A hybrid-dimensional compositional two-phase flow model in fractured porous media with phase transitions and Fickian diffusion

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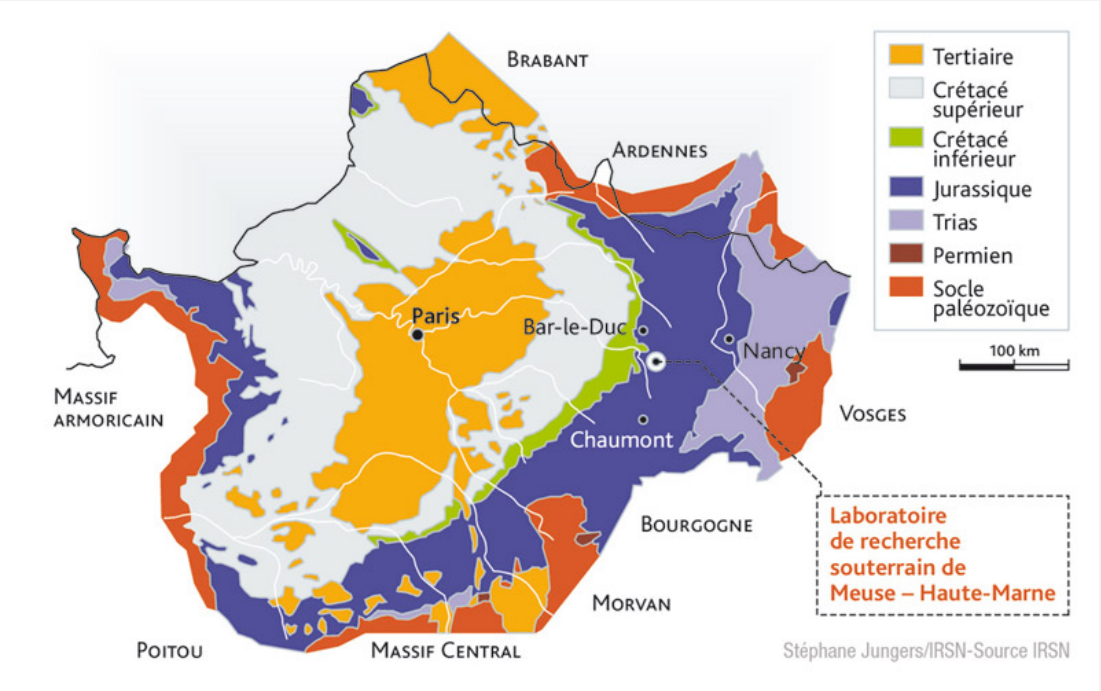
Contexte

Cigéo project (Andra)



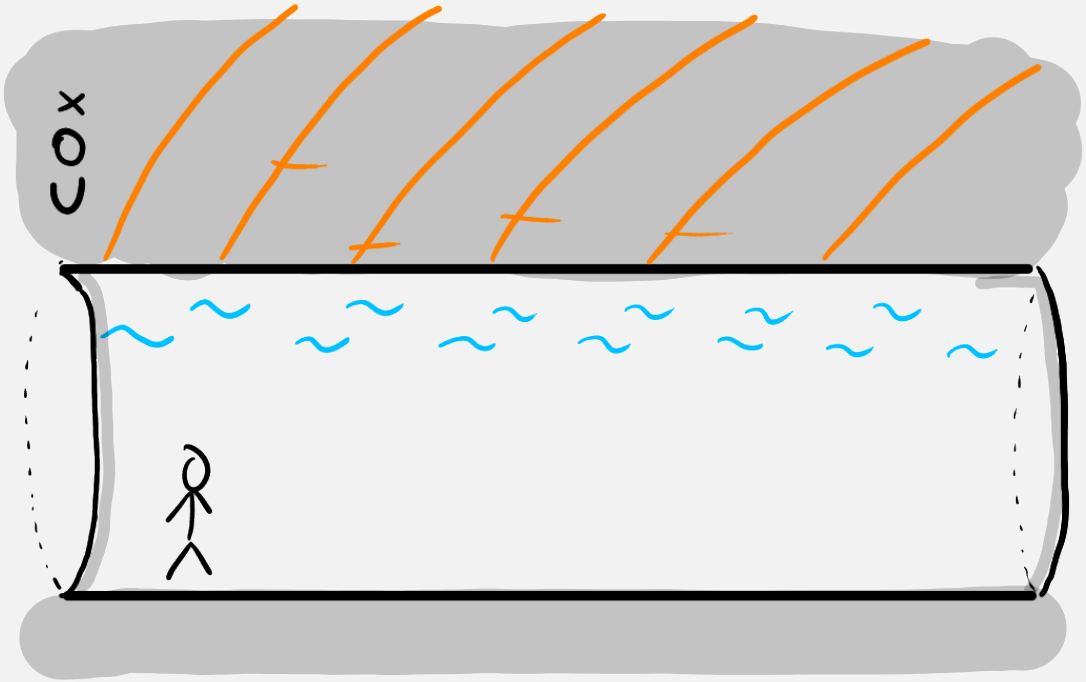
About Cigéo :

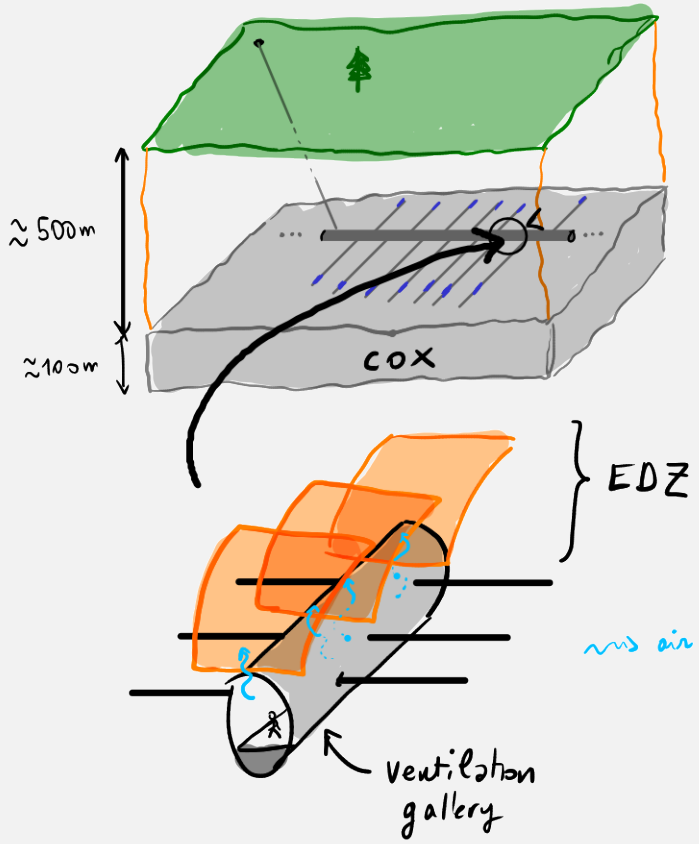
- Launched in the 90s
- Deep storage of HA [1] radioactive waste
- Effective storage starts around 2025
- Operating time before closure ≈ 100 years

1. highest radioactive waste

Contexte

A ventilation gallery





About COx & galeries :

- Ventilation to ensure air quality
- COx has very low permeability : 10^{-20} to $10^{-22} m^2$
- $\rightsquigarrow$ very low conductivity of water

$\approx$ 1cm/Ka

Porous media

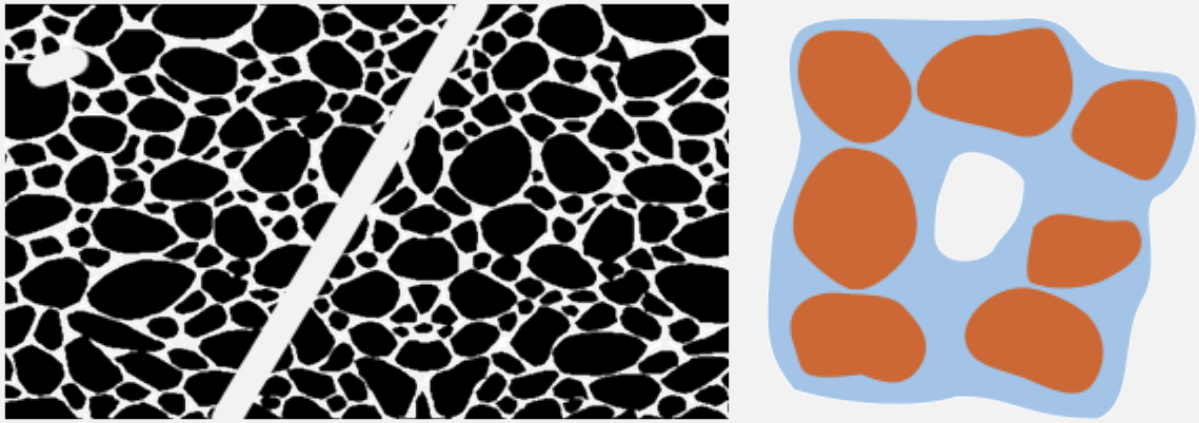


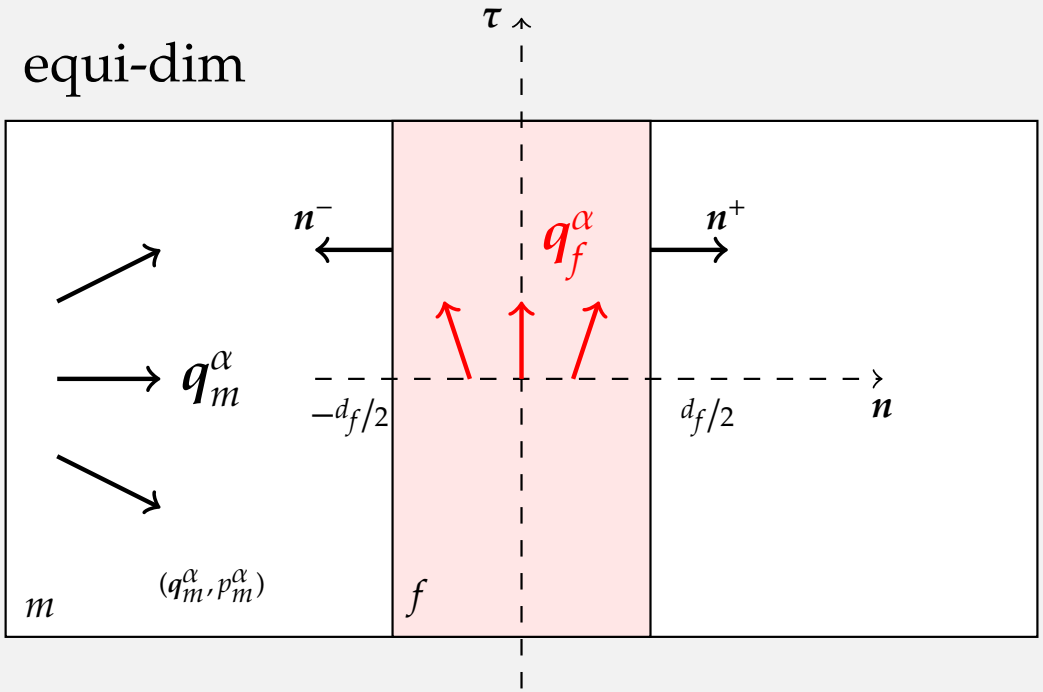
Figure – Porous media with a fracture (left); two-phase flow in a porous media (right)

Saturation s^α is

$$s^\alpha := \frac{\text{volume occupied by the phase inside the pores}}{\text{vol. pores}} \qquad \alpha \in \{\ell, g\},$$

Porosity is denoted $\phi := \frac{\text{vol. pore}}{\text{total vol.}}$

Equi-dimensional model



Volume conservation eqns

- $\phi_m \partial_t s_m^\alpha + \mathrm{div}(\boldsymbol{q}_m^\alpha) = 0$
- $\phi_f \partial_t s_f^\alpha + \mathrm{div}(\boldsymbol{q}_f^\alpha) = 0$

Notations :

phase : $\alpha = \ell, g$

p^α : phase pressure

$\boldsymbol{\Lambda}_i$: absolute permeability

k^α : relative permeability

ϕ_i : porosity

μ^α : fluid viscosity

Darcy velocities

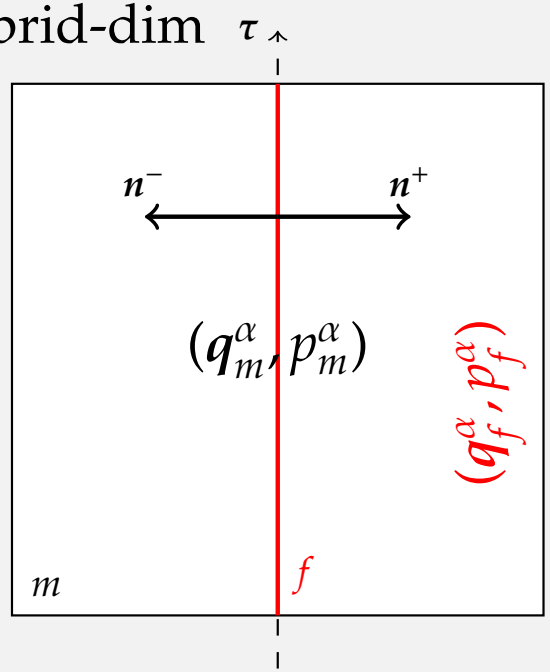
- $\boldsymbol{q}_m^\alpha := -\frac{k_m^\alpha(s_m^\alpha)}{\mu^\alpha} \boldsymbol{\Lambda}_m (\nabla p_m^\alpha - \rho^\alpha \boldsymbol{g})$
- $\boldsymbol{q}_f^\alpha := -\frac{k_f^\alpha(s_f^\alpha)}{\mu^\alpha} \boldsymbol{\Lambda}_f (\nabla p_f^\alpha - \rho^\alpha \boldsymbol{g})$

Reduced model

Dimensional hybridizing [1]

The Darcy flux in the fracture is integrated along the cross section of the fracture width.

hybrid-dim



Darcy velocities

$$q_m^\alpha := -k_m^\alpha(s_m^\alpha)\Lambda_m(\nabla p_m^\alpha - \rho^\alpha g)$$

$$q_f^\alpha := -\, d_f\, k_f^\alpha(s_f^\alpha)\Lambda_{f,\tau}(\nabla_\tau p_f^\alpha - \rho^\alpha g_\tau)$$

Volume conservation equations

$$\phi_m \partial_t s_m^\alpha + \mathrm{div}(q_m^\alpha) = 0$$

$$\phi_f\, d_f\, \partial_t s_f^\alpha + \mathrm{div}_\tau(q_f^\alpha) - \gamma_{n^+} q_m^\alpha - \gamma_{n^-} q_m^\alpha = 0$$

1. [Granet *et al.* 2001], [Jaffré *et al.* 2002,2005], [Bogdanov *et al.* 2003], [Faille *et al.* 2003], [Karimi-Fard 2004]

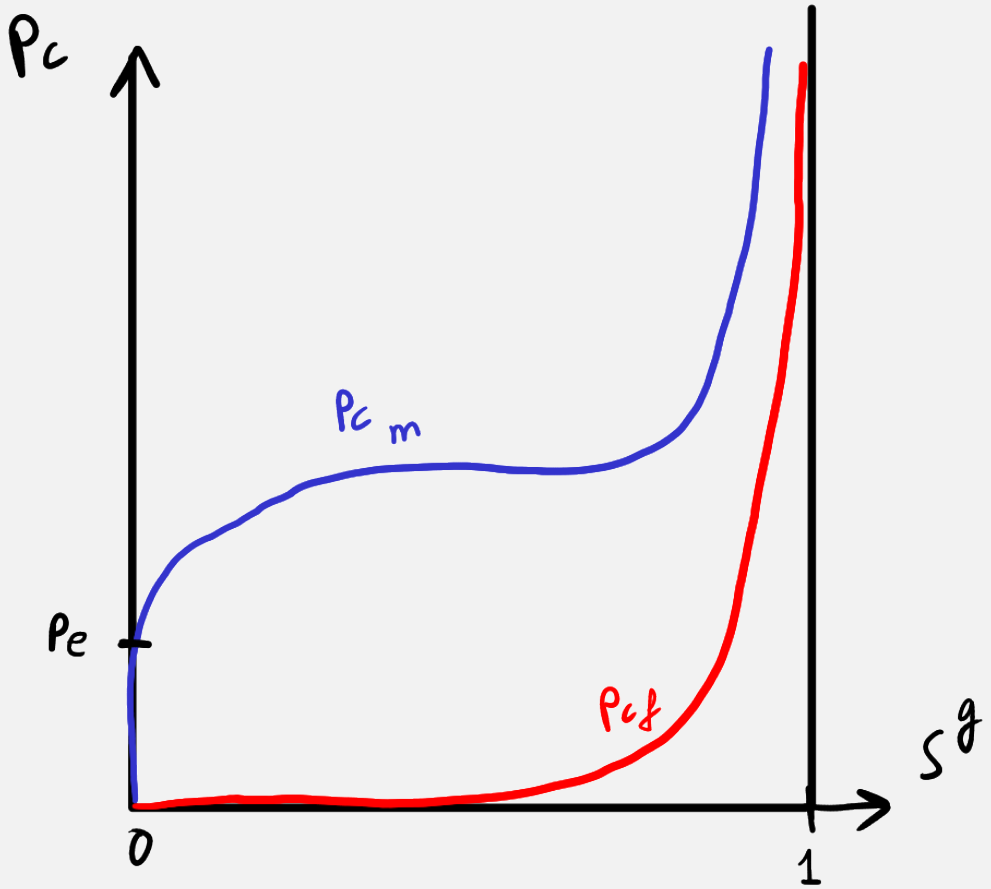
The immiscible two-phase DFM

Immiscible model :

1. $\phi_m \partial_t s_m^\alpha + \mathrm{div}(\boldsymbol{q}_m^\alpha) = 0,$
2. $\phi_f d_f \partial_t s_f^\alpha + \mathrm{div}_\tau(d_f \boldsymbol{q}_f^\alpha) + [\![\boldsymbol{q}_m^\alpha]\!] = 0,$
3. $s_\nu^{\mathrm{g}} + s_\nu^\ell = 1,$
4. $p_\nu^{\mathrm{g}} - p_\nu^\ell = \mathrm{Pc}_\nu(s_\nu^{\mathrm{g}})$,
5. $\gamma_n(\boldsymbol{q}_m^\alpha) + q_f = 0,$

$\alpha \in \{\mathrm{g}, \ell\} \quad \nu \in \{m, f\}$

Capillary pressure relation



highly nonlinear,
can be treated as a graph [Brenner et al. '17]

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Transmission conditions :

$$\gamma_n(\vec{q}_m^{\,\alpha}) + q_f = 0$$

TPFA

$$M(s_{up}^\alpha)(p_m^\alpha - p_i^\alpha) + M(s_{down}^\alpha)(p_f^\alpha - p_i^\alpha) = 0$$

"upwind" "continuous" "discontinuous"

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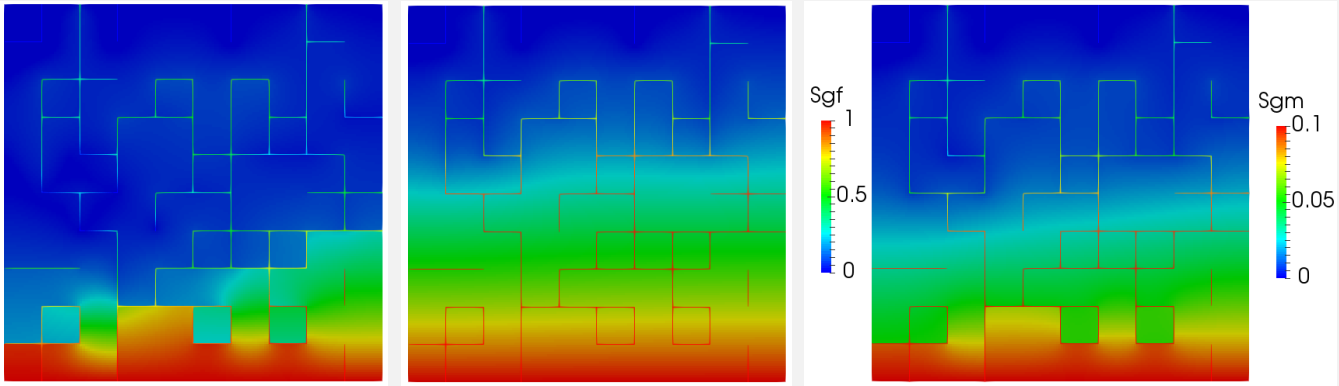
"upwind" "continuous" "discontinuous"

[JA *et al.* '19]



upwind vs continuous vs discontinuous

Fick flux

COx has vey low permeability : $\approx 10^{-20}$ to $10^{-22} m^2$

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for every chemical component c_i^α

$\longrightarrow$ compositional model,
$\longrightarrow$ barrier effect ?

Compositional model I

- Based on the model [Beaude *et al.* '18], unknowns are

$$\text{pressure } p^\alpha, \ \text{ saturation } s^\alpha, \ \ \text{molar fractions } c_i^\alpha.$$

- Conservation of moles $\mathfrak{n}_i$ for each comp. $i \in \mathcal{C}$

$$\begin{aligned} &(mat) - \ \phi_m \partial_t \mathfrak{n}_{i,m} + \mathrm{div}\mathbf{q}_{i,m} = 0, \\ &(frac) - \ \phi_f d_f \partial_t \mathfrak{n}_{i,f} + \mathrm{div}_\tau(d_f \mathbf{q}_{i,f}) - [\![\mathbf{q}_{i,m}]\!] = 0. \end{aligned}$$

with the component molar flux def. as

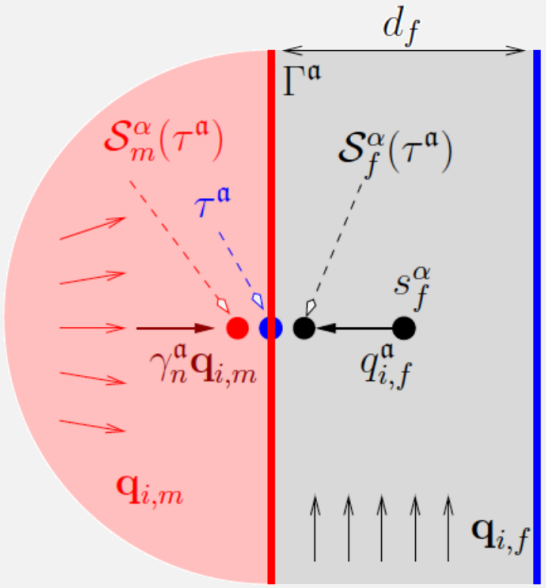
$$\mathbf{q}_{i,\nu} = \sum_{\alpha \in \mathcal{P}} (c_{i,\nu}^\alpha \mathbf{V}_\nu^\alpha + \mathbf{F}_{i,\nu}^\alpha), \quad \nu \in \{m, f\}, \qquad \mathfrak{n}_i := \sum_{\alpha \in \mathcal{P}} \zeta^\alpha s^\alpha c_i^\alpha$$

- Darcy and Fick fluxes are defined as

  - $\mathbf{V}_\nu^\alpha = -\dfrac{\zeta^\alpha(p_\nu^\alpha, c_\nu^\alpha) k_{r,\nu}^\alpha(s_\nu^\alpha)}{\mu^\alpha(p_\nu^\alpha, c_\nu^\alpha)} \mathbf{\Lambda}_\nu \nabla_\nu \left(p_\nu^\alpha - \rho^\alpha(p_\nu^\alpha, c_\nu^\alpha)\mathbf{g}_\nu\right)$

  - $\mathbf{F}_{i,\nu}^\alpha = -\phi_\nu s_\nu^\alpha \zeta^\alpha(p_\nu^\alpha, c_\nu^\alpha) \dfrac{\mathcal{D}^\alpha}{\mathcal{T}_\nu^2} \nabla_\nu c_{i,\nu}^\alpha.$

Compositional model II



- Capillary relation
  - $p_\nu^{\mathrm{g}} - p_\nu^{\ell} = \mathrm{Pc}_\nu(s_\nu^{\mathrm{g}})$,
  - $s_\nu^{\mathrm{g}} + s_\nu^{\ell} = 1, \quad \nu \in \{m, f\}$
- Thermodynamical equilibrium
  - $\mathrm{f}_i^{\mathrm{g}}(\gamma^{\mathfrak{a}} p_m^{\mathrm{g}}, \gamma^{\mathfrak{a}} c_m^{\mathrm{g}}) = \mathrm{f}_i^{\ell}(\gamma^{\mathfrak{a}} p_m^{\ell}, \gamma^{\mathfrak{a}} c_m^{\ell}), \quad i \in \mathcal{C}$,
  - $\min\left(1 - \sum_{i\in\mathcal{C}} \gamma^{\mathfrak{a}} c_{i,m}^{\mathrm{g}},\ \tau^{\mathfrak{a}} - \tau_0\right) = 0$,
  - $\min\left(1 - \sum_{i\in\mathcal{C}} \gamma^{\mathfrak{a}} c_{i,m}^{\ell},\ \tau_1 - \tau^{\mathfrak{a}}\right) = 0$,

- Transmission conditions : continuity of $\boldsymbol{q}^{\alpha} \cdot \boldsymbol{n}$ at mf interface :

$$\gamma_n^{\mathfrak{a}} \mathbf{q}_{i,m} + q_{i,f}^{\mathfrak{a}} = 0,$$

where $\gamma_n^{\mathfrak{a}}$ the normal trace operator. Two-point approximation inside fracture :

$$q_{i,f}^{\mathfrak{a}} = \sum_{\alpha\in\mathcal{P}} (V_{i,f}^{\alpha,\mathfrak{a}} + F_{i,f}^{\alpha,\mathfrak{a}}),$$

Compositional model III

Fick flux in the fracture :

$$F_{i,f}^{\alpha,\mathfrak{a}} = \frac{\zeta^\alpha(p_f^\alpha, c_f^\alpha) + \zeta^\alpha(\gamma^\mathfrak{a} p_m^\alpha, \gamma^\mathfrak{a} c_m^\alpha)}{2} \left(\frac{2 s_f^\alpha \, \mathcal{S}_f^\alpha(\tau^\mathfrak{a})}{s_f^\alpha + \mathcal{S}_f^\alpha(\tau^\mathfrak{a})} \right) \frac{\phi_f \mathcal{D}^\alpha}{\mathcal{T}_f^2} \frac{(c_{i,f}^\alpha - \gamma^\mathfrak{a} c_{i,m}^\alpha)}{d_f/2}.$$

$\longrightarrow$ Harmoning averaging to take account for vanishing saturation

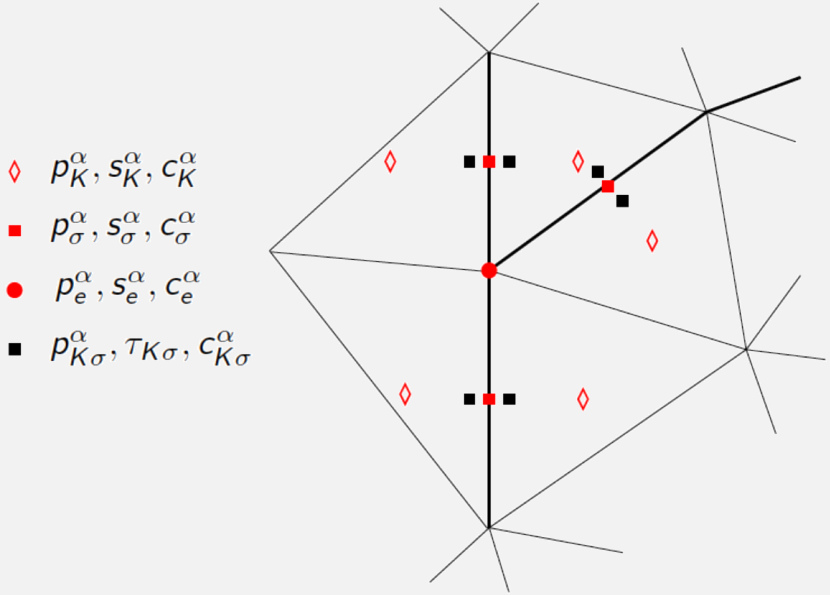
Darcy flux :

$$V_{i,f}^{\alpha,\mathfrak{a}} = c_{i,f}^\alpha \, \frac{\zeta^\alpha}{\mu^\alpha}(p_f^\alpha, c_f^\alpha) \, k_{r,f}^\alpha(s_f^\alpha) \, (V_f^{\alpha,\mathfrak{a}})^+ - \gamma^\mathfrak{a} c_{i,m}^\alpha \, \frac{\zeta^\alpha}{\mu^\alpha}(\gamma^\mathfrak{a} p_m^\alpha, \gamma^\mathfrak{a} c_m^\alpha) \, k_{r,f}^\alpha(\mathcal{S}_f^\alpha(\tau^\mathfrak{a})) \, (V_f^{\alpha,\mathfrak{a}})^-$$

with

$$V_f^{\alpha,\mathfrak{a}} = \lambda_{f,n} \left(\frac{(p_f^\alpha - \gamma^\mathfrak{a} p_m^\alpha)}{d_f/2} + \frac{\rho^\alpha(p_f^\alpha, c_f^\alpha) + \rho^\alpha(\gamma^\mathfrak{a} p_m^\alpha, \gamma^\mathfrak{a} c_m^\alpha)}{2} \mathbf{g}_f \cdot \mathbf{n}^\mathfrak{a} \right),$$

Discrete model I



Degrees of freedom :

- gaz pressure p_κ^g,
- saturation s_κ^g,
- molar fraction c_κ^α,
- interface variable τ_κ.

Remarks :

- Interfaces unknowns provides physically consistent approximations of *mf* fluxes ; Regularized harmonic mean in the discrete Fick flux ;
- Adding porous volume at interfaces for robustness on nonlinear solver ;
- parametrization of pc curves using a switch parameter τ [Brenner *et al.* '17] :

$$\tau > 1 : \text{matrix side} \quad \tau < 1 : \text{fracture side}$$

Discrete model II

Molar fraction conservation eqns :

$$\text{(cells)} \quad \frac{\mathfrak{n}_{i,K}^n - \mathfrak{n}_{i,K}^{n-1}}{\Delta t^n} + \sum_{\sigma \in \mathcal{F}_K \setminus \mathcal{F}_\Gamma} q_{i,K,\sigma}^n + \sum_{\sigma \in \mathcal{F}_K \cap \mathcal{F}_\Gamma} q_{i,K,K\sigma}^n = 0,$$

$$\text{(frac)} \quad \frac{\mathfrak{n}_{i,\sigma}^n - \mathfrak{n}_{i,\sigma}^{n-1}}{\Delta t^n} + \sum_{e \in \mathcal{E}_\sigma} q_{i,\sigma,e}^n + \sum_{K \in \mathcal{M}_\sigma} q_{i,\sigma,K\sigma}^n = 0,$$

$$\text{(edges)} \quad \frac{\mathfrak{n}_{i,e}^n - \mathfrak{n}_{i,e}^{n-1}}{\Delta t^n} - \sum_{\sigma \in \mathcal{F}_e \cap \mathcal{F}_\Gamma} q_{i,\sigma,e}^n = 0,$$

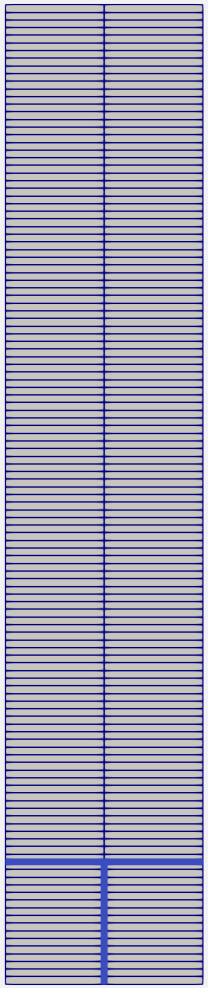
$$\text{(intf)} \quad \frac{\mathfrak{n}_{i,K\sigma}^n - \mathfrak{n}_{i,K\sigma}^{n-1}}{\Delta t^n} - q_{i,K,K\sigma}^n - q_{i,\sigma,K\sigma}^n = 0.$$

+ min **constraints and thermodynamical equilibrium.**

Remarks

TPFA for every fluxes ; **Fully implicit** Scheme ; Solver : using **Newton-min** algorithm [Kraütle '11, Ben Gharbia & Jaffré '13] ;

Simplified suction case : description



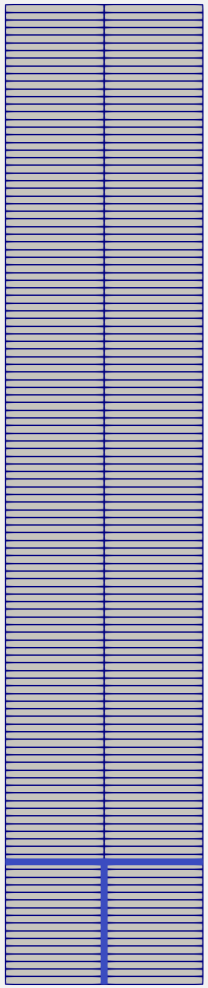
$(0, 20m) \times (0, 100m)$

2×128 grid

Desatuwration by suction :

- m, f initially saturated by pure water liquid phase,
- boundary conditions :
  - **bottom** thermo. eq. with $p^g = p^\ell = 10^5$ Pa, $H_r = 0.5$
  - **top** pure water,
  - **lateral** zero flux (impervious).
- Permeabilities : $\Lambda_m = 10^{-4}$ Darcy, $\Lambda_f = 10^6 \Lambda_m$
- Porosities : $\phi_m = 0.15$, $\phi_f = 0.4$,
- Simulation time : 200 years,
- Brooks- Corey laws,
- Rel. mob. : $k_{r,f}(s^\alpha) = s^\alpha$; $k_{r,m}(s^\ell) = (s^\ell)^2$; $k_{r,m}(s^g) = (s^g)^2$,

Simplified suction case : description



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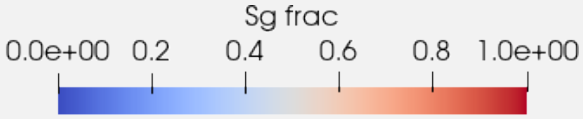
Comparison of three settings :

- No fick fluxes : $\mathcal{D}^\alpha = 0$ (`nofick`);
- Only on gas phase : $\mathcal{D}^g > 0$ and $\mathcal{D}^\ell = 0$ (`partialfick`);
- With Fick fluxes $\mathcal{D}^g > 0$ and $\mathcal{D}^\ell > 0$ (`fick`);

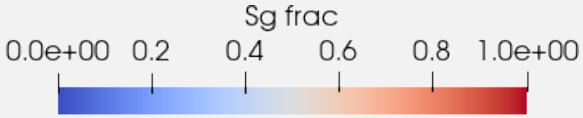
Simplified suction case : results



(`nofick`)

(`nofick`) Barrier effect due to fractures filled by gas, as in the immiscible case.

Simplified suction case : results



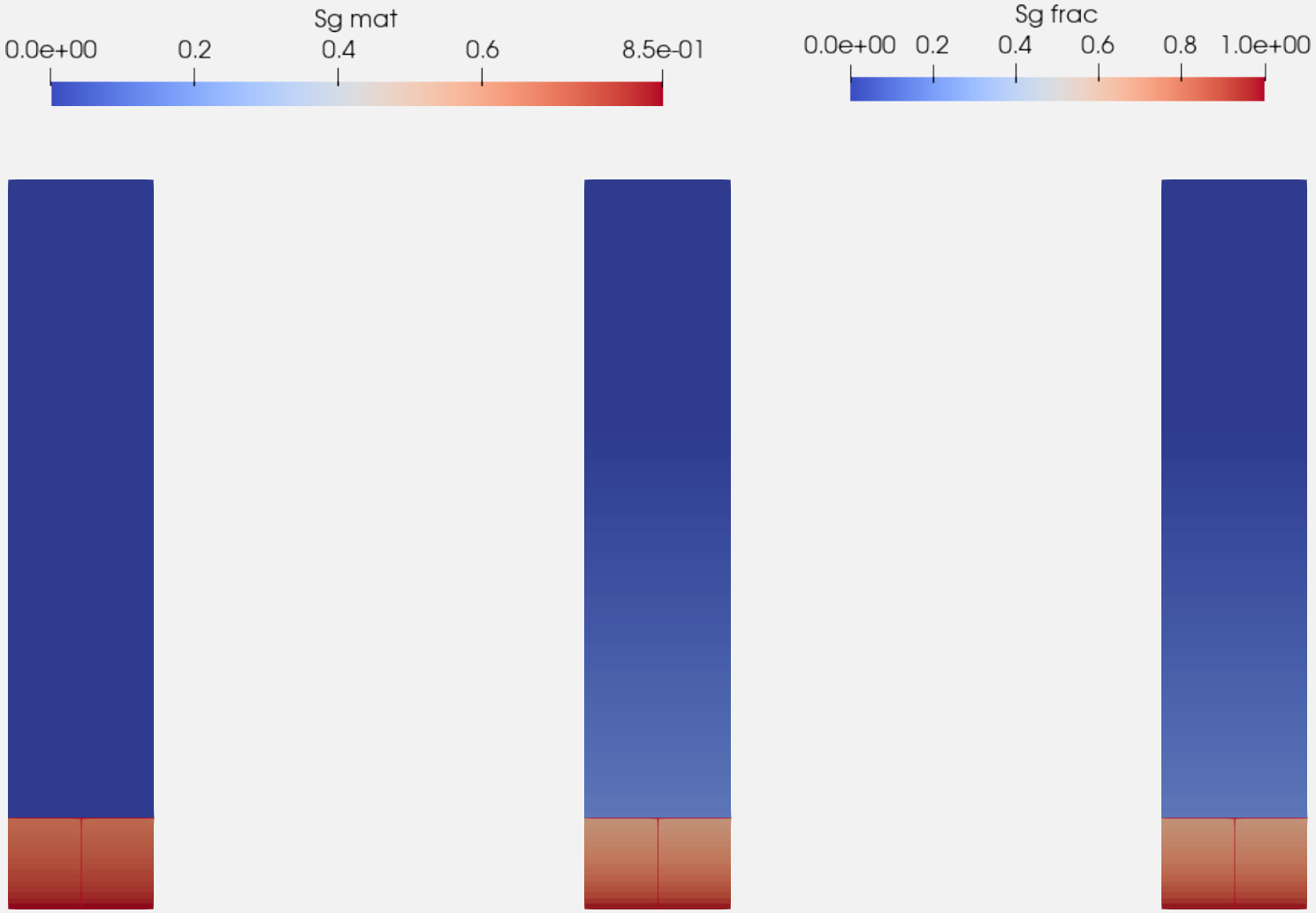
(`fick`) : Barrier effect is removed.

Depending on g or ℓ ?

(`nofick`)

$\mathcal{D}^{\ell} > 0$
$\mathcal{D}^{g} > 0$
(`fick`)

Simplified suction case : results

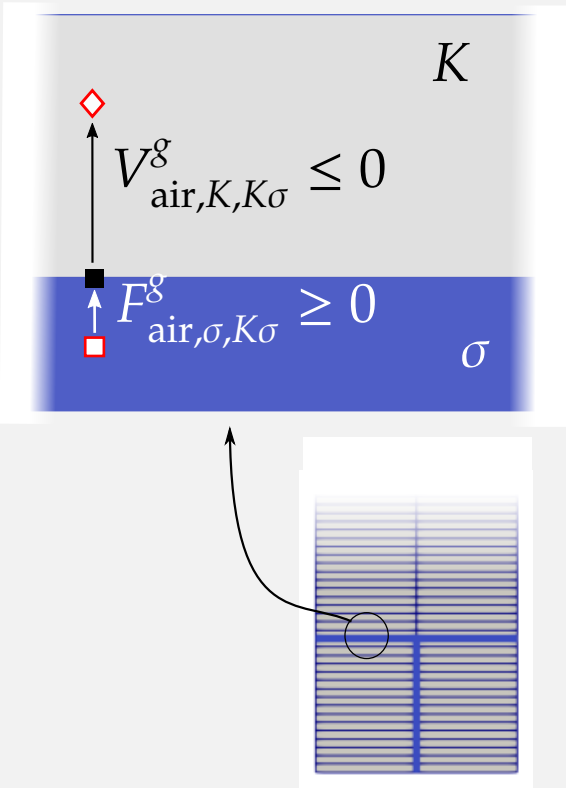


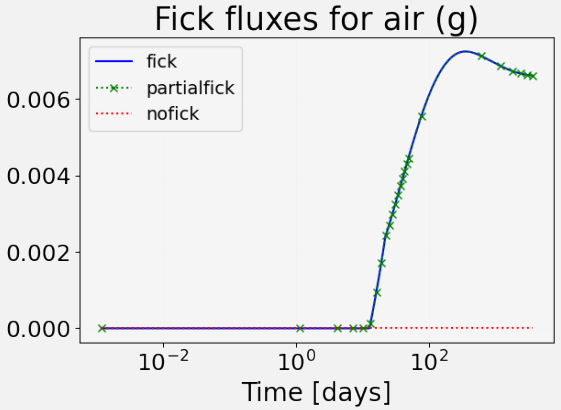
(nofick)

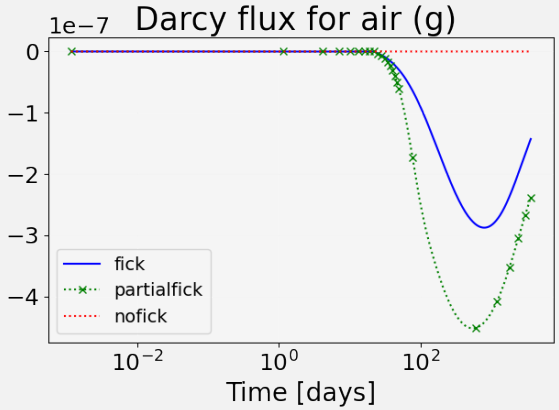
$\mathcal{D}^\ell = 0$
$\mathcal{D}^g > 0$
(partialfick)

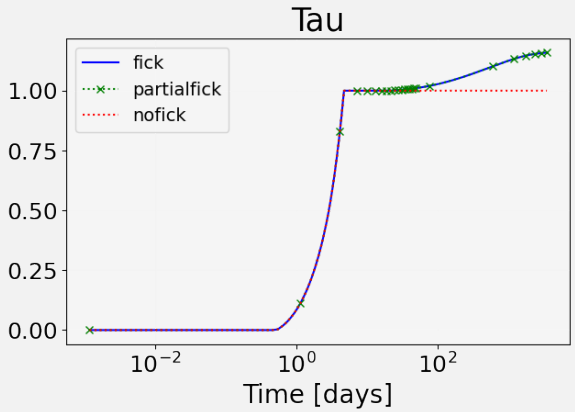
$\mathcal{D}^\ell > 0$
$\mathcal{D}^g > 0$
(fick)

Simplified suction case : results





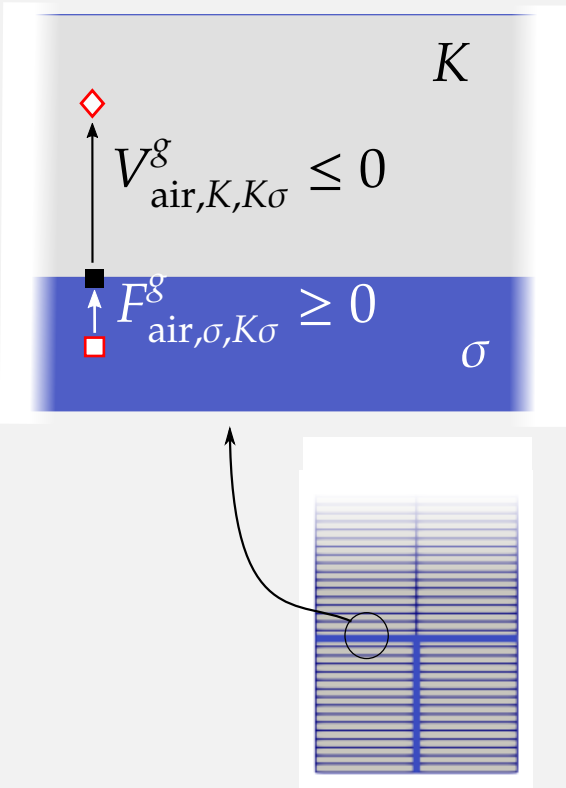


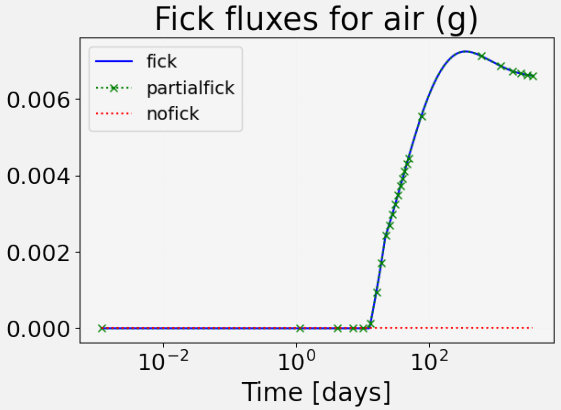


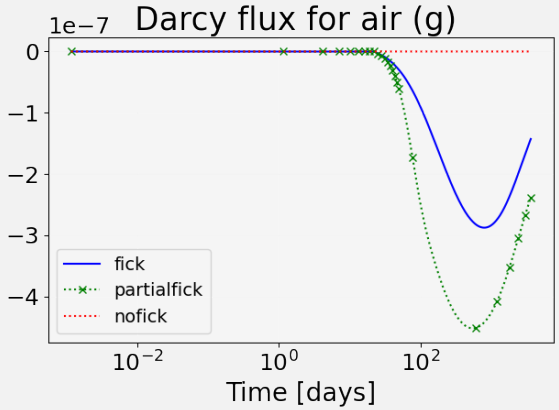
Interplay of Darcy and Fick fluxes

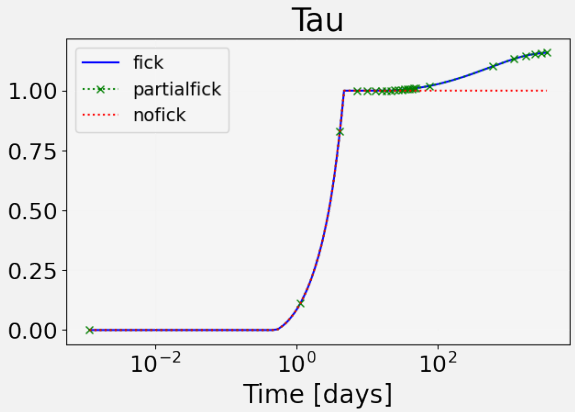
1. Air component is transported from fracture (□) to interface (■)

Simplified suction case : results





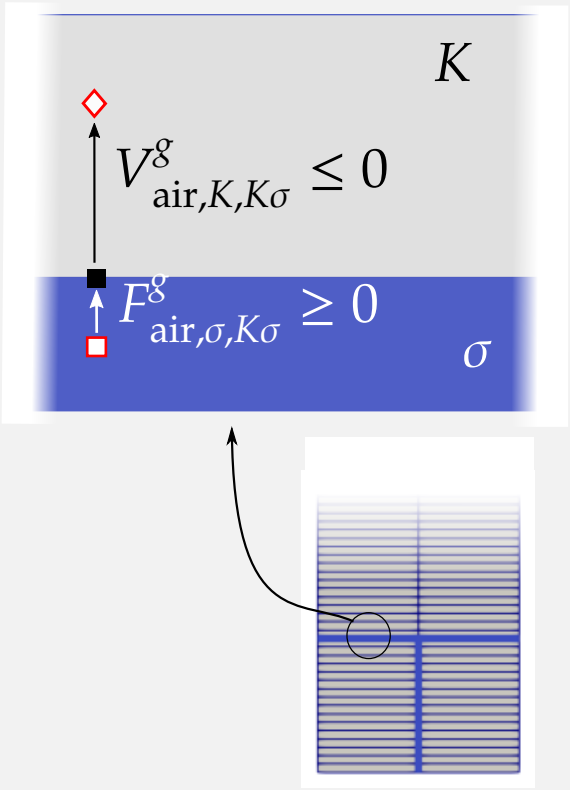


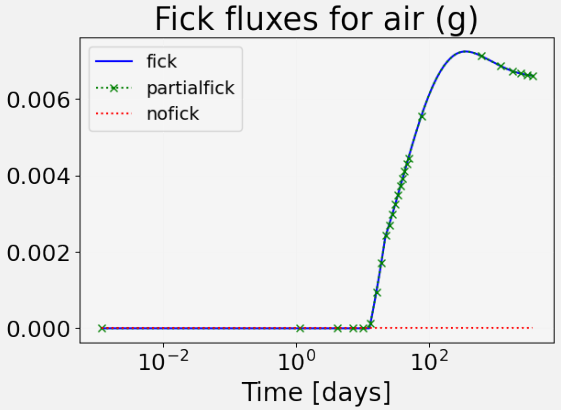


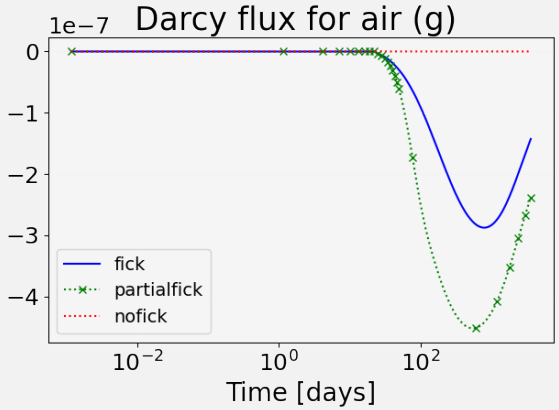
Interplay of Darcy and Fick fluxes

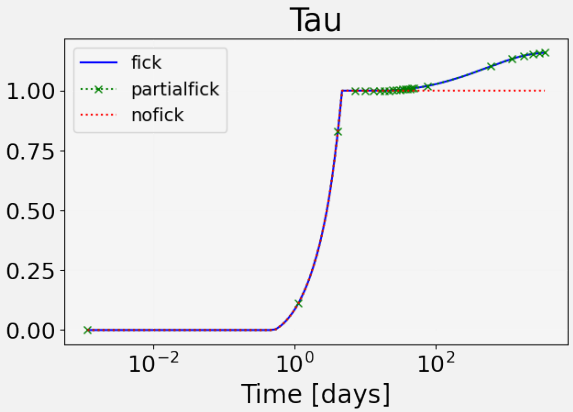
1. Air component is transported from fracture (□) to interface (■) ⇝ gas appearance at interface on matrix side ($\tau > 1$).

Simplified suction case : results







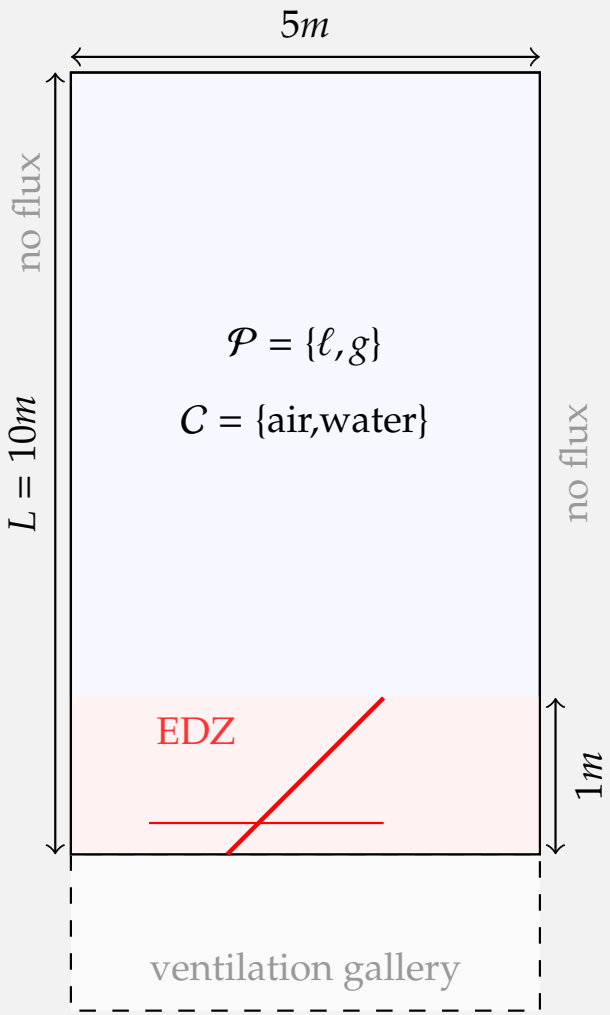


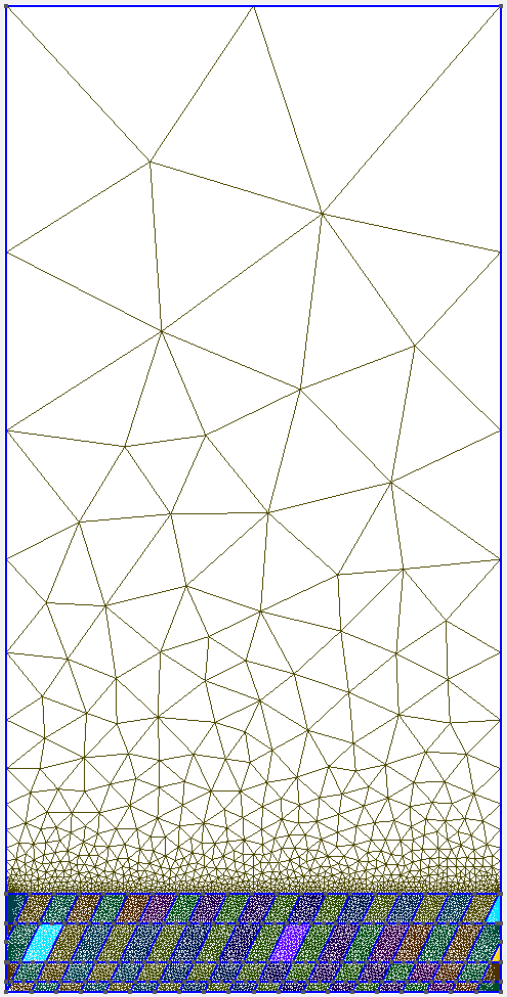
Interplay of Darcy and Fick fluxes

1. Air component is transported from fracture (□) to interface (■) ⇝ gas appearance at interface on matrix side ($\tau > 1$).
2. Gas is then transported to the upper cell (◊) by Darcy flux.

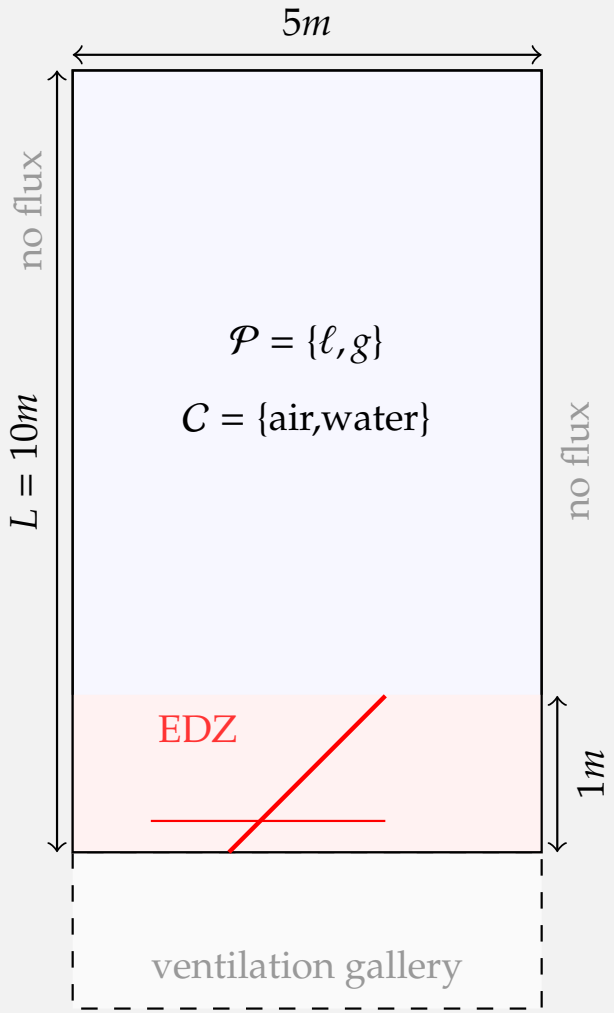
Application : domain

Desaturation by suction of a Callovo-Oxfordian argilite rock





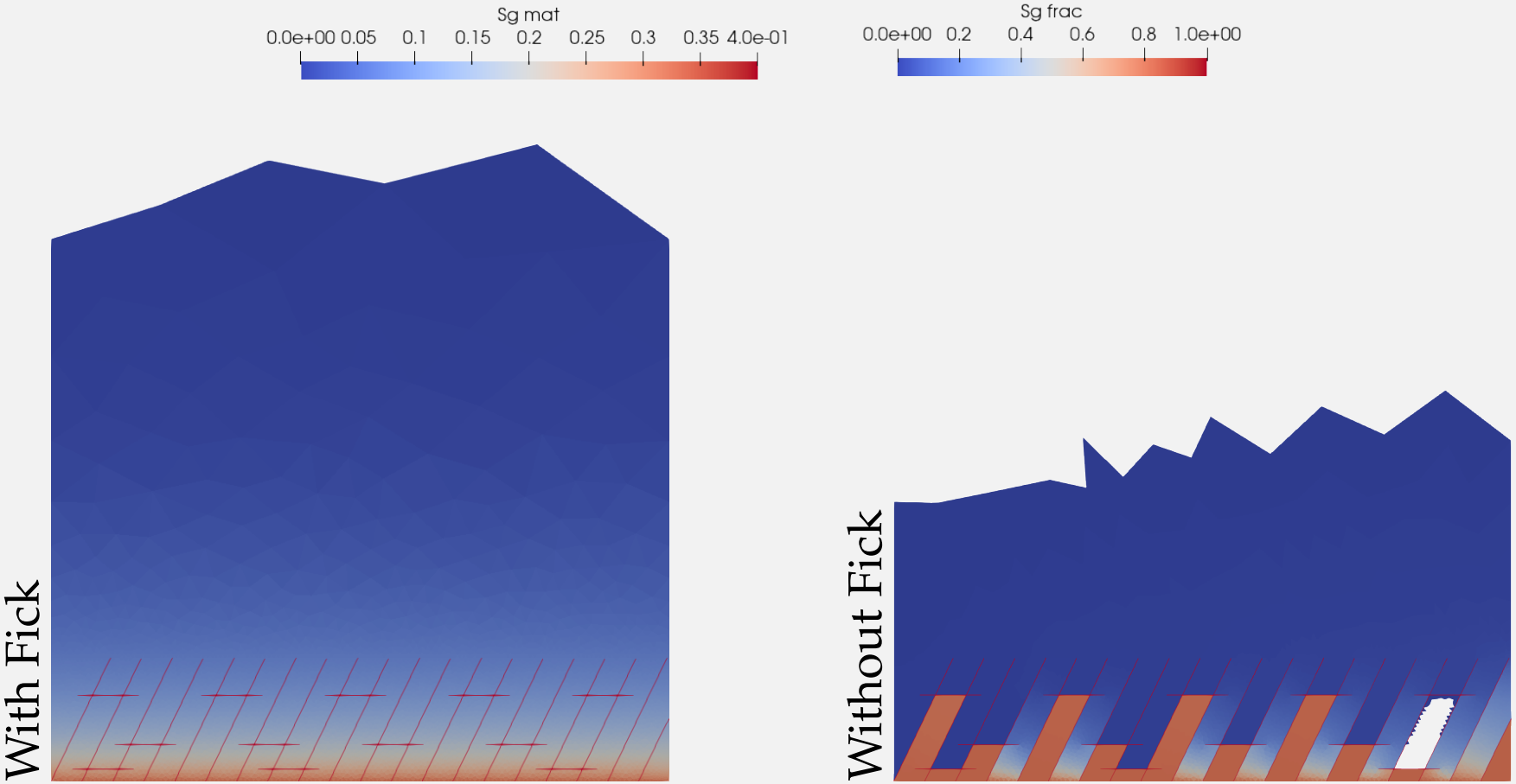
Application : settings



- Relative humidity $H_r = 0.6$
- Fractures sizes
  - obliques $d_f = 1\text{mm}$,
  - horizontal $d_f = 0.01\text{mm}$,
- $\Lambda_m = 5 \cdot 10^{-8}$ Darcy, $\quad \Lambda_f = \frac{d_f^2}{12}$
- $\phi_m = 0.15, \quad \phi_f = 1,$
- Van Genuchten CP laws $n = 1.49$, $m = 1 - \frac{1}{n}$,
- Fick diffusion coefficients :
  - $\mathcal{D}^g = 2.5 \cdot 10^{-5}\,\text{m}^2.s^{-1}$
  - $\mathcal{D}^\ell = 3 \cdot 10^{-9}\,\text{m}^2.s^{-1}$

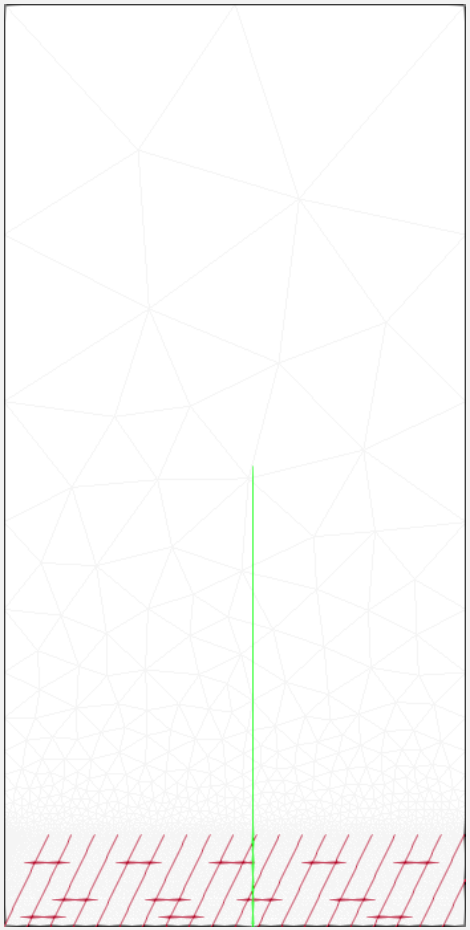
Application : results I

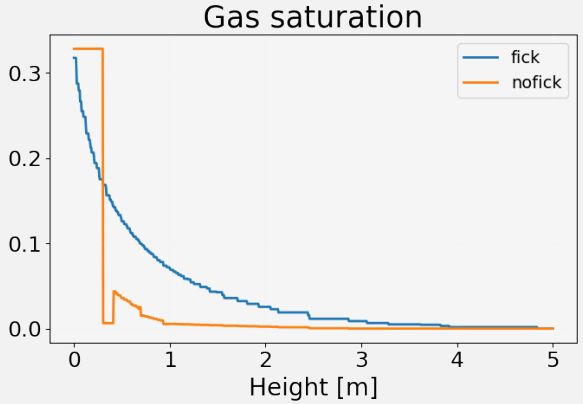
Saturation field at final time $T = 200$ yrs ($s^{\alpha} > 10^{-6}$)

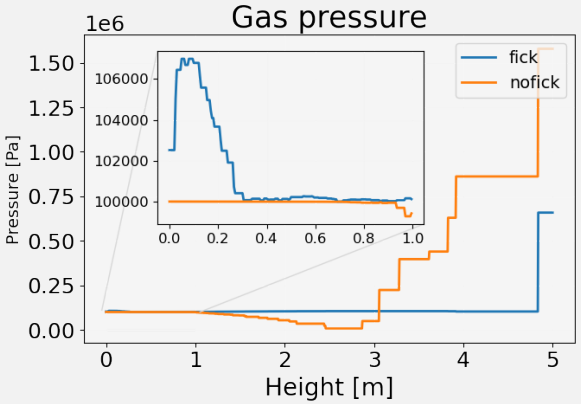


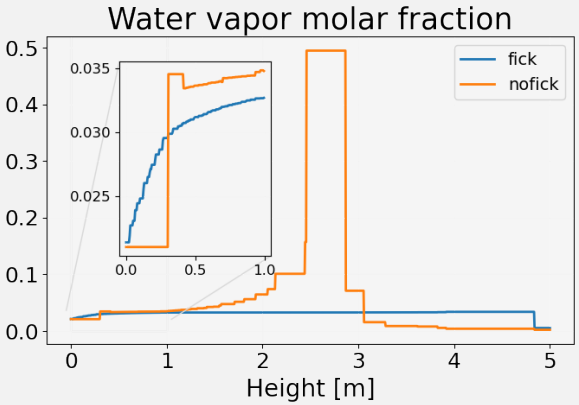
Fick diff.	**Nb Cells**	Cpu Time [s]	$N_{\Delta t}$	N_{Chop}	N_{Newton}
with	11549	403.08	384	34	7.18
without	11549	259.6	280	6	5.62

Application : results II









Solution at final time : cuts along $(2.7, 0)$ to $(2.7, 5)$

Conclusion

In brief :

- A new hybrid dimensional compositional two-phase model accounting for
  - Fickian diffusion,
  - phase transitions.
- Transmission conditions are designed to be physically consistent
- Takes account saturation jumps thanks to graph representation of capillary pressures.
- Same accuracy than equi-dimensional models.

Perspectives : Extend to general meshes, permeability anisotropy tensor using a face based approach.

Thank you for your attention!