EURAD2 ANNUAL EVENT 9-11 SEPTEMBER 2025, BOLOGNA

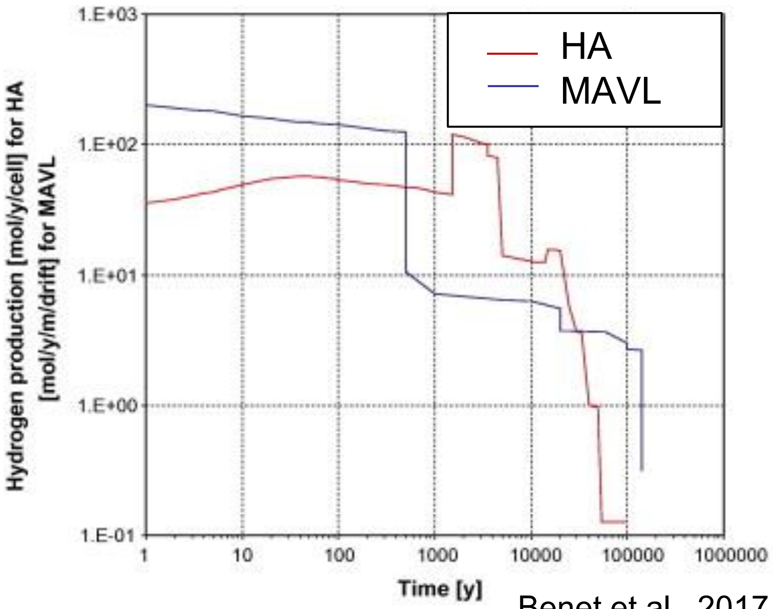
MACROSCOPIC AND PORE-SCALE MODELLING OF GAS TRANSPORT

MAGDALENA DYMITROWSKA

01

CONTEXT : WHY GAS MAY BE AN ISSUE ?

GAS PRODUCTION IN A DEEP REPOSITORY



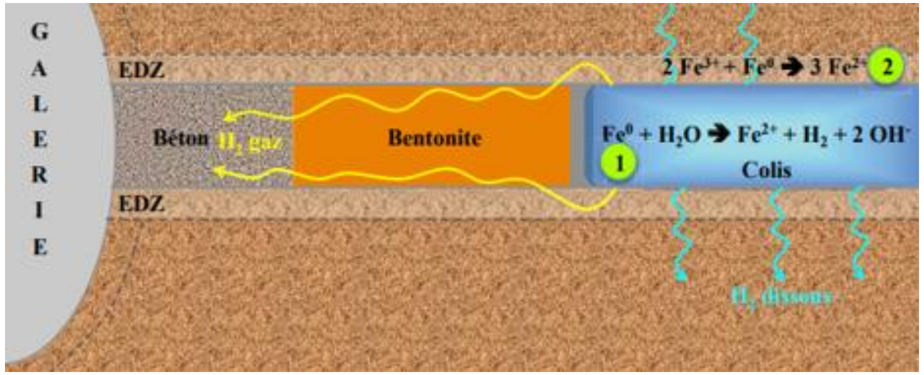
Benet et al., 2017

GAS SOURCE TERM

- mainly H_2 (also CH_4, CO_2..)
- ~ 300 mol/year/cell HA
- very slow > 10 000 years
- exact rates uncertain

HOST ROCK

- low permeability $k \sim 10^{-21}$ m^2
- high saturation $S_w > 0.9$
- strong capillarity $P_c > 5$MPa
- Reynolds number << 1
- heterogeneities (interfaces)
- THM coupling



POSSIBLE PERTURBATIONS

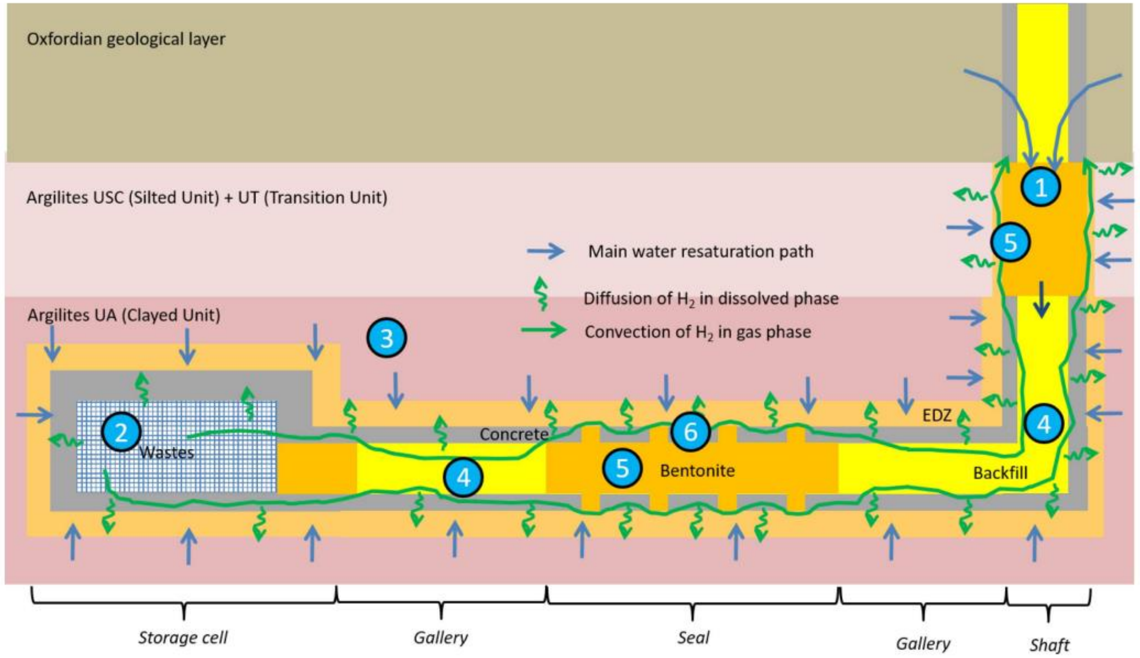
- hydraulic gradient

→ water and RN transport
- mechanical damage of HR & EB
- seals resaturation
- chemical state of close field
- ATEX risks during operation

02

CONTINUOUS SCALE MODELLING

GAS MIGRATION ON DISPOSAL SCALE



S. Levasseur et al(2022)

2-phase flow transport by diffusion and advection

- ➢ advection = generalised Darcy model

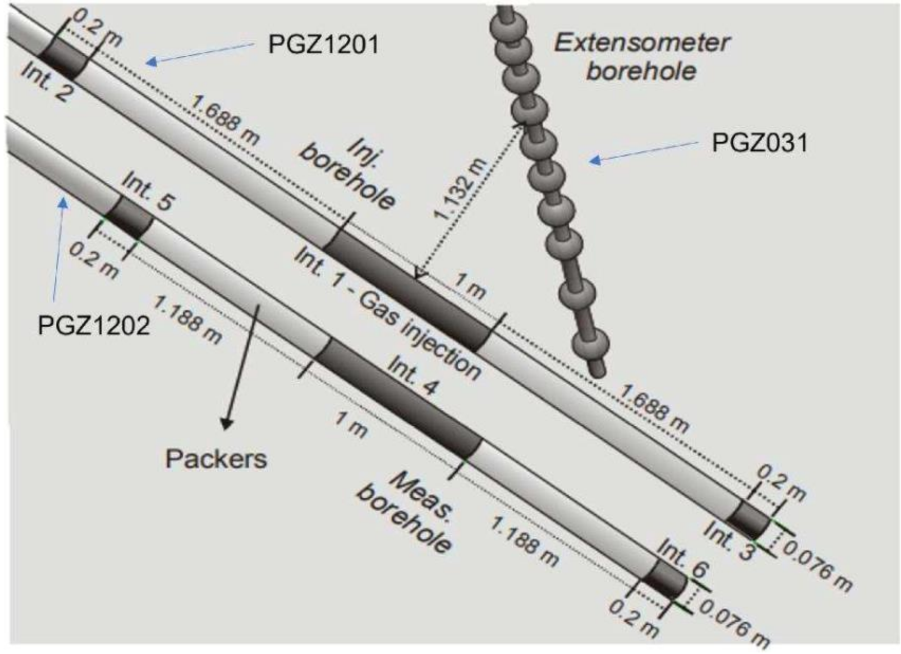
(sand columns in public fountains in DIJON ~1850)

$$\overrightarrow{F_\beta} = \rho_\beta \overrightarrow{\nu_\beta} = = -\frac{k k_{r,\beta}(S_\beta)}{\mu_\beta}(\vec{\nabla} P_\beta + \rho_\beta g \vec{\nabla} z)$$

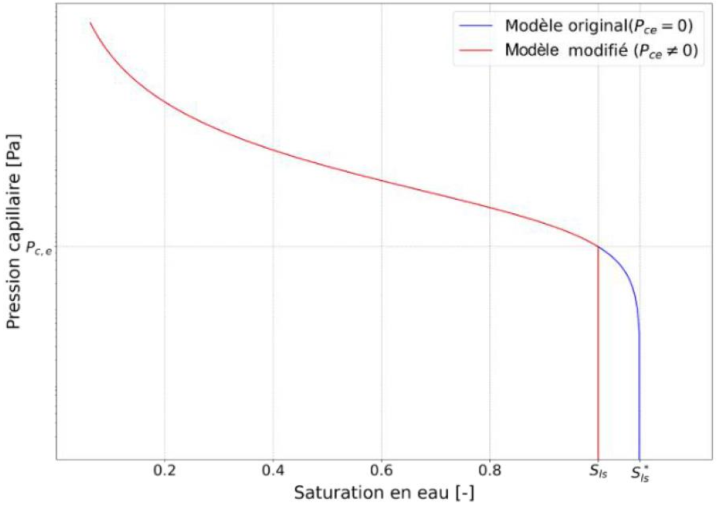
- ➢ unsaturated diffusion models

- ✓ well tested for more permeable materials
- ✓ solvable at grand scale

- → all materials must be characterised/parametrised
- → very limited HM coupling (linear elasticity)
- → zero entry pressure
- → experimental difficulties (results dispersion, representativity, models)



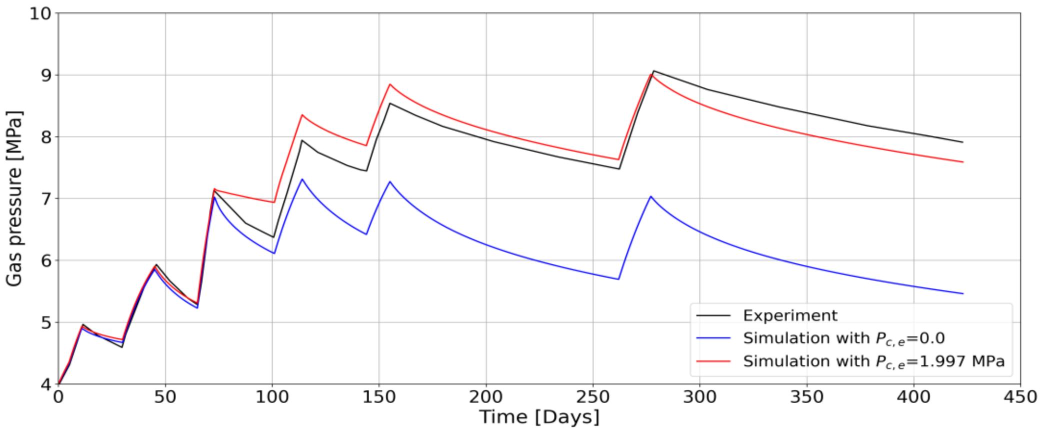
Harington et al 2012



SIMULATION OF PGZ1 EXPERIMENT WITH NO ZERO ENTRY PRESSURE

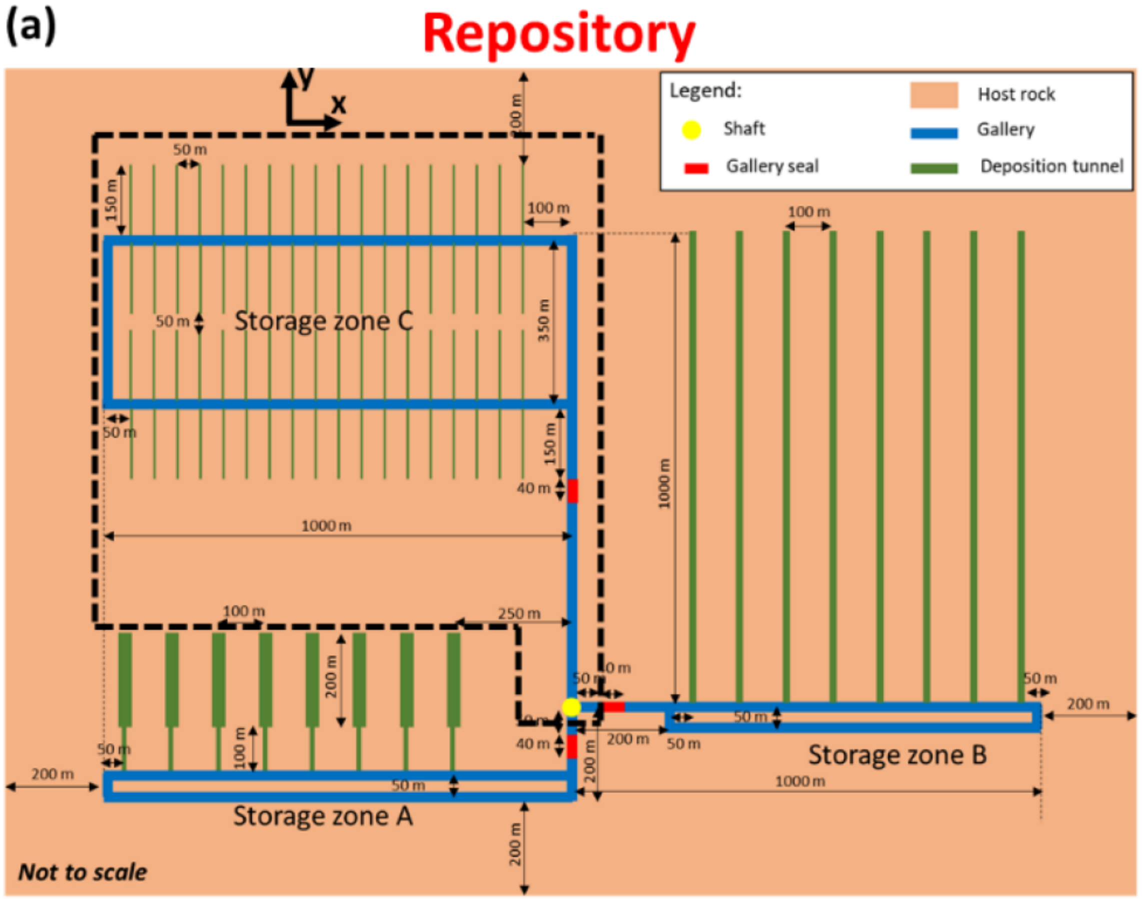
- IN-SITU GAS INJECTION EXPERIMENT IN COX BY ANDRA
- GAZ PRESSURE MONITORING IN INJECTION CHAMBER

- GAS ENTRY PRESSURE IN TOUGHII
- NEW PC-KR DATA ADJUSTMENT
- STRONG EFFECT ON PRESSURE EVOLUTION



Amri et al 2022

GAS MIGRATION ON MODULE SCALE



Wendling et al 2019 (EURAD Gas D6.9)

EURAD1 WP GAS

- GENERIC REPOSITORY WITH PARTS INSPIRED BY 3 NATIONAL PROGRAMS
- THgas 3D SIMULATION OF HA MODULE
- TOUGHII-MP/EOS5 WITH PERSISTENT VARIABLES

- 100K YEARS SIMULATED
- 276K ELEMENTS
- SIMULATION DURATION ~3 WEEKS ON 32CPU

GAS MIGRATION ON MODULE SCALE

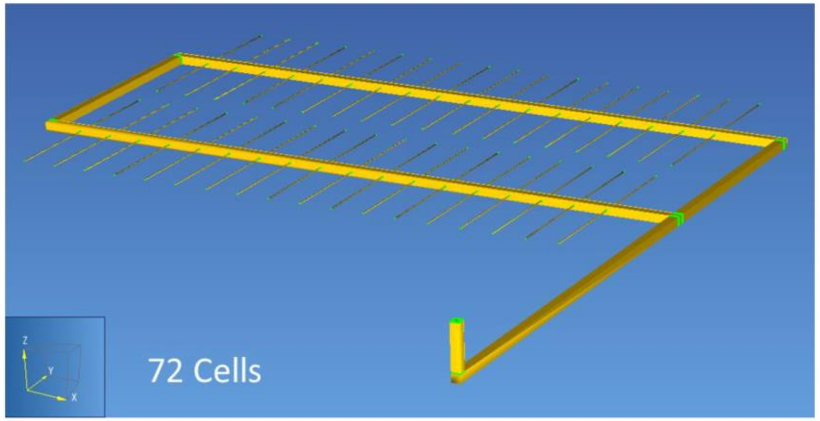
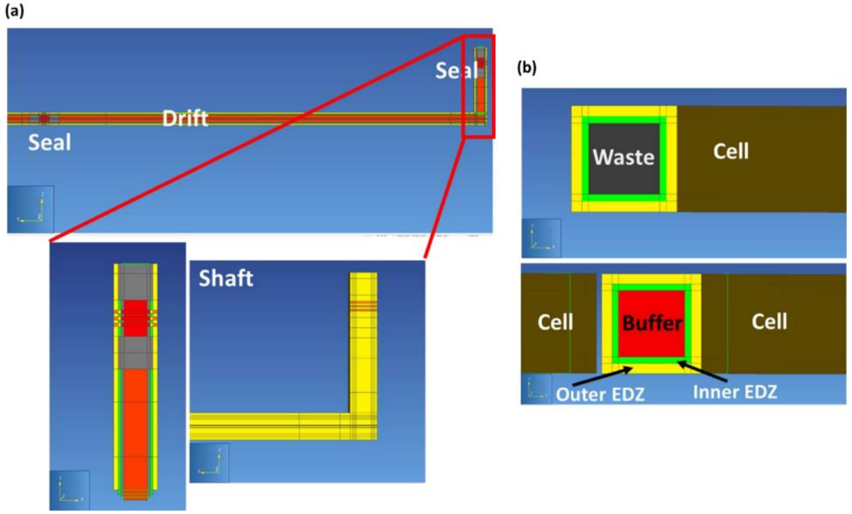


Figure 5-2 – 3D view of the stand-alone module of 72 HLW cells with shaft embedded within the host rock layer (PetraSim preprocessing; Thunderhead engineering inc.).

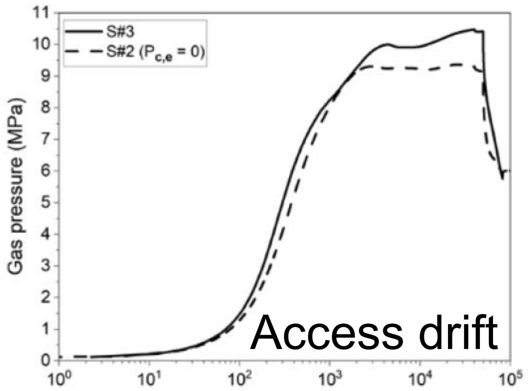


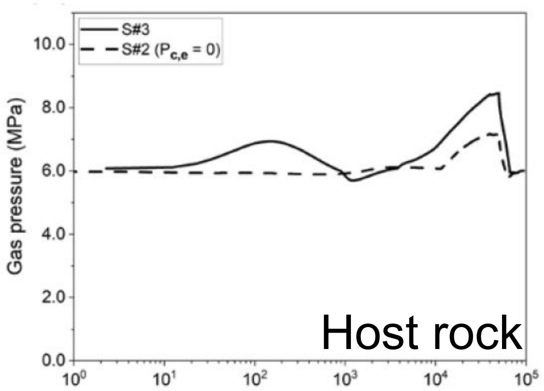
Wendling et al 2024
(EURAD Gas D6.9)

- 3D very important !
- onion-like structure

- no interfaces (voids)
- Millington-Quirk diffusion
- with/without entry pressure

- 1.5MPa increase of Pg with no 0 entry pressure
- Suction curve linearised





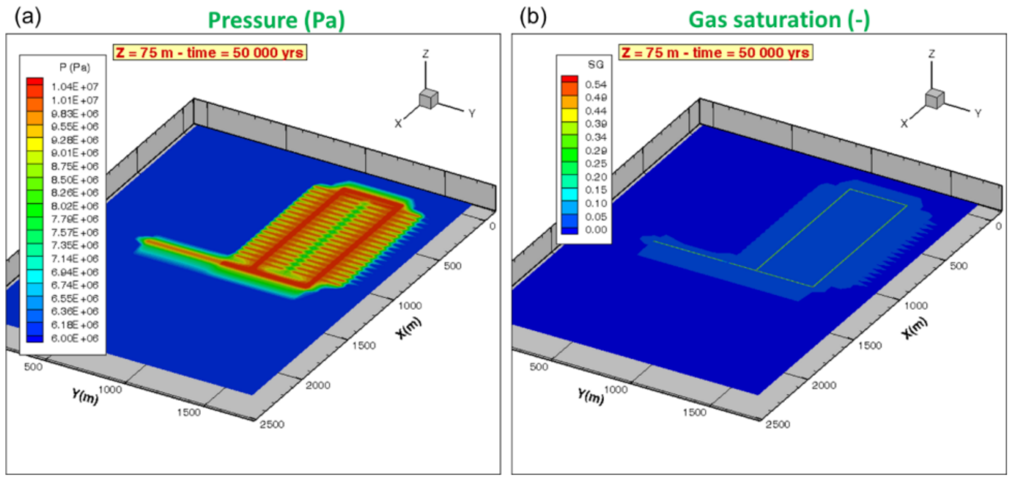
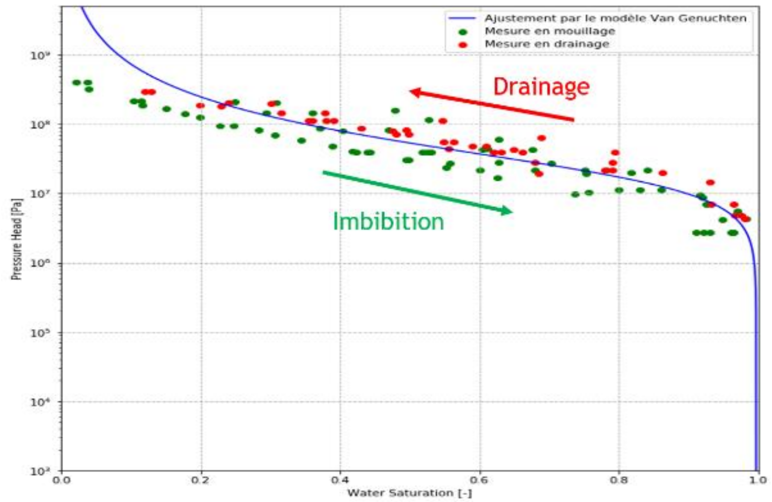
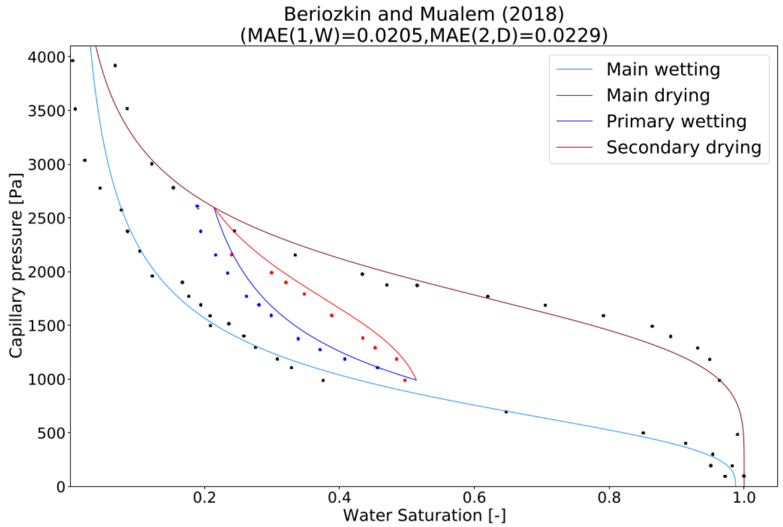


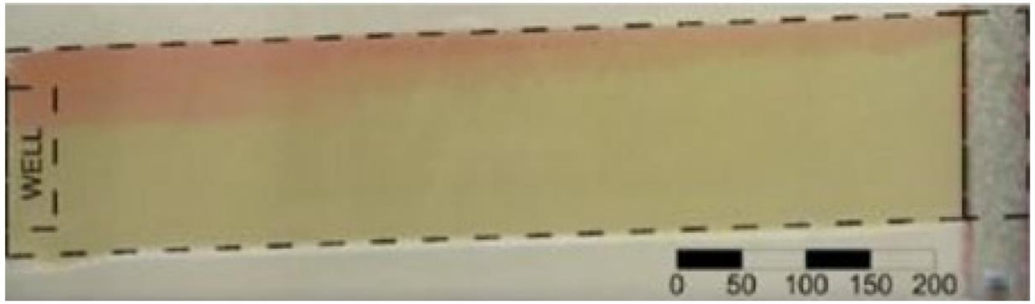
Figure 5-14– Simulated profiles of (a) pressure and (b) gas saturation at the slice plane z = 75 m simulated by scenario#3 ($P_{c,e} \neq 0$) at time 50 000 y.

HYSTERESIS MODEL FOR TWO-PHASE FLOW

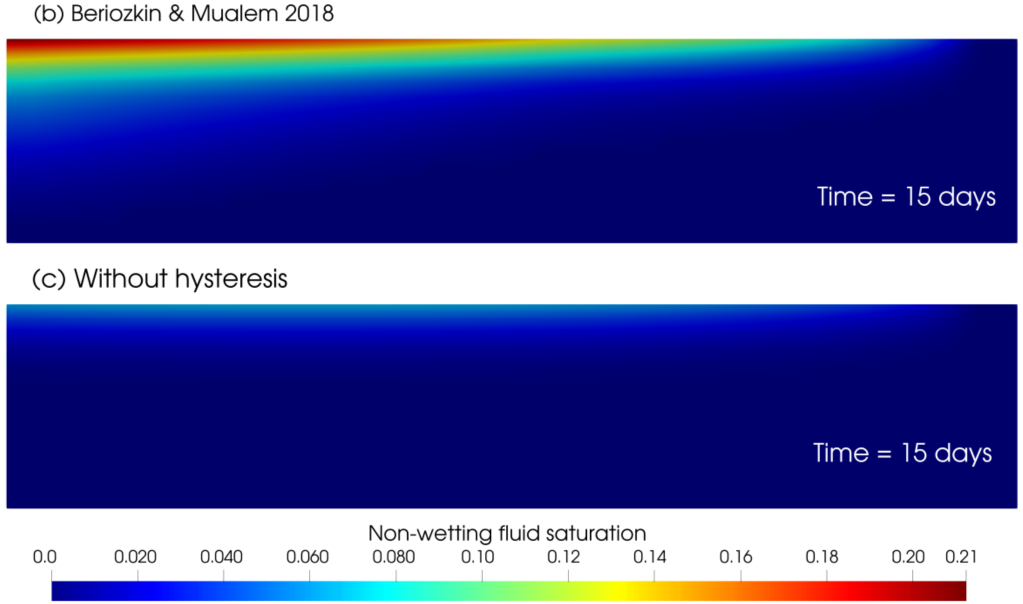
91*61*6 CM³ SLAB OF SAND+WATER WITH SOLTROL-220 INJECTION







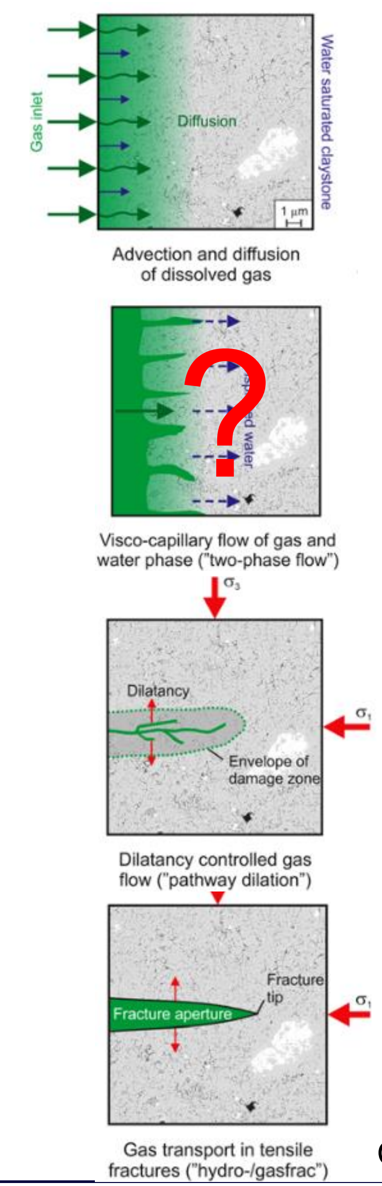
Trevisan et al 2014



Amri et al 2024

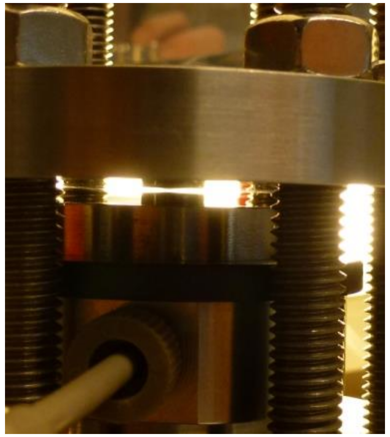
03

PORE SCALE MODELLING

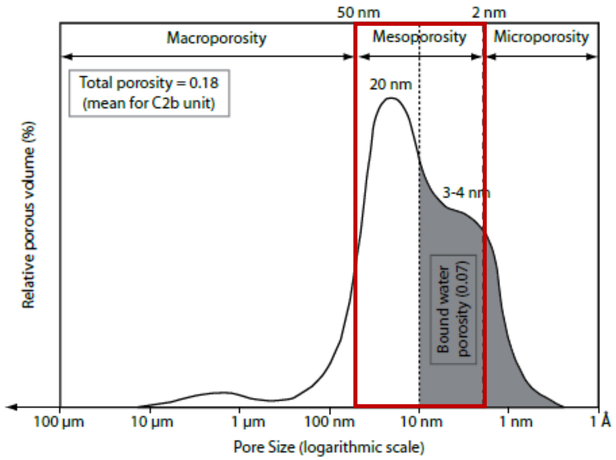


Cuss et al., 2014

UNDERSTANDING GAS MIGRATION AT S_W~1

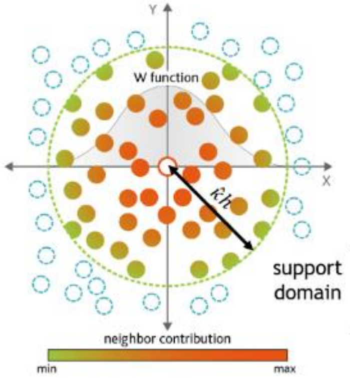


- EXPERIMENTAL RESULTS INDICATING DILATANT GAS FLOW
  - **Localised paths, no water movement, sample expansion**
  - **Need for a model different from Darcy**
- GAS FLOW IN EDZ VERY COMPLEX
  - **Indication of over-fracturing (Cuss et al. 2015)**
  - **Difficult to get REV samples**
- SATURATED BENTONITES MIXTURES:
  - **Consolidation**
  - **Swelling/gas entry pressure**
  - **HMgas models insufficient**
- MODELLING NO-PREDICTIVE (TODAY)



Pore size distribution of COx (ANDRA, 2005)

SMOOTH PARTICLE HYDRODYNAMICS CODE



$$f_{SPH}(x_i,t) \approx \sum_j f(x_j,t) * W(xij,h)$$

$$\nabla f_{SPH}(x_i,t) \approx \sum_j f(x_j,t) * \nabla W(xij,h)$$

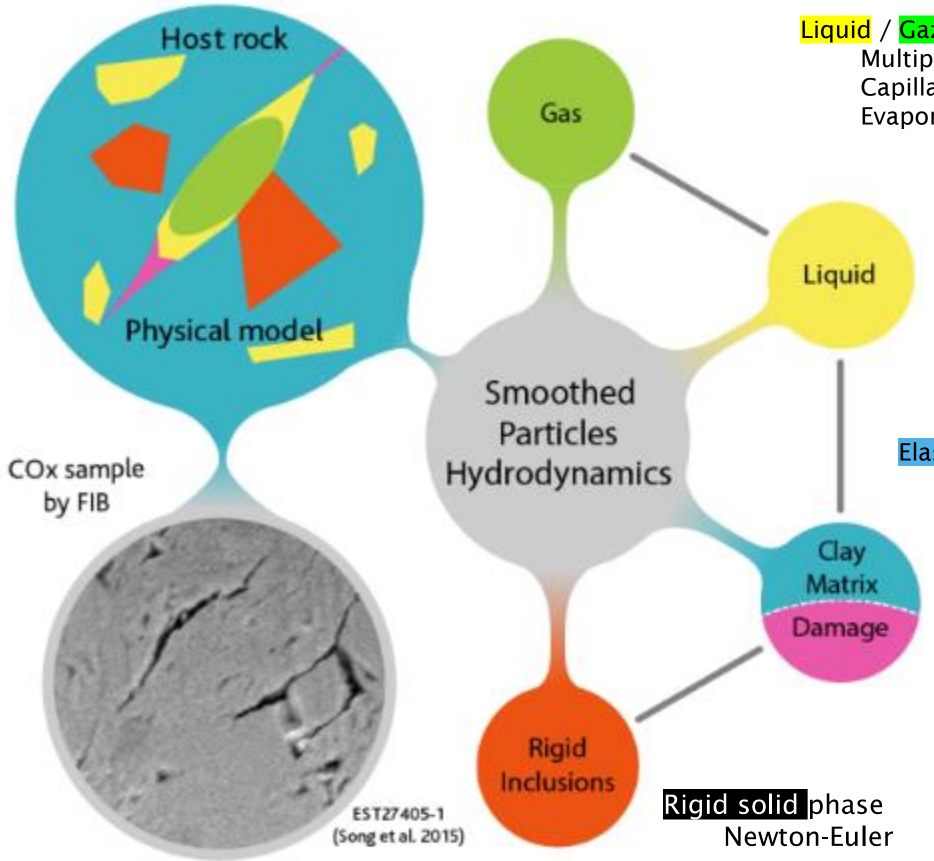
- General EDP solver
- Mesh-free, lagrangien, quasi-local

- 2 phases Navier-Stokes inside pores
- fluids quasi-incompressible

- Linear elasticity with rigid inclusions
- Damage models

- Input parameters : surface tension, contact angle, Young modulus…

- Massively parallelisable (GPU)

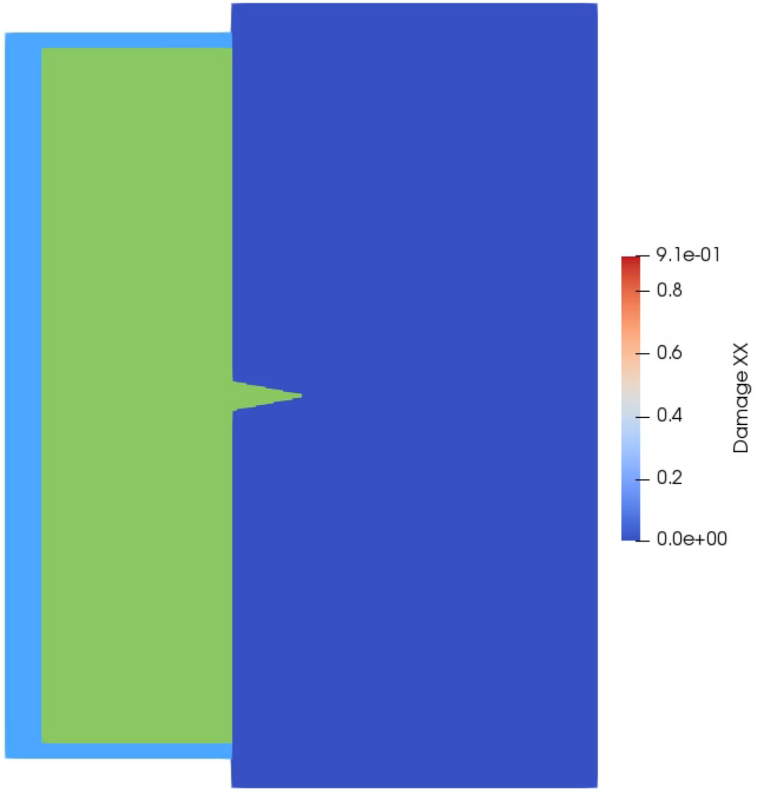


Liquid / Gaz Phases
Multiphase Navier-Stokes
Capillarity
Evaporation/condensation

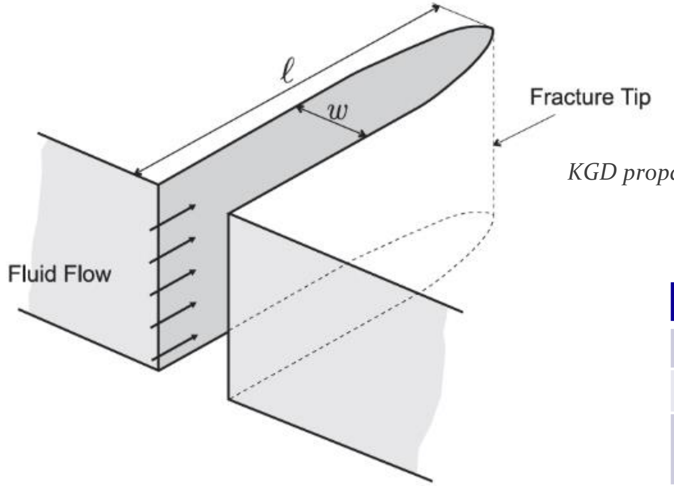
Elastic solid phase
Dynamic linear elasticity
Damage model

Rigid solid phase
Newton-Euler

SPH HYDROFRACTURING



Amrofel PhD 2024

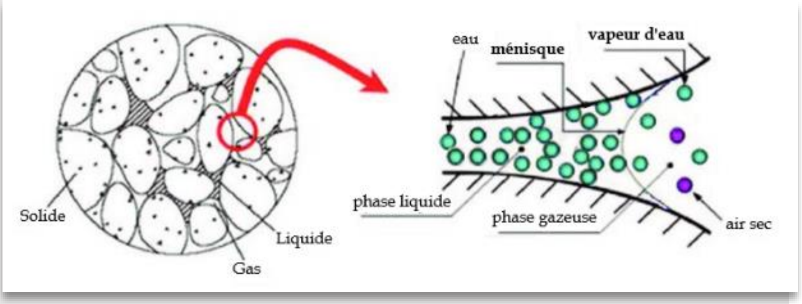


*KGD propagation **model** (Adachi et al., 2007)*

Young modulus	E	30 kPa
Poisson coefficient	ν	0,2
Volume mass	ρ	2450 kg/m
Critical energy yield	Y_c^0	135 Pa
Piston speed	v_p	1.10-4 m.s-1
Length of hatch	l_0	1.10-3 m
Domain width	l	5.10-3 m
Domain length	L	1,07. 10-2 m
Width of injection zone	L_i	9,5.10-3 m
Time step	Δt	1.10-6 s
Smoothing length	h	1.10-4 m
Points density	$/h$	4

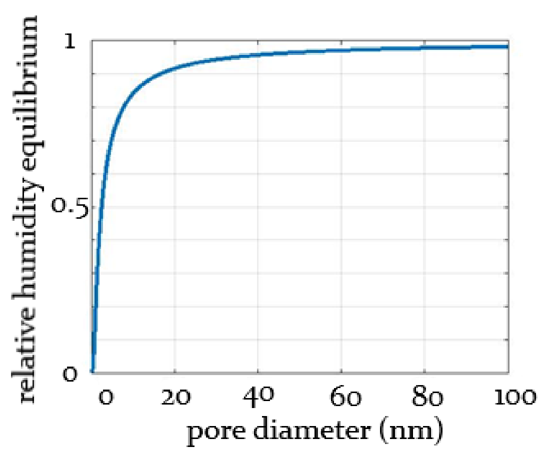
- ▲ Proof of concept ok
- ▲ Initiation pressure ok – 5%
- ▼ Propagation speed too high
- ▼ Low elasticity parameters !

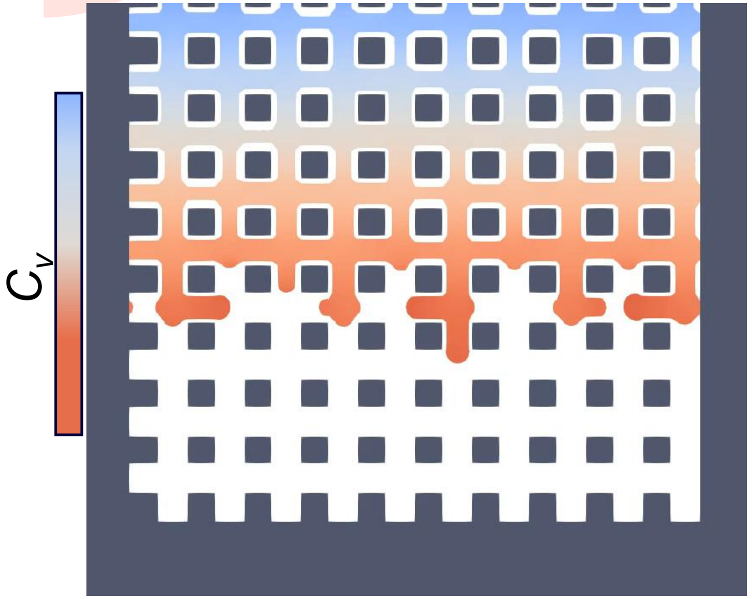
DRYING OF HETEROGENEOUS PORE NETWORK



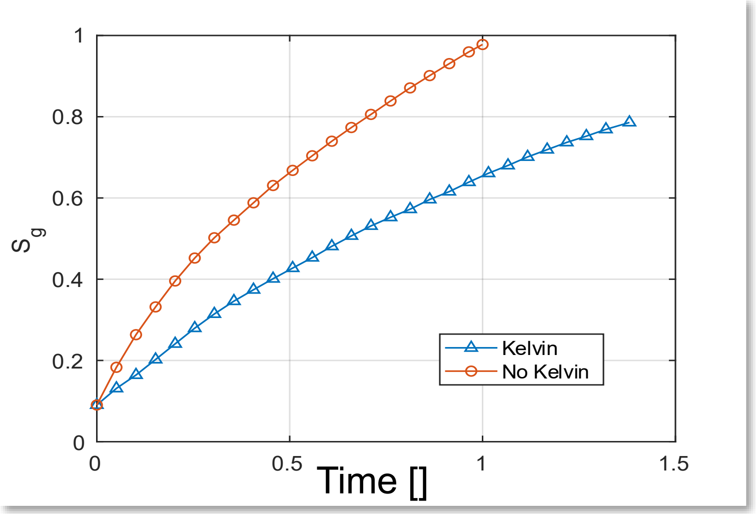
Mchirgui, 2012

Kelvin equation : $C_v = C_{vs} e^{-\frac{P_C M}{\rho_W R T}}$





Network parameters	Value	Unity
Pore size	13	nm
Throat size	5 - 10	nm
h	1.10^{-4}	m



Amrofel et al 2024

436000 PARTICLES

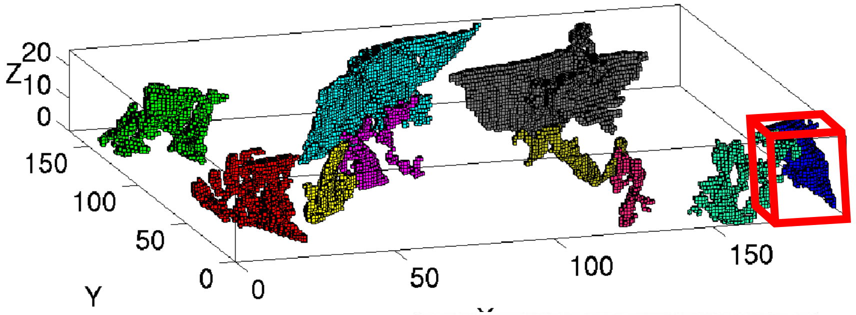
COMPUTATION TIME 9 DAYS

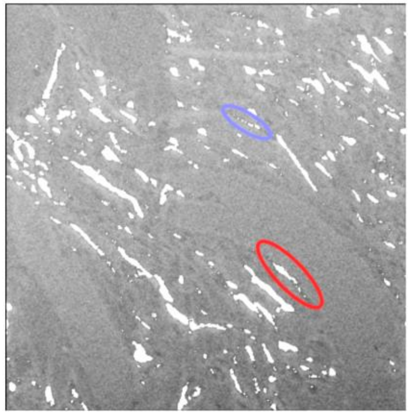
DRAINAGE IN COx CLAY MATRIX

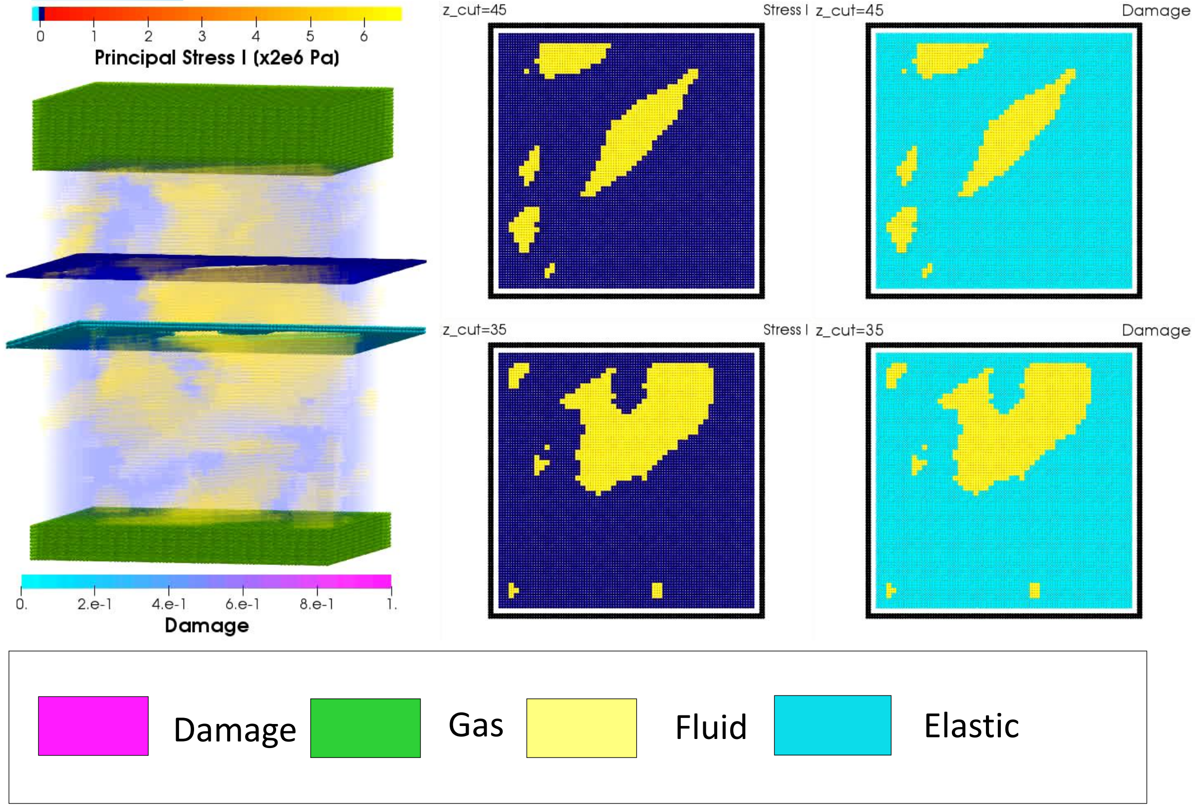
COx sample (FIB-SEM):

- Voxel size ~ (10 nm)^3
- Porosity ~ 3,07%

Song at al. 2015







Fully saturated COx

Poor pore connectivity

Damage model to connect

Flow diagrams :

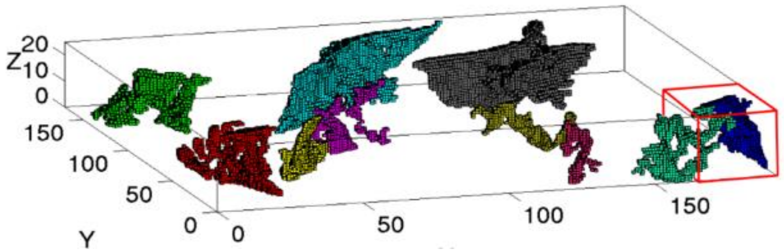
	P_g-P_w [MPa]				
Applied stress [MPa]	2,5	5	8	10	15
6	x	✓	✓	✓	✓
8	x	x	✓	✓	✓
10	x	x	✓	✓	✓
12	x	x	x	✓	✓

Deptulski PhD 2021

04

BRIDGING THE GAP µ↔M

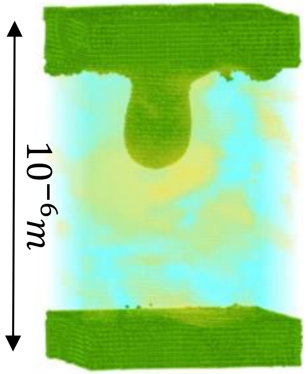
UPSCALING PATH(S)



K.Ganeshalingan 2025 (in préparation)

Effective behavior of clay matrix (poromechanics)

- Refined geometry
- Multiple observation windows
- Whole sample corse grained



A.Pazdniakou et al, 2018

R. Deptulski 2021

Individual pore

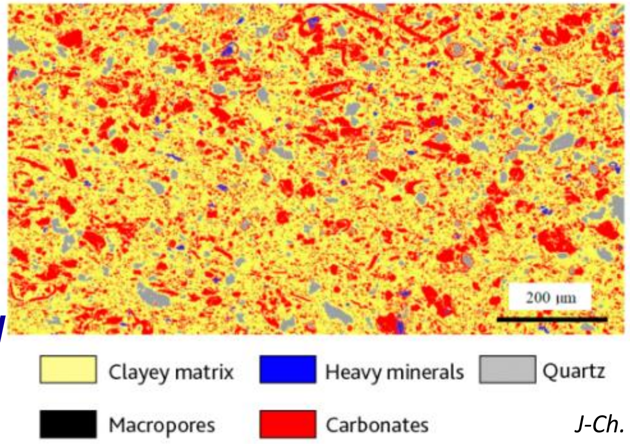
nm

µm

mm

cm

Argilite model

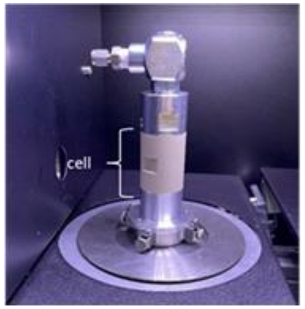


J-Ch. Robinet, 2008

- Post-doc HERMES (end 2025-)
  - ***speed-up SPH avec DNN***
  - ***PINNS***
  - ***reduced order methods***

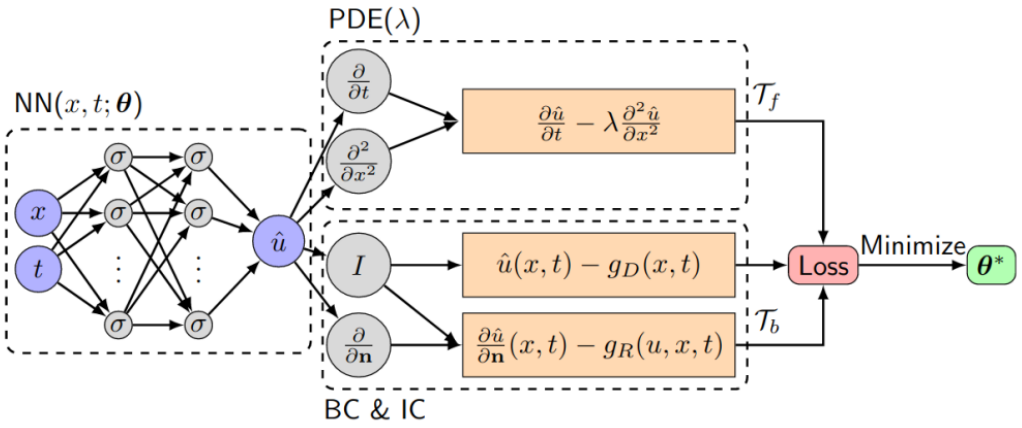
Small lab exp

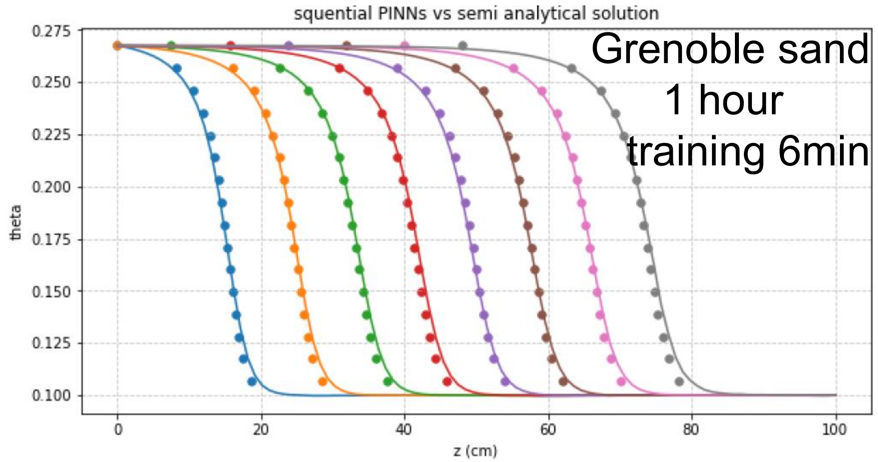
- PhD 2025-

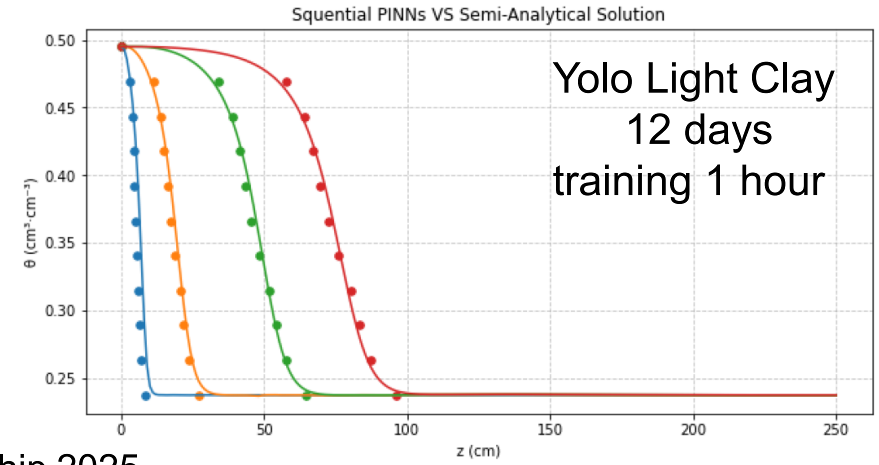


USING PHYSICALY INFORMED NN FOR RICHARDS EQUATION

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\Big[K(h)\,(\partial_z h - 1)\Big]$$







1D infiltration pb with semi-analytical Philip solution

- Recurrent PINNS version
- Adaptative collocation points
- Add convolutional block for feature extraction

Khlifi internship 2025

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NEEDS

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THANK YOU!