

# A nonlinear Domain Decomposition Method to couple compositional liquid gas Darcy and free gas flows

Nabil Birgale<sup>1</sup>, Roland Masson<sup>1</sup>, Laurent Trety<sup>2</sup>

<sup>1</sup> Université Côte d'Azur, LJAD, INRIA, CNRS

<sup>2</sup> Andra

Séminaire d'Analyse Numérique, Université de Genève,  
21 mars 2017, Genève

# Drying problems

From Defraeye 2014

## EXCHANGE PROCESSES

### Heat

- Convection
- Radiation (infrared & solar)
- Phase change (latent heat of evaporation)
- Conduction (in contact with solid)

### Liquid water

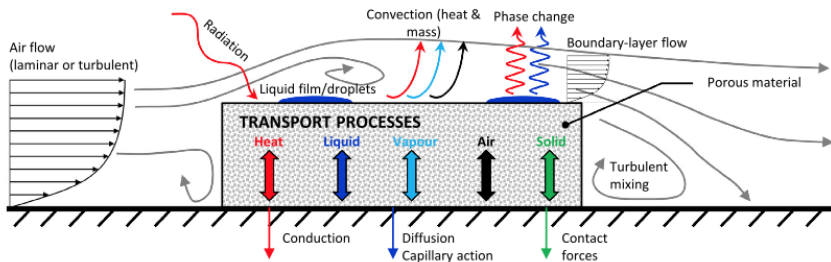
- Phase change (evaporation)
- Diffusion (e.g. osmotic dehydration)
- Capillary action

### Water vapour & Air

- Convection

### Solid

- Contact forces

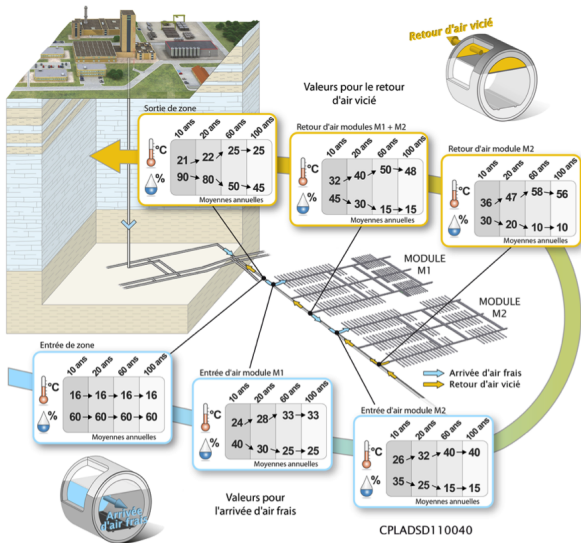


# Motivations

- ▶ Land atmosphere interaction, soil evaporation and evapotranspiration
- ▶ Drying problems in engineering: food, wood, paper, ceramic
- ▶ Radioactive waste geological storage

# Main motivation of this work: radioactive waste geological storage

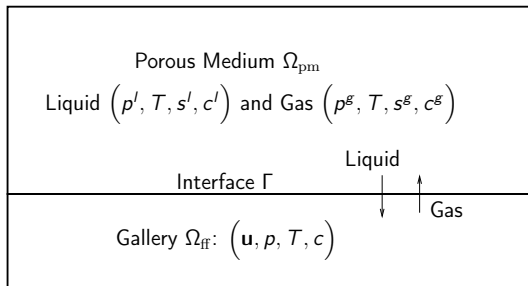
- ▶ Tens of kilometers of ventilated galleries
- ▶ Modelization of the mass and energy exchanges between the storage and the galleries
- ▶ Objectives
  - ▶ Guarantee safe air for workers
  - ▶ Study the desaturation induced by the ventilation



# Outline

- ▶ Model
- ▶ Nonlinear domain decomposition for a simplified model
- ▶ Extension to the compositional model
- ▶ Numerical results

# Model



- ▶ Starting point: model proposed by [Helmig et al. 2011]
- ▶ Liquid gas compositional Darcy flow
- ▶ RANS compositional free gas flow
- ▶ Non-isothermal model

# Single phase Darcy flow

$$\left\{ \begin{array}{l} \text{Darcy law:} \quad \mathbf{V} = -\frac{\mathbf{K}(\mathbf{x})}{\mu}(\nabla p - \rho(p)\mathbf{g}), \\ \text{Mole conservation:} \quad \phi \partial_t \zeta(p) + \text{div}(\zeta(p)\mathbf{V}) = 0. \end{array} \right.$$

$p$ : pressure (Pa)

$\mathbf{V}$ : Darcy Velocity ( $\text{m}\cdot\text{s}^{-1}$ )

$\mathbf{K}$ : permeability tensor of the porous medium ( $\text{m}^2$ ) (1 Darcy =  $10^{-12}$   $\text{m}^2$ )

$\phi$ : porosity of the porous medium

$\mu$ : viscosity of the fluid (Pa.s)

$\zeta$ : molar density of the fluid ( $\text{mol}\cdot\text{m}^{-3}$ )

$\rho$ : mass density of the fluid ( $\text{kg}\cdot\text{m}^{-3}$ )

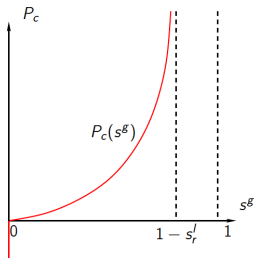
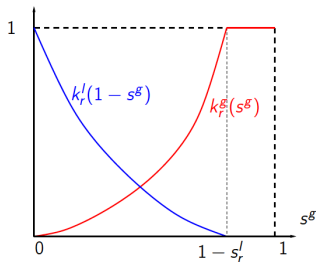
# Two phase Darcy velocities

$\alpha = g, l$ : phases

$s^\alpha$ : volume fractions

$p^\alpha$ : pressures

$$\left\{ \begin{array}{l} \mathbf{V}^\alpha = -\frac{k_r^\alpha(s^\alpha)}{\mu^\alpha} \mathbf{K}(\mathbf{x}) (\nabla p^\alpha - \rho^\alpha \mathbf{g}), \\ P_c(s^g) = p^g - p^l, \\ s^g + s^l = 1. \end{array} \right.$$

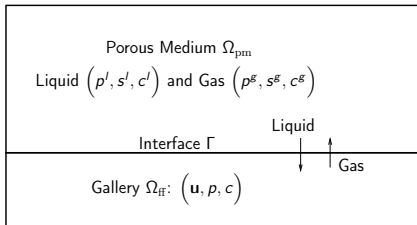


## Porous medium model on $\Omega_{\text{pm}}$ (isothermal)

- ▶ Set of components  $i \in \mathcal{C} = \{\text{water}, \text{air}\}$
- ▶ 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:

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

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



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

$$s^l + s^g = 1,$$

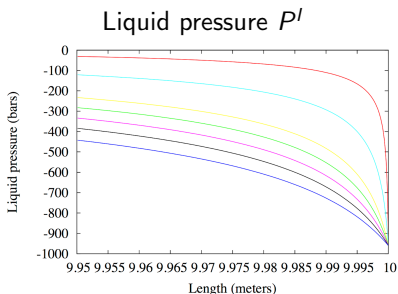
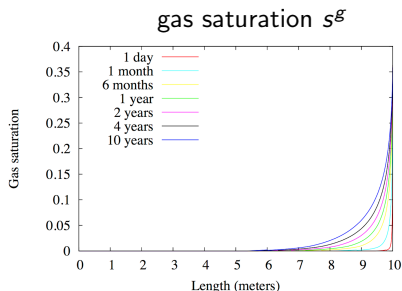
$$p^g - p^l = p_c(s^g),$$

$$\sum_{i \in \mathcal{C}} c_i^\alpha = 1 \text{ if phase } \alpha \text{ present,}$$

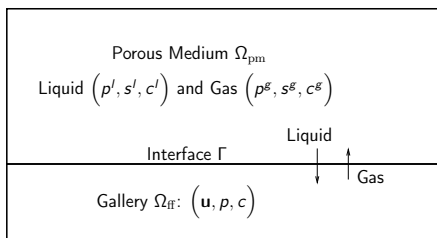
Thermodynamical equilibrium.

# Example of uncoupled solution in 1D

- ▶ Two components: air (a) and  $H_2O$  (w)
- ▶ Initial condition: :  $p^l = 4$  Mpa,  $s^l = 1$ , pure water
- ▶ Left boundary condition:  $p^l = 4$  Mpa,  $s^l = 1$ , pure water
- ▶ Right boundary condition (interface  $\Gamma$ ):
  - ▶  $p^g = 10^5$  Pa, relative humidity  $H_r = \frac{p^g c_e^g}{p_{sat}(T_e)} = 0.5$
  - ▶  $p^l, c^l, s^g$  computed using the gas liquid equilibrium



## Free flow model on $\Omega_{\text{ff}}$ (isothermal)



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

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

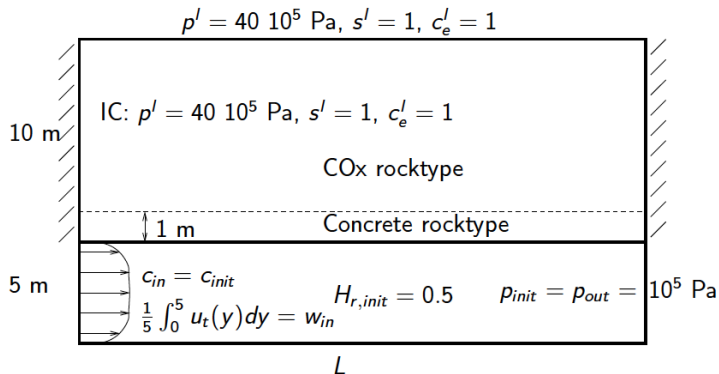
- ▶  $\mu_t, D_t$ : turbulence closure
- ▶ Quasi stationary solutions (porous medium time scale)

# Coupling conditions at the interface $\Gamma$ [Helmig et al. 2011] (isothermal)

$$\left\{ \begin{array}{l} \mathbf{V}_i \cdot \mathbf{n} = \mathbf{W}_i \cdot \mathbf{n}, \quad i \in \mathcal{C} : \text{molar flux continuity,} \\ c_i^g = c_i, \quad i \in \mathcal{C} : \text{gas molar fractions continuity,} \\ \text{Liquid Gas thermodynamical equilibrium,} \\ p^g = \mathbf{n} \cdot \mathbb{T} \mathbf{n}, \\ \mathbf{u} \cdot \boldsymbol{\tau} = 0 : \text{no slip condition.} \end{array} \right.$$

# Andra test case

- ▶ Two components: H<sub>2</sub>O (w) and air (a),  $T = 303$  K



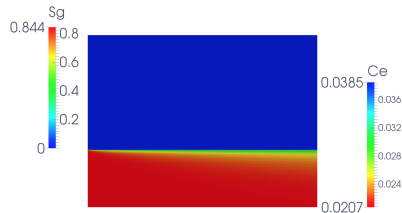
# Andra test case: evolution of $c_w$ and $s^g$

- ▶  $L = 100$  m,  $w_{in} = 0.5$  m/s
- ▶ Simulation time: 200 years

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



$t = 0.15$  day



$t = 1.1$  days



$t = 200$  years



## Andra test case: evolution of $c_w$ and $s^g$

- ▶  $L = 100$  m,  $w_{in} = 0.5$  m/s
- ▶ Simulation time: 200 years

Loading video...

# State of the art

- ▶ One way coupling algorithms using convective transfer coefficients
- ▶ Dirichlet Neumann sequential algorithms [Defraeye 2014]
- ▶ Fully coupled algorithms [Helmig et al 2011–2017]
- ▶ Domain Decomposition Methods
  - ▶ Many works for single phase Darcy - Navier Stokes coupling [Discacciati, Quarteroni et al 2003–]

# Richards model in the Darcy flow domain

Assumptions:  $p^g \simeq p_{atm}$ ,  $\zeta^l \gg \zeta^g$ ,  $c_e^l \sim 1$ .

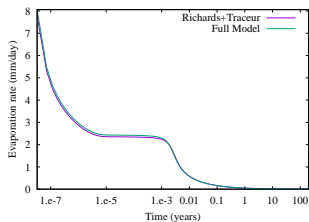
$$\left\{ \begin{array}{l} \text{Liquid saturation: } s^l(p^l) = 1 - P_c^{-1}(p^{atm} - p^l), \\ \text{Liquid Darcy velocity: } \mathbf{V}^l = -\frac{k_r^l(s^l(p^l))}{\mu^l} \mathbf{K}(\mathbf{x}) (\nabla p^l - \rho^l \mathbf{g}), \\ \text{Conservation of H2O: } \phi \partial_t (\zeta^l s^l(p^l)) + \text{div}(\zeta^l \mathbf{V}^l) = 0 \end{array} \right.$$

# Approximate coupled model: Richards + Tracer

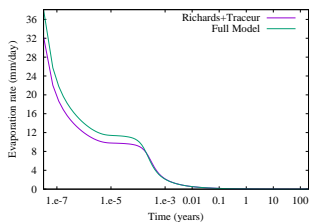
$\mathbf{u}_t$ : given uncoupled velocity with  $\text{div}(\zeta^g \mathbf{u}_t) = 0$  on  $\Omega_{\text{ff}}$  and  $\mathbf{u}_t \cdot \mathbf{n} = 0$  on  $\Gamma$ .

$$\left\{ \begin{array}{ll} \phi \partial_t (\zeta^l s^l(p^l)) + \text{div}(\zeta^l \mathbf{V}^l) = 0 & \text{on } \Omega_{\text{pm}} \quad (\text{Richards equation for } p^l), \\ \text{div}(\zeta^g c_w \mathbf{u}_t - \zeta^g D_t \nabla c_w) = 0 & \text{on } \Omega_{\text{ff}} \quad (\text{tracer equation for } c_w), \\ \zeta^l \mathbf{V}^l \cdot \mathbf{n} = -\zeta^g D_t \nabla c_w \cdot \mathbf{n} & \text{on } \Gamma \quad (\text{flux continuity}), \\ c_w = f(p^l) = \frac{p_{\text{sat}}(T)}{p_{\text{atm}}} e^{\frac{p^l - p_{\text{atm}}}{\zeta^l R T}} & \text{on } \Gamma \quad (\text{liq. vap. equilibrium}). \end{array} \right.$$

$T = 303 \text{ K}$



$T = 333 \text{ K}$



# Robin Robin Schwarz method

Given  $\beta_{\text{pm}}(x) \geq 0$  and  $\beta_{\text{ff}}(x) \geq 0$ ,  $\beta_{\text{pm}}(x)\beta_{\text{ff}}(x) \neq 0$ ,  $x \in \Gamma$ , solve for  $k = 1, \dots$  until convergence:

$$\left\{ \begin{array}{l} \phi \zeta^l \frac{s^l(p^{l,k})}{\Delta t} + \text{div}(\zeta^l \mathbf{V}^{l,k}) = \phi \zeta^l \frac{s^l(p^{l,n-1})}{\Delta t} \quad \text{on } \Omega_{\text{pm}}, \\ \beta_{\text{pm}} f(p^{l,k}) - \zeta^l \mathbf{V}^{l,k} \cdot \mathbf{n}_{\text{pm}} = \beta_{\text{pm}} c_w^{k-1} - \zeta^g D_t \nabla c_w^{k-1} \cdot \mathbf{n}_{\text{pm}} \quad \text{on } \Gamma, \end{array} \right.$$

$$\left\{ \begin{array}{l} \text{div}(\zeta^g c_w^k \mathbf{u}_t - \zeta^g D_t \nabla c_w^k) = 0 \quad \text{on } \Omega_{\text{ff}}, \\ \beta_{\text{ff}} c_w^k - \zeta^g D_t \nabla c_w^k \cdot \mathbf{n}_{\text{ff}} = \beta_{\text{ff}} f(p^{l,k}) - \zeta^l \mathbf{V}^{l,k} \cdot \mathbf{n}_{\text{ff}} \quad \text{on } \Gamma. \end{array} \right.$$

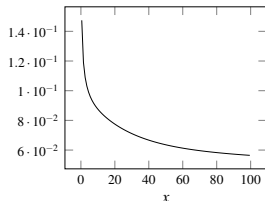
# Computation of $\beta_{\text{pm}}$ : diagonal approximation of the DtN operator in $\Omega_{\text{ff}}$

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

$$\left\{ \begin{array}{l} \operatorname{div}\left(c_w \zeta^g \mathbf{u}_t - \zeta^g D_t \nabla c_w\right) = 0 \text{ on } \Omega_{\text{ff}}, \\ c_w = c_{w,\Gamma} \text{ on } \Gamma, \\ c_w = c_{w,in} \text{ on } \Gamma_{in}, \\ \nabla c_w \cdot \mathbf{n} = 0 \text{ on } \partial\Omega_{\text{ff}} \setminus (\Gamma \cup \Gamma_{in}) \end{array} \right.$$

and compute

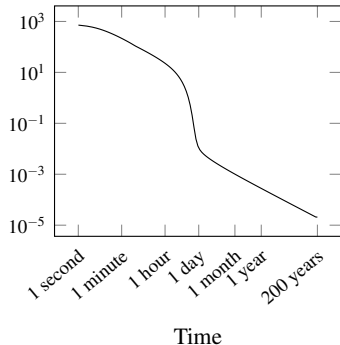
$$\beta_{\text{pm}}(x) = \frac{-\zeta^g D_t \nabla c_w \cdot \mathbf{n}(x)}{c_{w,\Gamma} - c_{w,in}} > 0 \text{ on } \Gamma.$$



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

## Computation of $\beta_{ff}$ : diagonal approximation of the DtN operator in $\Omega_{pm}$

- ▶ Linearized Richards equation with frozen coefficients at the interface  $\Gamma$
- ▶  $\beta_{ff}(x, t) =$  order 0 Taylor approximation of the DtN operator



Plot of  $\frac{\int_{\Gamma} \beta_{ff}(x, t) dx}{\int_{\Gamma} dx}$  function of time.

## Extension to the compositional model - Coupling conditions at the interface $\Gamma$ (isothermal)

$$\left\{ \begin{array}{l} \mathbf{V}_i \cdot \mathbf{n} = \mathbf{W}_i \cdot \mathbf{n}, \quad i \in \mathcal{C} : \text{molar flux continuity,} \\ c_i^g = c_i, \quad i \in \mathcal{C} : \text{gas molar fractions continuity,} \\ p^g = \mathbf{n} \cdot \mathbb{T} \mathbf{n}, \\ \mathbf{u} \cdot \boldsymbol{\tau} = 0 : \text{no slip condition.} \end{array} \right.$$

$$\sum_{i \in \mathcal{C}} \mathbf{V}_i \cdot \mathbf{n} = \sum_{i \in \mathcal{C}} \mathbf{W}_i \cdot \mathbf{n} = \zeta^g \mathbf{u} \cdot \mathbf{n}.$$

## Extension to the compositional model (isothermal)

- ▶ Porous medium flow on  $\Omega_{\text{pm}}$  with Robin and Dirichlet boundary conditions on  $\Gamma$

$$\beta_{\text{pm}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{pm}} - c_i^{g,k} \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k = \beta_{\text{pm}} c_i^{k-1} - \mathbf{W}_i^{k-1} \cdot \mathbf{n}_{\text{pm}}, \quad i \in \mathcal{C},$$

$$p^{g,k} = \mathbf{n} \cdot \mathbb{T}^{k-1} \mathbf{n}.$$

- ▶ RANS flow on  $\Omega_{\text{ff}}$  with Dirichlet boundary condition on  $\Gamma$

$$\zeta_{\text{ff}}^{g,k} \mathbf{u}^k \cdot \mathbf{n}_{\text{ff}} = \sum_{i \in \mathcal{C}} \mathbf{V}_i^k \cdot \mathbf{n}_{\text{ff}} = \zeta_{\text{ff}}^{g,k-1} \mathbf{u}^{k-1} \cdot \mathbf{n}_{\text{ff}} + \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k,$$

$$\mathbf{u}^k \cdot \boldsymbol{\tau} = 0.$$

- ▶ Convection diffusion equations on  $\Omega_{\text{ff}}$  with Robin boundary conditions on  $\Gamma$

$$\beta_{\text{ff}} c_i^k - \mathbf{W}_i^k \cdot \mathbf{n}_{\text{ff}} = \beta_{\text{ff}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{ff}}, \quad i \in \mathcal{C}.$$

## Extension to the compositional model (isothermal)

Porous medium flow on  $\Omega_{\text{pm}}$  with Robin boundary conditions on  $\Gamma$ : compute  $p^\alpha, s^\alpha, c^\alpha, \delta_{\mathbf{u}}$  such that

$$\frac{\phi}{\Delta t}(n_i^k - n_i^{k-1}) + \nabla \cdot \mathbf{V}_i^k = 0, \quad \text{in } \Omega_{\text{pm}},$$

$$\beta_{\text{pm}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{pm}} - c_i^{g,k} \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k = \beta_{\text{pm}} c_i^{k-1} - \mathbf{W}_i^{k-1} \cdot \mathbf{n}_{\text{pm}}, \quad \text{on } \Gamma,$$

$$p^{g,k} = \mathbf{n} \cdot \mathbb{T}^{k-1} \mathbf{n}, \quad \text{on } \Gamma,$$

+ thermodynamical equilibrium and other closure laws,

with  $\zeta_{\text{pm}}^{g,k} = \zeta^g(p^{g,k}, c^{g,k})$ .

## Extension to the compositional model (isothermal)

RANS flow on  $\Omega_{\text{ff}}$  with Dirichlet boundary condition on  $\Gamma$ : compute the pressure  $p^k$  and the gas velocity  $\mathbf{u}^k$  such that

$$\nabla \cdot (\rho_{\text{ff}}^{g,k} \mathbf{u}^k \otimes \mathbf{u}^k - \mu_t (\nabla \mathbf{u}^k + \nabla^t \mathbf{u}^k)) + \nabla p^k = \rho_{\text{ff}}^{g,k} \mathbf{g}, \quad \text{in } \Omega_{\text{ff}},$$

$$\nabla \cdot (\zeta_{\text{ff}}^{g,k} \mathbf{u}^k) = 0, \quad \text{in } \Omega_{\text{ff}},$$

$$\zeta_{\text{ff}}^{g,k} \mathbf{u}^k = \zeta_{\text{ff}}^{g,k-1} \mathbf{u}^{k-1} + \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k \mathbf{n}_{\text{ff}}, \quad \text{on } \Gamma,$$

with  $\zeta_{\text{ff}}^{g,k} = \zeta^g(p^k, c^{k-1})$  and  $\rho_{\text{ff}}^{g,k} = \rho^g(p^k, c^{k-1})$ .

## Extension to the compositional model (isothermal)

Convection diffusion equations on  $\Omega_{\text{ff}}$  with Robin boundary conditions on  $\Gamma$ :  
compute  $c^k$  such that for all  $i \in \mathcal{C}$

$$\nabla \cdot \mathbf{W}_i^k = 0, \quad \text{in } \Omega_{\text{ff}},$$

$$\beta_{\text{ff}} c_i^k - \mathbf{W}_i^k \cdot \mathbf{n}_{\text{ff}} = \beta_{\text{ff}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{ff}}, \quad \text{on } \Gamma,$$

with  $\mathbf{W}_i^k = \zeta_{\text{ff}}^{g,k} (c_i^k \mathbf{u}^k - D_t \nabla c_i^k)$ .

## Extension to the compositional model (non-isothermal)

Porous medium flow on  $\Omega_{\text{pm}}$  with Robin boundary conditions on  $\Gamma$ : compute  $p^\alpha, T_{\text{pm}}, s^\alpha, c^\alpha, \delta_{\mathbf{u}}$  such that for all  $i \in \mathcal{C}$ :

$$\frac{\phi}{\Delta t} (n_i^k - n_i^{k-1}) + \nabla \cdot \mathbf{V}_i^k = 0, \quad \text{in } \Omega_{\text{pm}},$$

$$\frac{E^k - E^{k-1}}{\Delta t} + \nabla \cdot \mathbf{V}_e^k = 0, \quad \text{in } \Omega_{\text{pm}},$$

$$\beta_{\text{pm}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{pm}} - c_i^{g,k} \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k = \beta_{\text{pm}} c_i^{k-1} - \mathbf{W}_i^{k-1} \cdot \mathbf{n}_{\text{pm}}, \quad \text{on } \Gamma,$$

$$\gamma_{\text{pm}} T_{\text{pm}}^k - \mathbf{V}_e^k \cdot \mathbf{n}_{\text{pm}} - h_{\text{pm}}^{g,k} \zeta_{\text{pm}}^{g,k} \delta_{\mathbf{u}}^k = \gamma_{\text{pm}} T_{\text{ff}}^{k-1} - \mathbf{W}_e^{k-1} \cdot \mathbf{n}_{\text{pm}}, \quad \text{on } \Gamma,$$

$$p^{g,k} = \mathbf{n} \cdot \mathbb{T}^{k-1} \mathbf{n}, \quad \text{on } \Gamma,$$

+ thermodynamical equilibrium and other closure laws,

with  $\zeta_{\text{pm}}^{g,k} = \zeta^g(p^{g,k}, T_{\text{pm}}^k, c^{g,k})$ ,  $h_{\text{pm}}^{g,k} = h^g(p^{g,k}, T_{\text{pm}}^k, c^{g,k})$ .

## Extension to the compositional model (non-isothermal)

RANS flow on  $\Omega_{\text{ff}}$  with Dirichlet boundary condition on  $\Gamma$ : compute the pressure  $p^k$  and the gas velocity  $\mathbf{u}^k$  such that

$$\nabla \cdot (\rho_{\text{ff}}^{\mathbf{g},k} \mathbf{u}^k \otimes \mathbf{u}^k - \mu_t (\nabla \mathbf{u}^k + \nabla^t \mathbf{u}^k)) + \nabla p^k = \rho_{\text{ff}}^{\mathbf{g},k} \mathbf{g}, \quad \text{in } \Omega_{\text{ff}},$$

$$\nabla \cdot (\zeta_{\text{ff}}^{\mathbf{g},k} \mathbf{u}^k) = 0, \quad \text{in } \Omega_{\text{ff}},$$

$$\zeta_{\text{ff}}^{\mathbf{g},k} \mathbf{u}^k = \zeta_{\text{ff}}^{\mathbf{g},k-1} \mathbf{u}^{k-1} + \zeta_{\text{pm}}^{\mathbf{g},k} \delta_{\mathbf{u}}^k \mathbf{n}_{\text{ff}}, \quad \text{on } \Gamma,$$

with  $\zeta_{\text{ff}}^{\mathbf{g},k} = \zeta^{\mathbf{g}}(p^k, T_{\text{ff}}^{k-1}, c^{k-1})$  and  $\rho_{\text{ff}}^{\mathbf{g},k} = \rho^{\mathbf{g}}(p^k, T_{\text{ff}}^{k-1}, c^{k-1})$ .

## Extension to the compositional model (non-isothermal)

Convection diffusion equations on  $\Omega_{\text{ff}}$  with Robin boundary conditions on  $\Gamma$ :  
compute  $c^k$ ,  $T_{\text{ff}}^k$  such that for all  $i \in \mathcal{C}$

$$\nabla \cdot \mathbf{W}_i^k = 0, \quad \text{in } \Omega_{\text{ff}},$$

$$\nabla \cdot \mathbf{W}_e^k = 0, \quad \text{in } \Omega_{\text{ff}},$$

$$\beta_{\text{ff}} c_i^k - \mathbf{W}_i^k \cdot \mathbf{n}_{\text{ff}} = \beta_{\text{ff}} c_i^{g,k} - \mathbf{V}_i^k \cdot \mathbf{n}_{\text{ff}}, \quad \text{on } \Gamma,$$

$$\gamma_{\text{ff}} T_{\text{ff}}^k - \mathbf{W}_e^k \cdot \mathbf{n}_{\text{ff}} = \gamma_{\text{ff}} T_{\text{pm}}^k - \mathbf{V}_e^k \cdot \mathbf{n}_{\text{ff}}, \quad \text{on } \Gamma,$$

with  $\mathbf{W}_i^k = \zeta_{\text{ff}}^{g,k} (c_i^k \mathbf{u}^k - D_t \nabla c_i^k)$  and  $\mathbf{W}_e^k = \sum_{i \in \mathcal{C}} h_i^{g,k}(p^k, T_{\text{ff}}^k) \mathbf{W}_i^k - \lambda_t \nabla T_{\text{ff}}^k$ .

where we have used that  $h^g(p, T, c) = \sum_{i \in \mathcal{C}} h_i^g(p, T) c_i$ .

# Computation of $\gamma_{\text{pm}}$ : diagonal approximation of the DtN operator in $\Omega_{\text{ff}}$

Given two constants  $T_{\Gamma} \neq T_{in}$  and  $C_{p,i} = \langle \partial_T h_i^g(p, T) \rangle_{\Gamma}$ , solve

$$\left\{ \begin{array}{l} \operatorname{div} \left( \sum_{i \in \mathcal{C}} C_{p,i} T \mathbf{W}_i - \lambda_t \nabla T \right) = 0 \text{ on } \Omega_{\text{ff}}, \\ T = T_{\Gamma} \text{ on } \Gamma, \\ T = T_{in} \text{ on } \Gamma_{in}, \\ \nabla T \cdot \mathbf{n} = 0 \text{ on } \partial\Omega_{\text{ff}} \setminus (\Gamma \cup \Gamma_{in}) \end{array} \right.$$

and compute

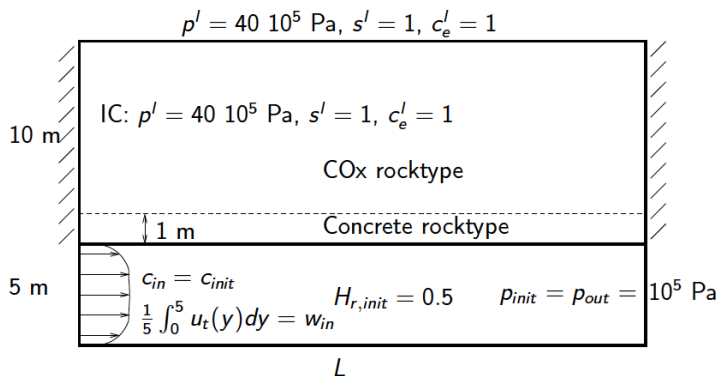
$$\gamma_{\text{pm}}(x) = \frac{\left( \sum_{i \in \mathcal{C}} C_{p,i} T_{\Gamma} \mathbf{W}_i - \lambda_t \nabla T \right) \cdot \mathbf{n}(x)}{T_{\Gamma} - T_{in}} > 0 \text{ on } \Gamma.$$

which is independent of  $T_{\Gamma}$  and  $T_{in}$

## Computation of $\gamma_{\text{ff}}$ : diagonal approximation of the DtN operator in $\Omega_{\text{pm}}$

- ▶ Linearized energy conservation equation with frozen coefficients at the interface  $\Gamma$
- ▶  $\gamma_{\text{ff}}(x, t) =$  order 0 Taylor approximation of the DtN operator

## Andra test case

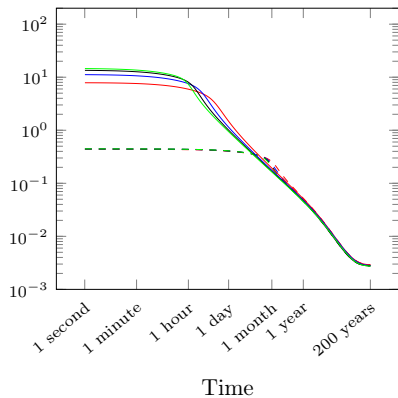


- ▶ Two components: H<sub>2</sub>O (w) and air (a)
- ▶  $L = 100 \text{ m}$
- ▶ Input gas:  $T_{in} = 303$  and  $H_{r,in} = 0.5$
- ▶  $w_{in} = 5 \text{ m/s}$  or  $0.05 \text{ m/s}$
- ▶ Initial temperature in  $\Omega_{pm}$ :  $T_{init} = 303$  or  $333 \text{ K}$ .
- ▶ Simulation time: 200 years

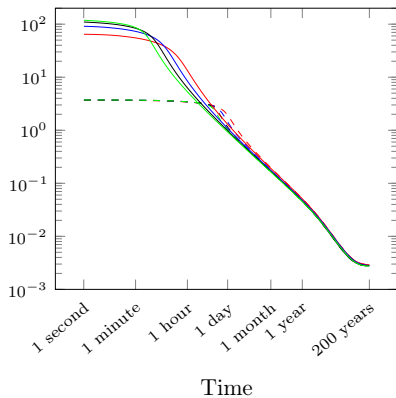
# Andra test case: evaporation rates in $\text{mm}/\text{day}/\text{m}^2$

—— :  $w_{in} = 5 \text{ m/s}$ ,  
- - - :  $w_{in} = 0.05 \text{ m/s}$

(a)  $T^0 = 303 \text{ K}$



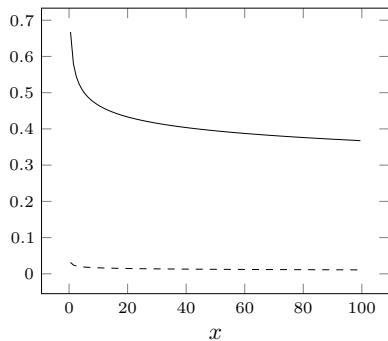
(b)  $T^0|_{\Omega_{pm}} = 333 \text{ K}$



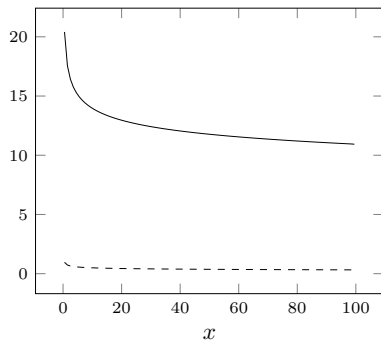
# Andra test case: Robin coefficients $\beta_{pm}$ and $\gamma_{pm}$

— :  $w_{in} = 5$  m/s,  
- - - :  $w_{in} = 0.05$  m/s

(a)  $\beta_{pm}$



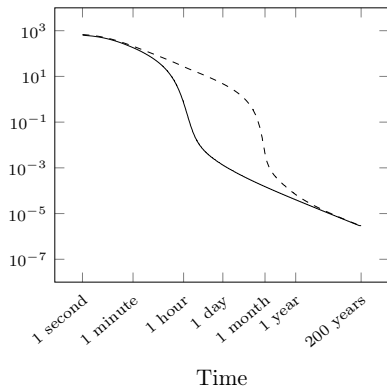
(b)  $\gamma_{pm}$



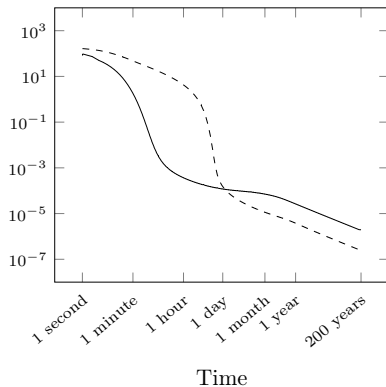
# Andra test case: Robin coefficients $\beta_{ff}$

— :  $w_{in} = 5$  m/s,  
- - - :  $w_{in} = 0.05$  m/s

(a)  $T^0 = 303$  K



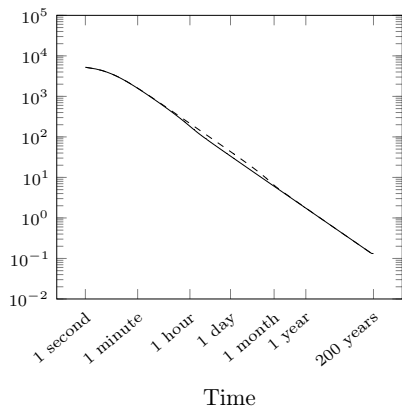
(b)  $T^0|_{\Omega_{pm}} = 333$  K



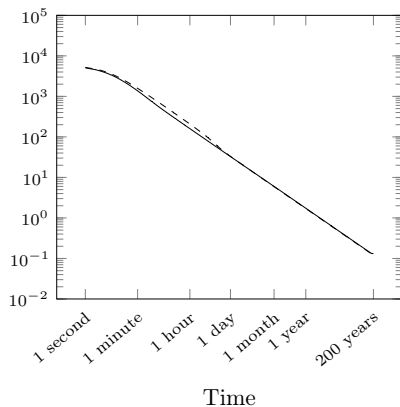
# Andra test case: Robin coefficients $\gamma_{ff}$

— :  $w_{in} = 5$  m/s,  
- - - :  $w_{in} = 0.05$  m/s

(a)  $T^0 = 303$  K



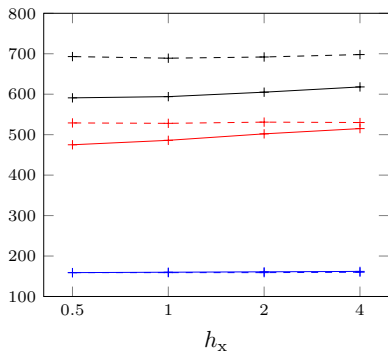
(b)  $T^0|_{\Omega_{pm}} = 333$  K



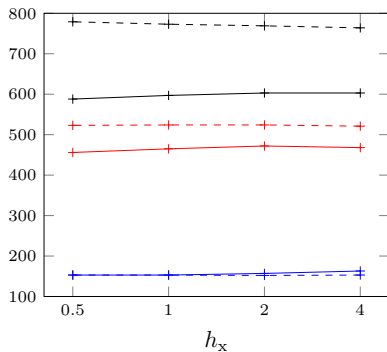
# Andra test case: total number of DDM iterations for 115 time steps

— :  $w_{in} = 5$  m/s,  
- - - :  $w_{in} = 0.05$  m/s

(a)  $T^0 = 303$  K



(b)  $T^0|_{\Omega_{pm}} = 333$  K



# Conclusions and perspectives

## Conclusions

- ▶ Algorithm to solve the coupling between a liquid gas Darcy and a free gas flow
  - ▶ Provide an efficient nonlinear solver
  - ▶ Allow the use of separate codes in the porous and free flow domains

## Perspectives

- ▶ Code coupling
- ▶ Test cases with more complex geometries
- ▶ Acceleration by Newton method
- ▶ Convergence analysis

## **Acknowledgements:**

We would like to thank Andra for supporting this work.

**Thanks for your attention!**