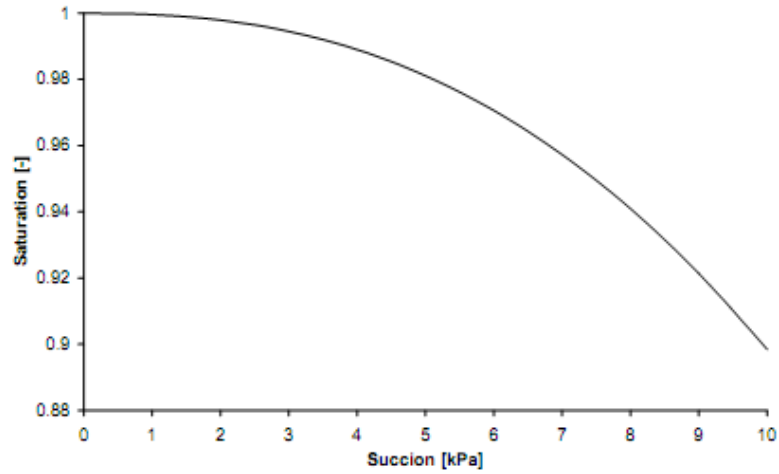
- JOMMI C., VAUNAT J., GENS A., GAWIN D. & SCHREFLER B. – Multiphase flow in porous media : a numerical benchmark – Proceedings NAFEMS World Congress Stuttgart, 1997.
- VAUNAT J., GENS A. & JOMMI C. – A Strategy for Numerical Analysis of the Transition between Saturated and Unsaturated Flow Conditions – Numerical Models in Geomechanics, pp. 297-302, 1997.



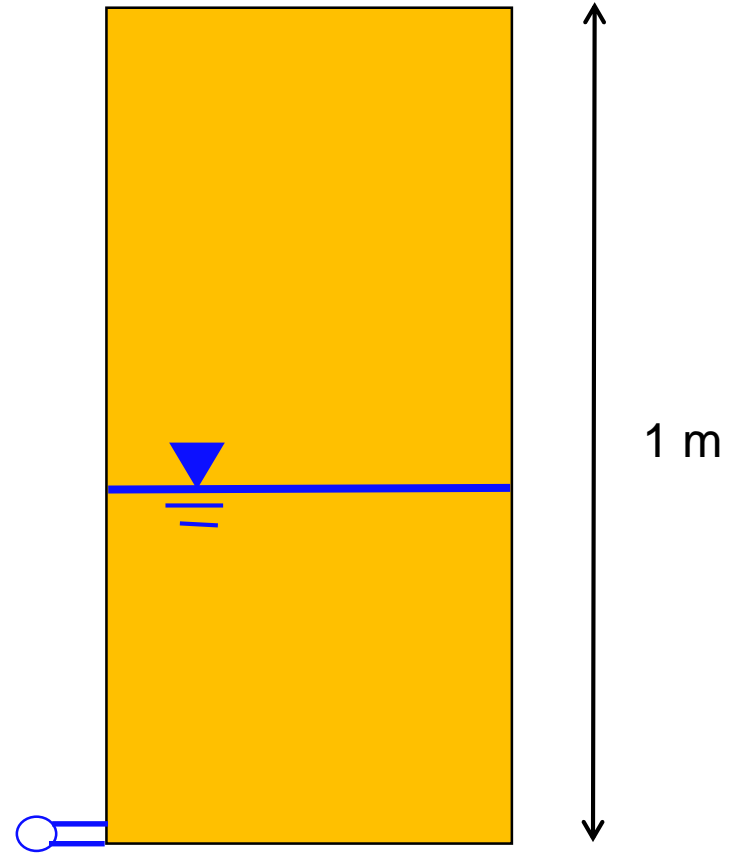
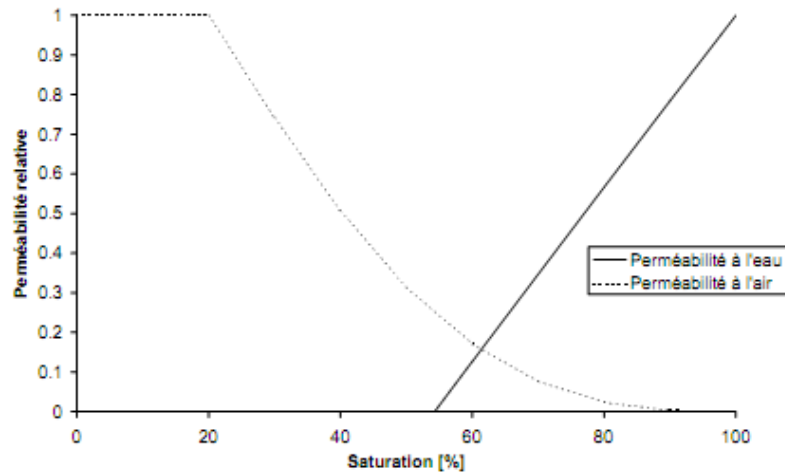
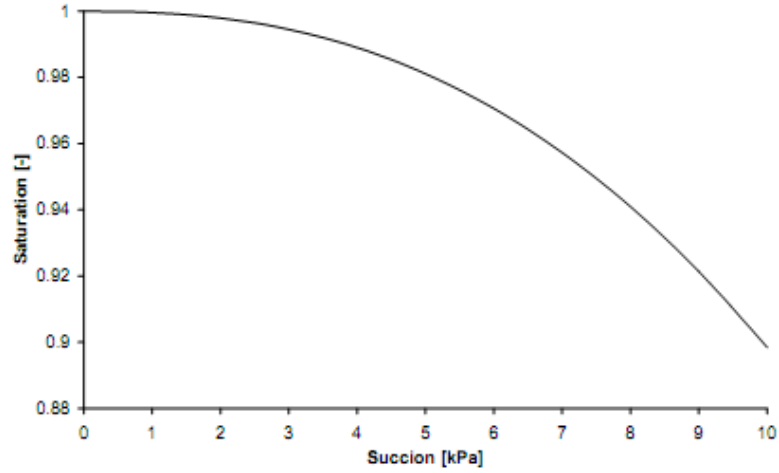
# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

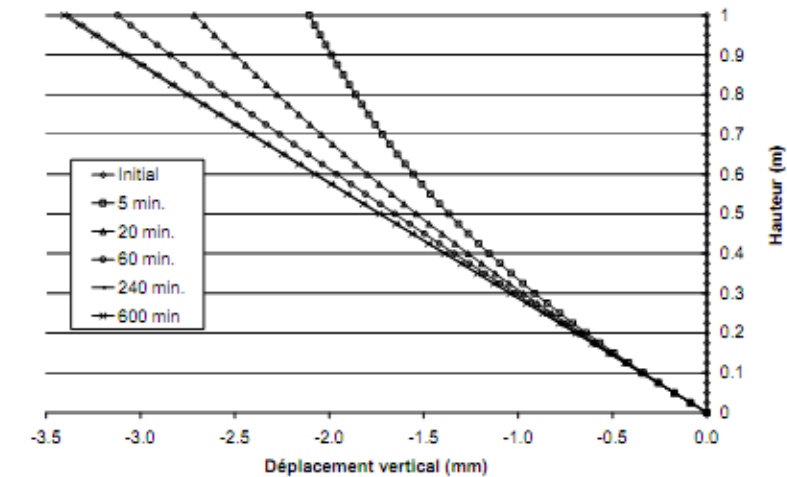
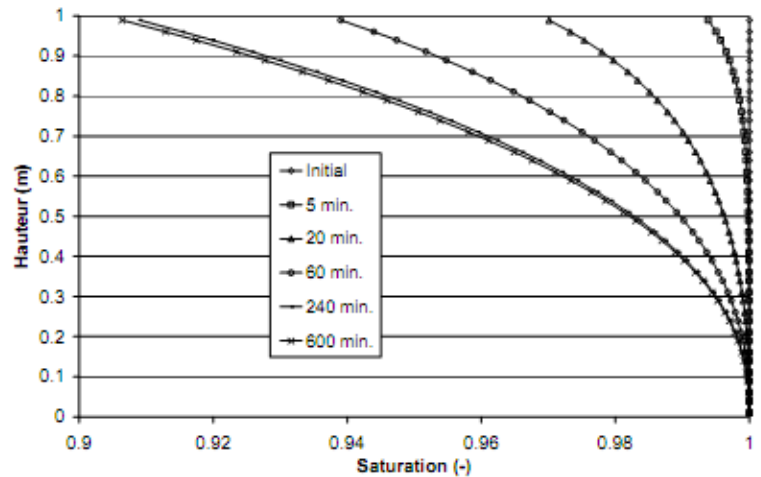
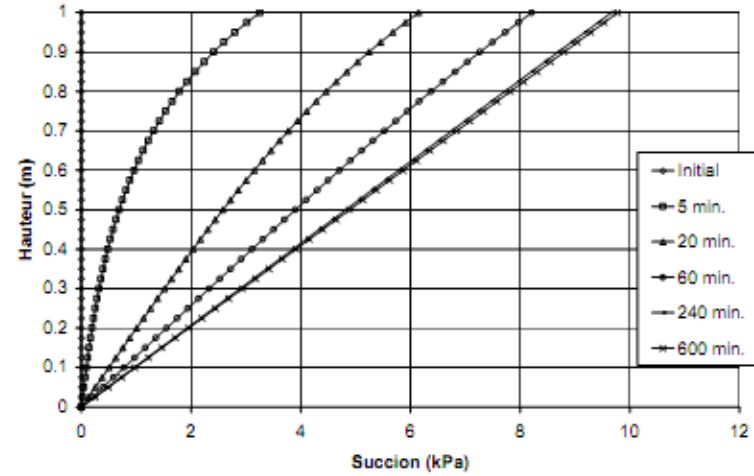
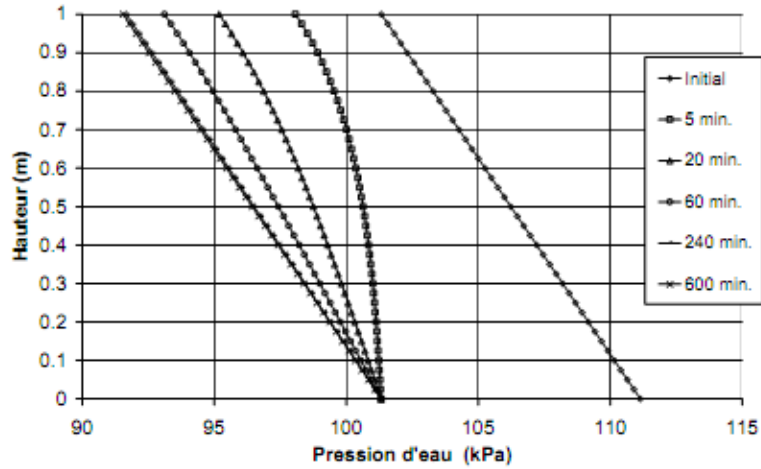


# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

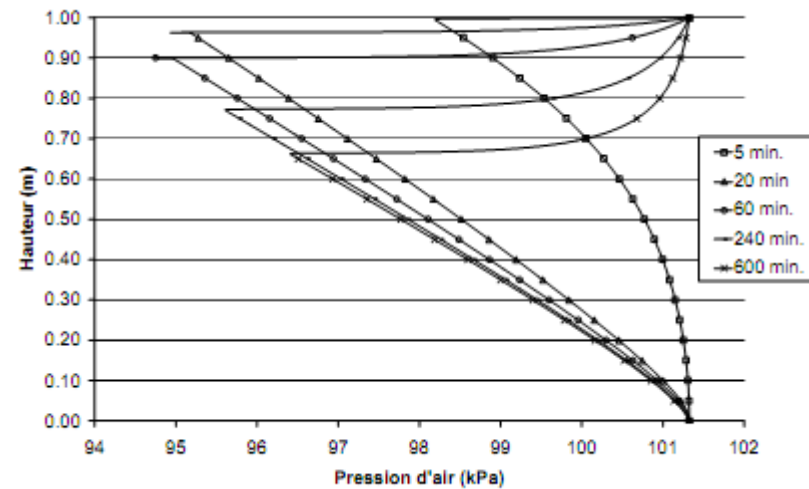
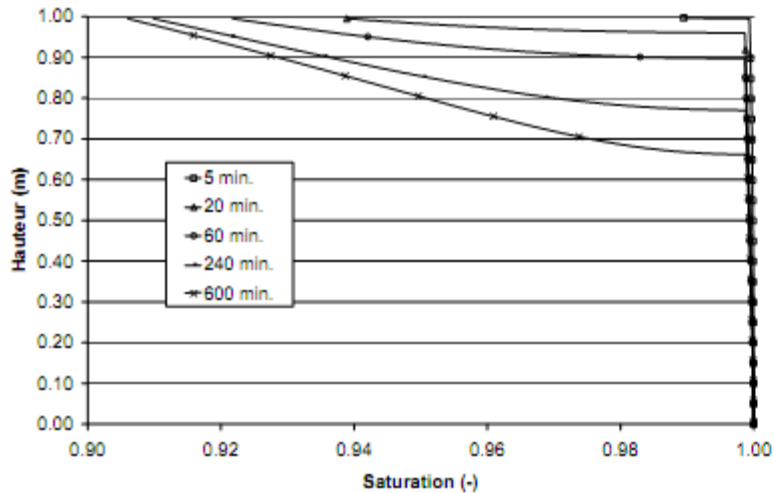
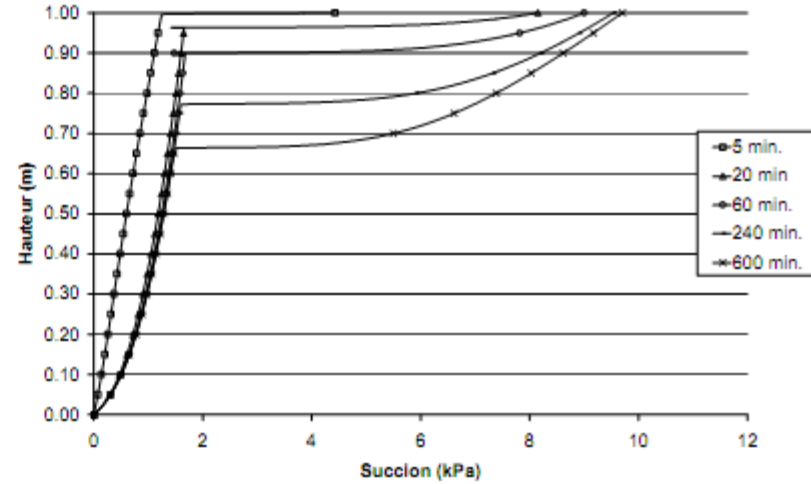
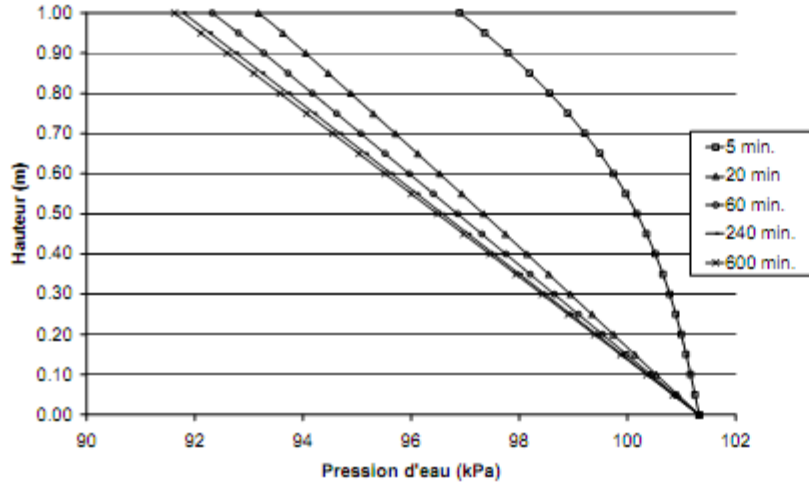
Modelling with fixed gas pressure





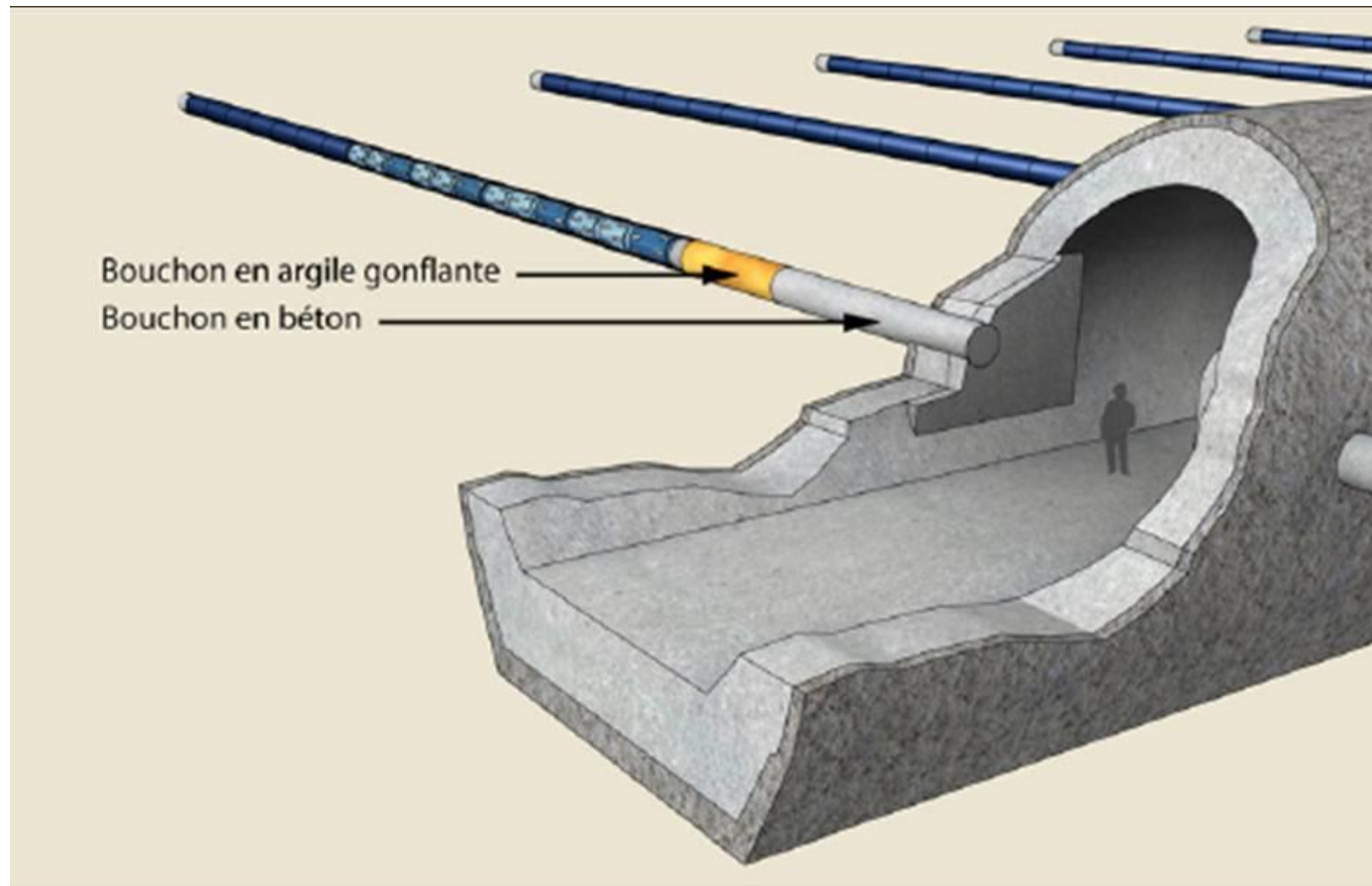
# UNSATURATED FLOW PROCESSES

Modelling with variable gas pressure (+dissolved gas)

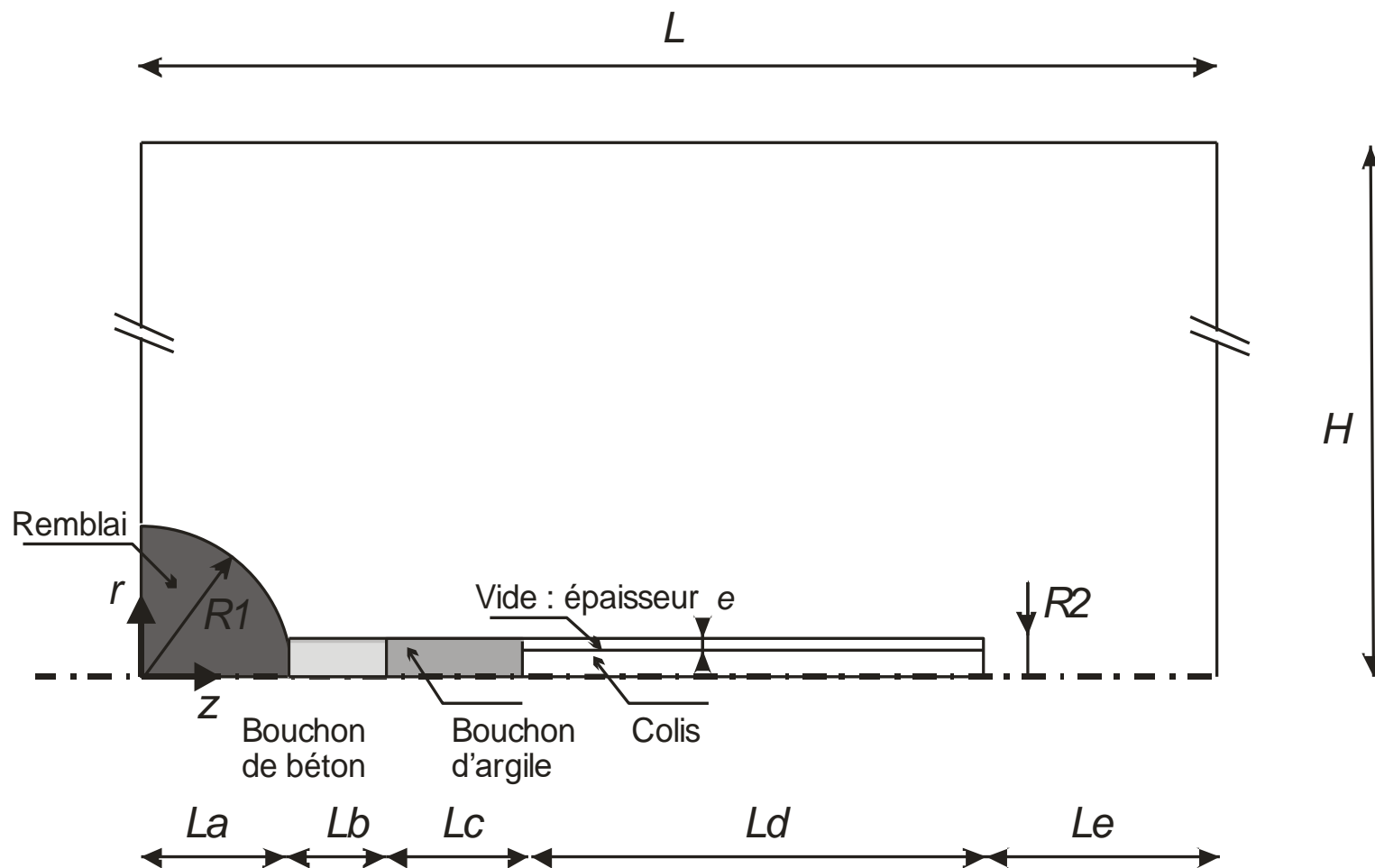


## UNSATURATED FLOW PROCESSES

Benchmark exercise to study the gas migration around a drift

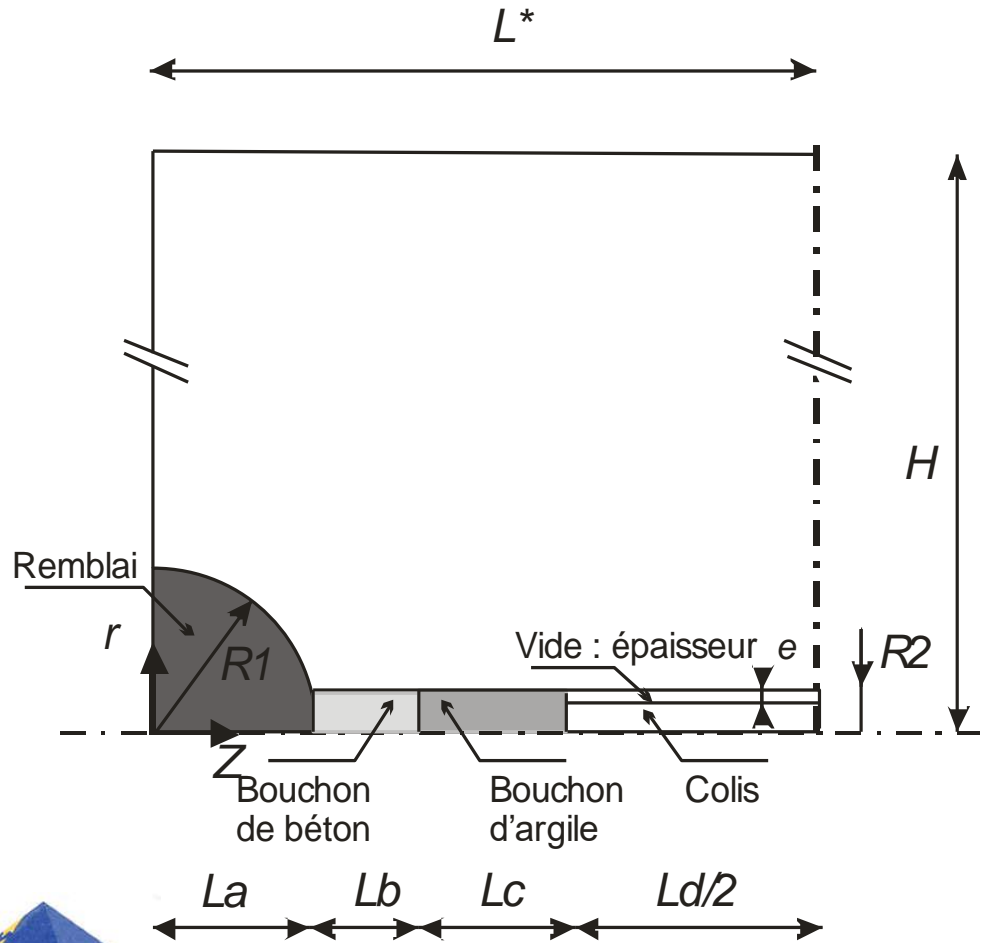


# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

## Geometry



$$H = 82 \text{ m}$$

$$L = 51 \text{ m}$$

$$R1 = La = 4 \text{ m}$$

$$Lb = 3.3 \text{ m}$$

$$Lc = 3 \text{ m}$$

$$Ld = 30.7 \text{ m}$$

$$Le = 10 \text{ m}$$

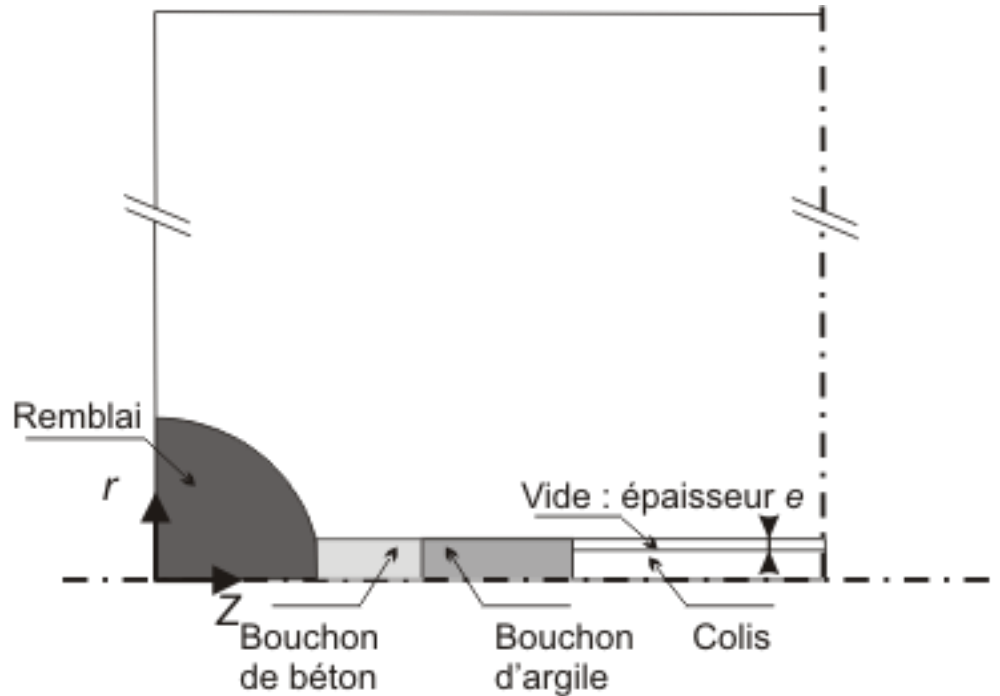
$$R2 = 0.35 \text{ m}$$

$$E = 0.0125 \text{ m}$$



# UNSATURATED FLOW PROCESSES

## Initial conditions



### Clay rock:

$\sigma_0 = 12.3 \text{ MPa}$   
 $P_w = 5 \text{ MPa}$   
 $P_g = 0.1 \text{ MPa}$   
 $T = 303^\circ\text{K}$

### Swelling clay:

$\sigma_0 = 0.1 \text{ MPa}$   
 $S_{r,w} = 0.80$   
 $P_g = 0.1 \text{ MPa}$   
 $T = 303^\circ\text{K}$

### Concrete plug:

$\sigma_0 = 0.1 \text{ MPa}$   
 $P_w = 0.1 \text{ MPa}$   
 $P_g = 0.1 \text{ MPa}$   
 $T = 303^\circ\text{K}$

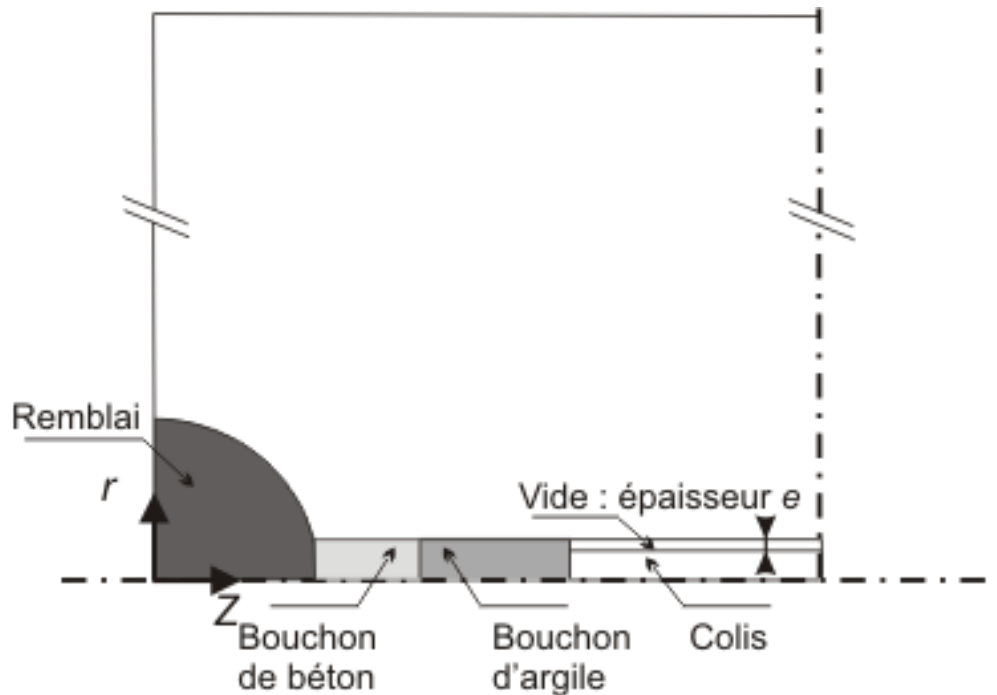
### Backfill:

$\sigma_0 = 0.1 \text{ MPa}$   
 $S_{r,w} = 0.80$   
 $P_g = 0.1 \text{ MPa}$   
 $T = 303^\circ\text{K}$



# UNSATURATED FLOW PROCESSES

## Modelling steps and boundary conditions

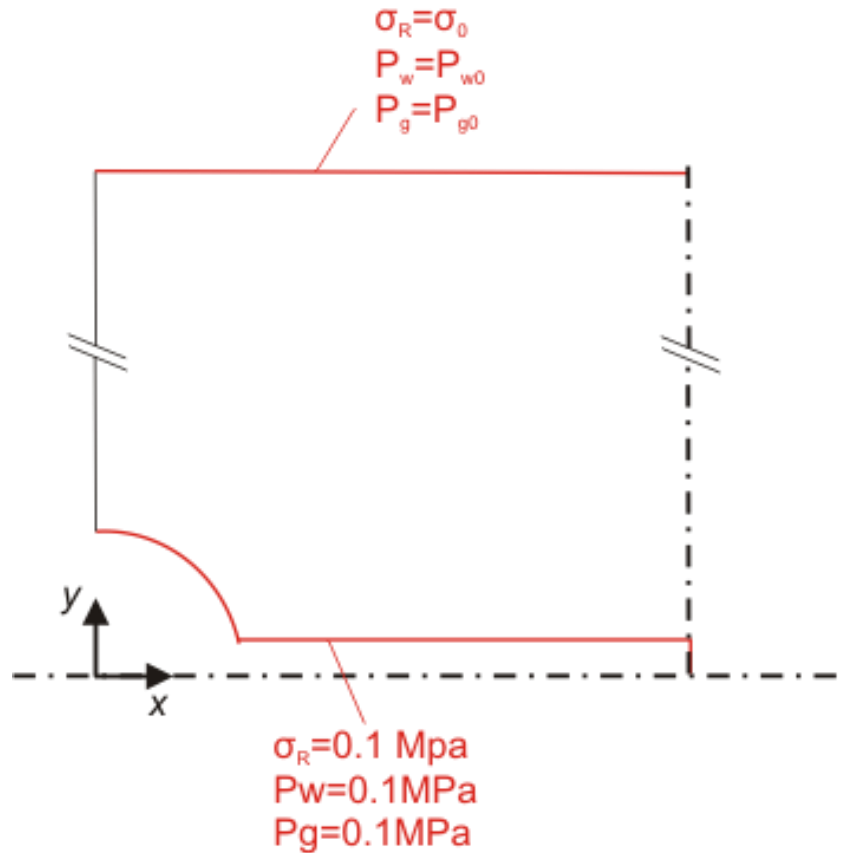


- **Step 1** : Excavation and waiting phase ( $\rightarrow$  2 years)
- **Step 2** : Water resaturation of the void space and activation of the plugs ( $\rightarrow$  3 years)
- **Step 3** : Hydrogene production and backfilling ( $\rightarrow$  100 000 years)



# UNSATURATED FLOW PROCESSES

## Boundary conditions - Step 1 : Excavation + Waiting phase



Simultaneous excavation of the main drift and the alveole ( $\rightarrow$  3 days) :

Deconfinement  $\rightarrow \sigma_R$  decreased at the wall down to  $P_{atm}$

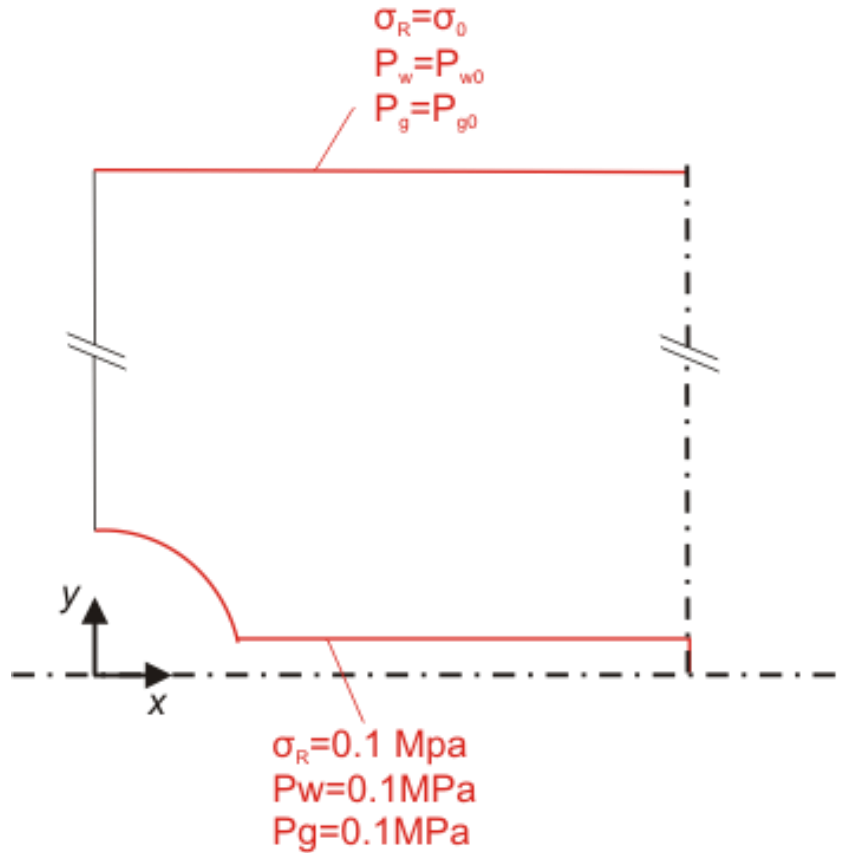
Drained condition  $\rightarrow P_w$  decreased to  $P_{atm}$

$P_g$  fixed



# UNSATURATED FLOW PROCESSES

## Boundary conditions - Step 1 : Excavation + Waiting phase



Waiting phase ( $\rightarrow$  2 years) :

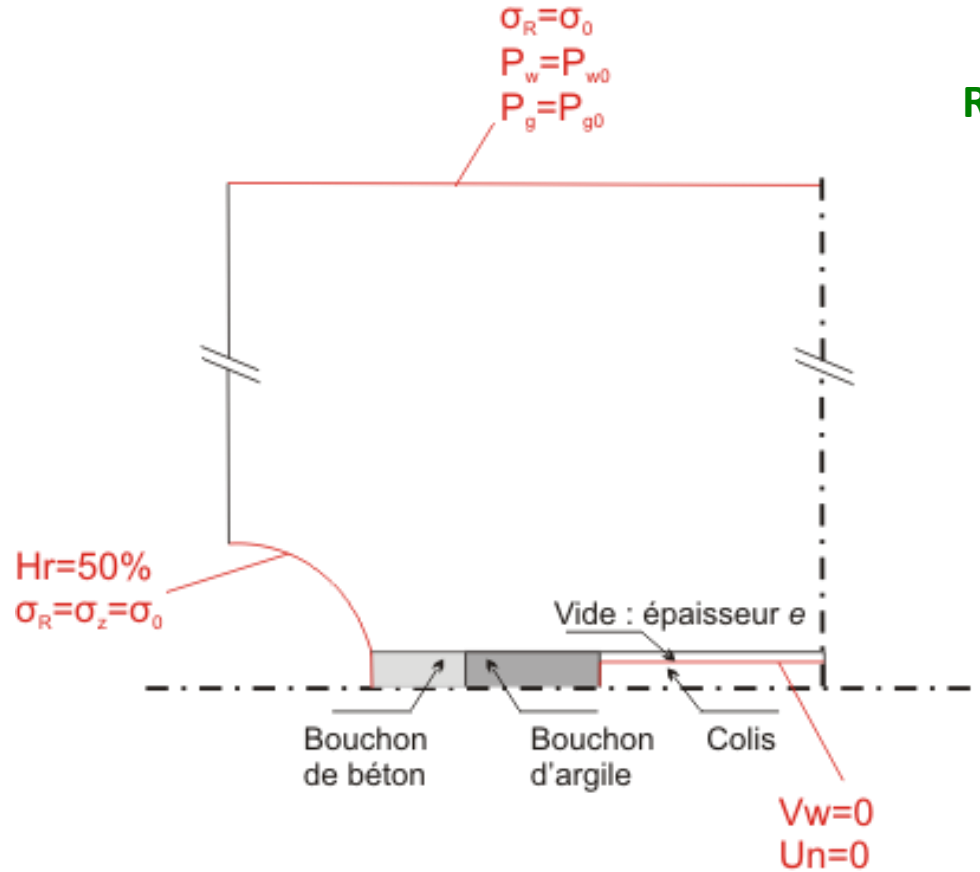
$$\sigma_R = 0.1 \text{ MPa}$$

Drained condition

$P_g$  fixed

# UNSATURATED FLOW PROCESSES

Boundary conditions - Step 2 : Activation of the plugs and the cannisters  
+ water Resaturation of the void space



Resaturation of the void space ( $\rightarrow$  3 years):

$P_g$  fixed

Main shaft

Constant relative humidity

$\sigma_R = \sigma_z = 0.1 \text{ MPa}$

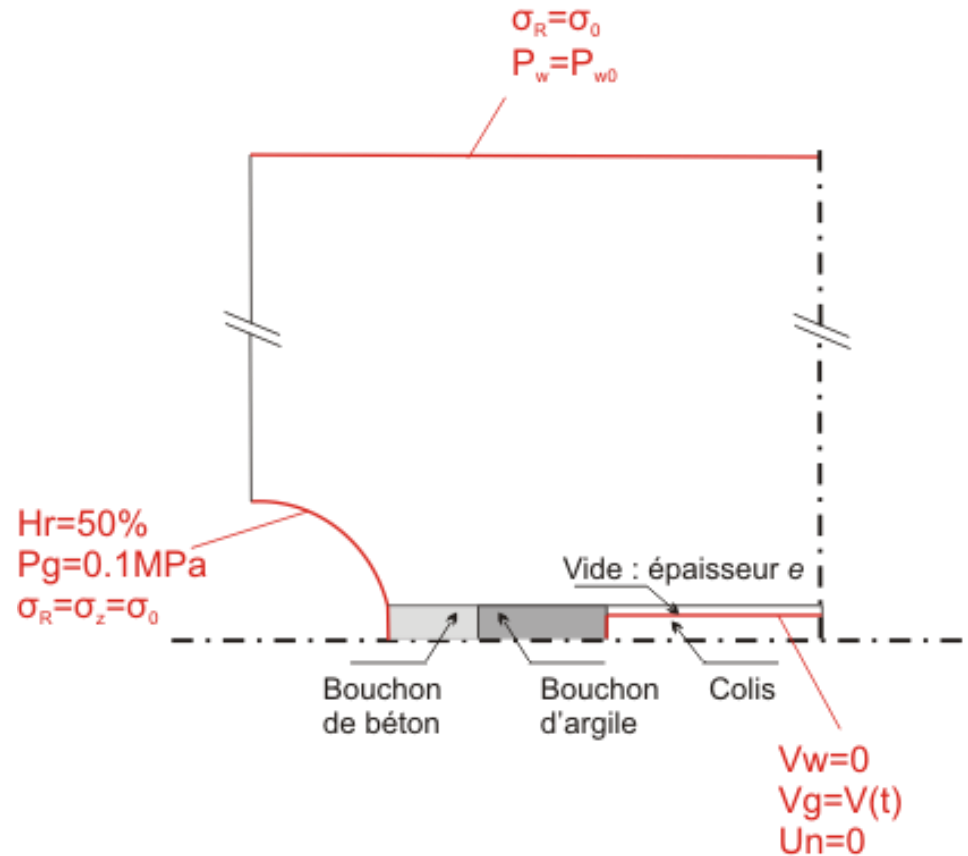
Alveole

Cannister: impervious to fluids  $\rightarrow$  Resaturation of the void space

Fixed radial displacement

# UNSATURATED FLOW PROCESSES

## Boundary conditions - Step 3 : Hydrogene Injection + Backfilling



### Hydrogene Injection without backfill (3 → 100 years):

#### Main drift

Constant relative humidity

$P_g = 0.1 \text{ MPa}$  at the wall

$\sigma_R = \sigma_z = 0.1 \text{ MPa}$

#### Alveole

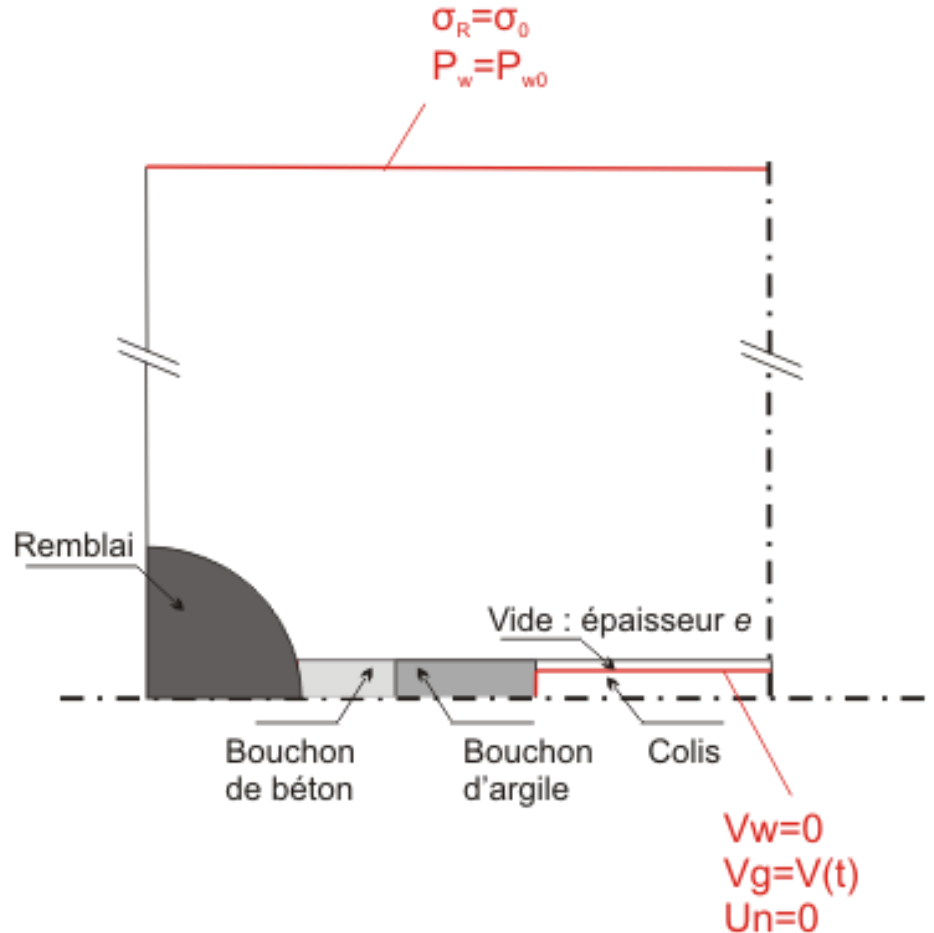
Cannister impervious to fluid

Hydrogene flux imposed at the wall

Fixed radial displacement

# UNSATURATED FLOW PROCESSES

## Boundary conditions - Step 3 : Hydrogene Injection + Backfilling



Hydrogene injection with the backfill  
(100 → 100 000 years):

Main drift

-

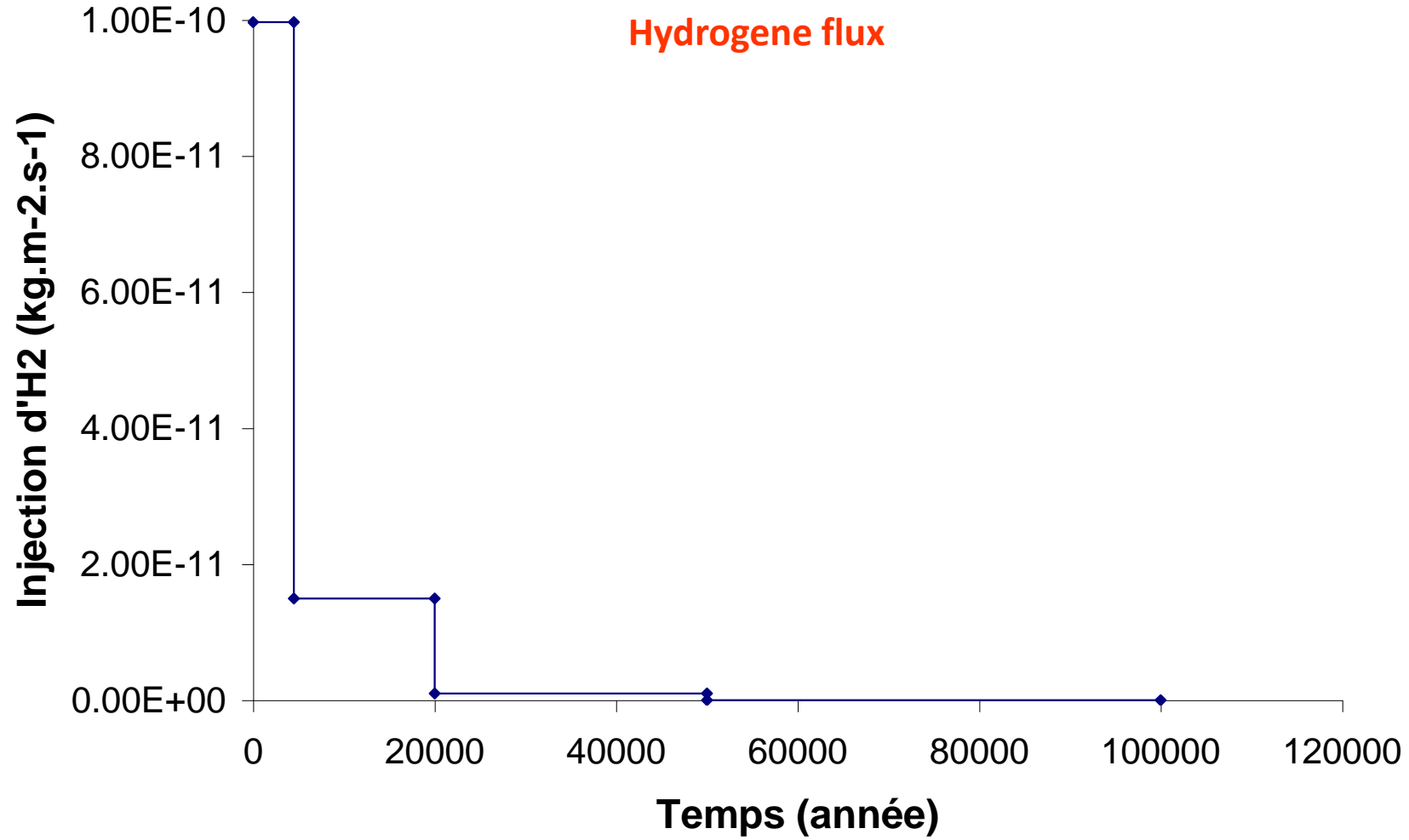
Alveole

Cannister impervious to fluid

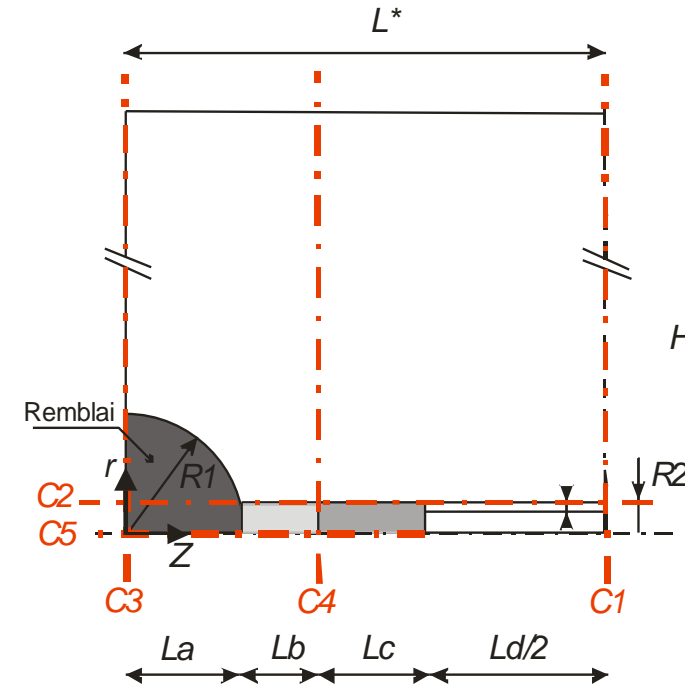
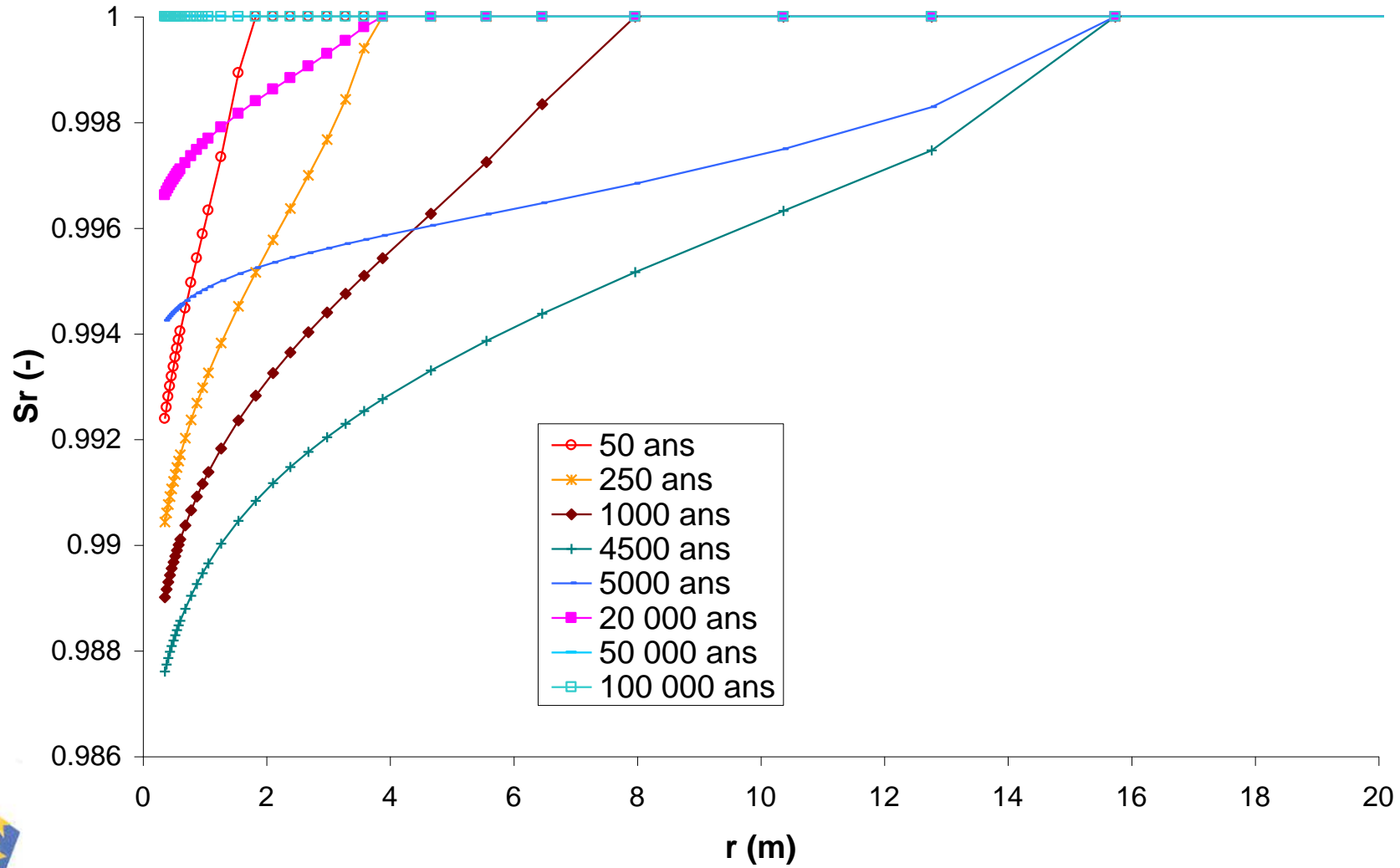
Hydrogene flux imposed at the wall

Fixed radial displacement

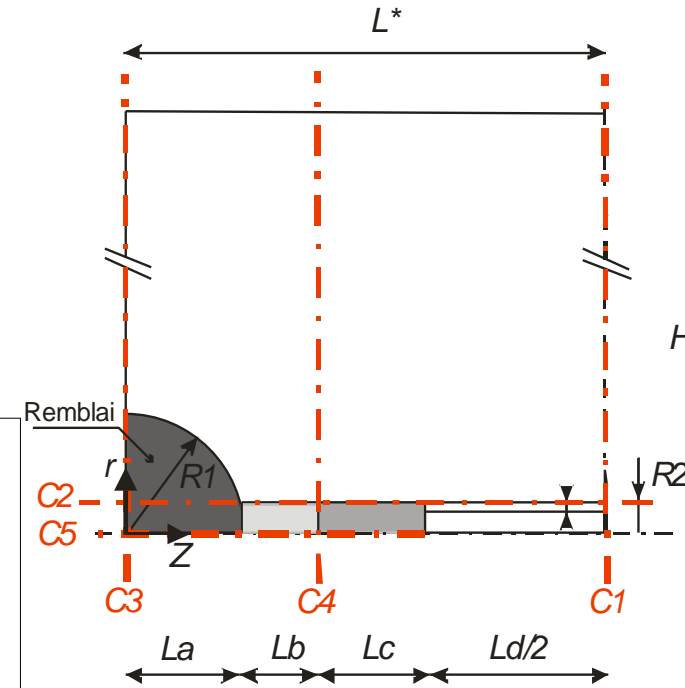
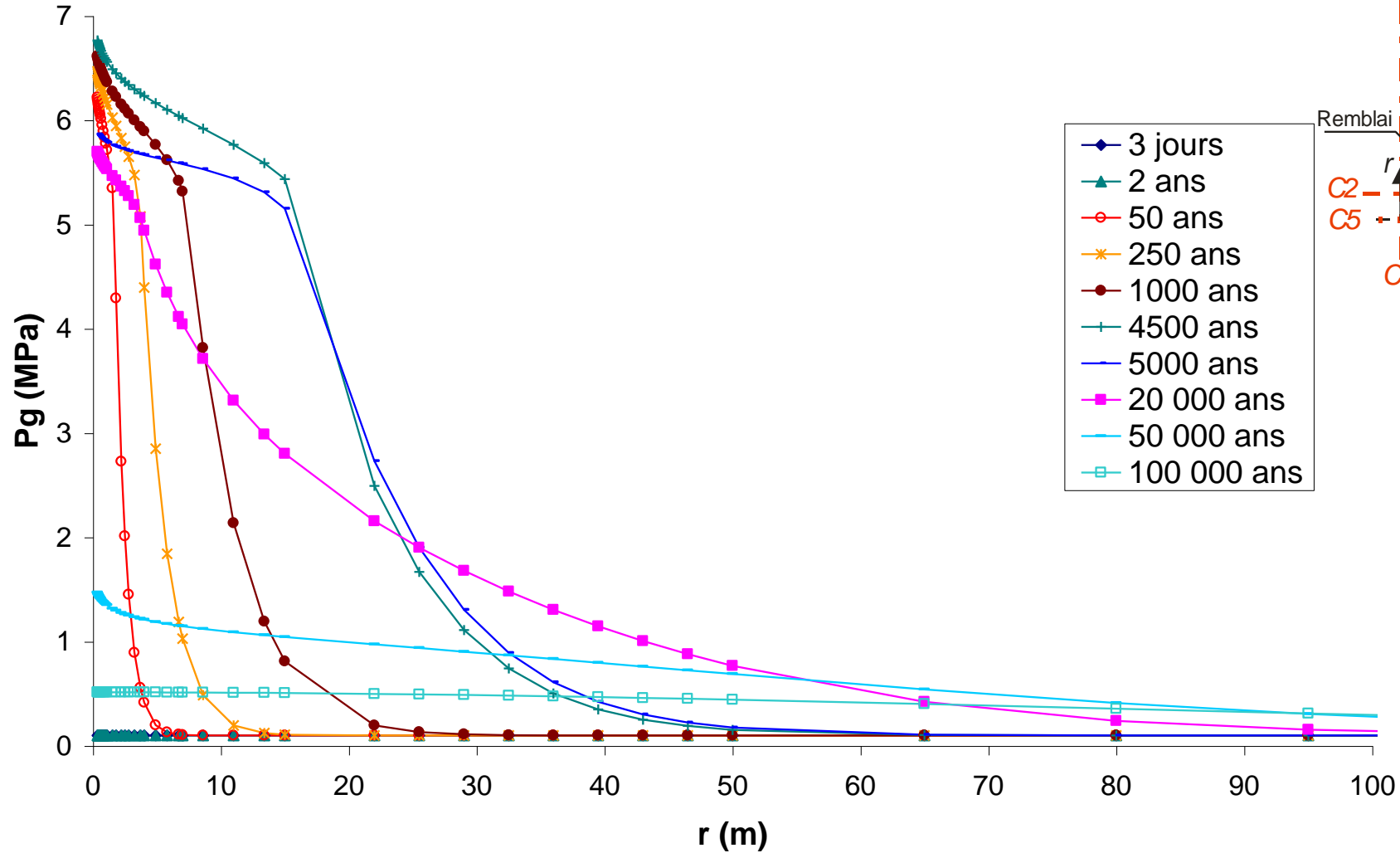
# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

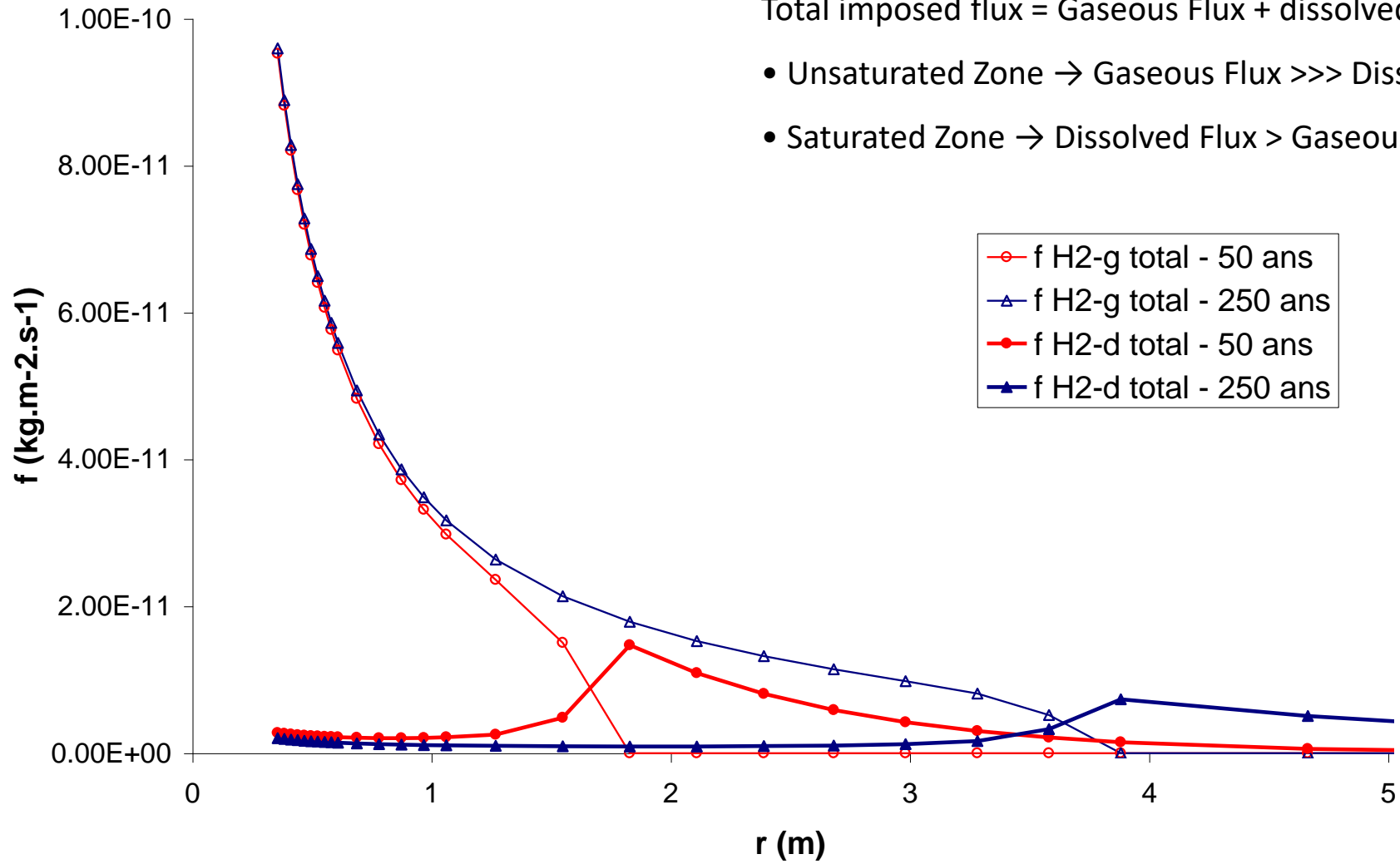


# UNSATURATED FLOW PROCESSES





# UNSATURATED FLOW PROCESSES

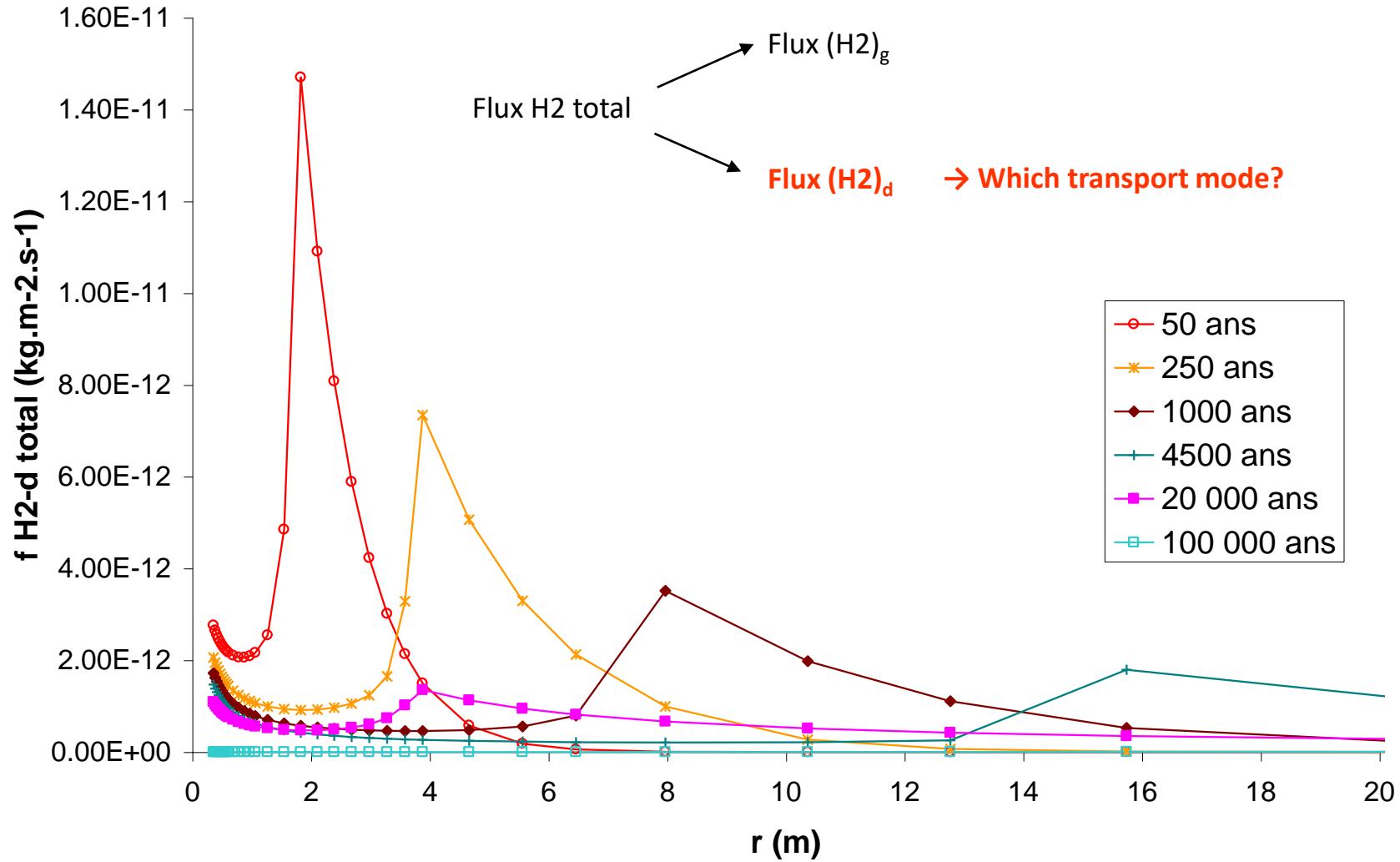


Total imposed flux = Gaseous Flux + dissolved Flux

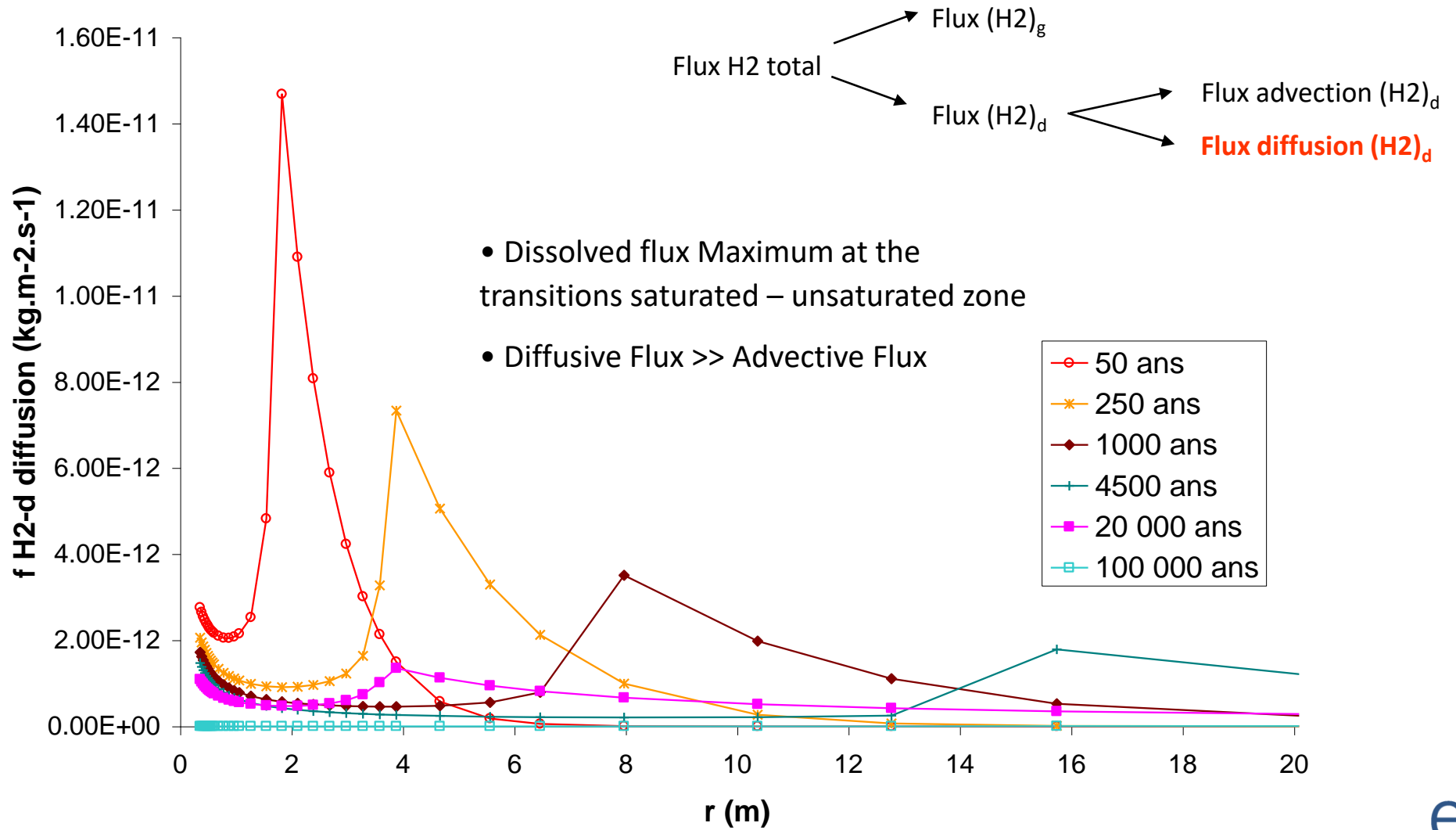
- Unsaturated Zone  $\rightarrow$  Gaseous Flux  $\gg$  Dissolved Flux
- Saturated Zone  $\rightarrow$  Dissolved Flux  $>$  Gaseous Flux



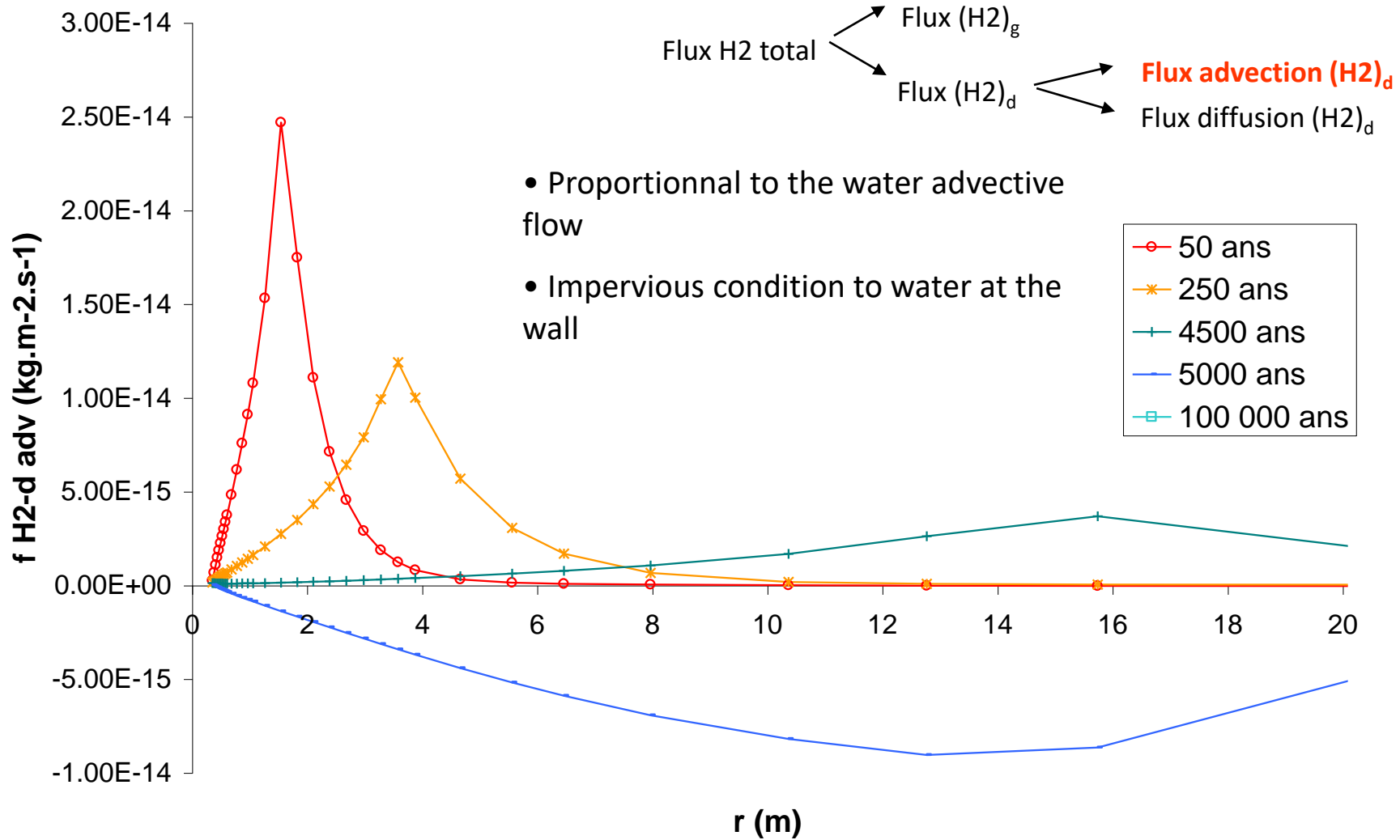
# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

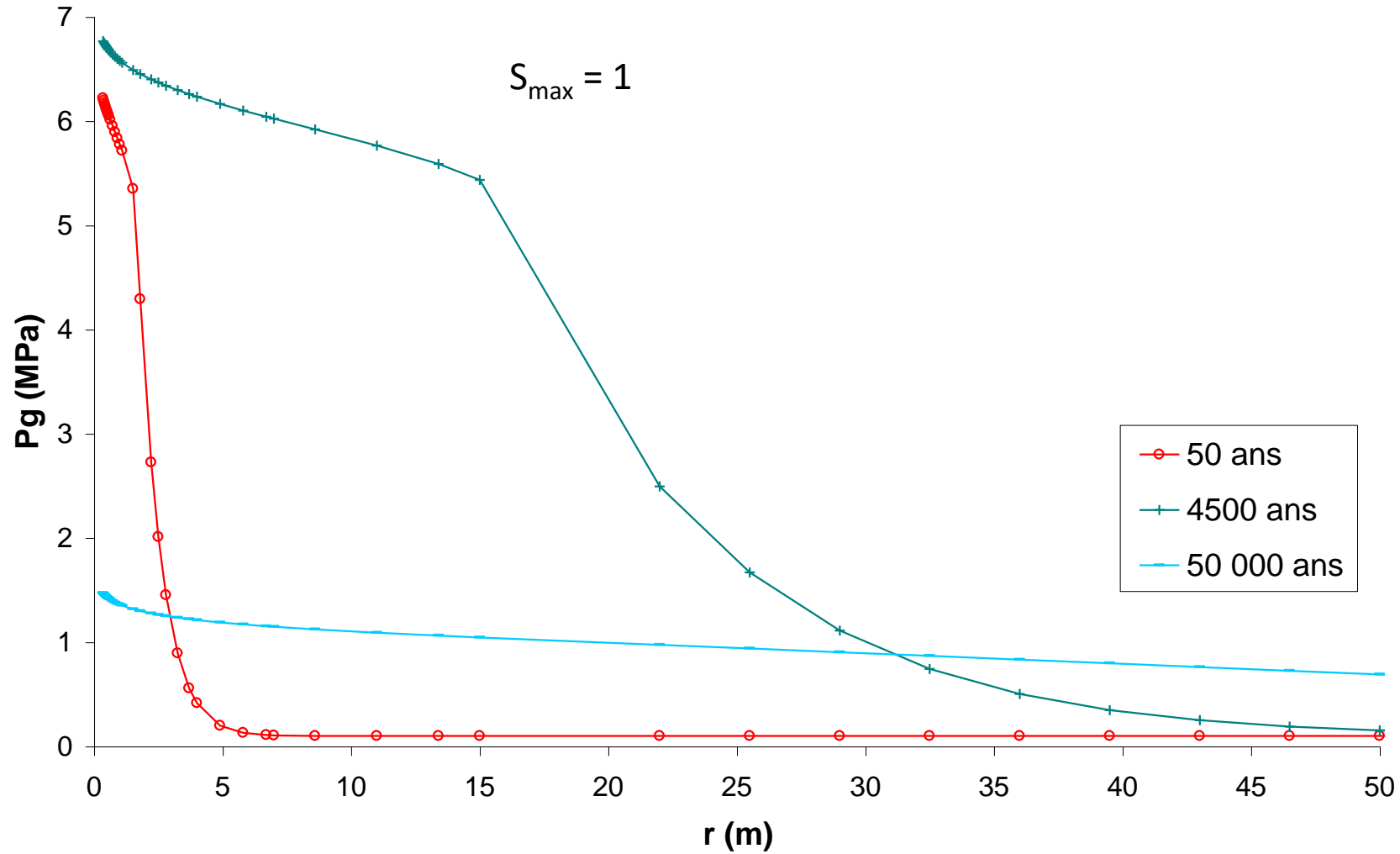
## Retention curve

$$S_{r,w} = S_{res} + \frac{S_{max} - S_{res}}{\left[1 + \left(\frac{p_c}{P_r}\right)^n\right]^m}$$

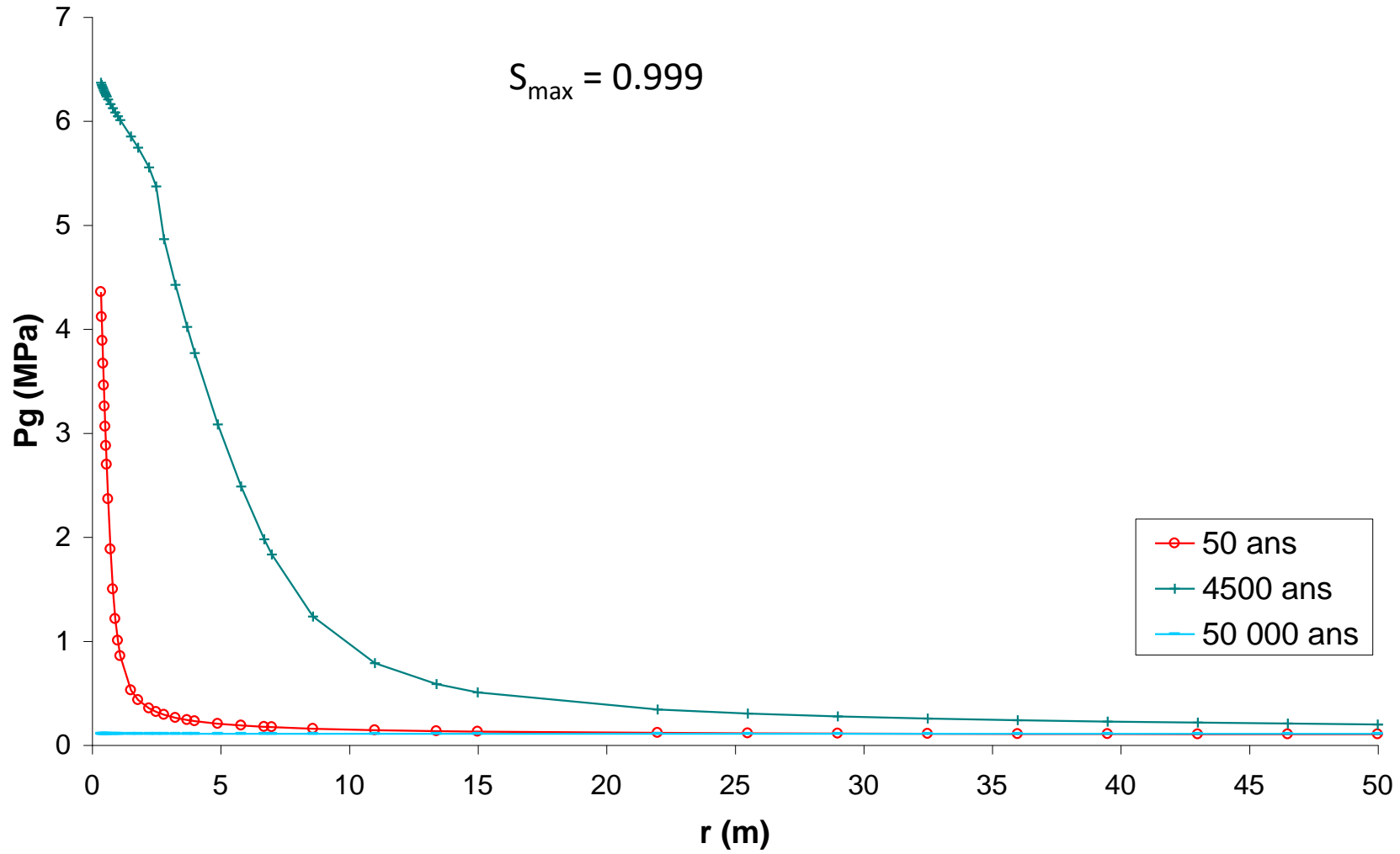
If  $S_{max} < 1 \rightarrow H_2$  injection is easier  
 $\rightarrow P_g \downarrow$



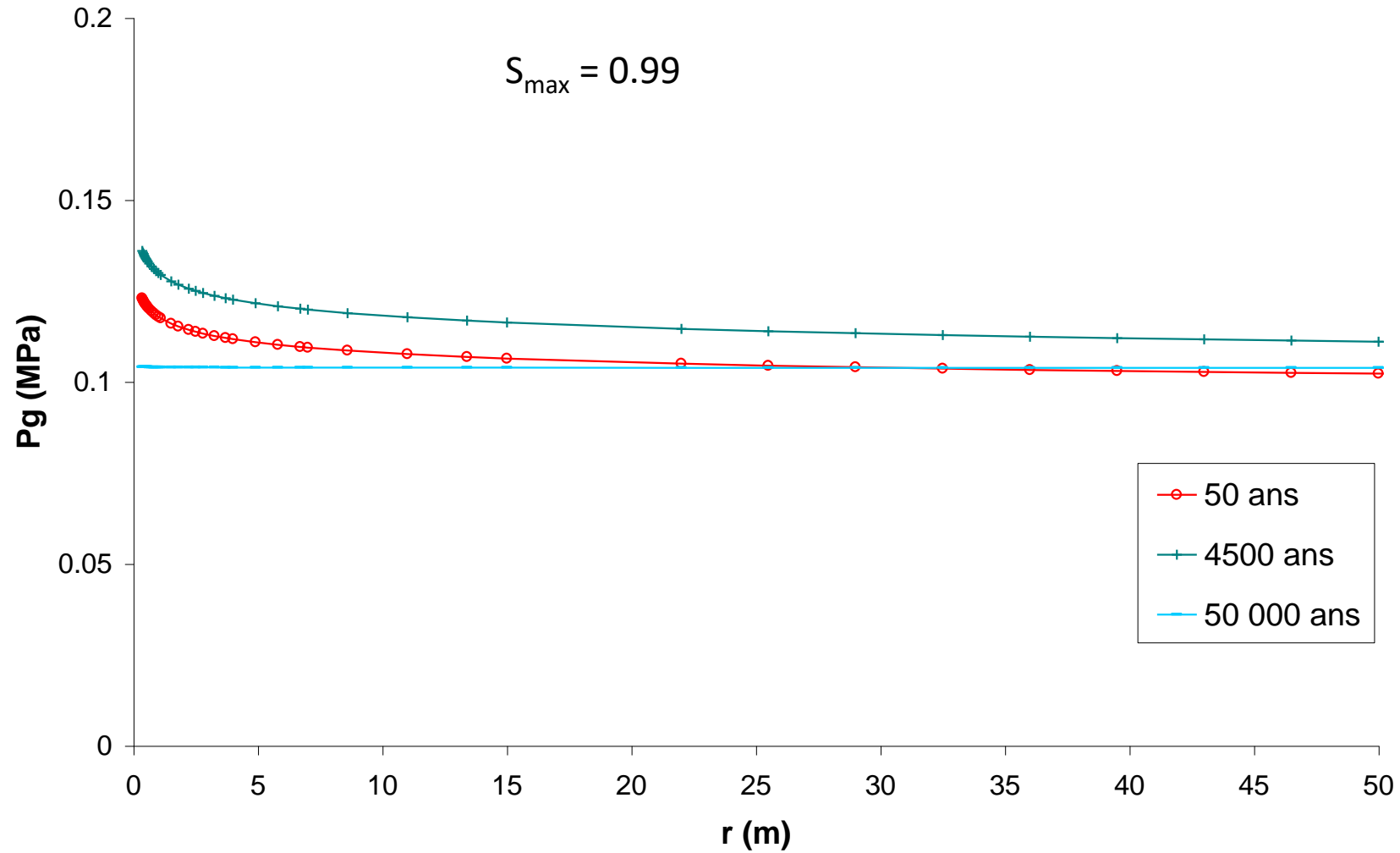
# UNSATURATED FLOW PROCESSES



# UNSATURATED FLOW PROCESSES

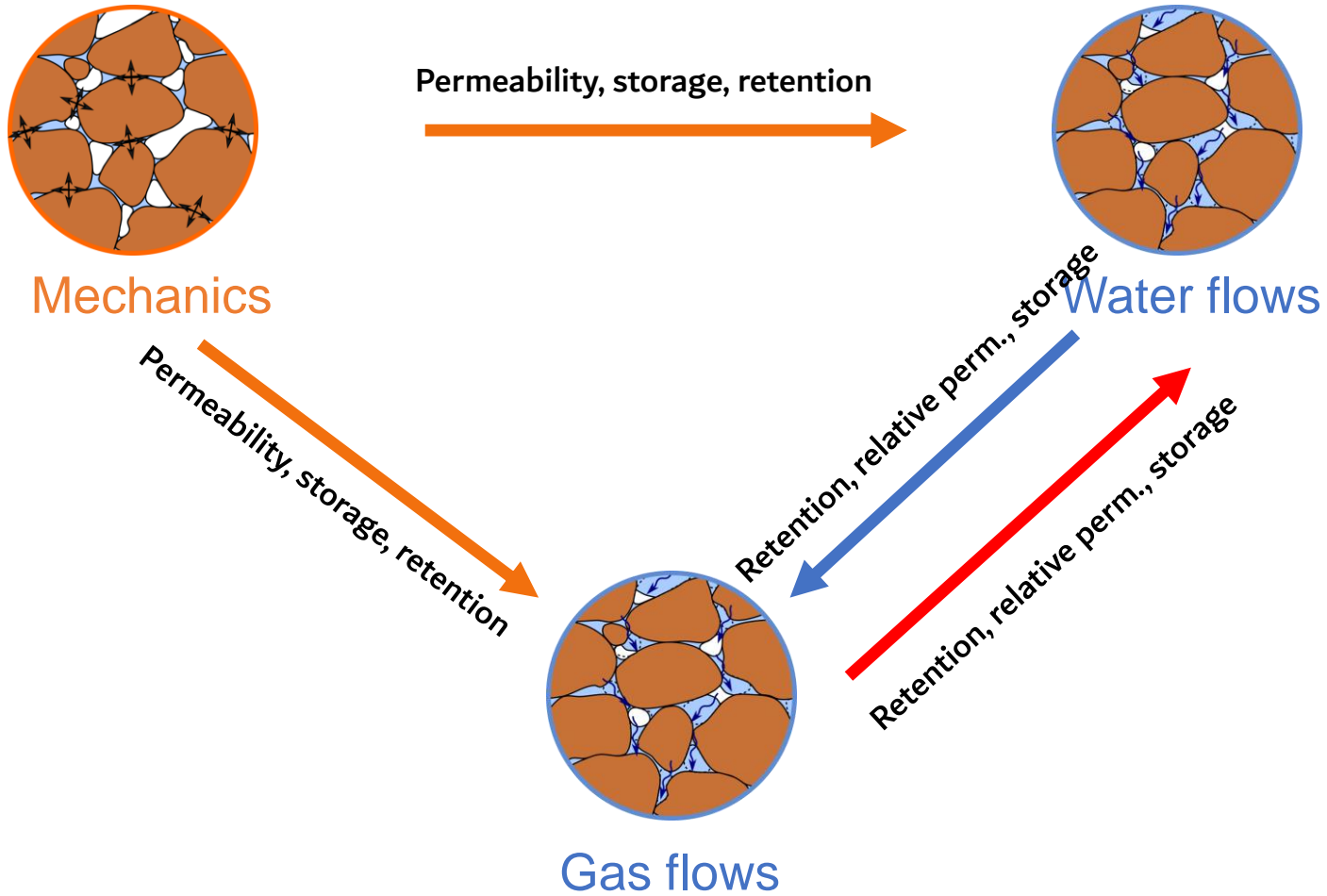


# UNSATURATED FLOW PROCESSES





# UNSATURATED FLOW PROCESSES





## TABLE OF CONTENT

1. WELCOME
2. INTRODUCTION
3. THERMO-HYDRAULIC PROCESSES (saturated conditions)
4. UNSATURATED FLOW PROCESSES
- 5. THMG PROCESSES**





## THMG PROCESSES

### Mechanical behaviour

The mechanical behaviour of a gematerial is by essence highly complex:

- Non linear
- Reversible/Permanent deformation
- Time dependent behaviour
- Cyclic behaviour

In geomeachnics, the stress increment is generally computed from the strain increment as:

$$d\sigma = D(\sigma, \epsilon, \dot{\epsilon}, \kappa)d\epsilon$$

Where  $\sigma$  is the stress tensor,  $\epsilon$  the strain tensor,  $\kappa$  the internal variables





## THMG PROCESSES

### Mechanical behaviour

Contrary to classic continuous media, the mechanical behaviour of porous media is not only controlled by the total stress, but it is also influenced by the fluids occupying the porous space. Therefore, alternative stress variable(s) should be defined. In the case of saturated porous media, the concept of effective stress was early introduced by Terzaghi (1936).

Terzaghi (1936) introduced the concept of effective stress to describe the mechanical behavior of fully saturated porous media. The effective stress transforms a real multiphase porous medium into a mechanically equivalent single-phase continuum. It is defined as:

$$\sigma'_{ij} = \sigma_{ij} - u_w \delta_{ij}$$

And the previous relationship is written as:

$$d\sigma' = D(\sigma', \epsilon, \dot{\epsilon}, \kappa) d\epsilon$$

Where  $\sigma'$  is the effective stress tensor,  $\epsilon$  the strain tensor,  $\kappa$  the internal variables





## THMG PROCESSES

### Mechanical behaviour in unsaturated medium

The choice of constitutive variables is an inevitable issue in modelling unsaturated soils. Over the years, the choice of appropriate stress variables to model the behaviour of unsaturated soils has indeed been an intensively debated issue. Two main approaches are generally distinguished:

- The extension of the effective stress definition for saturated porous media towards unsaturated states;
- The definition of two independent stress variables (while only one, the effective stress, is used for saturated media).

Each of these two approaches has advantages and drawbacks. They are briefly described in the next two sections. Further discussion and historical review can be found in Khalili et al. (2004) and Nuth & Laloui (2008b).





## THMG PROCESSES

### Mechanical behaviour in unsaturated medium

#### *Extension of the effective stress definition*

In the effective stress approach, Terzaghi's definition of the effective stress is extended to the partial saturation domain. One of the most famous definition was proposed by Bishop (1959). It is given by:

$$\sigma'_{ij} = \sigma_{ij} - u_a \delta_{ij} + \chi(u_a - u_w) \delta_{ij}$$

where  $\chi$  is a material parameter, called Bishop's parameter, which depends on the degree of saturation. It takes the value of 1 for fully saturated states and 0 for totally dry states. Experimental results on unsaturated soils evidence the relation between  $\chi$  and the degree of saturation (Jennings & Burland, 1962; Fredlund & Rahardjo, 1993). Note that, since Bishop's stress depends on the material properties, it is not strictly speaking an effective stress (Sheng et al., 2008b).





## THMG PROCESSES

### **Mechanical behaviour in unsaturated medium**

#### *Extension of the effective stress definition*

When working with constitutive models for unsaturated soils, the main advantage of the effective stress approach is that the models previously developed for saturated soils are straightforwardly extended to the unsaturated domain. In addition, there is a continuous and smooth transition from saturated to unsaturated states. However, the determination of the different model parameters from laboratory tests is often complex.

The effective stress approach has shown limitations in representing the important swelling of compacted clays and bentonites. The approach is also incapable of reproducing the collapse phenomenon upon wetting paths under high stress levels. Indeed, upon hydration, the fluid pressure increases, producing a decrease in the effective stress. Accordingly, the material swells, while compaction is observed experimentally.

In order to overcome this issue, constitutive models written in terms of a generalized effective stress generally introduce suction as a variable and define a Loading-Collapse curve, similarly to the Barcelona Basic Model.





## THMG PROCESSES

### Mechanical behaviour in unsaturated medium

#### *Independent variable approach*

According to Fredlund & Rahardjo (1993), the number of independent variables is directly linked to the number of phases. For a saturated porous material, only one variable is required: the effective stress. For partially saturated soils, Coleman (1962), Bishop & Blight (1963), Fredlund & Morgenstern (1977) and Alonso et al. (1990), among others, showed that two independent variables enable to overcome the limitations of the single effective stress. In particular, Fredlund & Morgenstern (1977) demonstrated that any pair of net stress, effective stress and suction.

$$\bar{\sigma}_{ij} = \sigma_{ij} - u_a \delta_{ij}$$

The couple of variables net stress and suction is primarily justified by the fact that the variables are directly accessible during experimental tests. Once that the material is saturated, the effective stress is often used instead of the net stress.



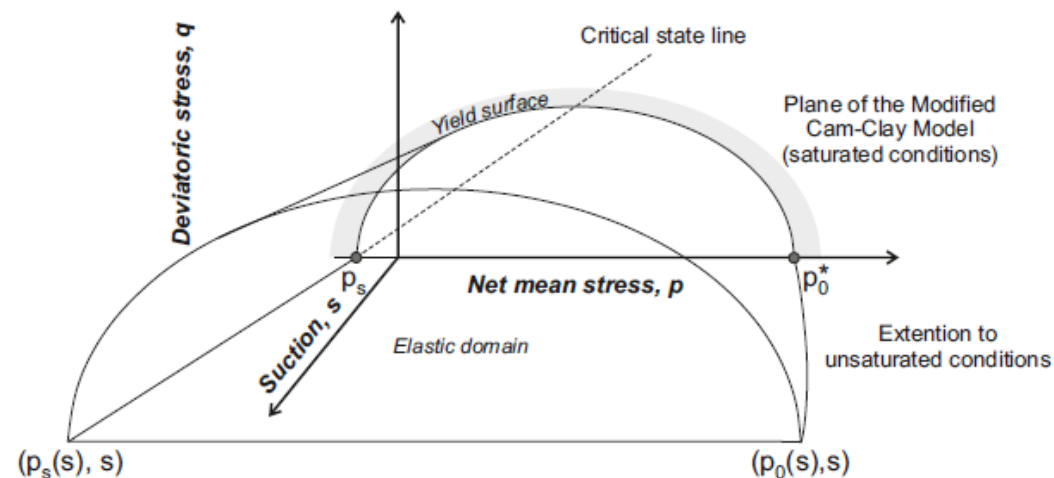


## THMG PROCESSES

### Mechanical behaviour in unsaturated medium

#### *Independent variable approach*

The first and most famous complete constitutive model for unsaturated soils is the Barcelona Basic Model (BBM) developed by Alonso et al. (1990). The model uses suction and net stress as independent variables. As an extension of the Modified Cam-Clay model (Roscoe & Burland, 1968), the Barcelona Basic Model is formulated in the framework of elastoplasticity theory and critical state models. An important contribution of the BBM is the definition of the Loading-Collapse (LC) curve.



Three dimensional yield surface of Barcelona Basic Model (Alonso et al., 1990).



## THMG PROCESSES

### Mechanical behaviour in unsaturated medium and non-isothermal conditions

Following the same approach of independent variables:

$$d\bar{\sigma} = D(\bar{\sigma}, \epsilon, \dot{\epsilon}, \kappa, s, T)d\epsilon + hds + \beta dT$$

Where  $h$  constitutive vector net stress-suction and  $\beta$  is the constitutive vector net stress temperature.





## THMG PROCESSES

### Mechanical behaviour in unsaturated medium and non-isothermal conditions

#### *Mechanical problem*

Soils and rocks have a non linear behaviour and may undergo very large deformations. Lagamine code has been developed in the context of large strain, large displacement problems.

In this case, the initial configuration is different from the actual one. One may write the balance equations in the initial configuration or in the current one.

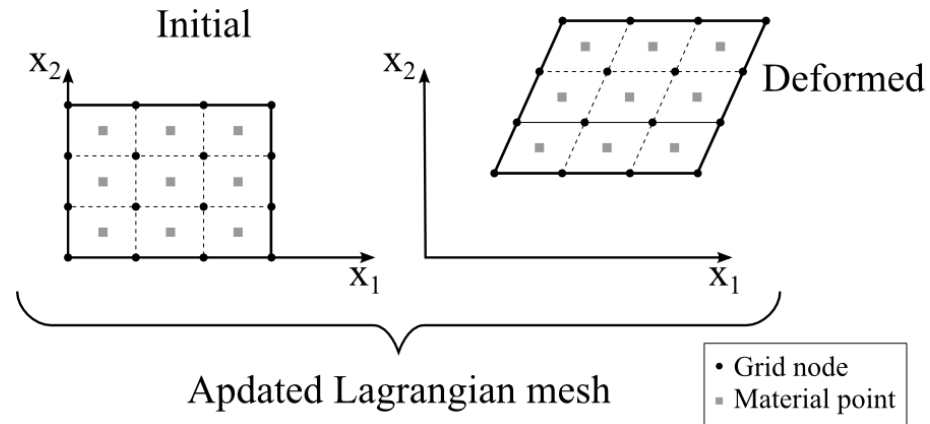
This latter choice is made in Lagamine code: we use the actualised deformed configuration as reference one (**Up-dated Lagrangian formulation**).

The flow problem is also written in this actualised deformed configuration and the modification of water storage due to solid displacement is therefore implicitly taken into account.



## THMG PROCESSES

### Mechanical behaviour in unsaturated medium and non-isothermal conditions



Among the different types of stress formulation (and the deformations associated with them), we will use the Cauchy stress tensor and the Cauchy strain rate defined as:

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left( \frac{\partial \dot{u}_i}{\partial x_j} + \frac{\partial \dot{u}_j}{\partial x_i} \right)$$

### Solid Mass Balance

As far as the reference configuration follows the solid phase, the solid mass balance equation is automatically met.

It provides the porosity evolution equation:

$$d\varphi = (b - \varphi) \cdot \left( d\varepsilon_v + \frac{S_{r,w} \cdot dp_w + S_{r,g} \cdot dp_g + (p_g - p_w) dS_{r,w}}{K_s} - 3\alpha_s dT \right)$$

### Linear momentum Balance

$$\text{div}(\sigma_{ij}) + \rho g_i = 0$$

Where  $\sigma_{ij}$  is the total stress tensor and  $\rho$  is the bulk density of the soil



### Water Mass Balance

$$\frac{\partial}{\partial t} (\rho_w n S_{rw}) + \text{div}(\underline{f}_w) + \frac{\partial}{\partial t} (\rho_v n S_{rg}) + \text{div}(\underline{f}_v) - Q_w = 0$$

Liquid water,  $S_{rw}$  water saturation degree

Water vapour,  $S_{rg} = 1 - S_{rw}$  gas saturation degree

Source term

### Gas Mass Balance

$$\frac{\partial}{\partial t} (\rho_{d,a} n S_{rw}) + \text{div}(\underline{f}_{d,a}) + \frac{\partial}{\partial t} (\rho_a n S_{rg}) + \text{div}(\underline{f}_a) - Q_a = 0$$

Dissolved air,  $S_{rw}$  water saturation degree

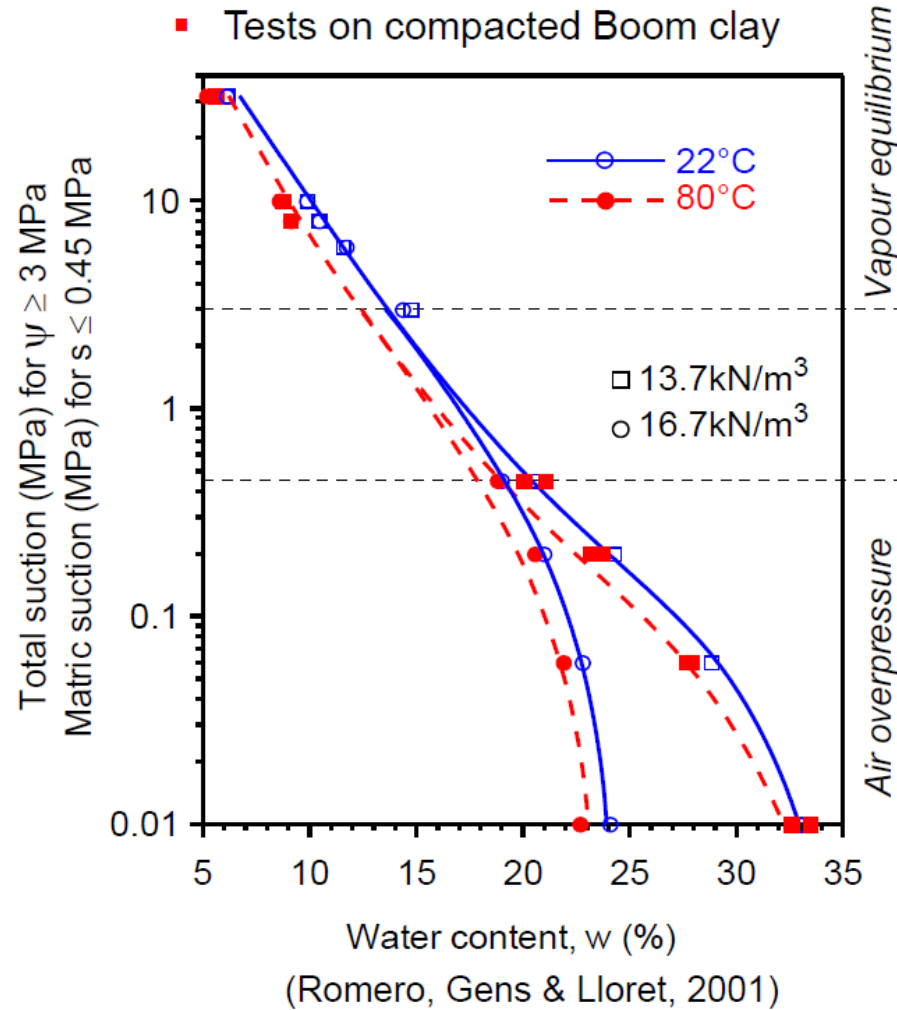
Dry air,  $S_{rg} = 1 - S_{rw}$  gas saturation degree

Source term



# THMG PROCESSES

## Retention properties: influence of the temperature



### Retention properties: influence of the temperature

In the Van Genuchten expression,  $P_r$  is a function of the air entry pressure depending on the max. pore radius and the surface tension:

$$P_r = \frac{2\sigma_{G-L}}{r}$$

And the surface tension depends on the temperature as:

$$\sigma_{G-L} = 0.0359 \exp\left(\frac{252.93}{T}\right)$$

The  $P_r$  parameter can thus be adapted as:

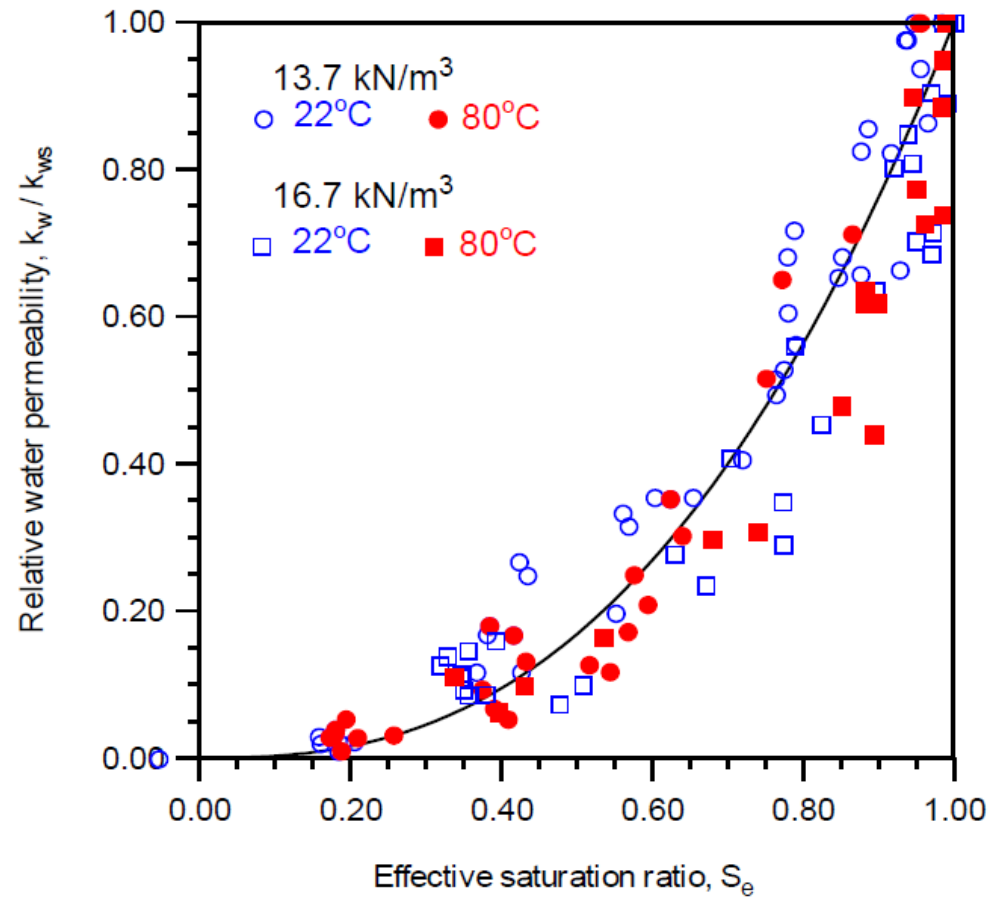
$$\frac{P_r(T)}{P_r(T_0)} = \frac{\sigma_{G-L}(T)}{\sigma_{G-L}(T_0)}$$





# THMG PROCESSES

## Relative water permeability: influence of the temperature



(Romero, Gens & Lloret, 2001)



Internal energy Balance

$$\frac{\partial S_T}{\partial t} + \text{div}(\underline{V}_T) + \dot{E}_{H_2O}^{w \rightarrow v} L - Q_T = 0$$

$$\begin{aligned} S_T &= n \rho_w S_{rw} c_{pw} (T - T_0) + n \rho_v S_{rg} c_{pv} (T - T_0) + n \rho_a S_{rg} c_{pa} (T - T_0) \\ &+ n \rho_{da} S_{rw} c_{pda} (T - T_0) + (1 - n) \rho_s c_{ps} (T - T_0) \end{aligned}$$

$$\underline{V}_T = -\Gamma \nabla T + c_{pw} \rho_w \underline{q}_l (T - T_0) + c_{pv} (\rho_v \underline{q}_g + \underline{i}_v) (T - T_0) + c_{pa} (\rho_a \underline{q}_g + \underline{i}_a) (T - T_0)$$

Water vapour mass balance equation :  $\frac{\partial S_v}{\partial t} + \text{div}(\underline{f}_v) - \dot{E}_{H_2O}^{w \rightarrow v} = 0$



## Internal energy Balance

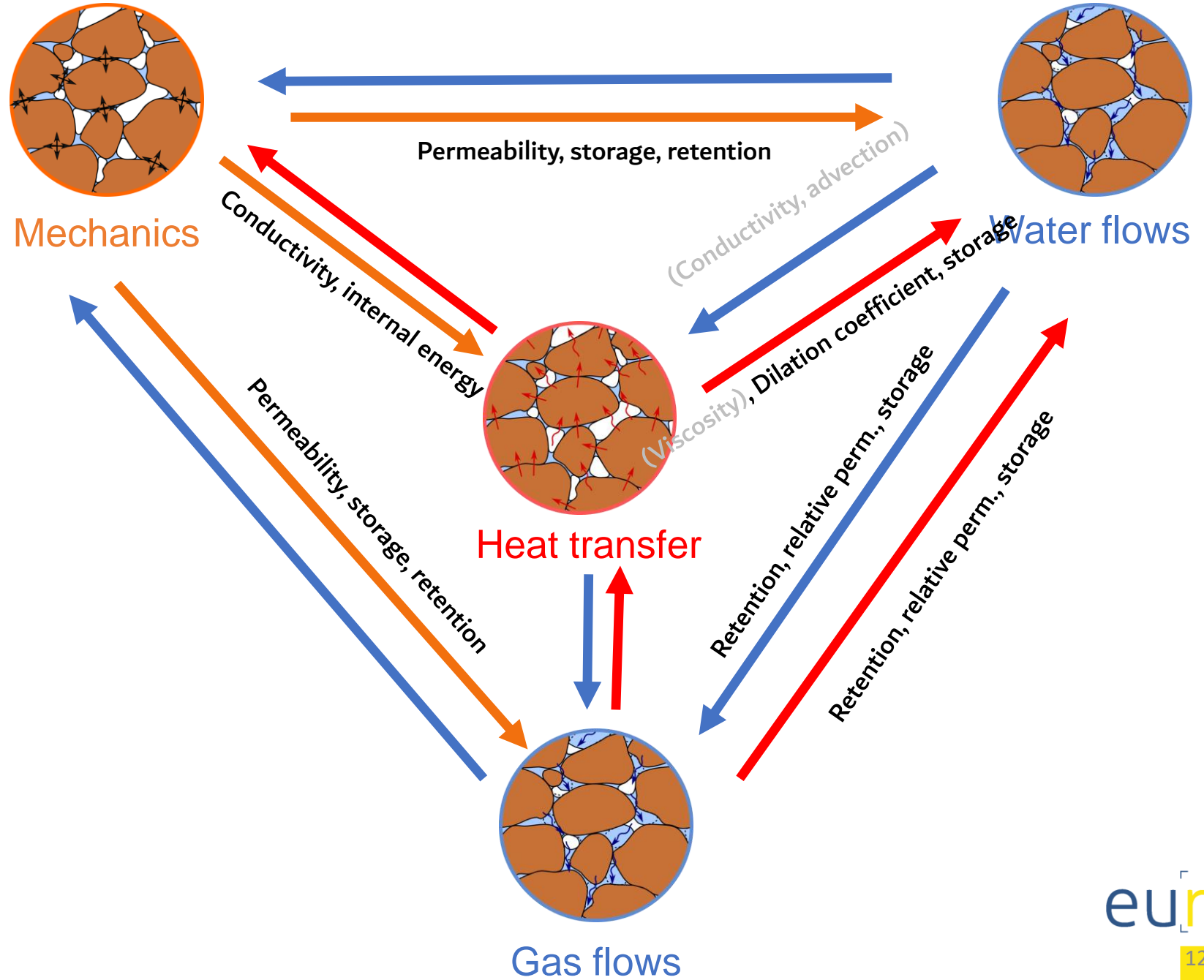
$$\frac{\partial S_T}{\partial t} + \text{div}(\underline{V}_T) + \left( \frac{\partial S_v}{\partial t} + \text{div}(\underline{f}_v) \right) L - Q_T = 0$$

$$S_T^* = n \rho_w S_{rw} c_{pw} (T - T_0) + n \rho_v S_{rg} c_{pv} (T - T_0) + n \rho_a S_{rg} c_{pa} (T - T_0) + n \rho_{da} S_{rw} c_{pda} (T - T_0) + (1 - n) \rho_s c_{ps} (T - T_0) + L n S_{rg} \rho_v$$

$$\begin{aligned} V_T^* &= -\Gamma \nabla T + c_{pw} \rho_w \underline{q}_l (T - T_0) + c_{pv} (\rho_v \underline{q}_g + \underline{i}_v) (T - T_0) \\ &+ c_{pa} (\rho_a \underline{q}_g + \underline{i}_a) (T - T_0) + (\rho_v \underline{q}_g + \underline{i}_v) L \end{aligned}$$



# THMG PROCESSES



# THMG PROCESSES

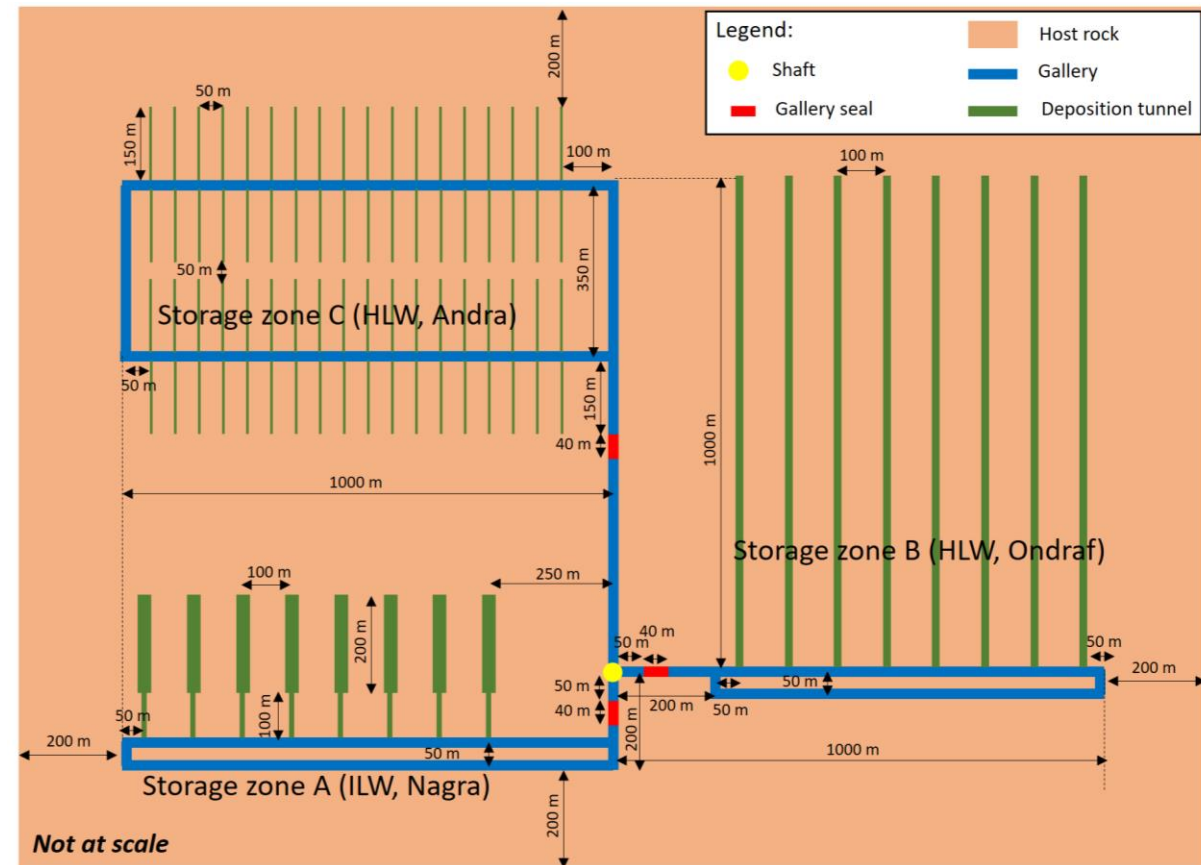
## TASK 4.2: MECHANISTIC UNDERSTANDING OF GAS TRANSPORT AT THE SCALE OF A REPOSITORY

- Preliminary Technical Information
  - Generic repository configuration with material parameters for three cases:
    - Storage Zone A (ILW, NAGRA)
    - Storage Zone B (HLW, ONDRAF)
    - Storage Zone C (HLW, ANDRA)
  - Initial boundary conditions in terms of  $T$ ,  $P_W$  and  $\sigma_{v/h}$
  - Time varying conditions

Stage	Scenario	Time scale
1.	Initial stage (No repository)	$T < 0$
2.	Instantaneous excavation	$T = 0$
3.	Ventilation	$T = 0$ to 50 Years
4.	Waste emplacement	$T = 50$

• Source terms for temperature and gas injection

Schematic horizontal slice at generic repository depth

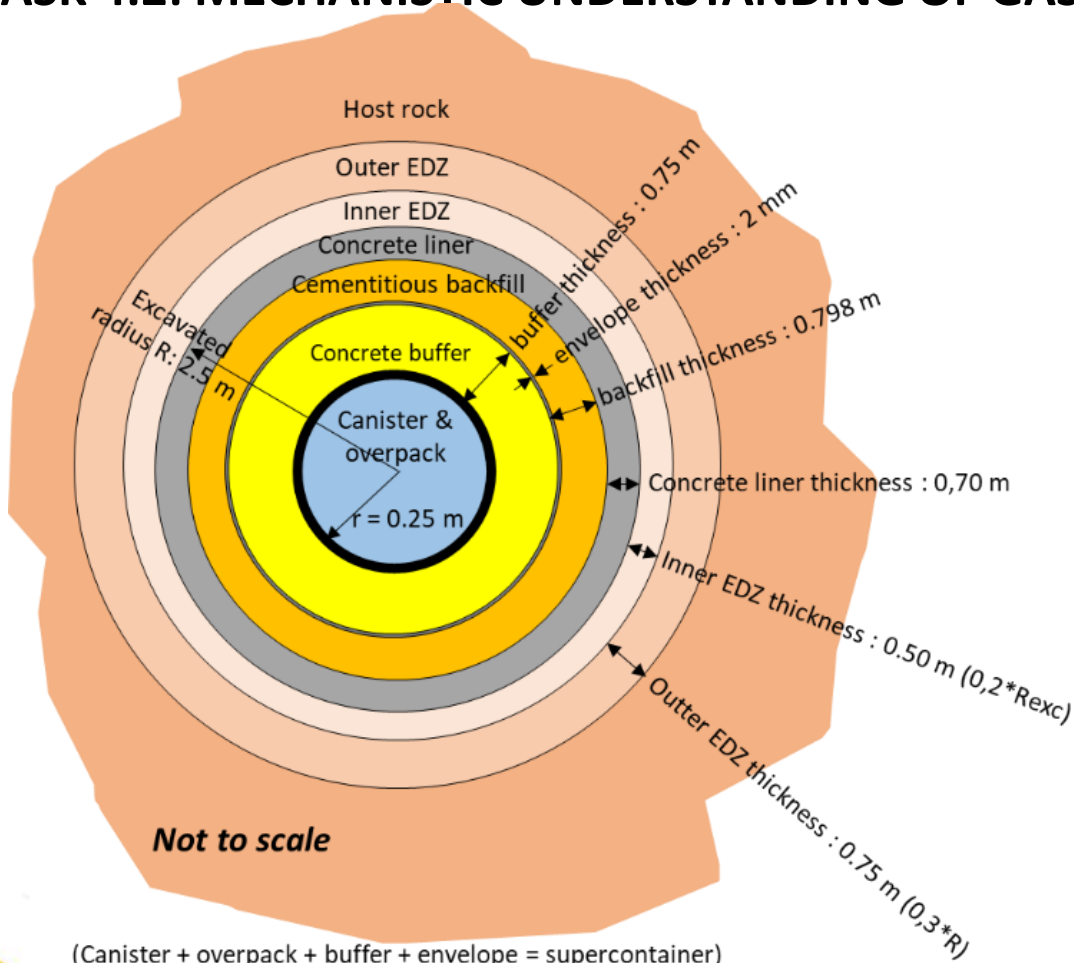


Not at scale

# THMG PROCESSES

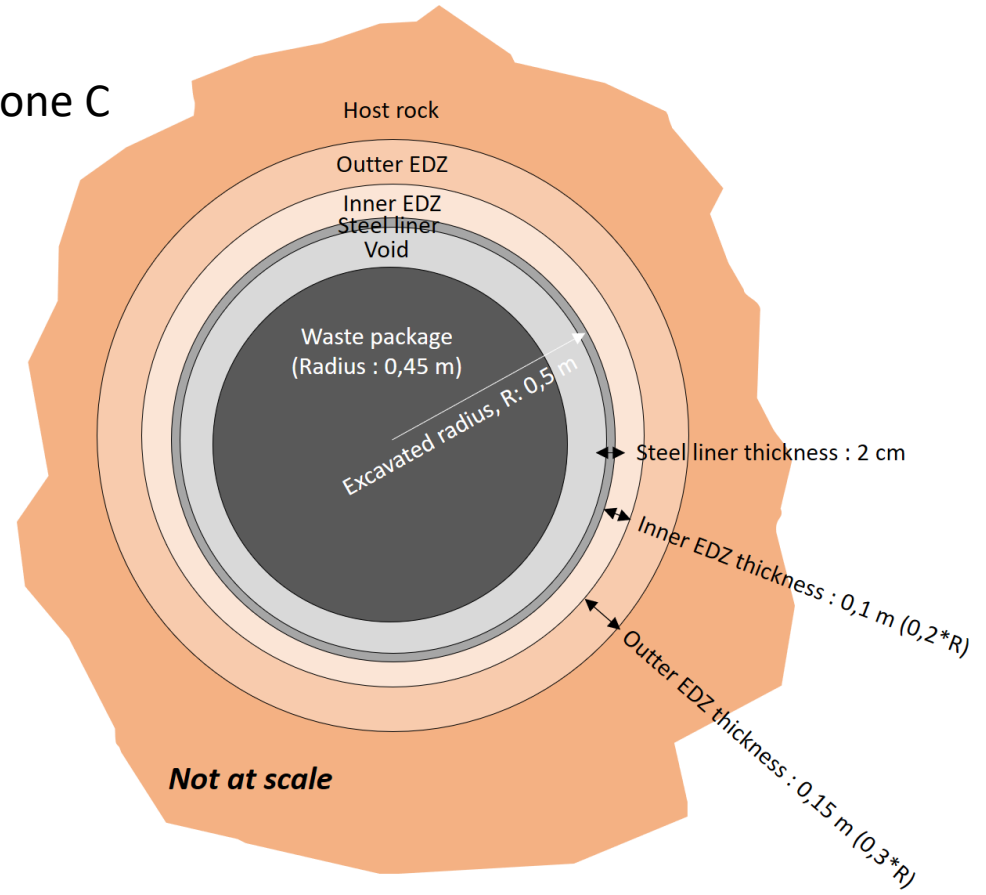
## TASK 4.2: MECHANISTIC UNDERSTANDING OF GAS TRANSPORT AT THE SCALE OF A REPOSITORY

Zone B



AA' vertical cross-section perpendicular to the axis of the tunnel

Zone C

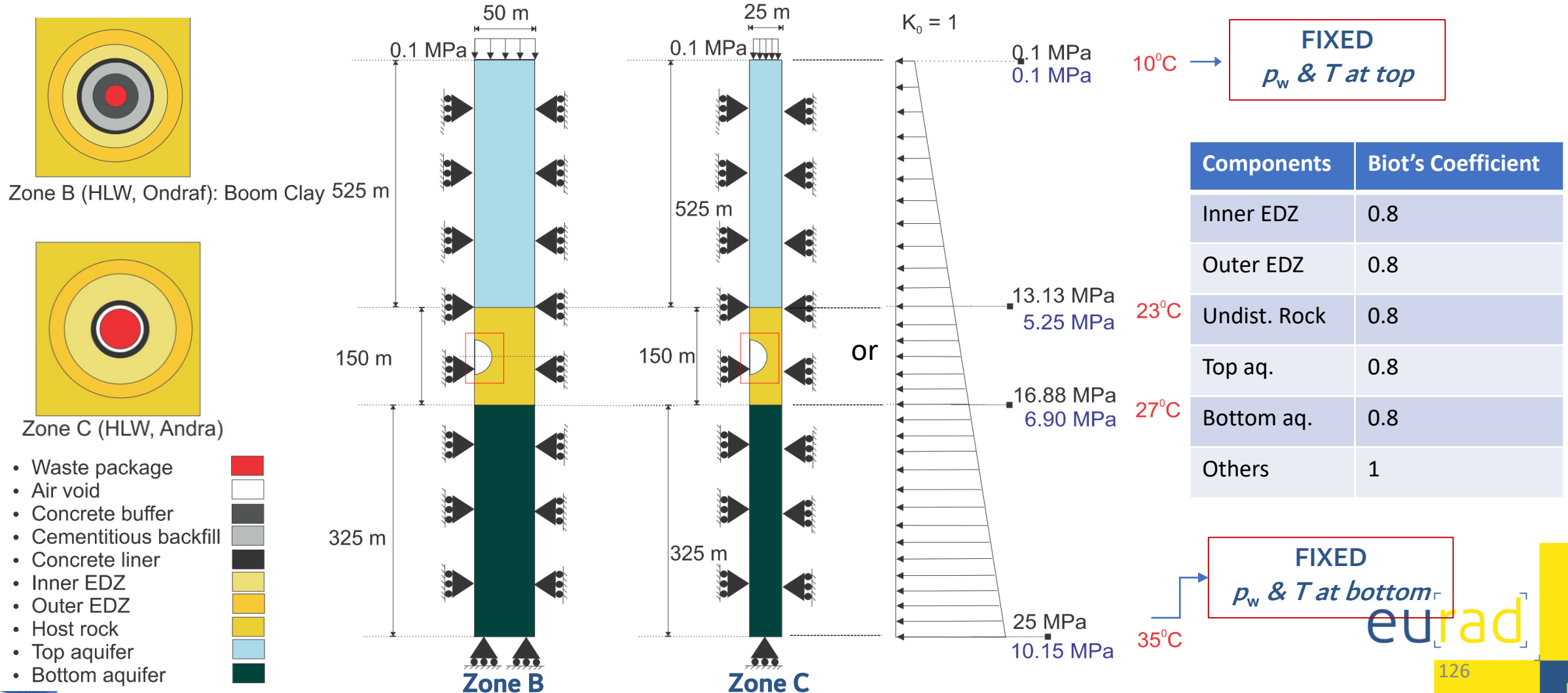


AA' vertical cut perpendicular to the axis of the tunnel



# THMG PROCESSES

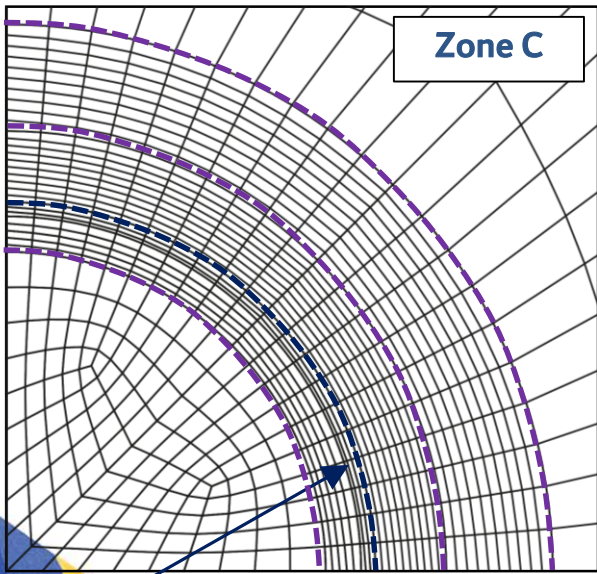
## TASK 4.2: MECHANISTIC UNDERSTANDING OF GAS TRANSPORT AT THE SCALE OF A REPOSITORY





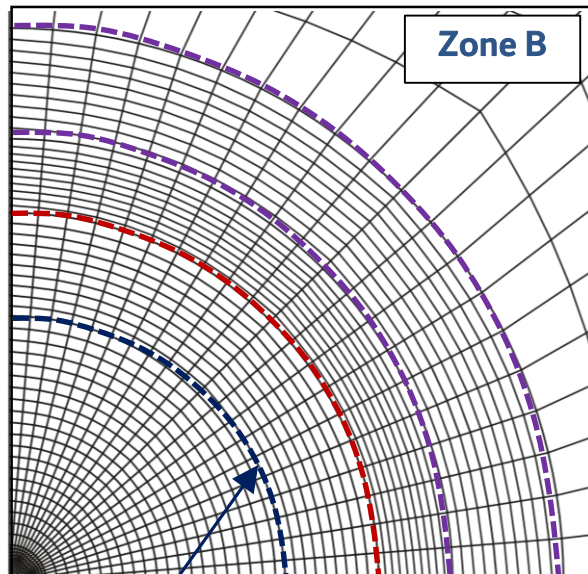
# THMG PROCESSES

Phase	Time [Years]	Scenario	Features
Initial	$T < 0$	No Repository (Instantaneous excavation)	<ul style="list-style-type: none"> <li>In-situ stress regime (<math>\sigma_v; \sigma_h</math>)</li> <li>Hydrostatic pressure (<math>p_w</math>)</li> <li>Natural geothermal field (<math>T</math>)</li> </ul>
Phase-I	$T = 0-50$	Ventilation (Zone B) Dewatering (Zone C)	<ul style="list-style-type: none"> <li>Ventilation/Dewatering effect                             <ul style="list-style-type: none"> <li>Zone B <math>\approx 80\%</math> RH (<math>s_t = 30.60</math> MPa)</li> <li>Zone C (<math>p_w \approx 0.1</math> MPa)</li> </ul> </li> </ul>
Phase-II	$T = 50-100,000$	Instantaneous waste emplacement	<ul style="list-style-type: none"> <li>Thermal load and gas generation (Hydrogen)</li> </ul>



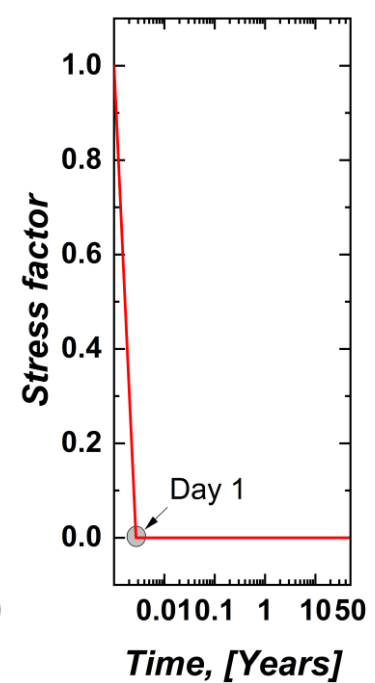
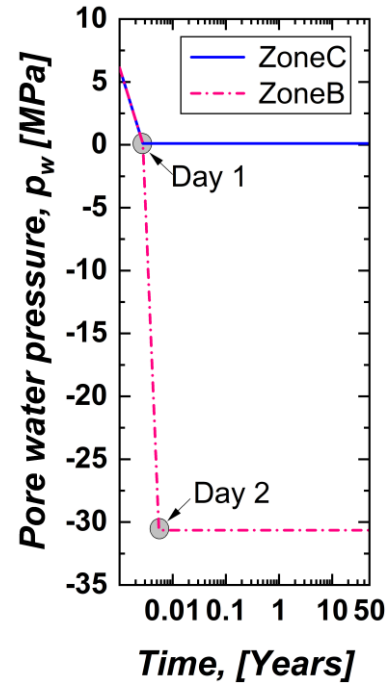
$p_w \approx 0.10$  MPa ( $r = 0.5$  m)

$R_{exc.} = 0.5$  m



$p_w = -30.60$  MPa ( $r = 1.8$  m)

$R_{exc.} = 2.5$  m

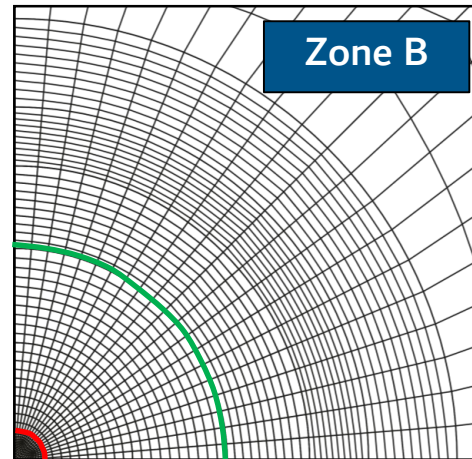




# THMG PROCESSES

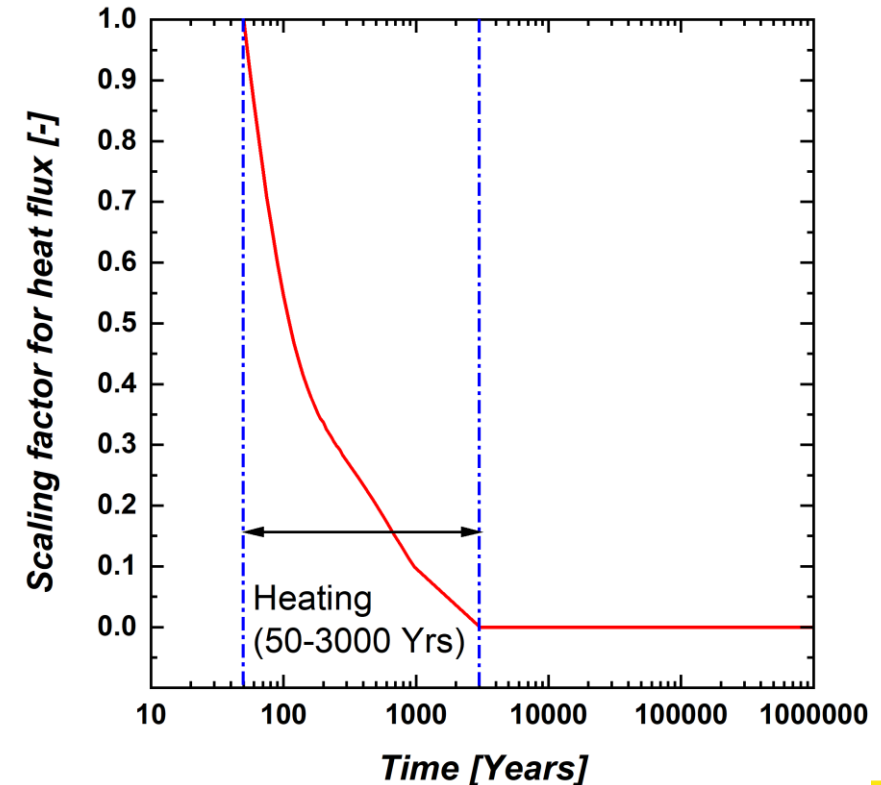
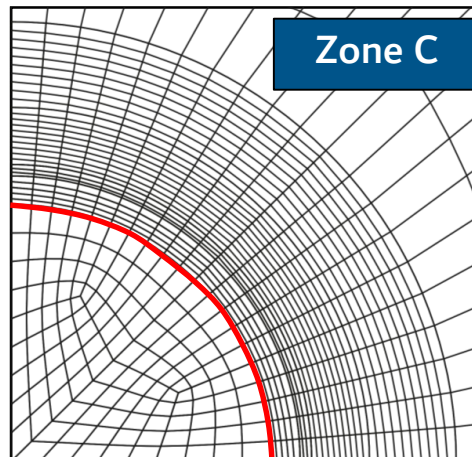
- **For Zone B (HLW, ONDRAF)**

- Gas-H<sub>2</sub> source term [mol/y] = 0.25 (per m of cell) for 100,000 years
- Gas flux-H<sub>2</sub> = 0.141E-11 [kg/s.m<sup>2</sup>] @ at liner intrados (r= 1.80 m)
- Max. heat flux = 123.00 [W/m<sup>2</sup>] along the canister circumference (r=0.25m)



- **For Zone C (HLW, ANDRA)**

- Gas-H<sub>2</sub> source term [mol/y] = 1.90 (per m of cell) for 40,000 years
- Gas flux-H<sub>2</sub> = 4.295E-11 [kg/s.m<sup>2</sup>] along the canister circumference (r=0.45m)
- Max. heat flux = 88.42 [W/m<sup>2</sup>] along the canister circumference (r=0.45m)



# THMG PROCESSES

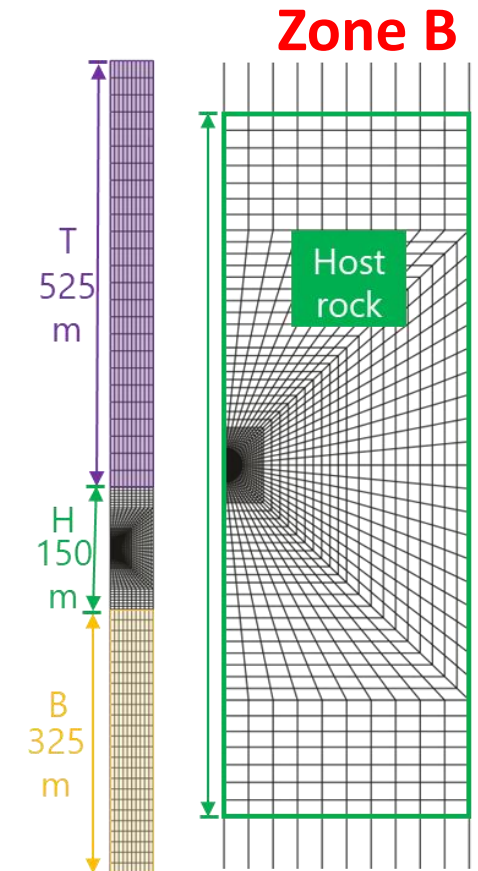
## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)

**Table:** Different cases for evaluating the effect of overlaying and underlaying aquifers.

Cases	Specified SWRC	Spec. Rel. Per. Funs.	Remark
Case 4	✓	✓	With Top/Bottom aquifers (THMG)
Case 5	✓	✓	Without Top/Bottom aquifer (THMG)

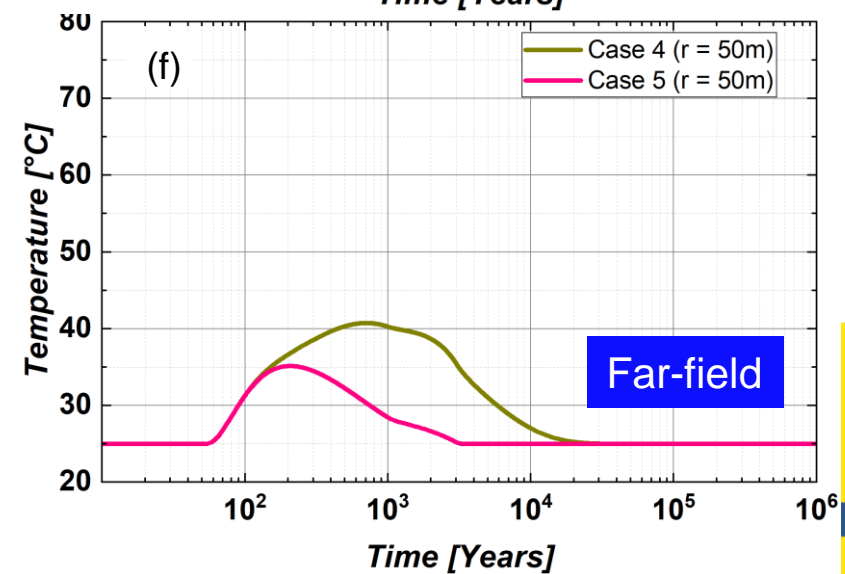
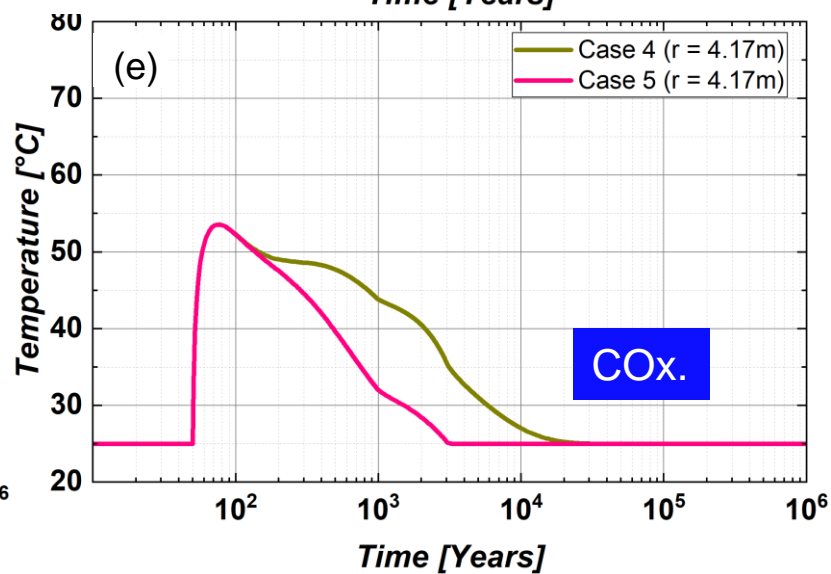
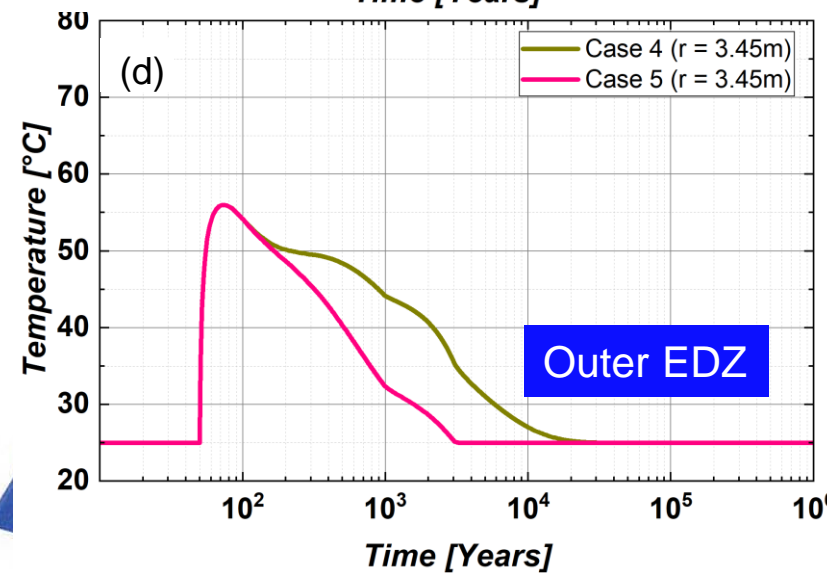
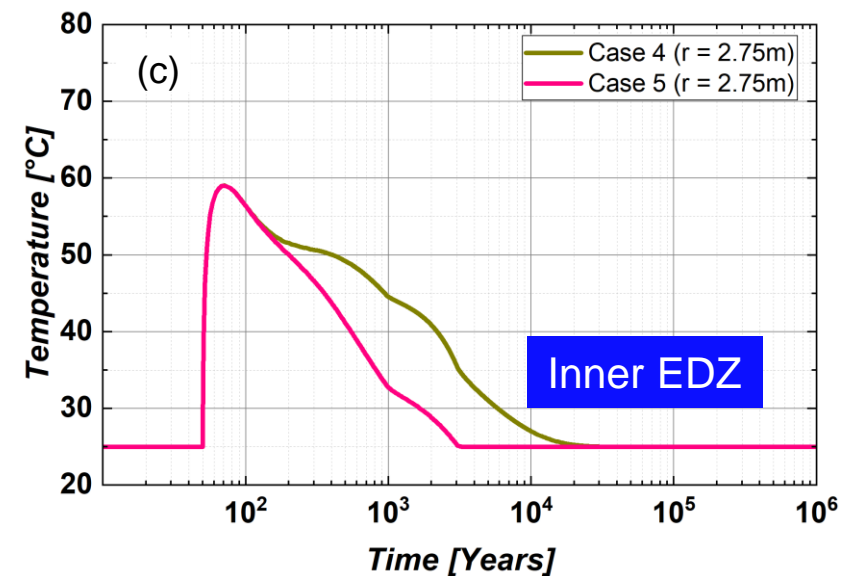
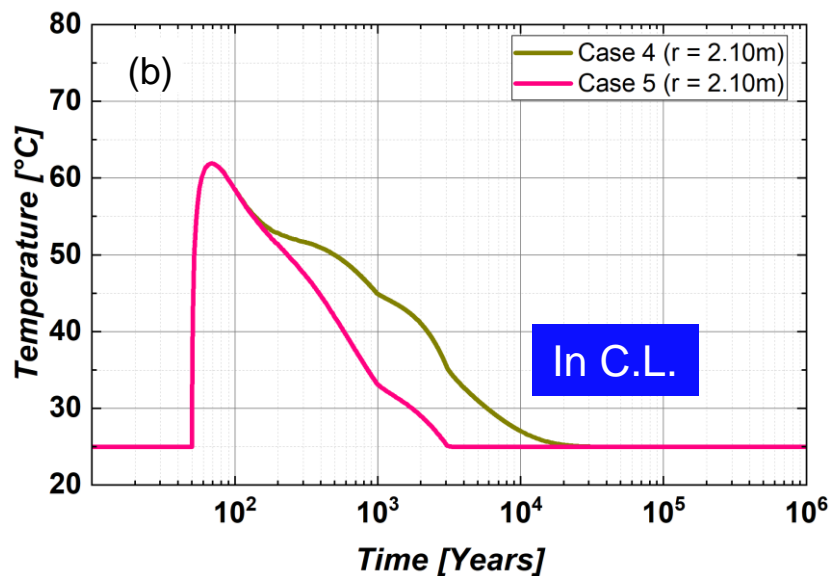
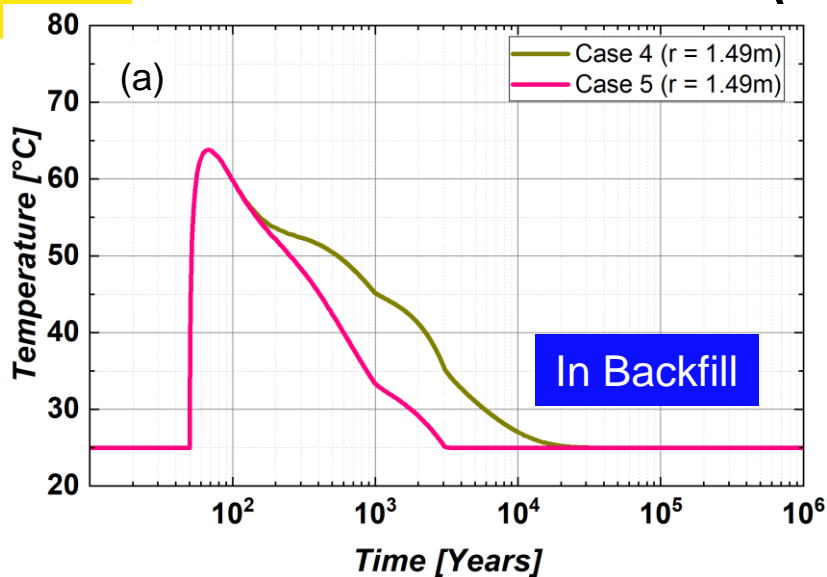
### In Case5:

Nodes in Top and bottom aquifers are fixed for  $p_w$ ,  $p_g$ , and T



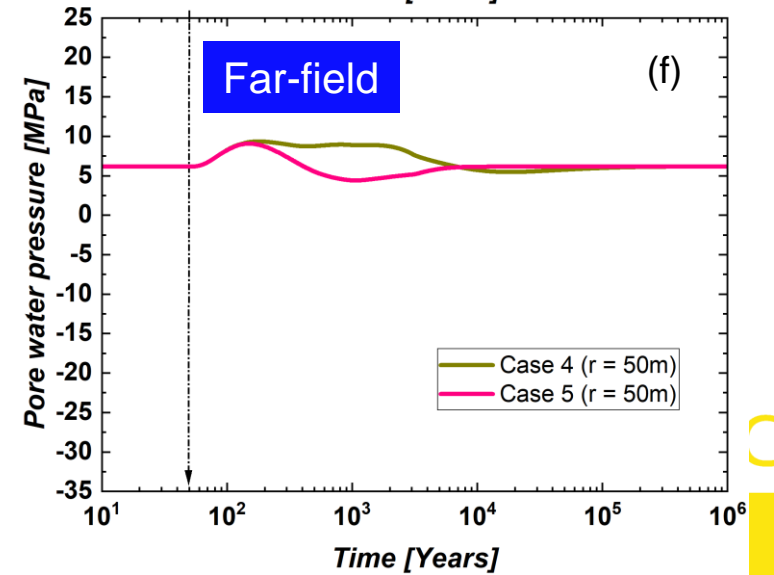
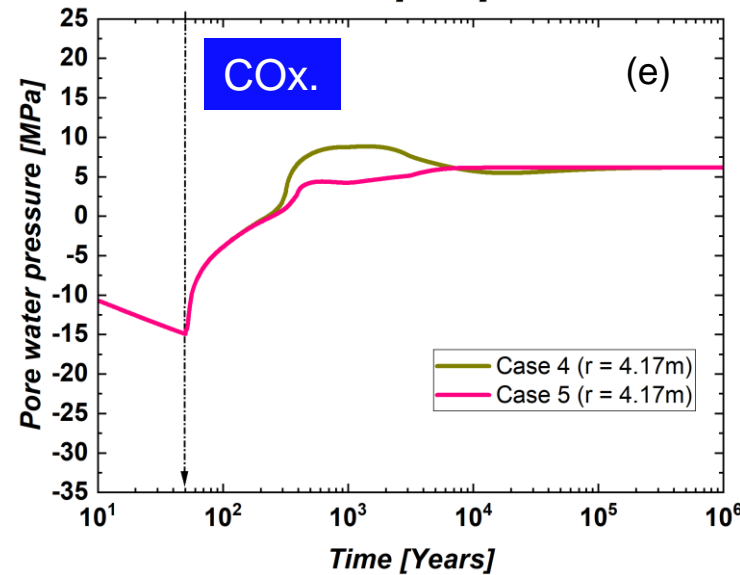
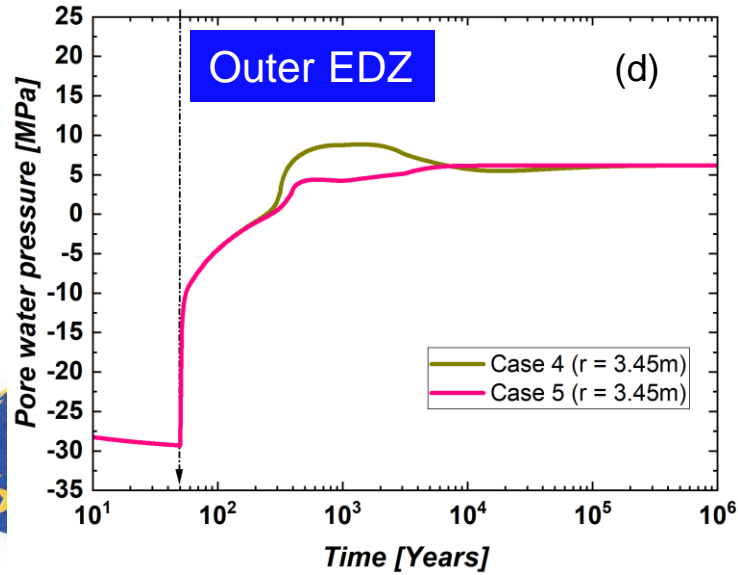
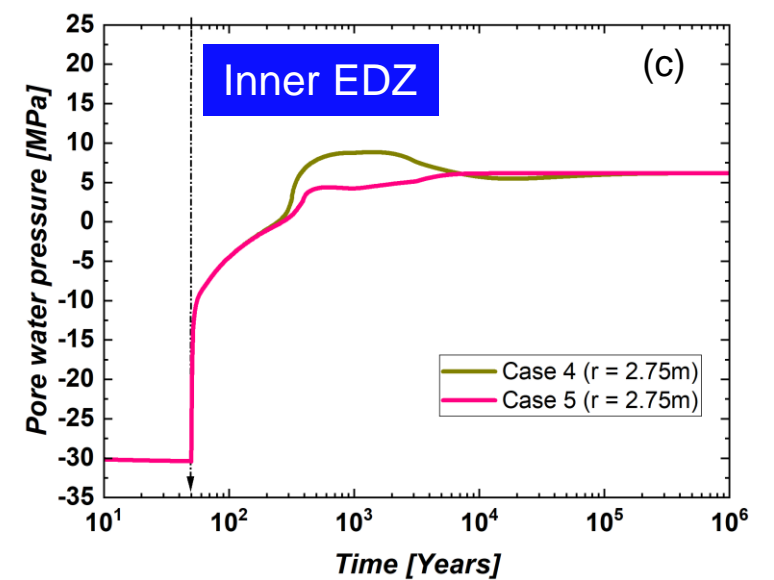
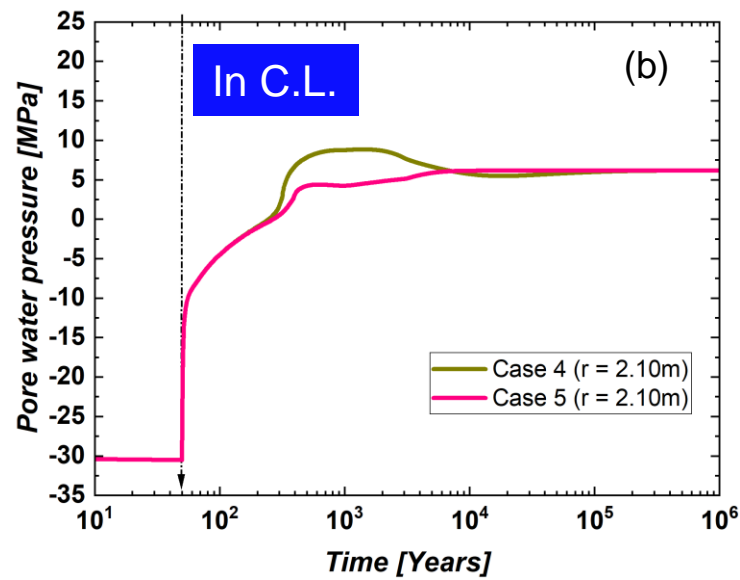
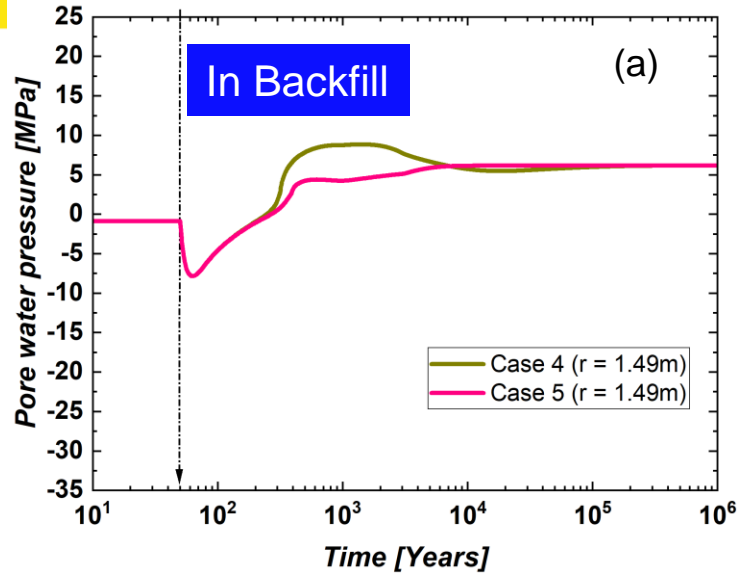
# THMG PROCESSES

## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)



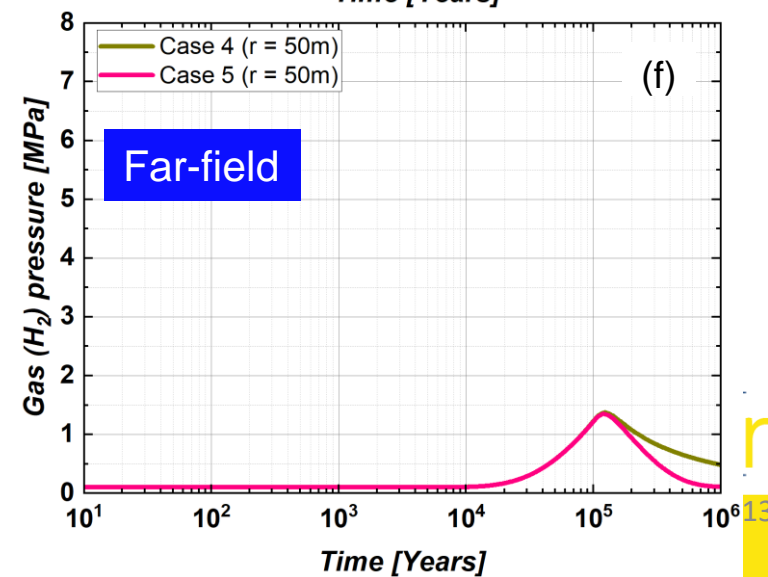
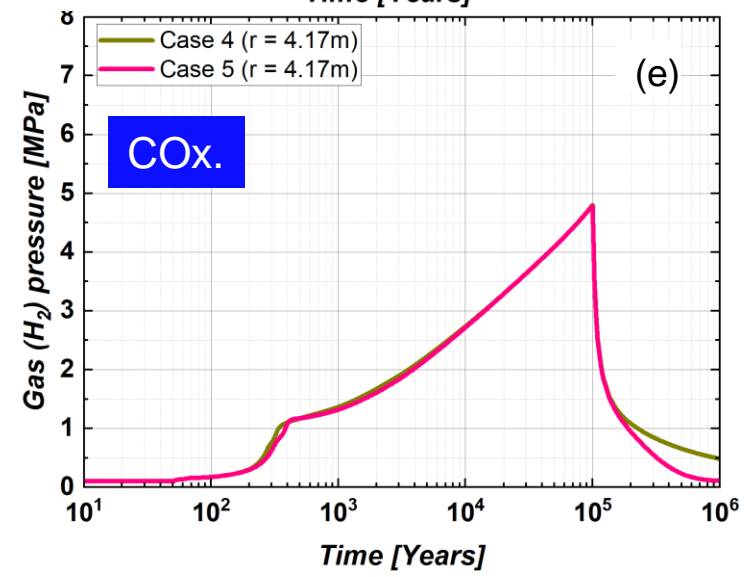
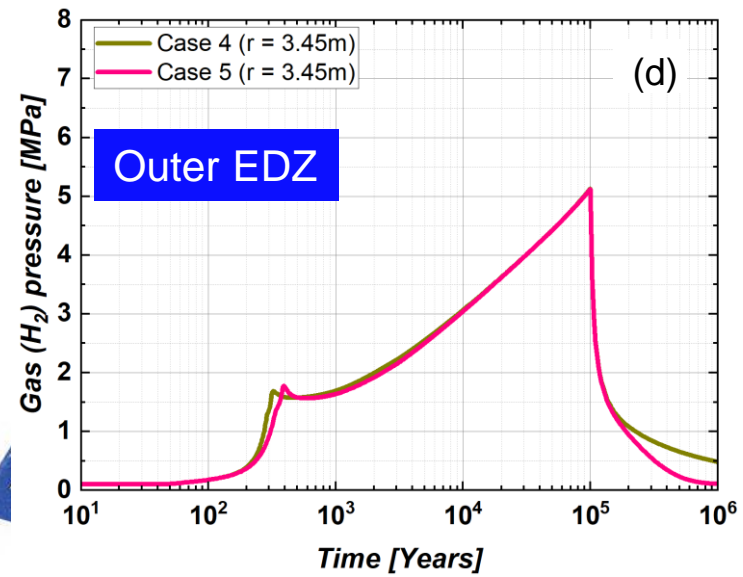
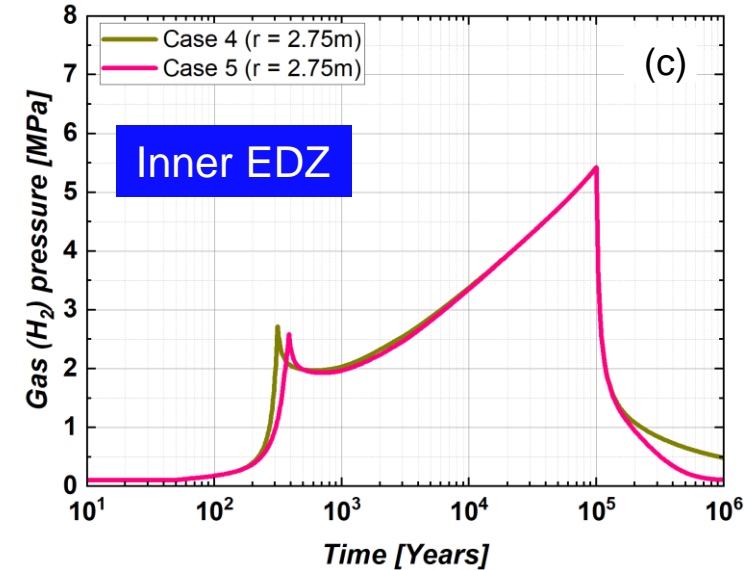
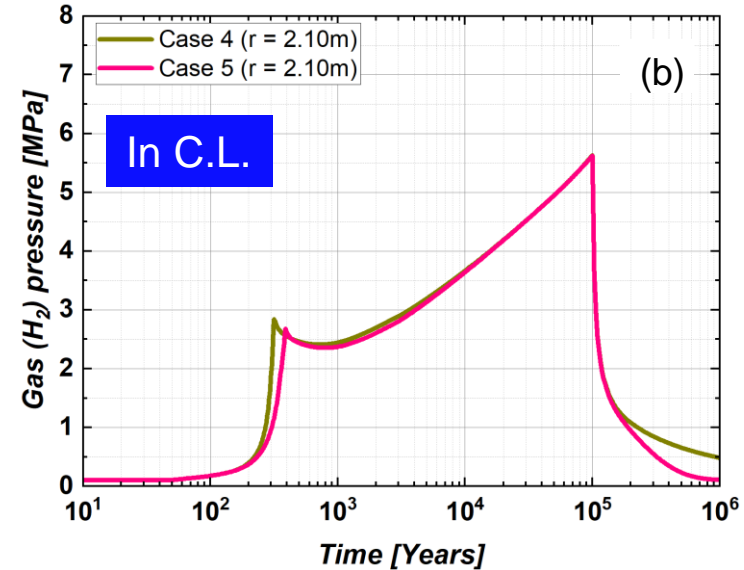
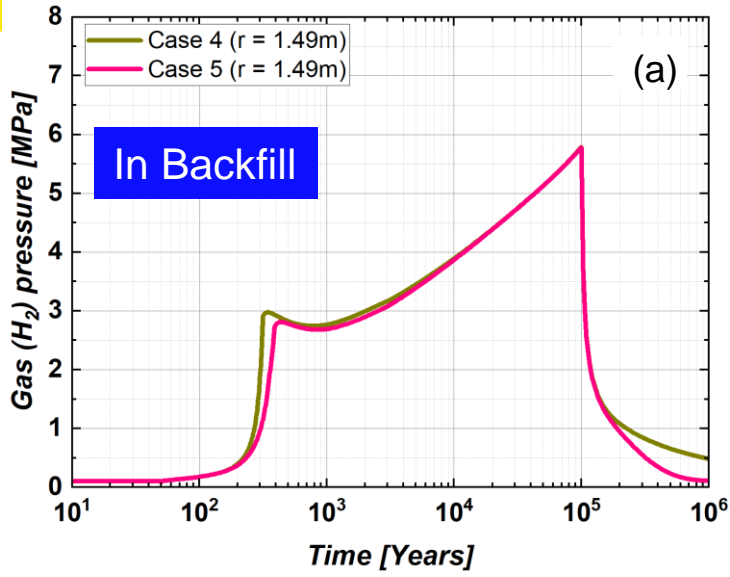
# THMG PROCESSES

## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)



# THMG PROCESSES

## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)





## THMG PROCESSES

### EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)

**Table:** Different cases for evaluating the effect of overlaying and underlying aquifers.

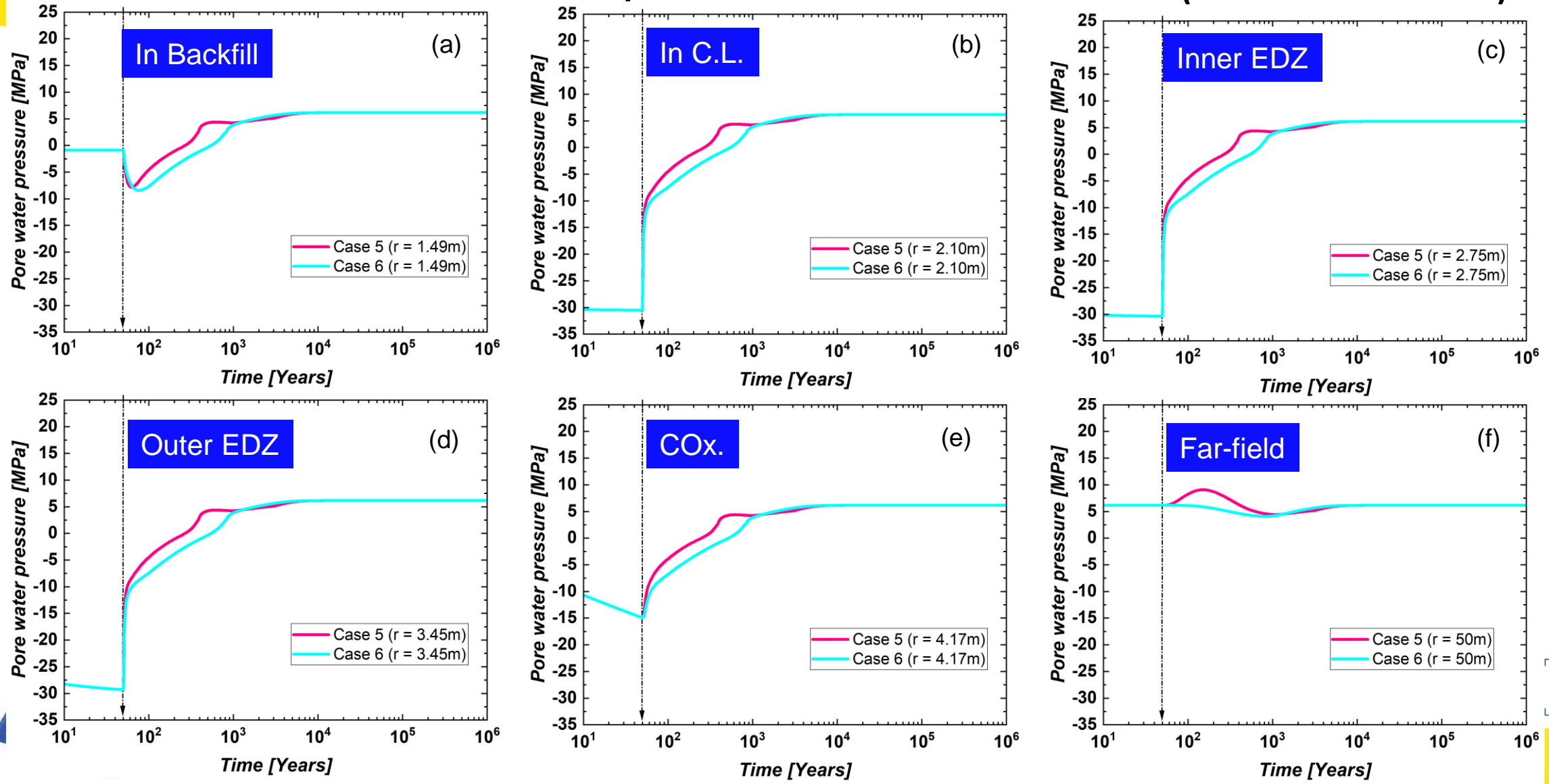
Cases	Specified SWRC	Spec. Rel. per. funs.	Remark	Coupling case
<i>Case 5</i>	✓	✓	Without Top/Bottom aquifer	THMG
<i>Case 6</i>	✓	✓	Without Top/Bottom aquifer	HMG- T is fixed at all the nodes





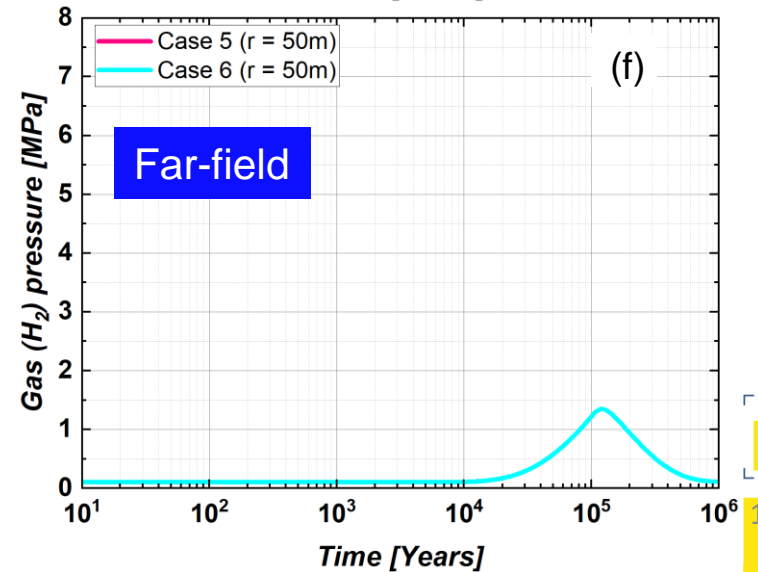
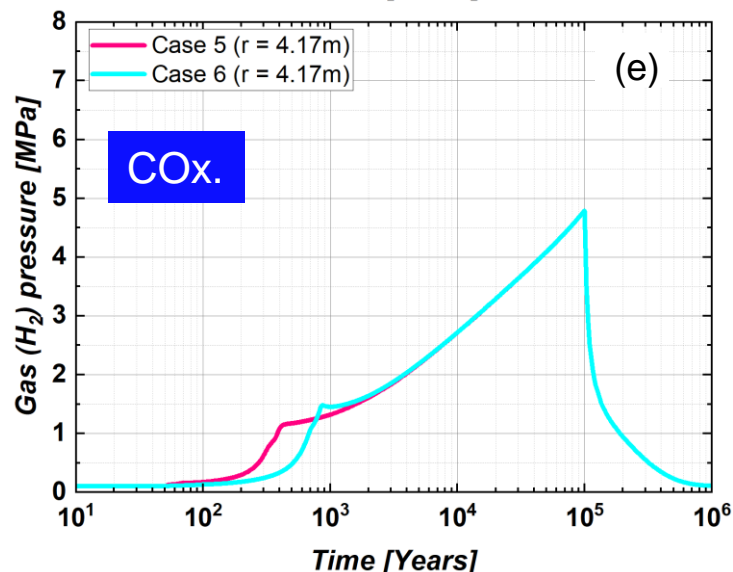
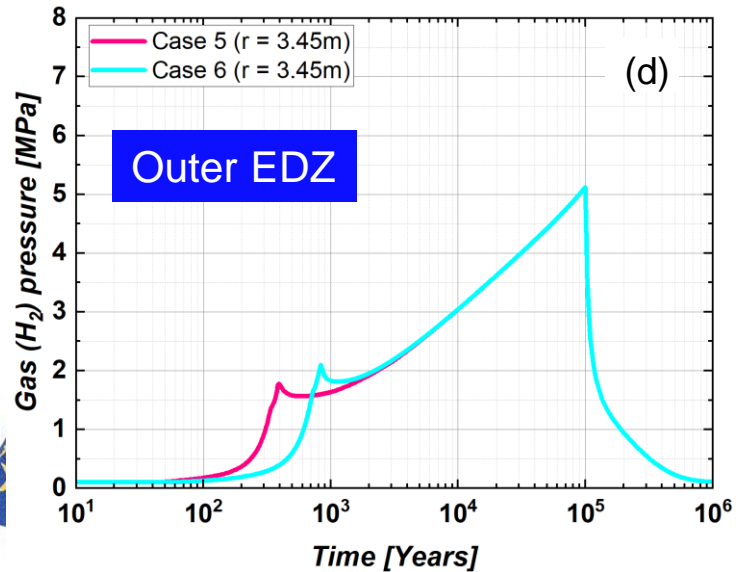
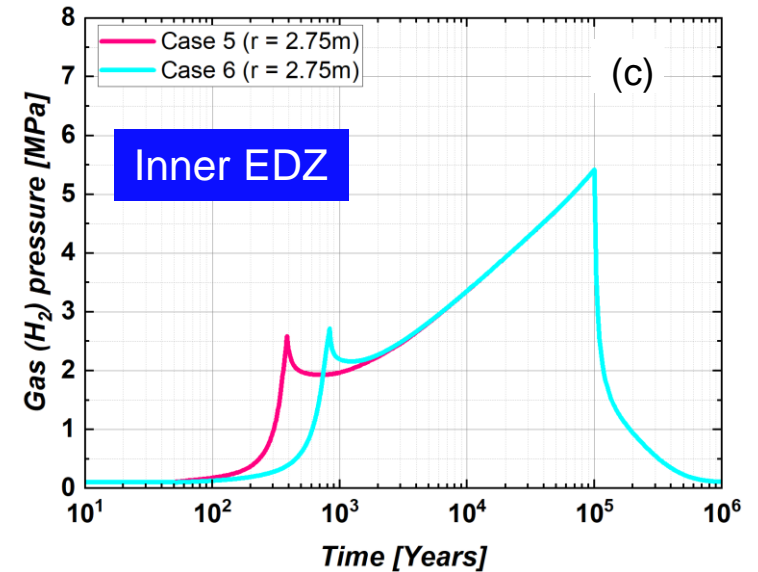
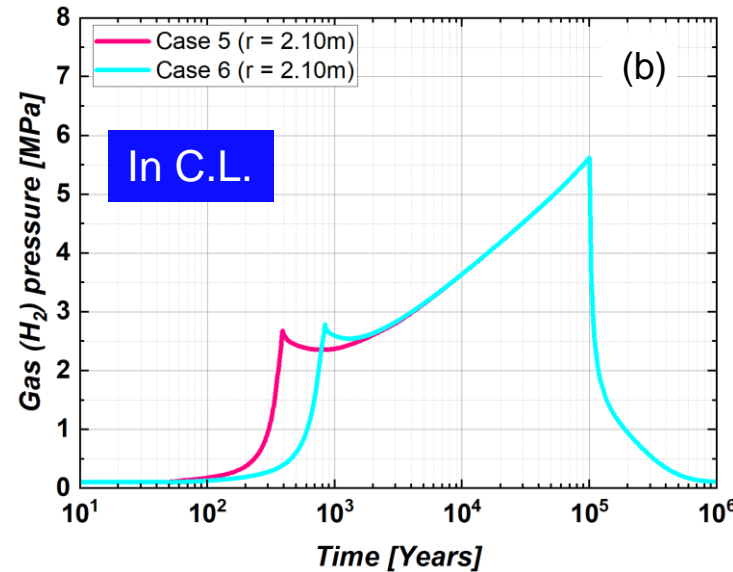
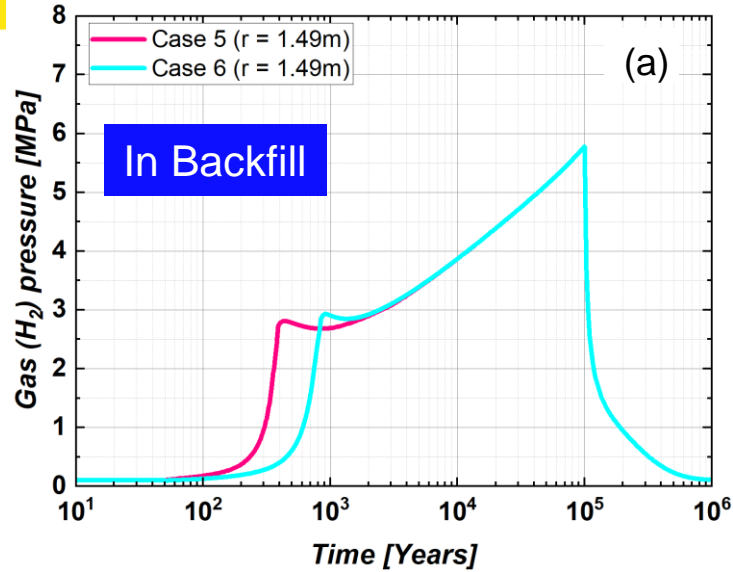
# THMG PROCESSES

## EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)



# THMG PROCESSES

## EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)







## THMG PROCESSES

### EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)

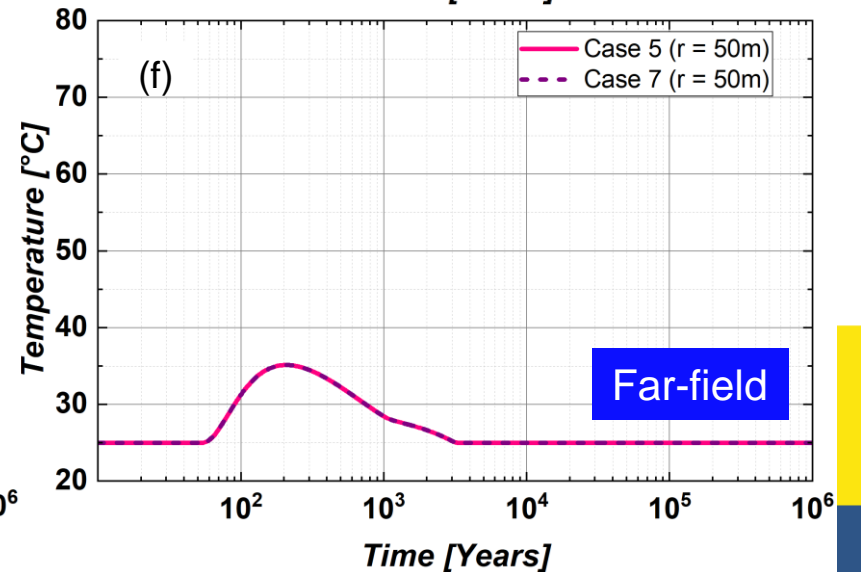
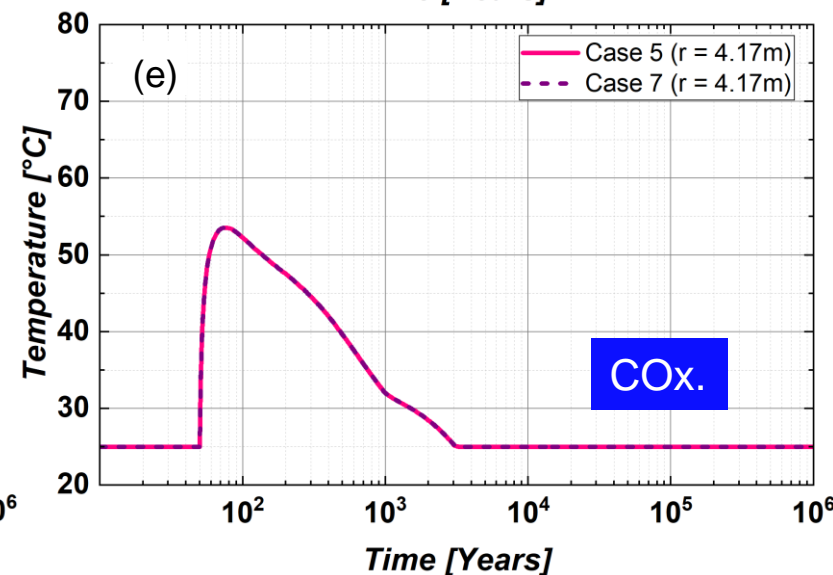
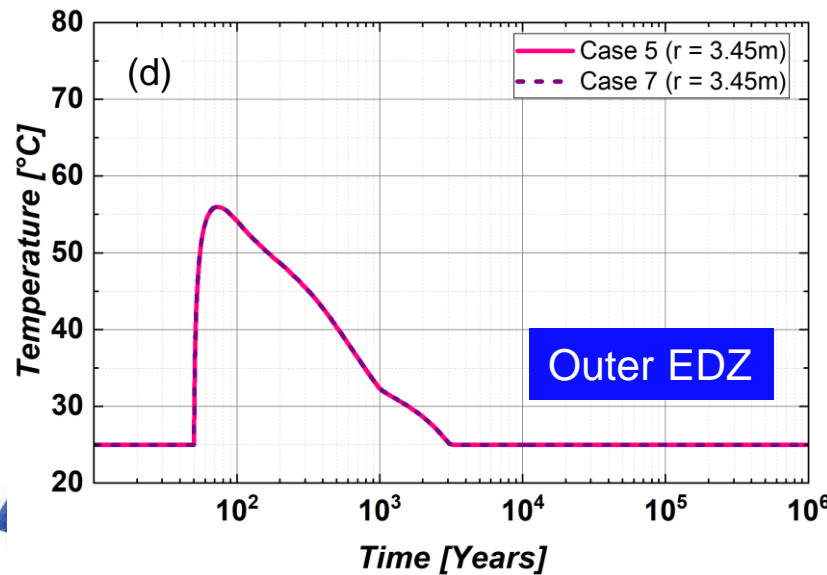
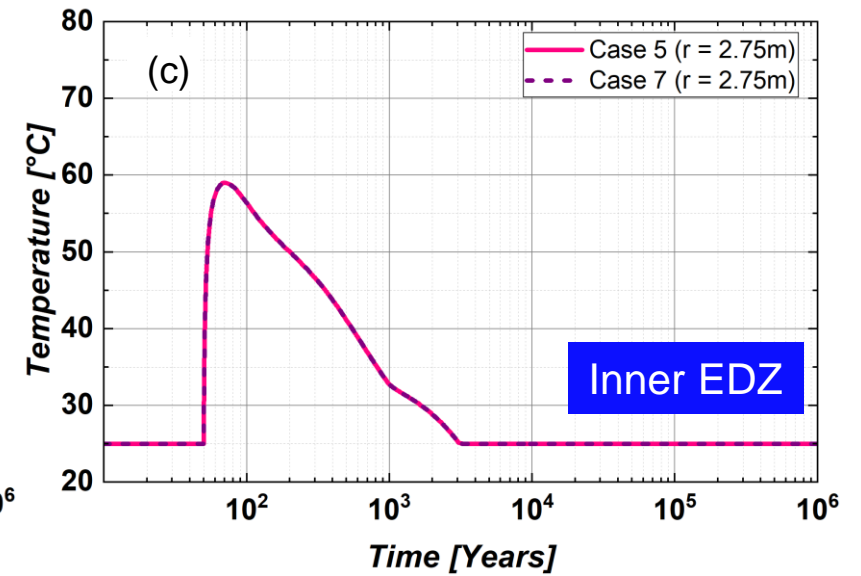
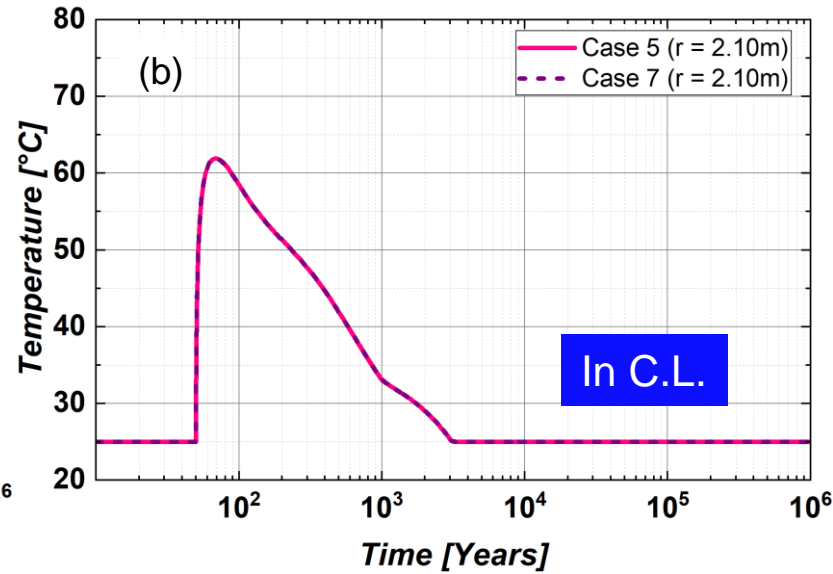
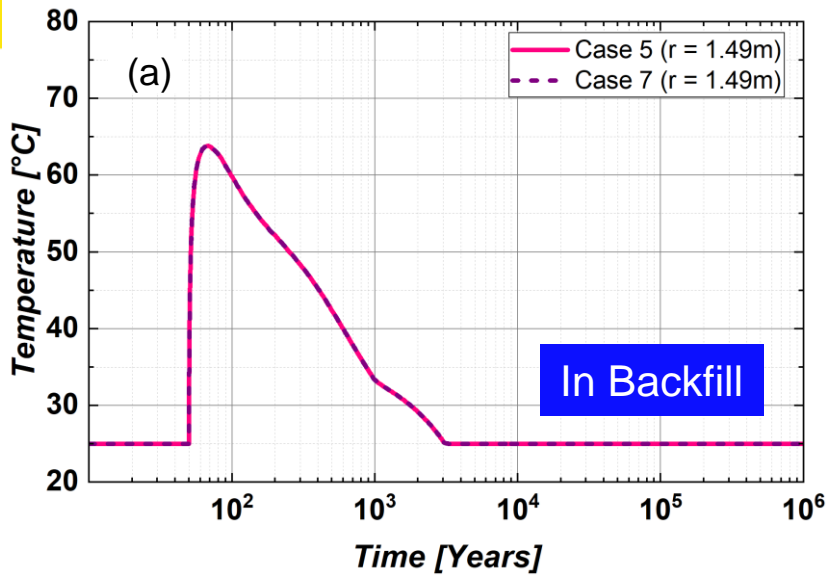
**Table:** Different cases for examining the effect of gas pressure on the porewater evolution.

Cases	Specified SWRC	Spec. Rel. per. funs.	Remark	Coupling case
<i>Case 5</i>	✓	✓	Without top/bottom aquifer	THMG
<i>Case 7</i>	✓	✓	Without top/bottom aquifer	THM (G is fixed at all the nodes)



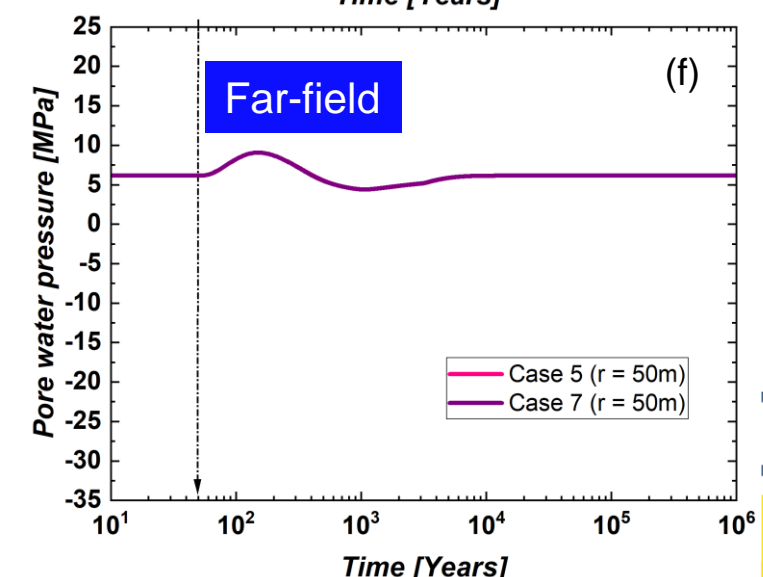
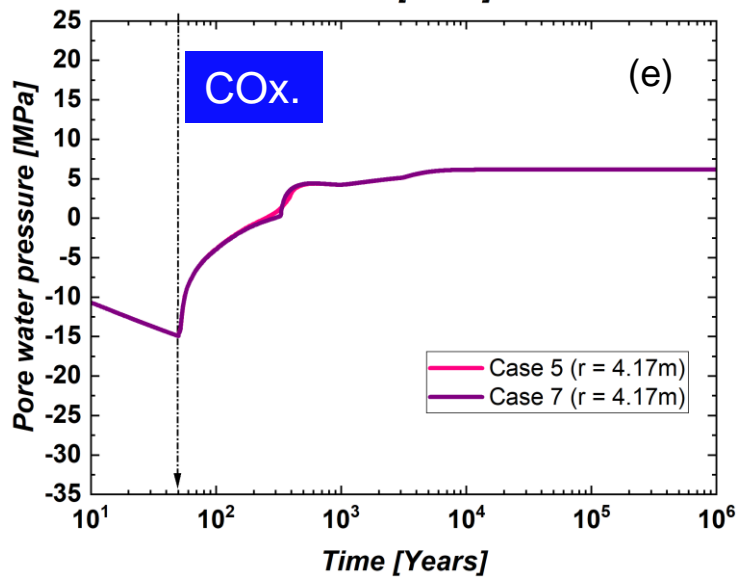
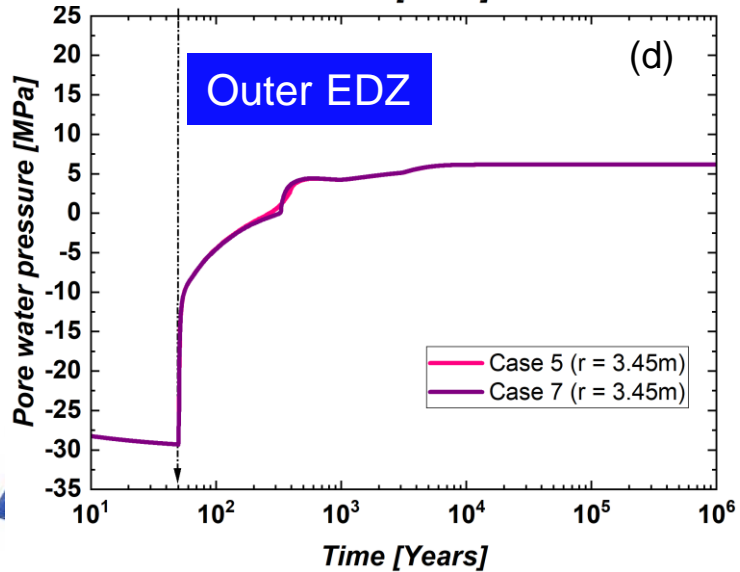
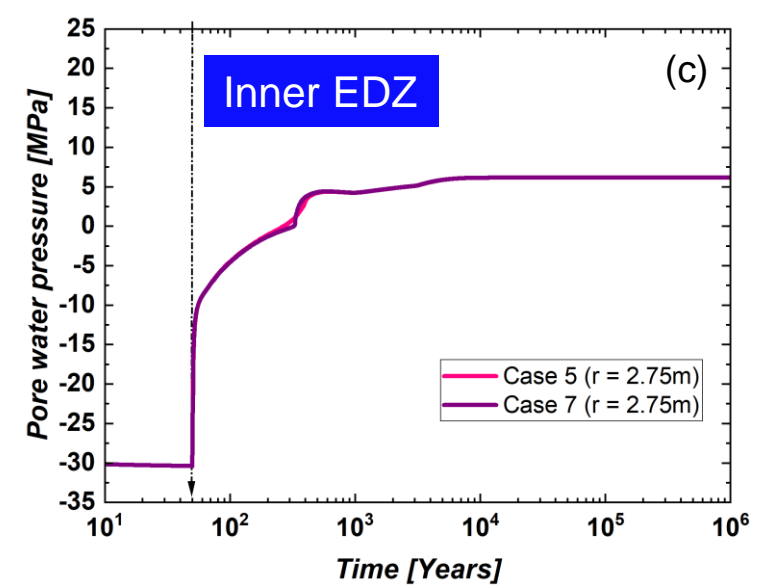
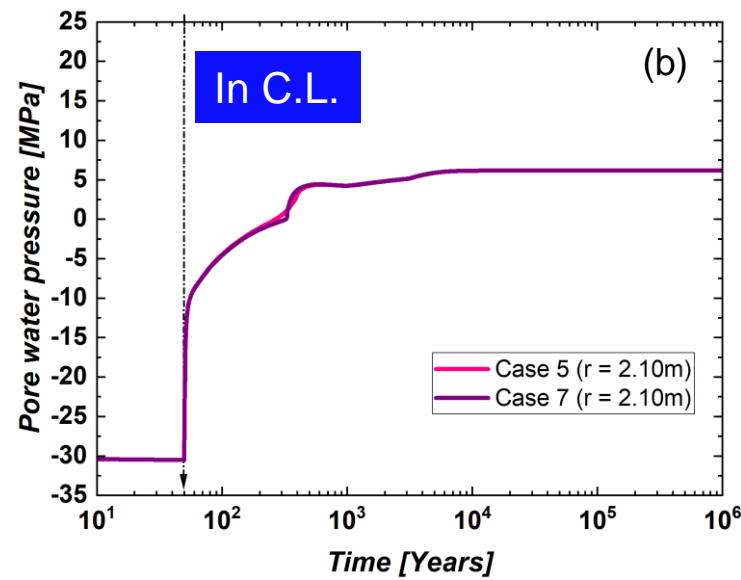
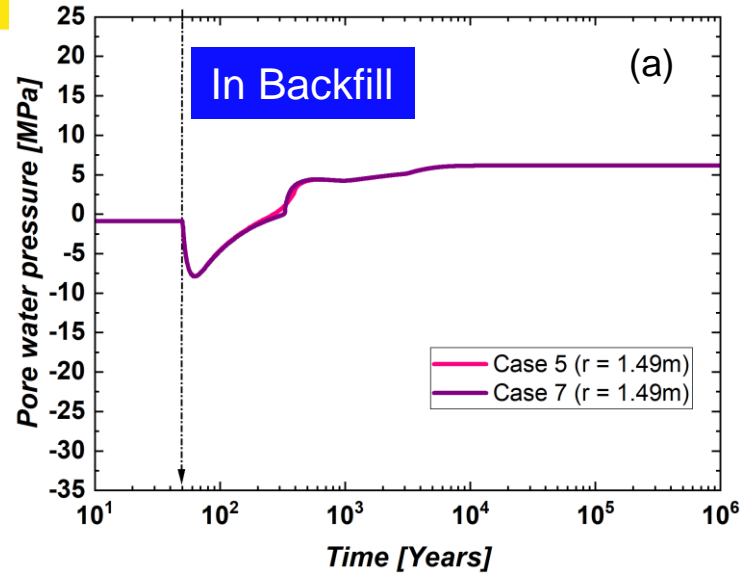
# THMG PROCESSES

## EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)



# THMG PROCESSES

## EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)



# THMG PROCESSES

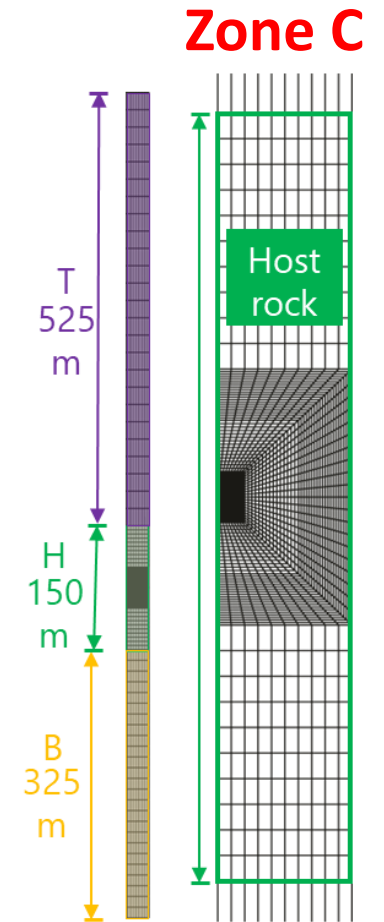
## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)

**Table:** Different cases for evaluating the effect of overlaying and underlaying aquifers.

Cases	Specified SWRC	Spec. Rel. Per. Funs.	Remark
Case 4	✓	✓	With Top/Bottom aquifers (THMG)
Case 5	✓	✓	Without Top/Bottom aquifer (THMG)

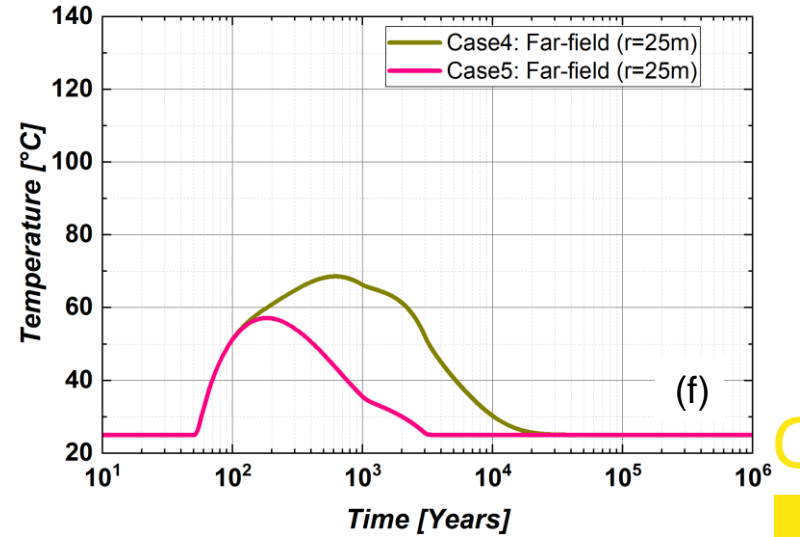
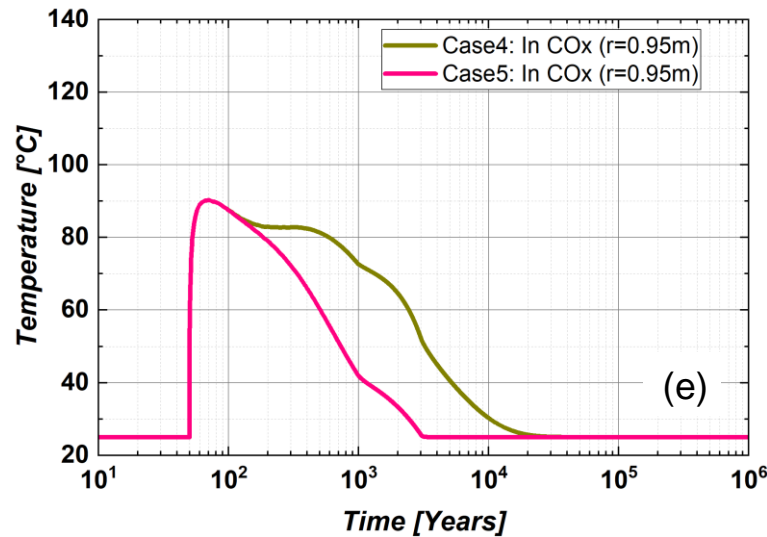
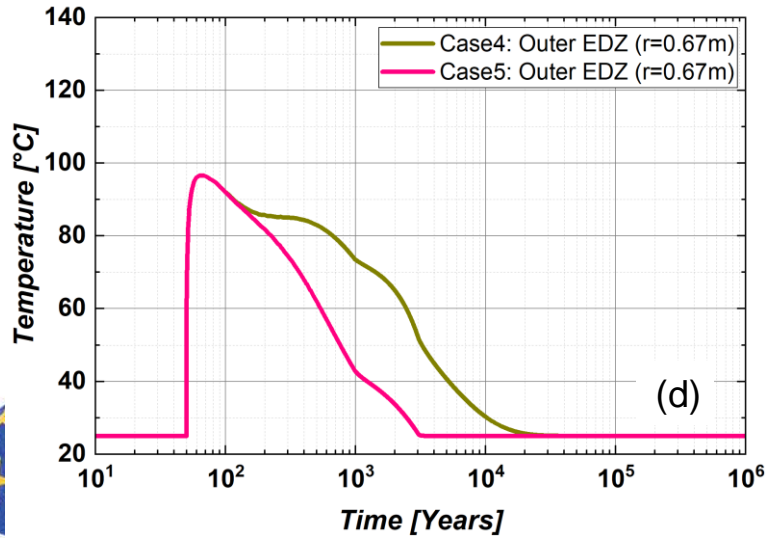
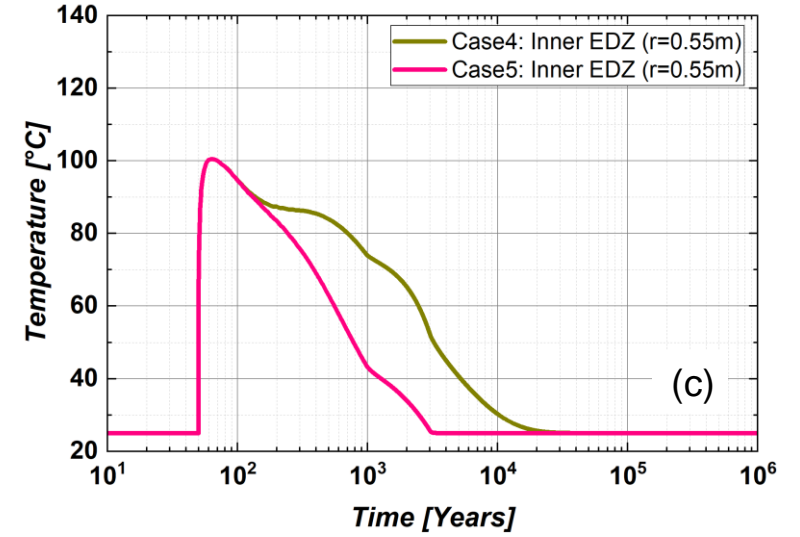
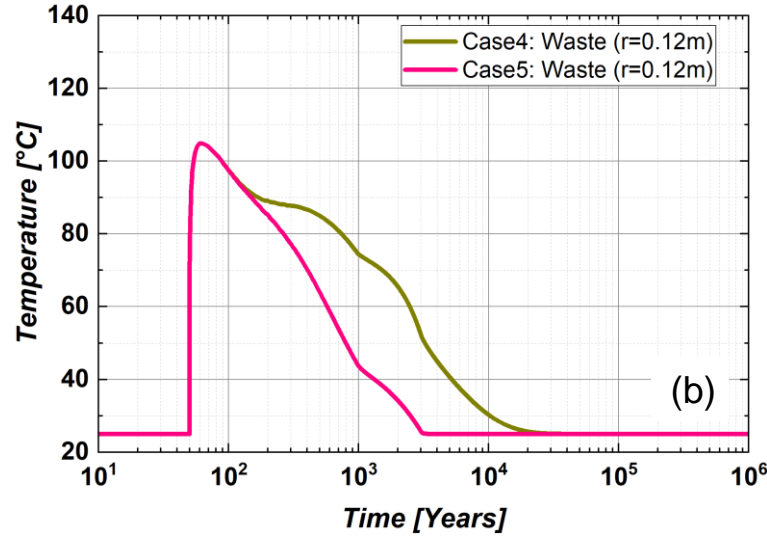
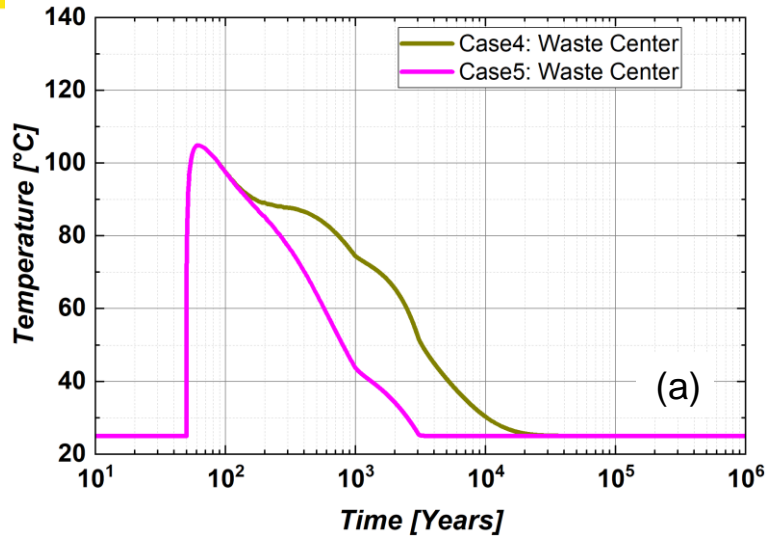
### In Case5:

Nodes in Top and bottom aquifers are fixed for  $p_w$ ,  $p_g$ , and T



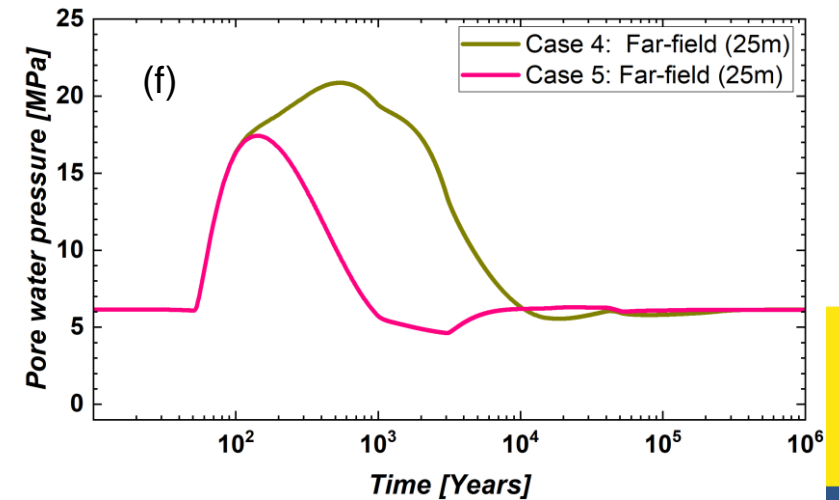
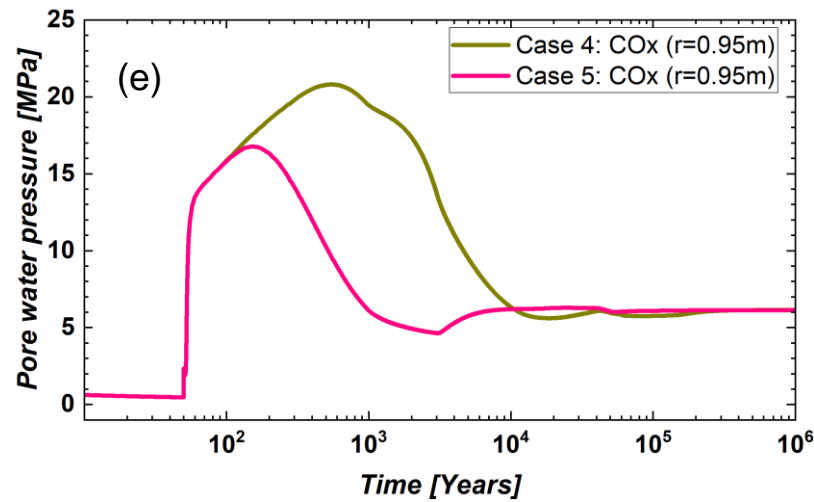
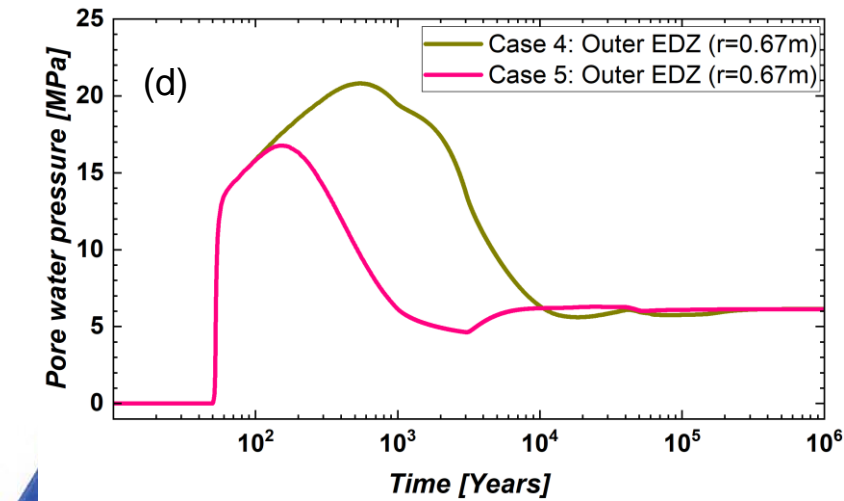
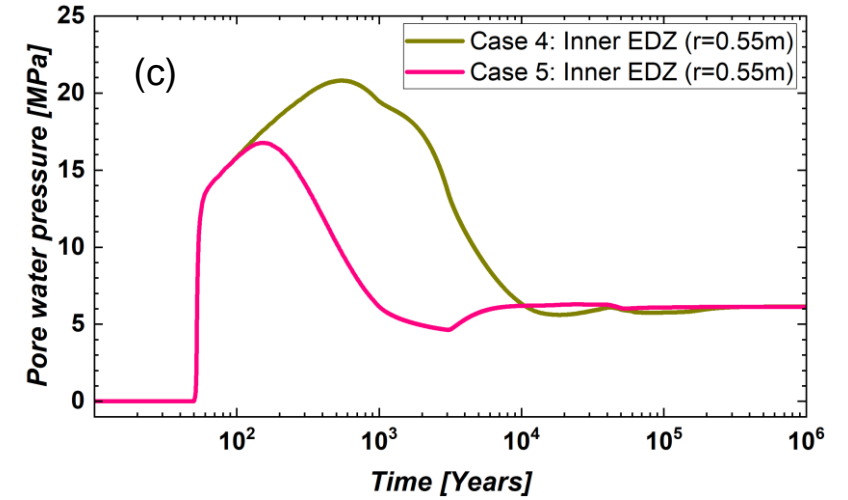
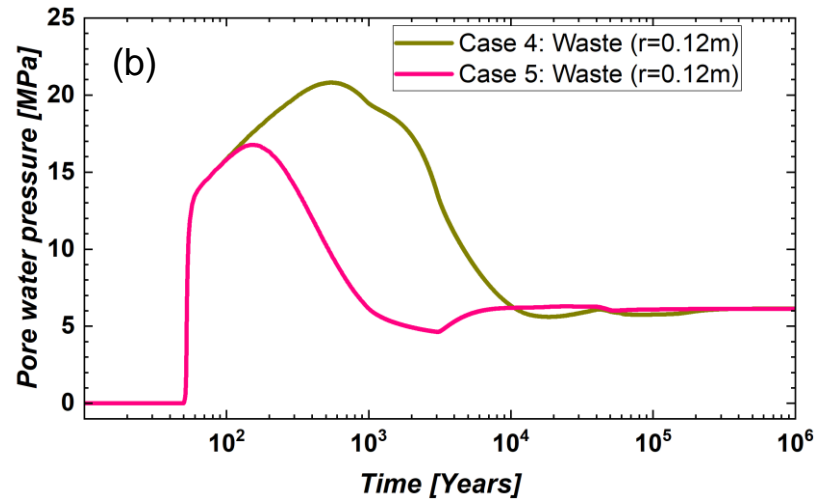
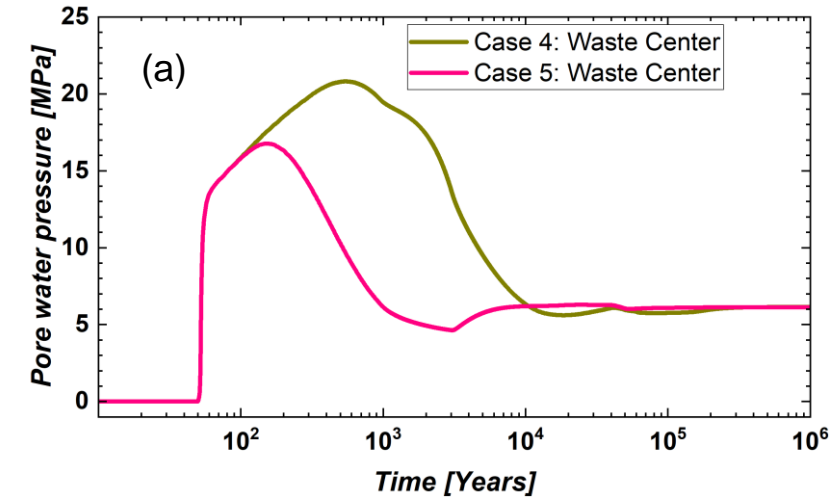
# THMG PROCESSES

## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)



# THMG PROCESSES

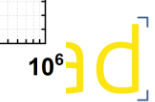
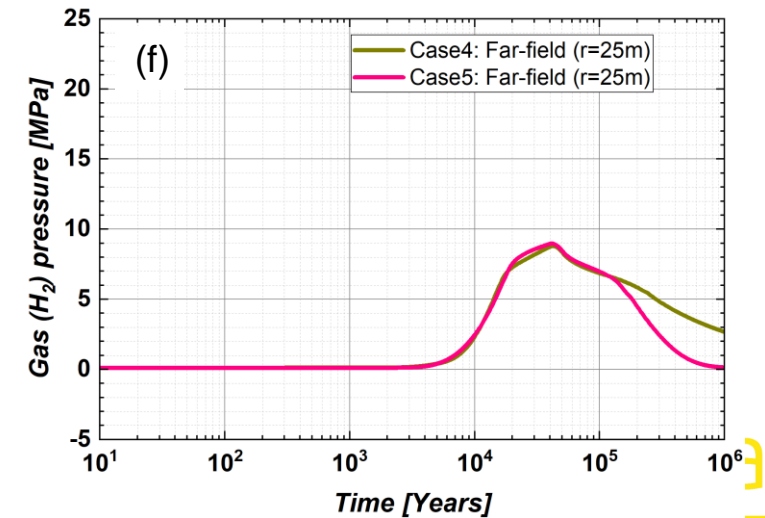
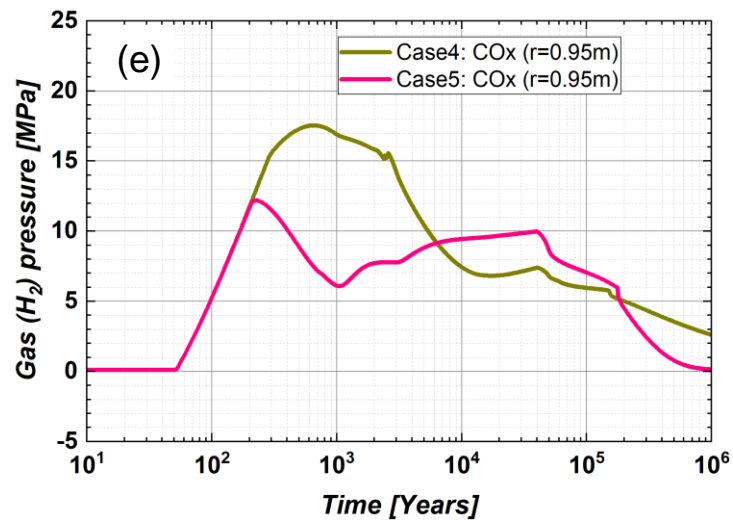
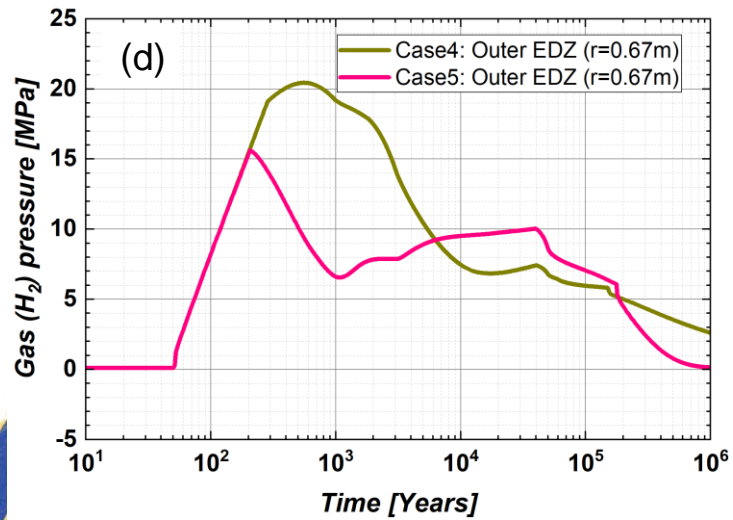
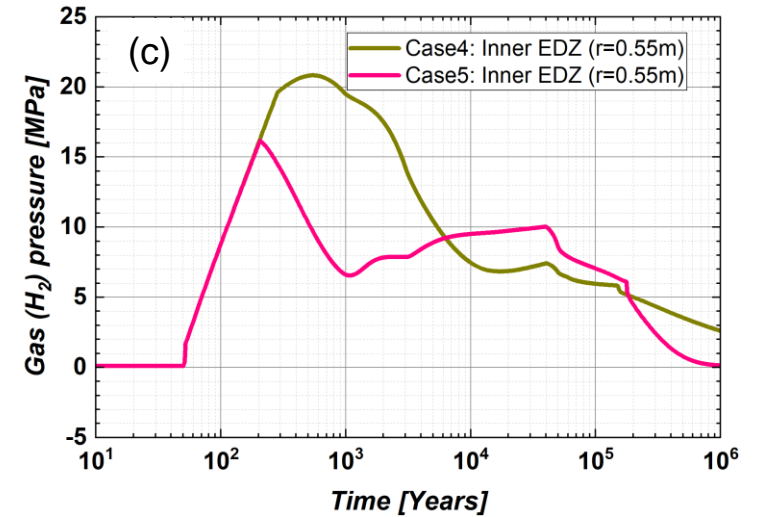
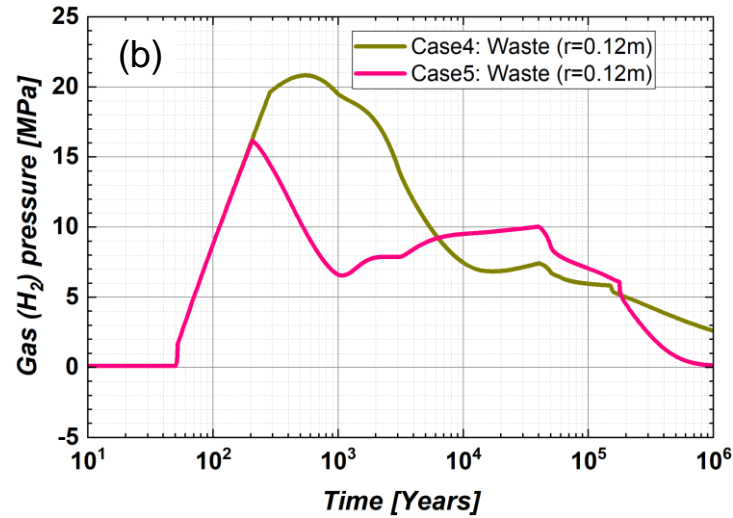
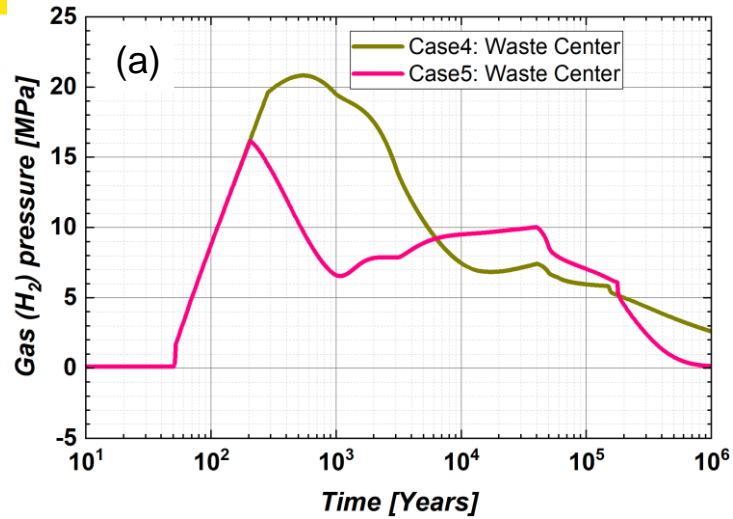
## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)





# THMG PROCESSES

## EFFECT OF THE GEOMETRY (TOP/BOTTOM AQUIFER)





## THMG PROCESSES

### EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)

**Table:** Different cases for evaluating the effect of overlaying and underlying aquifers.

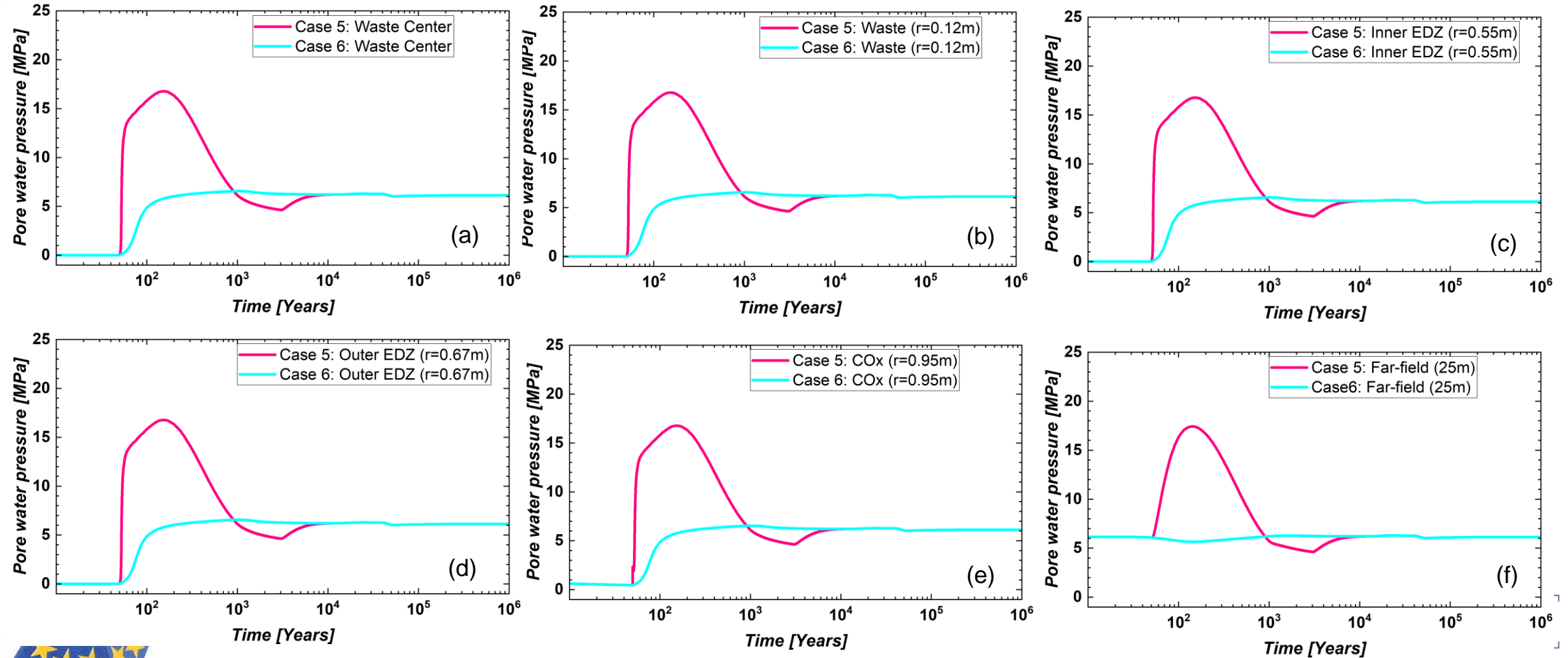
Cases	Specified SWRC	Spec. Rel. per. funs.	Remark	Coupling case
<i>Case 5</i>	✓	✓	Without Top/Bottom aquifer	THMG
<i>Case 6</i>	✓	✓	Without Top/Bottom aquifer	HMG- T is fixed at all the nodes





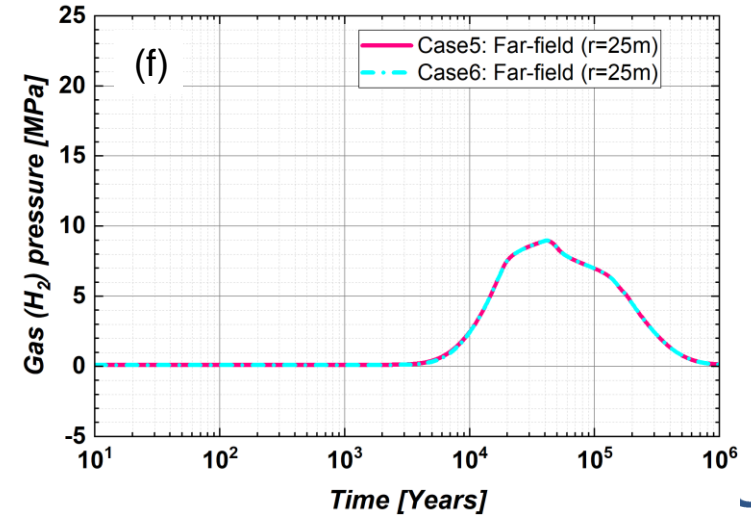
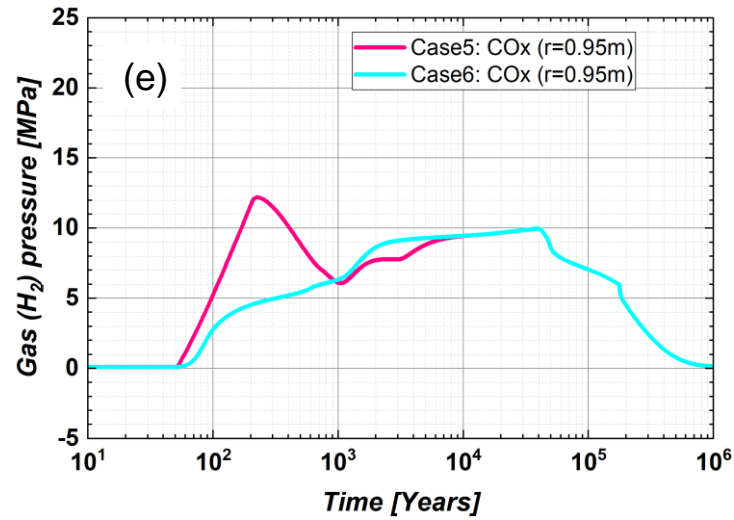
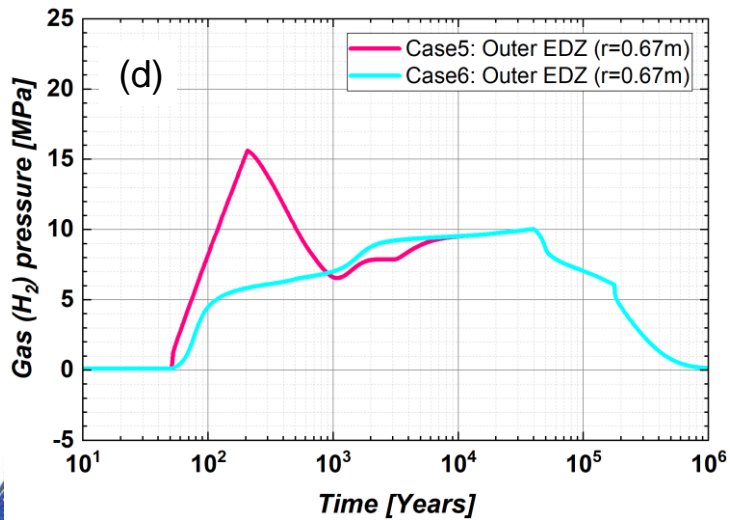
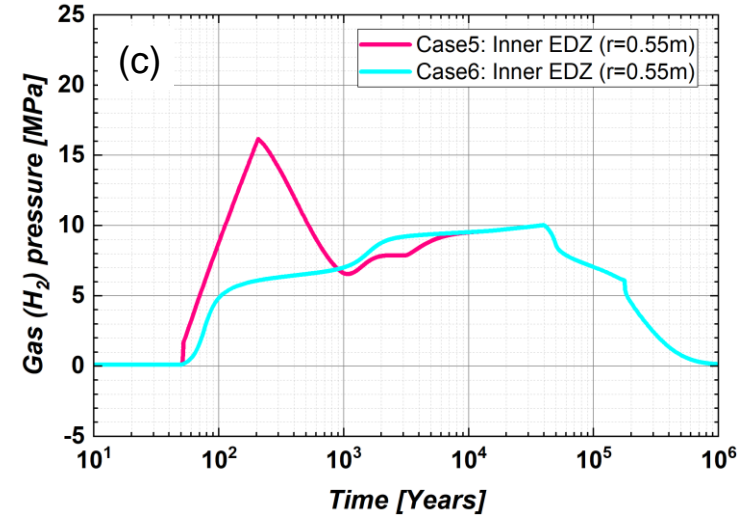
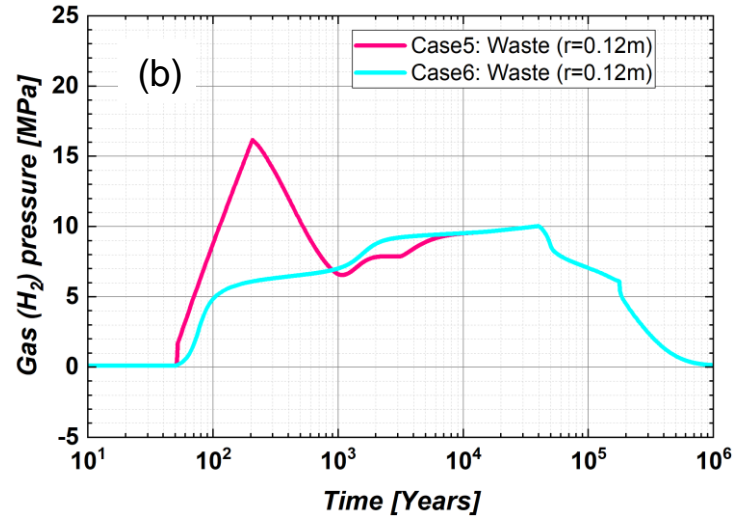
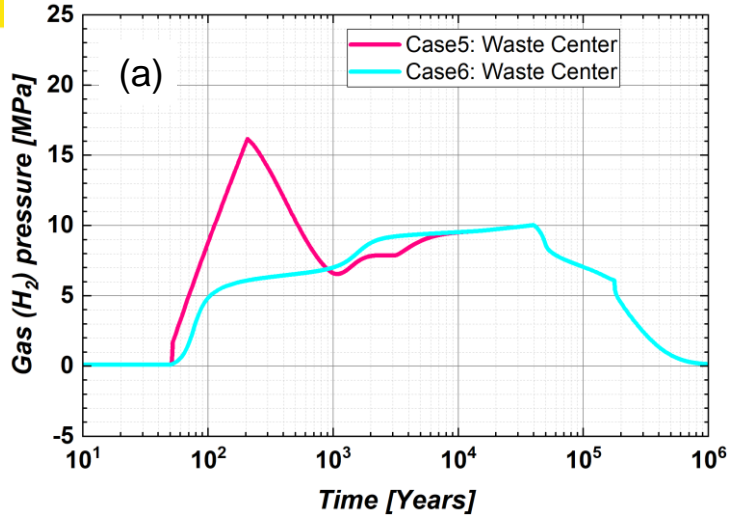
# THMG PROCESSES

## EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)



# THMG PROCESSES

## EFFECT OF TEMPERATURE ON GAS/POREWATER PRESSURE EVOLUTION (THMG VERSUS HMG)





## THMG PROCESSES

### EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)

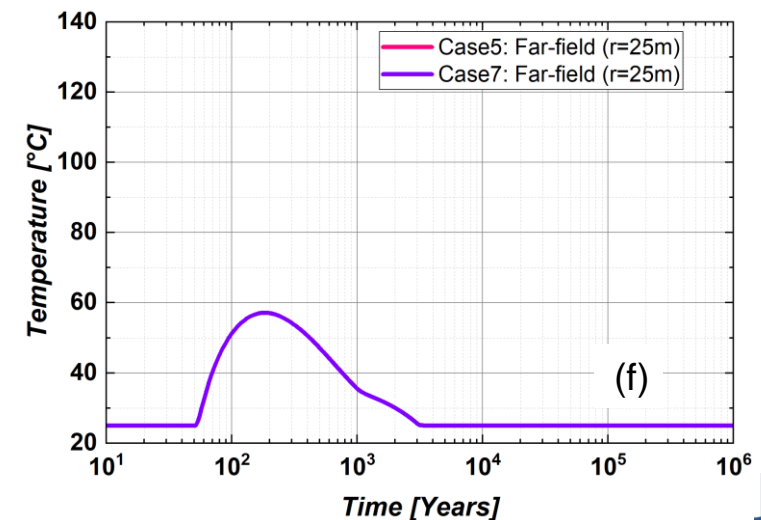
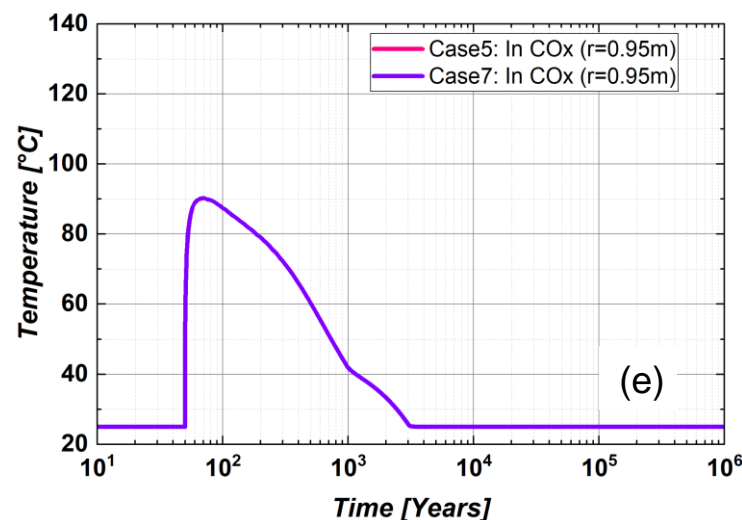
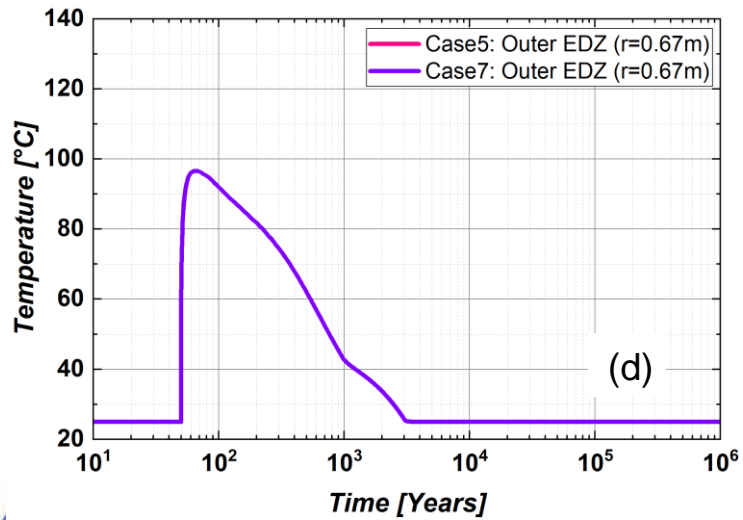
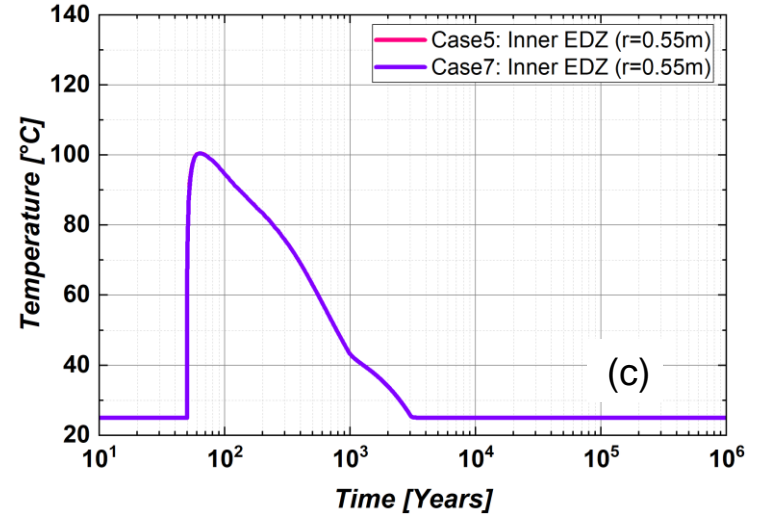
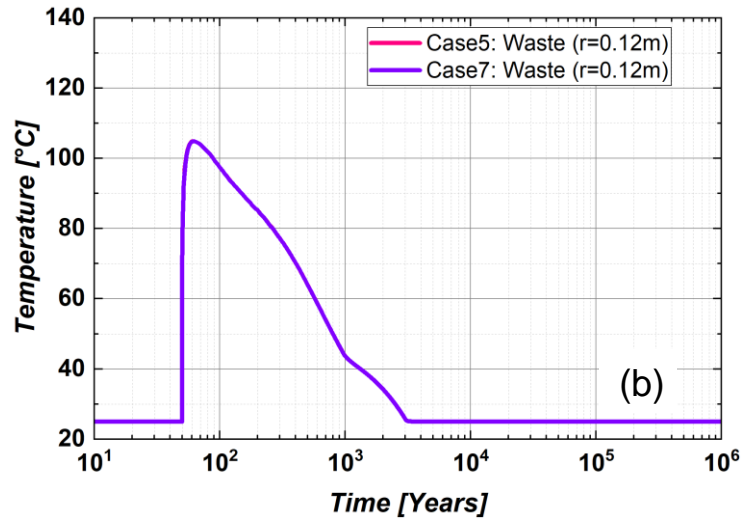
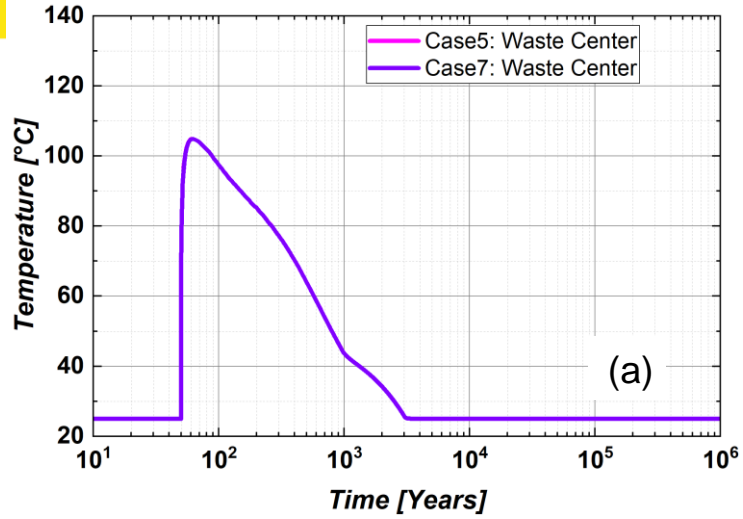
**Table:** Different cases for examining the effect of gas pressure on the porewater evolution.

Cases	Specified SWRC	Spec. Rel. per. funs.	Remark	Coupling case
<i>Case 5</i>	✓	✓	Without top/bottom aquifer	THMG
<i>Case 7</i>	✓	✓	Without top/bottom aquifer	THM (G is fixed at all the nodes)



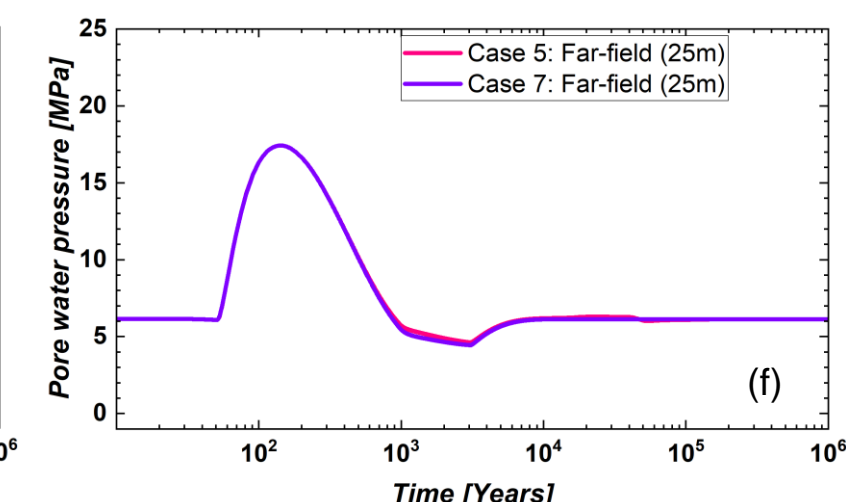
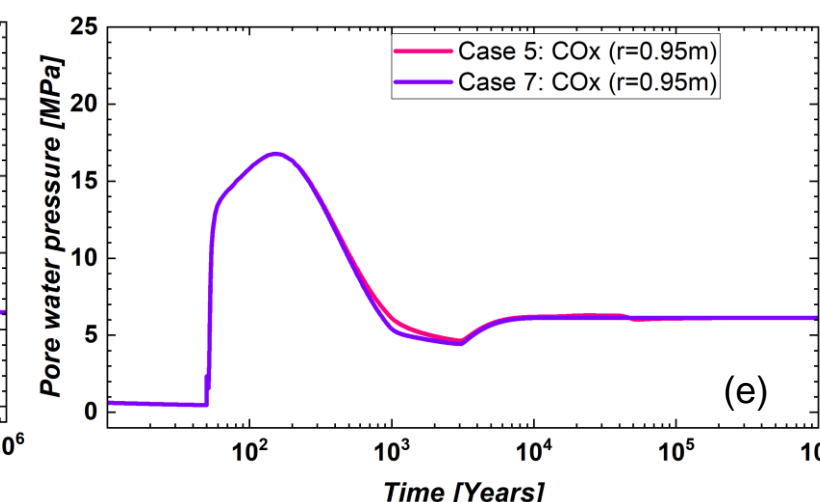
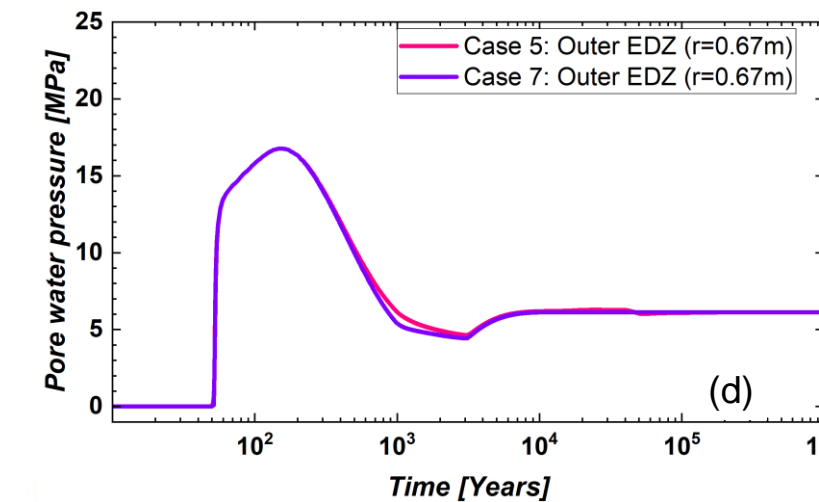
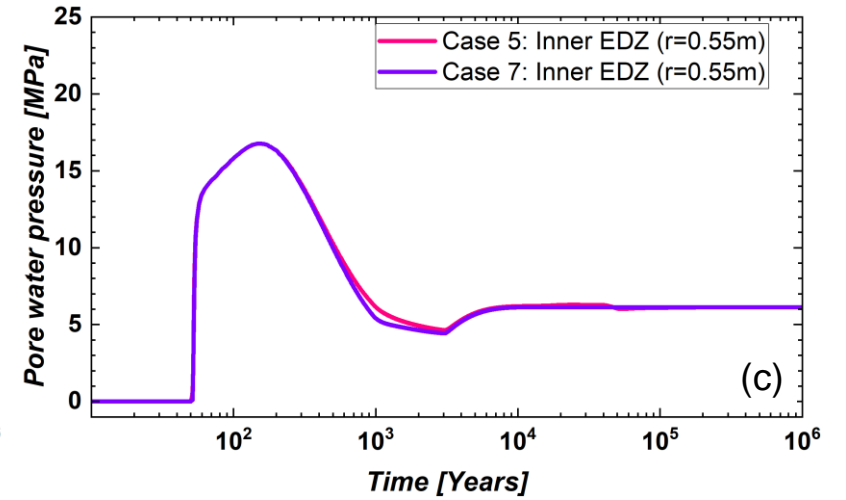
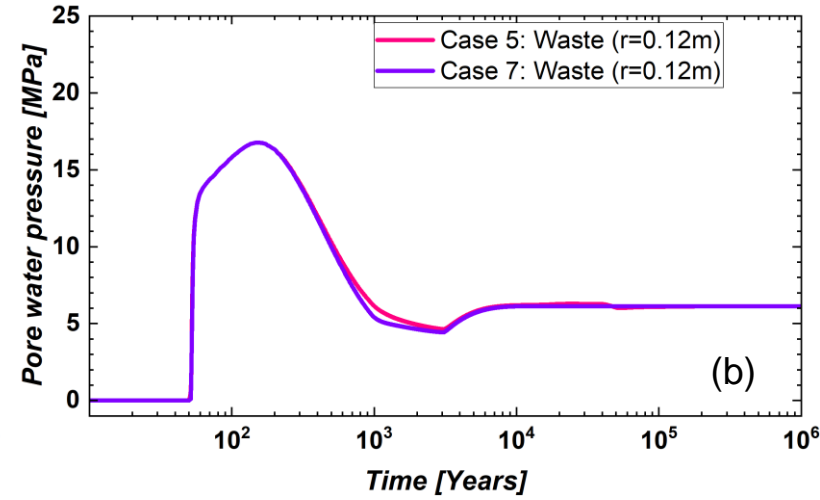
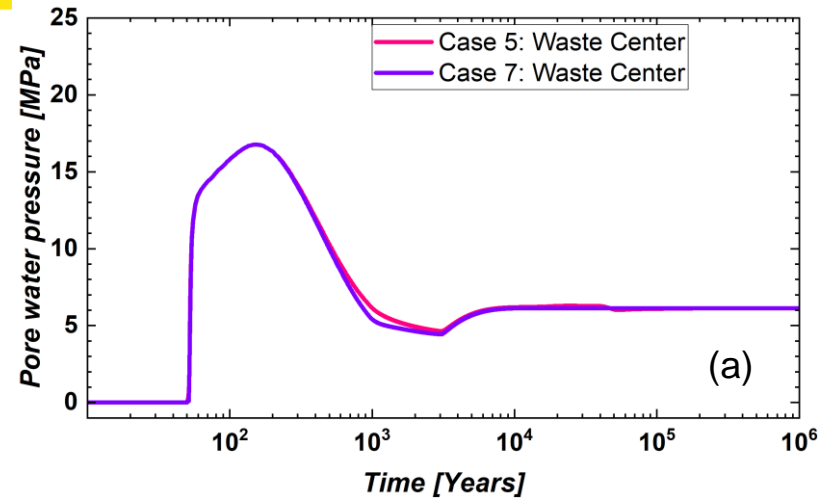
# THMG PROCESSES

## EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)



# THMG PROCESSES

## EFFECT OF GAS GENERATION (THMG VERSUS THM-COUPLING)





## THMG PROCESSES

### Effect of Geometry (Presence of Top/Bottom Aquifers):

- Primarily affect the thermal response (peak value, and post-peak distribution), as a result, a much shorter thermal period (3000 years) is observed without the top/bottom aquifers as compared to the opposite case (20,000 years).
- A change in the thermal response induces cascading effect on the PWP and Gas pressure evolution.

### Effect of Temperature on Gas/PWP Evolution (THMG versus HMG-coupling):

- Rise in the temperature induces excess PWP, thus affects the gas pressure ( $H_2$ ) evolution.
- As a result, higher PWP and Gas pressure are observed in THMG case as compared to HMG coupling scenario.

### Effect of Gas Pressure on PWP Evolution:

- The gas pressure does not affect the temperature or PWP evolution.





## CONCLUSIONS

- The different physical phenomena occurring in the geomaterials are by essence coupled.
- The effective existence of this coupling will depend on the nature, properties, environmental loads acting on the geomaterials
- Experimental (in the lab and in situ) are of paramount importance in order to assess the coupling between the processes. A process and a coupling both observed at lab scale and in situ is probably to be considered
- The next step to predict the long term behavior of the geomaterial is the development of constitutive models based on the lab observations.
- From a numerical perspective, the couplings are challenges that the numerical codes have to tackle. A step by step procedure in the modelling of THMG processes is often a reasonable approach.

