Coupling compositional liquid gas Darcy and free gas flows at porous and free-flow domains interface

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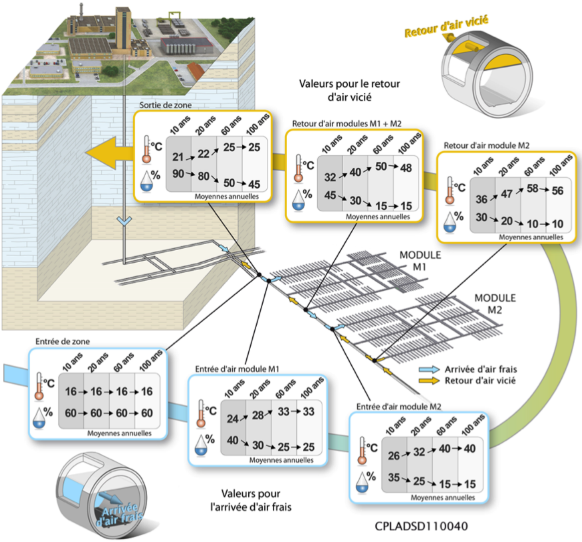
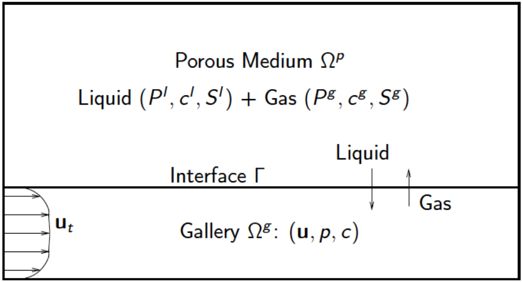
Motivation: radioactive waste geological storage

- Tens of kilometers of ventilated galleries
- Modelization of the mass and energy exchanges between the storage and the galleries
- Objectives
  - Guarantee safe air for workers
  - Study the desaturation induced by the ventilation



Model



- Starting point: model proposed by [Helmig et al. 2011]
- Liquid gas compositional Darcy flow coupled with a RANS compositional free gas flow
- Isothermal model

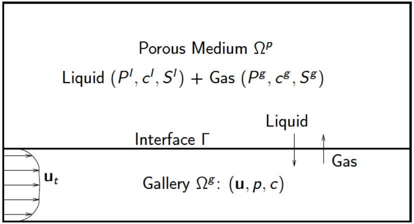
Outline

- Coupled model formulation
- Nonlinear solver for the coupled systems based on
  - A splitting algorithm
  - A nonlinear Domain Decomposition Method (DDM)

Porous medium model on Ω^p

- Set of components $i \in \mathcal{C} = \{water, air\}$
- Unknowns: $p^\alpha, s^\alpha, c^\alpha = (c_i^\alpha)_{i\in\mathcal{C}}$, $\alpha = l, g$
- $n_i = \sum_{\alpha=l,g} \zeta^\alpha s^\alpha c_i^\alpha$
- Darcy velocities:

$$\mathbf{V}^\alpha = \frac{k_r^\alpha(s^\alpha)}{\mu^\alpha}\mathbf{K}(\nabla p^\alpha - \rho^\alpha \mathbf{g})$$



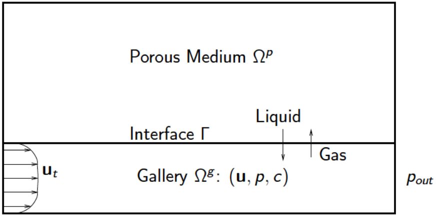
- $\mathbf{V}_i = \sum_{\alpha=l,g} c_i^\alpha \zeta^\alpha \mathbf{V}^\alpha$

$$\phi\partial_t n_i + \mathrm{div}(\mathbf{V}_i) = 0,\ i \in \mathcal{C},$$

$$s^l + s^g = 1,$$
$$p^g - p^l = p_c(s^g),$$
$$\sum_{i\in\mathcal{C}} c_i^\alpha = 1 \text{ if phase } \alpha \text{ present},$$

Thermodynamical equilibrium.

Free flow model on Ω^g



RANS model: find $(\mathbf{u}, p, c)$ such that

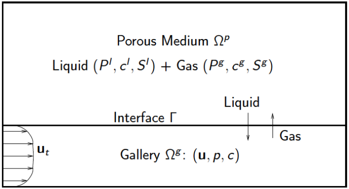
$$\left\{\begin{array}{l}\mathrm{div}\Big(\rho^g \mathbf{u}\otimes\mathbf{u}\Big) - \mathrm{div}\Big(\mu_t(\nabla\mathbf{u} + \nabla^t\mathbf{u})\Big) + \nabla p = 0,\\ \mathbf{U}_i = \zeta^g\Big(c_i\mathbf{u} - D_t\nabla c_i\Big), i\in\mathcal{C},\\ \mathrm{div}(\mathbf{U}_i) = 0, i\in\mathcal{C},\\ \sum_{i\in\mathcal{C}} c_i = 1.\end{array}\right.$$

- μ_t, D_t: turbulence closure
- Quasi stationary solutions (porous medium time scale)

Coupling conditions at the interface Γ [Helmig et al. 2011]

$$
\begin{cases}
\mathbf{V}_i \cdot \mathbf{n} = \mathbf{U}_i \cdot \mathbf{n},\ i \in \mathcal{C}: \ \text{molar flux continuity,} \\
c_i^g = c_i, i \in \mathcal{C}: \ \text{gas molar fractions continuity,} \\
\ \text{Liquid Gas thermodynamical equilibrium,} \\
p^g = p: \ \text{small pressure jump,} \\
\mathbf{u} \cdot \tau = 0: \ \text{no slip condition.}
\end{cases}
$$

Dominant physics of the coupling



- $(\mathbf{u}, p)$ weakly coupled to the porous medium
- Strong coupling between
  - the vaporisation rate of the liquid at the interface
  - the convection diffusion of the H_2O molar fraction c_w in the free gas flow

Splitting algorithm

Initialization at $t = 0$:

$\mathbf{u} = 0$ at Γ, $c = c^0$ on Ω^g

Compute $\mathbf{u} = \mathbf{u}_t$, $p = p_t$ in Ω^g (uncoupled velocity and pressure)

At each time step:

(1) Given $\mathbf{u}$, p in Ω^g, Compute $p^\alpha, s^\alpha, c^\alpha, \alpha = l, g$ in Ω^p, $\delta \mathbf{u} \cdot \mathbf{n}$ at Γ, c in Ω^g

$$\mathbf{u} \cdot \mathbf{n} \leftarrow \mathbf{u} \cdot \mathbf{n} + \delta \mathbf{u} \cdot \mathbf{n}$$

(2) Given $\mathbf{u} \cdot \mathbf{n}$ at Γ, $c \in \Omega^g$, Compute $\mathbf{u}$, p in Ω^g

Coupled system (1)

Given $\mathbf{u}$, p in Ω^g, Compute $p^\alpha, s^\alpha, c^\alpha, \alpha = l, g$ in Ω^p, $\delta \mathbf{u} \cdot \mathbf{n}$ at Γ, c in Ω^g

$$
\begin{cases}
\phi \partial_t n_i + \mathrm{div}(\mathbf{V}_i) = 0, \ i \in \mathcal{C}, & \text{on } \Omega^p, \\
\\
\mathrm{div}(\mathbf{U}_i) = 0, \ i \in \mathcal{C}, & \text{on } \Omega^g, \\
\mathbf{U}_i = \zeta^g \Big(c_i \mathbf{u} - D_t \nabla c_i \Big), \ i \in \mathcal{C}, & \text{on } \Omega^g, \\
\\
\mathbf{V}_i \cdot \mathbf{n} = \zeta^g (\delta \mathbf{u} \cdot \mathbf{n}) c_i + \mathbf{U}_i \cdot \mathbf{n}, \ i \in \mathcal{C}, & \text{on } \Gamma \\
c_i^g = c_i, \ i \in \mathcal{C}, & \text{on } \Gamma, \\
p^g = p, & \text{on } \Gamma \\
\\
+ \text{ Equilibrium } + \text{ other closure laws.}
\end{cases}
$$

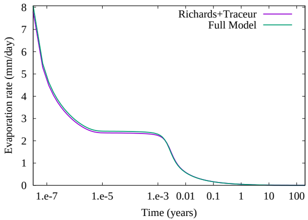
Objective: design a nonlinear DDM for this coupled system

DDM for an approximate model: Richards + Tracer

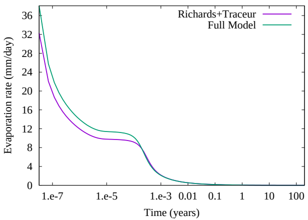
$\mathbf{u}_t$: uncoupled velocity

$$\begin{cases} \phi\partial_t\left(\zeta^l s^l(p^l)\right) + \mathrm{div}(\zeta^l \mathbf{V}^l) = 0 & \text{on } \Omega^p \quad \text{(Richards equation for } p^l\text{)}, \\ \mathrm{div}\left(\zeta^g c_w \mathbf{u}_t - \zeta^g D_t \nabla c_w\right) = 0 & \text{on } \Omega^g \quad \text{(tracer equation for } c_w\text{)}, \\ \zeta^l \mathbf{V}^l \cdot \mathbf{n} = -\zeta^g D_t \nabla c_w \cdot \mathbf{n} & \text{on } \Gamma \quad \text{(flux continuity)}, \\ c_w = f(p^l) = \frac{p_{sat}(T)}{p_{out}} e^{\frac{p^l - p_{out}}{\zeta^l RT}} & \text{on } \Gamma \quad \text{(thermodynamical equilibrium)}. \end{cases}$$

$T = 303$ K



$T = 333$ K



Robin Robin Schwarz method

Given $\gamma^{(g)}(x) \geq 0$ and $\gamma^{(p)}(x) \geq 0$, $\gamma^{(g)}(x)\gamma^{(g)}(x) \neq 0$, $x \in \Gamma$, solve for $k = 1, \cdots$ until convergence:

$$\begin{cases} \phi\zeta^l \dfrac{s^l(p^{l,k})}{\Delta t} + \mathrm{div}(\zeta^l \mathbf{V}^{l,k}) = \phi\zeta^l \dfrac{s^l(p^{l,n-1})}{\Delta t} & \text{on } \Omega^p, \\ \gamma^{(g)} f(p^{l,k}) - \zeta^l \mathbf{V}^{l,k} \cdot \mathbf{n}^p = \gamma^{(g)} c_w^{k-1} - \zeta^g D_t \nabla c_w^{k-1} \cdot \mathbf{n}^p & \text{on } \Gamma, \end{cases}$$

$$\begin{cases} \mathrm{div}\left(\zeta^g c_w^k \mathbf{u}_t - \zeta^g D_t \nabla c_w^k\right) = 0 & \text{on } \Omega^g, \\ \gamma^{(p)} c_w^k - \zeta^g D_t \nabla c_w^k \cdot \mathbf{n}^g = \gamma^{(p)} f(p^{l,k}) - \zeta^l \mathbf{V}^{l,k} \cdot \mathbf{n}^g & \text{on } \Gamma. \end{cases}$$

Computation of $\gamma^{(g)}$: diagonal approximation of the DtN operator in Ω^g

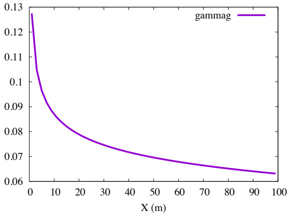
Given two constants $c_{w,\Gamma} \neq c_{w,in}$, solve

$$\begin{cases} \mathrm{div}\Big(c_w \mathbf{u}_t - D_t \nabla c_w\Big) = 0 \text{ on } \Omega^g, \\ c_w = c_{w,\Gamma} \text{ on } \Gamma, \\ c_w = c_{w,in} \text{ on } \Gamma_{in}, \\ \nabla c_w \cdot \mathbf{n} = 0 \text{ on } \partial\Omega^g \setminus (\Gamma \cup \Gamma_{in}) \end{cases}$$

and compute

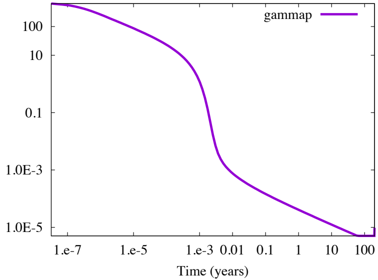
$$\gamma^{(g)}(x) = \frac{-\zeta^g D_t \nabla c_w \cdot \mathbf{n}(x)}{c_{w,\Gamma} - c_{w,in}} > 0 \text{ on } \Gamma.$$

which is independent of $c_{w,\Gamma}$ and $c_{w,in}$



Computation of $\gamma^{(p)}$: diagonal approximation of the DtN operator in Ω^p

- Linearized Richards equation with frozen coefficients at the interface Γ
- $\gamma^{(p)}(x,t)$ = order 0 Taylor approximation of the DtN operator



Plot of $\frac{\int_\Gamma \gamma^{(p)}(x,t)dx}{\int_\Gamma dx}$ function of time.

Extension of the DDM to the coupled model (1)

$\mathbf{u}$, p fixed in Ω^g.

Compute $p^\alpha, s^\alpha, c^\alpha, \alpha = l, g$ in Ω^p and $\delta \mathbf{u} \cdot \mathbf{n}$ at Γ:

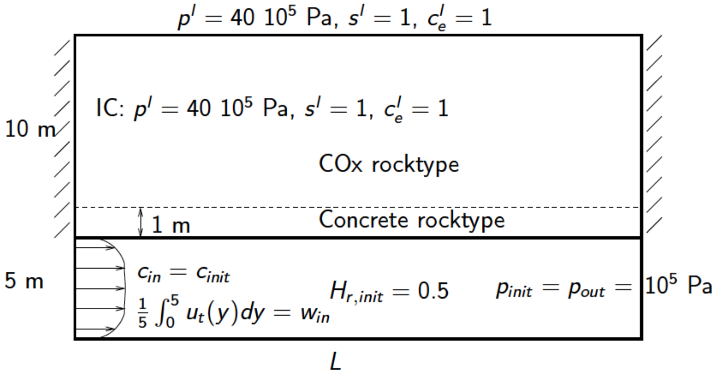
$$\begin{cases} \phi \dfrac{n_i^k - n_i^{n-1}}{\Delta t} + \mathrm{div}(\mathbf{V}_i^k) = 0,\ i \in \mathcal{C},\ \text{on } \Omega^p, \\ (\gamma^{(p)} + \zeta^g \delta \mathbf{u}^k \cdot \mathbf{n}^p) c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}^p = \gamma^{(p)} c_i^{k-1} - \mathbf{U}_i^{k-1} \cdot \mathbf{n}^p,\ i \in \mathcal{C},\ \text{on } \Gamma \\ p^{g,k} = p,\ \text{on } \Gamma \\ \ + \text{Equilibrium} + \text{other closure laws}, \end{cases}$$

Compute c in Ω^g:

$$\begin{cases} \mathrm{div}(\mathbf{U}_i^k) = 0,\ i \in \mathcal{C},,\ \text{on } \Omega^g, \\ \mathbf{U}_i^k = \zeta^g \left(c_i^k \mathbf{u} - D_t \nabla c_i^k \right),\ i \in \mathcal{C},\ \text{on } \Omega^g, \\ \gamma^{(g)} c_i^k - \mathbf{U}_i^k \cdot \mathbf{n}^g = \gamma^{(g)} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}^g + \zeta^g c_i^{g,k} \delta \mathbf{u}^k \cdot \mathbf{n}^g,\ i \in \mathcal{C},\ \text{on } \Gamma, \end{cases}$$

Andra test case

- Two components: H2O (w) and air (a)



Andra test case: evolution of c_w and s^g,

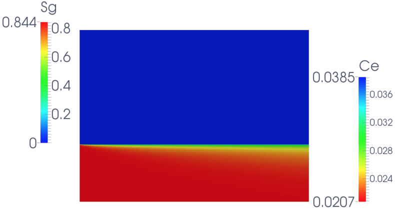
- Discretization: TPFA for Darcy + Tracer and MAC scheme for NVS
- $L = 100$ m, $w_{in} = 0.5$ m/s, Cartesian Mesh 100×200
- Simulation time: 200 years, time steps: from 1 s to 1 year

$t = 0$

Andra test case: evolution of c_w and s^g,

$t = 1.9\ 10^{-4}$ day

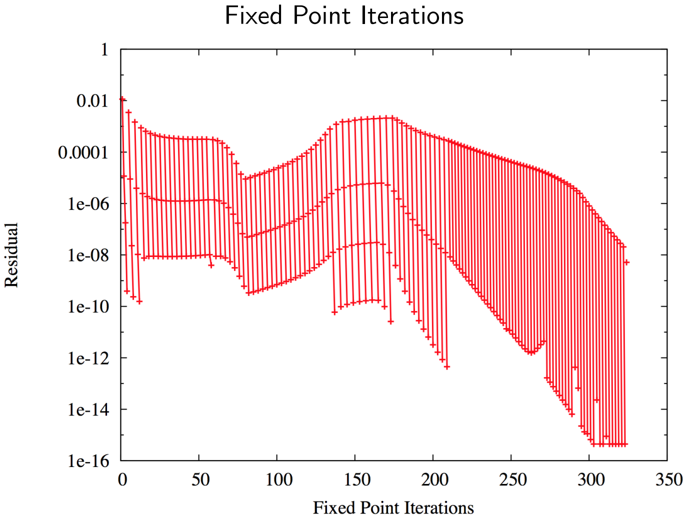
$t = 0.15$ day



$t = 1.1$ days

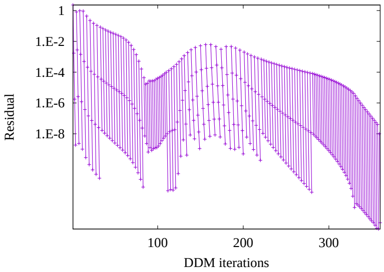
$t = 200$ years

Andra test case: $L = 100$ m, $w_{in} = 0.5$ m/s and mesh 100×200



Andra test case: DDM iterations

$T = 303$ K



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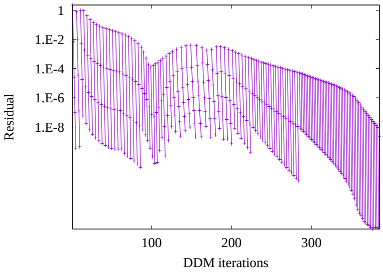
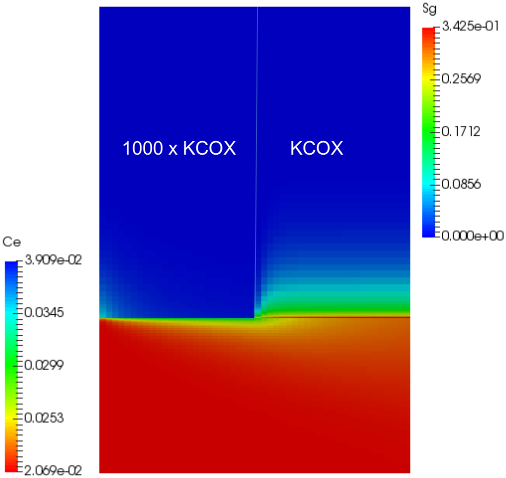
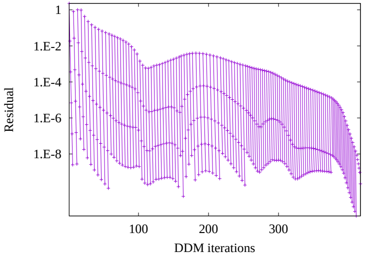
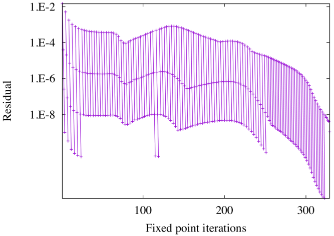


Heterogeneous porous medium along Γ







Conclusions and perspectives

Conclusions

- Algorithm to solve the coupling between a liquid gas Darcy and a free gas flow
  - Based on a splitting + a nonlinear Domain Decomposition Method
  - Provides an efficient nonlinear solver
  - Possibility to use separate codes in the porous and free flow domains

Perspectives

- Add the energy equation
- Test cases with more complex geometries

Acknowledgements:
We would like to thank Andra for supporting this work.

Thanks for your attention!