Coupling Liquid Gas Darcy flow and Gas Free Flow
Application to radioactive waste geological storage

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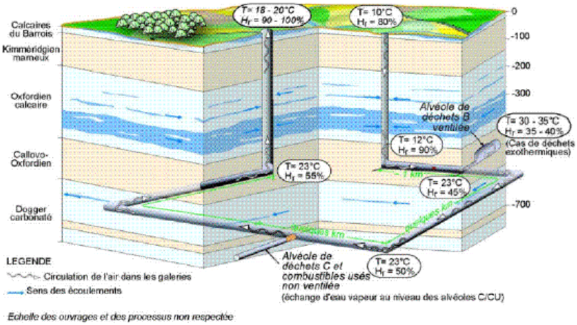
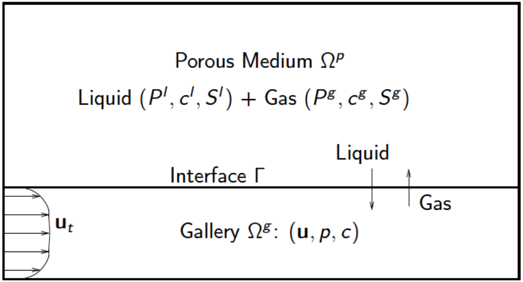
Motivation: radioactive waste geological storage

- Modelization of mass and energy exchanges between the storage and the excavated ventilated gallery
- A few tens of kilometers of ventilated gallery
- Objectives of the ventilation
  - safe air for workers
- Coupled simulations required by the safety case



Model



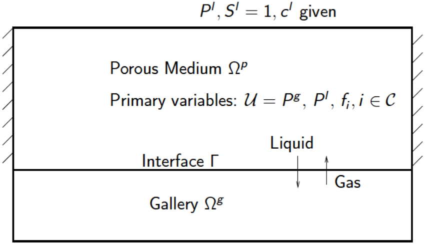
- Starting point: model proposed by [Helmig et al. 2011]
  - Liquid gas Darcy flow in Ω^p
  - Gas free flow in Ω^g
  - Coupling conditions at the interface Γ
- Our additional physical assumptions
  - Constant temperature T_e
  - Small perturbation of the velocity by the coupling

Outline

- Model formulation
- Splitting algorithm
- Reduced model: 1D in the gallery
- Numerical experiments
  - Andra test case with an horizontal gallery
  - Andra test case with a vertical gallery
  - Drying test case

Porous media model on Ω^p

- Phases $\alpha = g, l$
- Components: $i \in \mathcal{C}$
- Primary variables: $\mathcal{U} = (p^g, p^l, f)$
- Fugacities: $f = f^g(p^g, c^g) = f^l(p^l, p^g, c^l)$
  $\Rightarrow$ molar fractions $c^\alpha(\mathcal{U})$, $\alpha = g, l$
- $s^l = 1 - s^g = \mathcal{S}^l(\mathbf{x}, p^g - p^l)$.



Find $\mathcal{U} = (p^g, p^l, f)$ such that

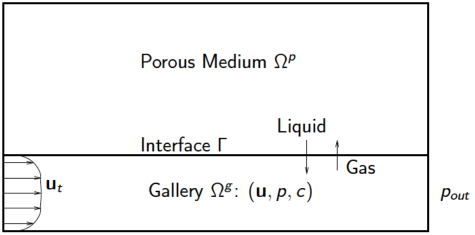
$$\phi \partial_t \sum_{\alpha=g,l} \zeta^\alpha(\mathcal{U}) s^\alpha c_i^\alpha(\mathcal{U}) + \mathrm{div}\Big(\sum_{\alpha=g,l} \zeta^\alpha(\mathcal{U}) c_i^\alpha(\mathcal{U}) \mathbf{V}^\alpha \Big) = 0, \; i \in \mathcal{C},$$

$$\sum_{i \in \mathcal{C}} c_i^\alpha(\mathcal{U}) = 1, \; \alpha = g, l,$$

coupled with the Darcy laws $\mathbf{V}^\alpha = -\dfrac{k_r^\alpha(\mathbf{x}, s^\alpha)}{\mu^\alpha(\mathcal{U})} \mathbf{K} \Big(\nabla p^\alpha - \rho^\alpha(\mathcal{U}) \mathbf{g} \Big)$, $\alpha = g, l$.

Free flow model on Ω^g

- Algebraic turbulent model
  - turbulent profile: $u_t(y)$
  - turbulent viscosity: $\mu_t(y)$
  - turbulent diffusion $D_t(y)$
- RANS model at fixed μ_t, D_t
- Constant ζ^g and ρ^g



Find $(\widetilde{\mathbf{u}}, \widetilde{p}, c)$ such that

$$\rho^g \mathrm{div}\Big(\mathbf{u}_t \otimes \widetilde{\mathbf{u}} + \widetilde{\mathbf{u}} \otimes \mathbf{u}_t + \widetilde{\mathbf{u}} \otimes \widetilde{\mathbf{u}}\Big) - \mathrm{div}\Big((\mu^g + \mu_t)(\nabla\widetilde{\mathbf{u}} + \nabla^t\widetilde{\mathbf{u}})\Big) + \nabla\widetilde{p} = 0,$$

$$\partial_t c_i + \mathrm{div}\Big(c_i(\mathbf{u}_t + \widetilde{\mathbf{u}})\Big) + \mathrm{div}\Big(-(D^g + D_t)\nabla c_i\Big) = 0, i \in \mathcal{C},$$

$$\sum_{i\in\mathcal{C}} c_i = 1.$$

$$\text{with } \mathbf{u} = \mathbf{u}_t(y) + \widetilde{\mathbf{u}}, \quad p = p_t(x,y) + \widetilde{p}, \quad \mathbf{u}_t = \begin{pmatrix} u_t(y) \\ 0 \end{pmatrix}$$

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

- No slip condition (small permeability of the storage)
- No gas pressure jump (small perturbation of the velocity profile)
- Vaporization of the liquid phase at the interface

$$\begin{cases} \displaystyle\sum_{\alpha=l,g} \zeta^\alpha(\mathcal{U}) c_i^\alpha(\mathcal{U}) \mathbf{V}^\alpha \cdot \mathbf{n} = \zeta^g \Big(c_i \mathbf{u} \cdot \mathbf{n} - D^g \nabla c_i \cdot \mathbf{n} \Big),\ i \in \mathcal{C} \\ \qquad\qquad\qquad\qquad \text{(molar flux continuity)}, \\ c_i^g(\mathcal{U}) = c_i, i \in \mathcal{C} \text{ (gas molar fractions continuity)}, \\ \displaystyle\sum_{i\in\mathcal{C}} c_i^l(\mathcal{U}) = 1 \text{ (liquid gas equilibrium)}, \\ \displaystyle\sum_{i\in\mathcal{C}} c_i^g(\mathcal{U}) = 1, \\ p^g = p \text{ (no pressure jump)}, \\ \mathbf{u} \cdot \tau = 0 \text{ (no slip condition)}. \end{cases}$$

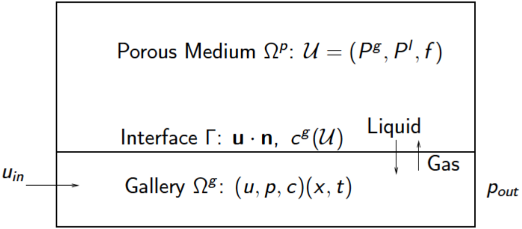
Splitting algorithm

- Typical approach will compute sequentially
  - Darcy flow at given p, c in the gallery
  - Free flow at given Darcy flux at the interface Γ
- Fails due to the strong coupling between c and Darcy flux at the interface Γ

Proposed splitting algorithm

- Step 1: Given $\boxed{\mathbf{u},\ p \text{ in } \Omega^g}$ Compute $\boxed{\mathcal{U} \text{ in } \Omega^p,\ \mathbf{u}\cdot\mathbf{n} \text{ at } \Gamma,\ c \text{ in } \Omega^g}$
- Step 2: Given $\boxed{\mathbf{u}\cdot\mathbf{n} \text{ at } \Gamma}$ Compute $\boxed{\mathbf{u},\ p \text{ in } \Omega^g}$
- Is used as a fixed point method for $\mathbf{u}\cdot\mathbf{n}$ at Γ with the stopping criteria $\|1 - \sum_{i\in\mathcal{C}} c_i\| \leq \epsilon$

Reduced model: 1D model in the gallery



New interface conditions on Γ:

$$\sum_{\alpha=g,l} \zeta^\alpha(\mathcal{U}) c_i^\alpha(\mathcal{U}) \mathbf{V}^\alpha \cdot \mathbf{n} = \zeta^g \Big(c_i^g(\mathcal{U})(\mathbf{u}\cdot\mathbf{n})^+ + c_i(\mathbf{u}\cdot\mathbf{n})^- + \frac{D^g}{\boxed{\delta}}(c_i^g(\mathcal{U}) - c_i) \Big),\ i \in \mathcal{C},$$

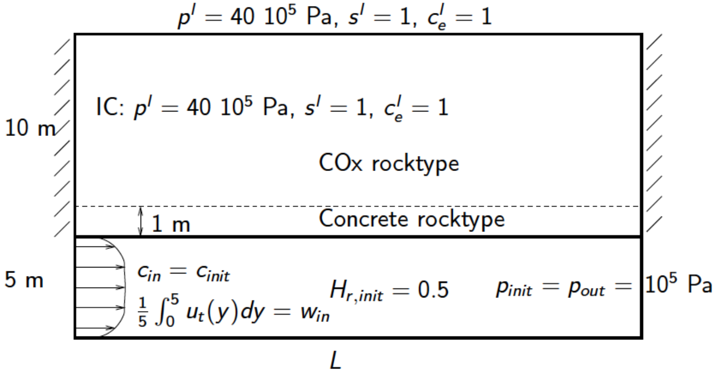
$$\sum_{i\in\mathcal{C}} c_i^\alpha(\mathcal{U}) = 1,\ \alpha = g, l, \quad p^g = p.$$

1D conservation equations along the gallery $x \in (0, L)$:

$$\partial_t\Big(|S|\zeta^g c_i\Big) + \partial_x\Big(|S|\zeta^g c_i u\Big) = \sum_{\alpha=g,l} \zeta^\alpha(\mathcal{U}) c_i^\alpha(\mathcal{U}) \mathbf{V}^\alpha \cdot \mathbf{n},\ i \in \mathcal{C},$$

$$\sum_{i\in\mathcal{C}} c_i = 1, \quad p = p_{out}.$$

Andra test case



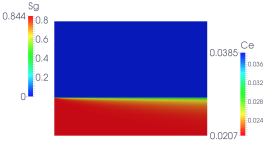
- Two components: H2O (e) and air (a), $T_e = 303$ K
- Fugacities
  - Gas: $f_i^g = c_i^g p^g$, $i = e, a$,
  - Liquid: $f_a^l = c_a^l H_a(T_e)$, $f_e^l = c_e^l P_{sat}(T_e)\exp\left(\frac{-(p^g - p^l)}{\zeta^l R T_e}\right)$
- Van Genuchten parameters accounting for COx and Concrete.

Andra test case: evolution of c_e 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 1s to 1 year

$t = 0$ day

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



$t = 0.15$ day

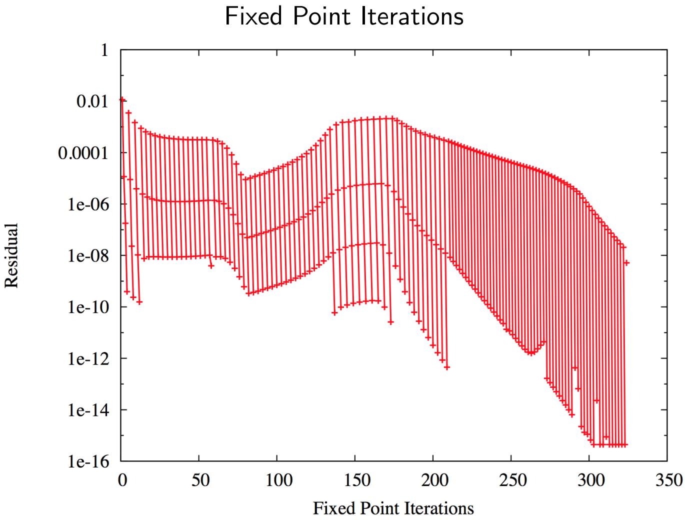
$t = 1.1$ days

$t = 125$ days

$t = 200$ years

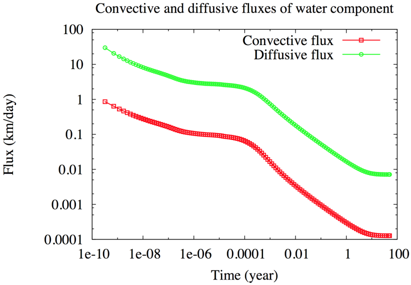
Andra test case: $L = 100$ m, $w_{in} = 0.5$ m/s and mesh 100×200

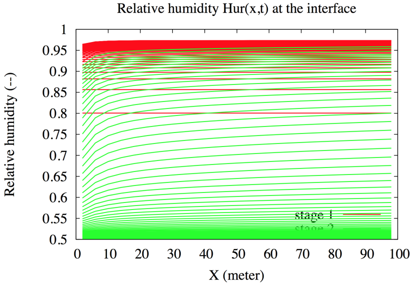
Stopping criteria: $\|1 - \sum_{i \in \mathcal{C}} c_i\|_\infty \leq 10^{-6}$



Comparison of the 2D-2D model and the 2D-1D model: how to choose δ ?

- $\zeta^g << \zeta^l$ and $ce << 1 \Rightarrow c_e \widetilde{\mathbf{u}} \cdot \mathbf{n} \sim -\frac{c_e}{1-c_e} D^g \nabla c_e \cdot \mathbf{n}$ at Γ
- We can check numerically that $c_e(x,t)$ depends weakly on x





Comparison of the 2D-2D model and the 2D-1D model: how to choose δ ?

For given constant $c_{e,\Gamma} \neq c_{e,in}$ solve the stationary convection diffusion problem:

$$\begin{cases} \cancel{\partial_t c_e} + \operatorname{div}\Big(c_e \mathbf{u}_t + \cancel{c_e \tilde{\mathbf{u}}} - (D^g + D_t) \nabla c_e \Big) = 0, \\ c_e = c_{e,\Gamma} \text{ on } \Gamma, \\ c_e = c_{e,in} \text{ on } \Gamma_{in}, \\ \nabla c_e \cdot \mathbf{n} = 0 \text{ on } \partial\Omega^g \setminus (\Gamma \cup \Gamma_{in}) \end{cases}$$

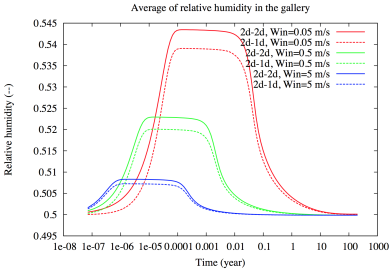
and compute

$$\delta(x) = \frac{c_{e,\Gamma} - \frac{1}{H}\int_0^H c_e(x,y)dy}{-\nabla c_e \cdot \mathbf{n}(x)} \text{ on } \Gamma.$$

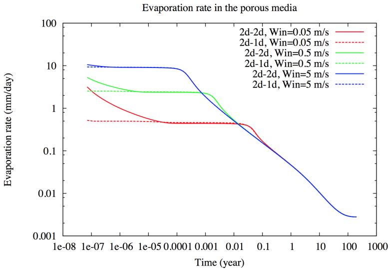
which is independent of $c_{e,\Gamma}$ and $c_{e,in}$

Andra test case: comparison of the 2D-2D model and the 2D-1D model $L = 100$ m

Relative Humidity $H_r = \frac{c_e^g p}{P_{sat}(T_e)}$

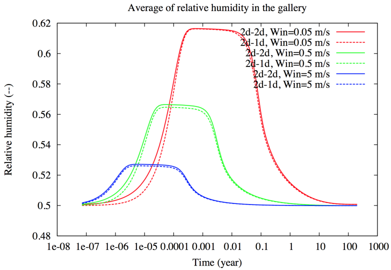


Evaporation rate in the porous medium

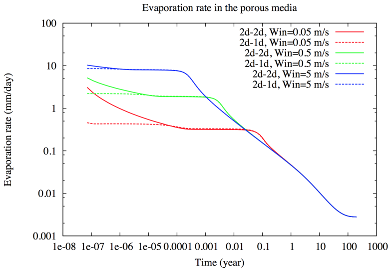


Andra test case: comparison of the 2D-2D model and the 2D-1D model with $L = 400$ m

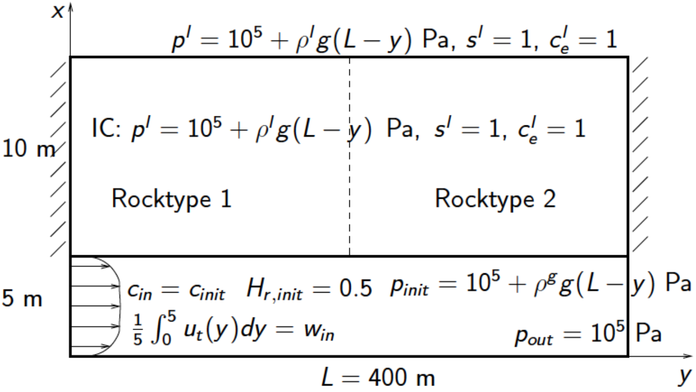
Relative Humidity $H_r = \dfrac{c_e^g p}{P_{sat}(T_e)}$



Evaporation rate in the porous medium

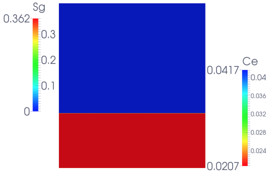


Andra test case with a vertical gallery

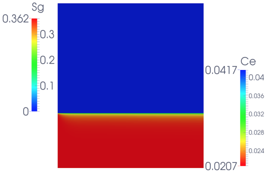


Andra test case with a vertical gallery: evolution of c_e and s^g

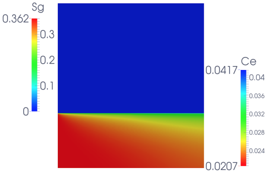
- $w_{in} = 0.5$ m/s, Cartesian Mesh 100×283
- Simulation time: 50 years, time steps: from 1s to 1 year



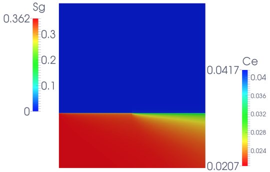
$t = 0$ day



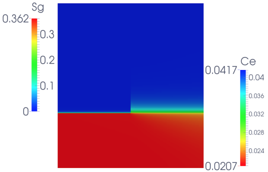
$t = 6.9\ 10^{-4}$ day



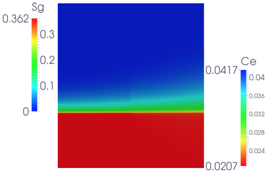
$t = 7.9\ 10^{-3}$ day



$t = 0.3$ days



$t = 14$ days

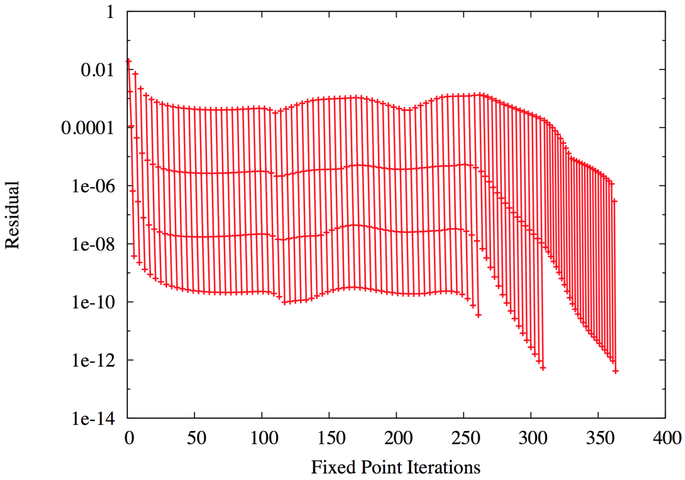


$t = 50$ years

Andra test case with a vertical gallery: $w_{in} = 0.5$ m/s and mesh 100×283

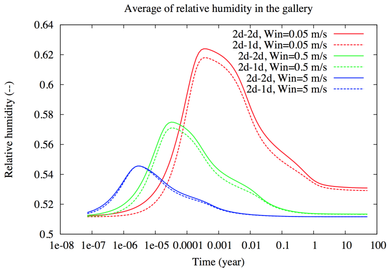
Stopping criteria: $\|1 - \sum_{i \in \mathcal{C}} c_i\|_\infty \leq 10^{-6}$

Fixed Point Iterations

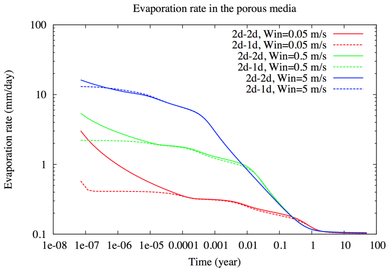


Andra test case with a vertical gallery: comparison of the 2D-2D model and the 2D-1D model

Relative Humidity $H_r = \dfrac{c_e^g p}{P_{sat}(T_e)}$

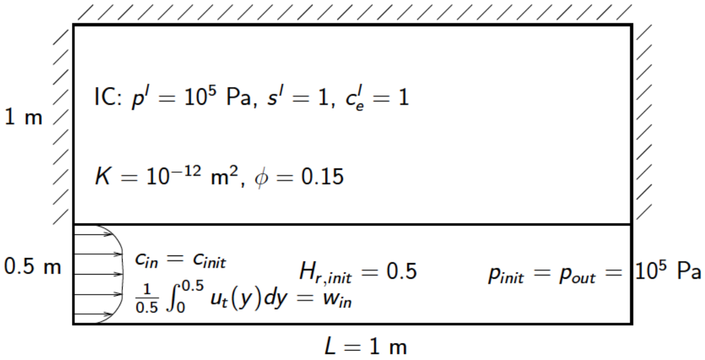


Evaporation rate in the porous medium



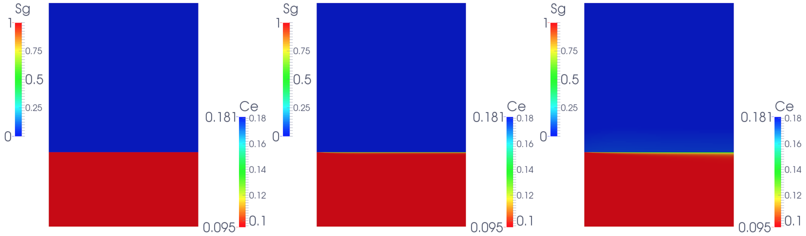
Drying test case

$T_e = 333$ K.

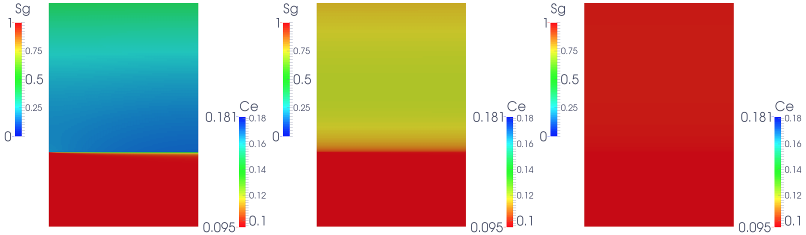


Drying test case: evolution of c_e and s^g

- $w_{in} = 10$ m/s, Cartesian Mesh 100×283
- Simulation time: 100 days, time steps: from 10^{-4}s to 1 day



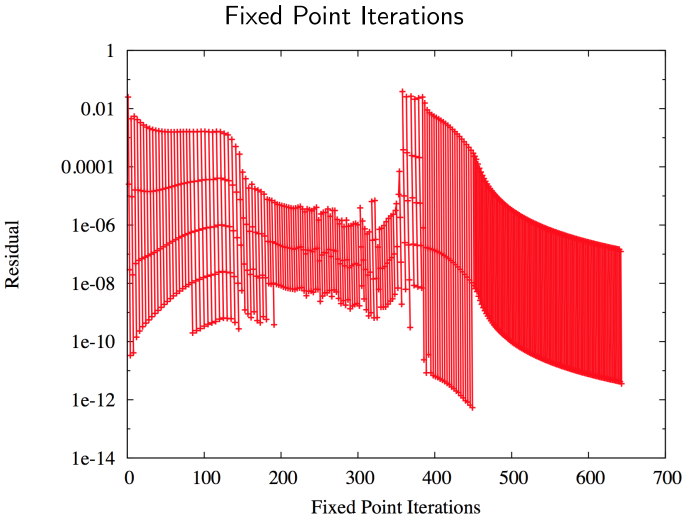
$t = 0$ day | $t = 3.1\ 10^{-7}$ day | $t = 2.9\ 10^{-3}$ day



$t = 0.11$ days | $t = 1$ days | $t = 100$ days

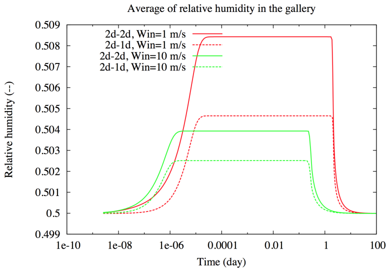
Drying test case: $w_{in} = 10$ m/s and mesh 100×283

Stopping criteria: $\|1 - \sum_{i \in \mathcal{C}} c_i\|_\infty \leq 10^{-6}$



Drying test case: comparison of the 2D-2D model and the 2D-1D model

Relative Humidity $H_r = \frac{c_e^g p}{P_{sat}(T_e)}$



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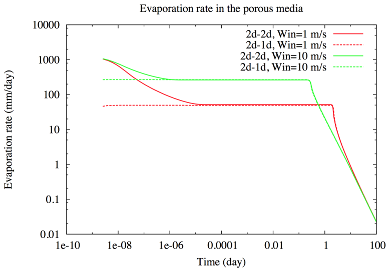

Conclusions and perspectives

Conclusions

- Splitting algorithm
  - Efficient thanks to the weak coupling with the velocity correction
- Reduced model
  - Provides good order of magnitudes
  - Easy to implement in existing Darcy flow codes

Perspectives

- Domain decomposition method
- Energy equation

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

Thanks for your attention!