Using COMSOL Multiphysics® to simulate heat exchanger fouling by heterogeneous barite crystallization

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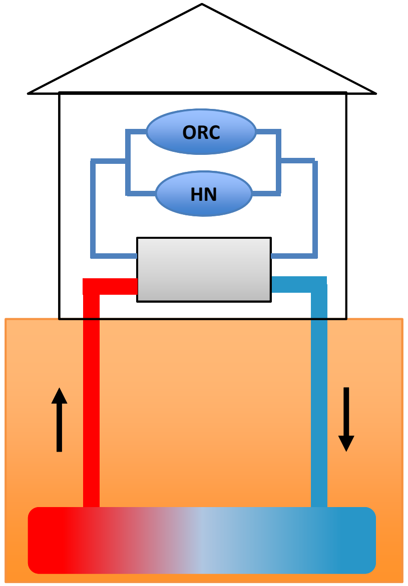
Comsol Conference - Lausanne

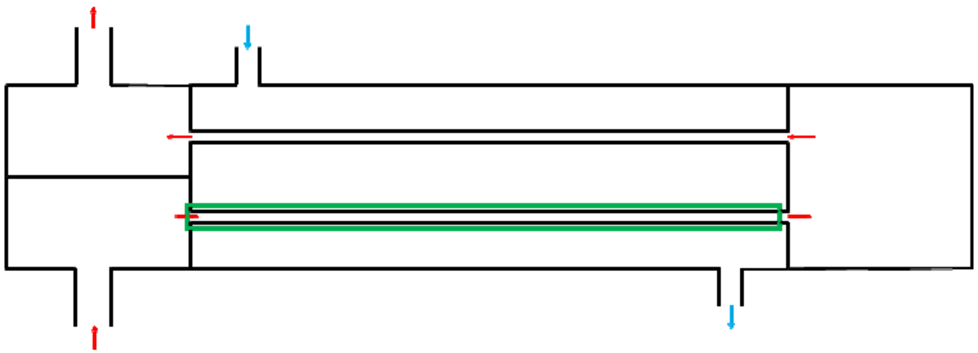
October 23th 2018

Context of the study

Main goals of CARPHYMCHEAU's project :

- Improving general knowledge on heat exchangers used in geothermal applications
- Study of the fouling phenomenon in the pipes





Outline

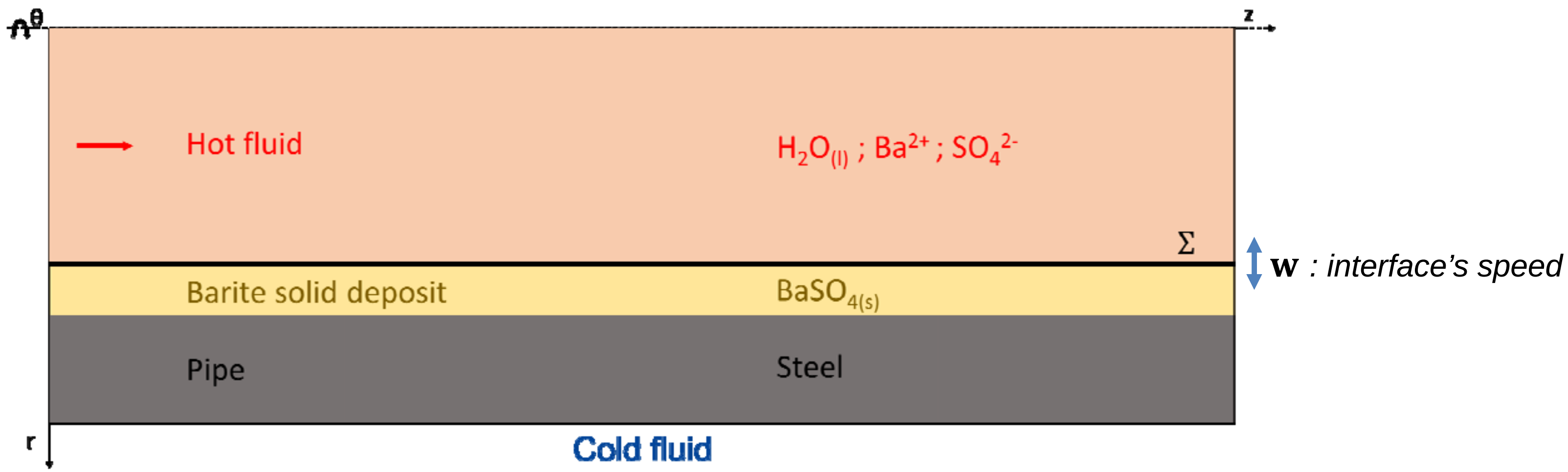
1. Case Study
2. Model
3. Simulation
4. Conclusion and prospects

Case study

Heterogeneous barite crystallization

Main assumptions

- Diluted species in the water
- Fluid density assumed constant equal to the water's



Model

Conservation laws - liquid phase

- Mass

$$\frac{\partial C_{li}}{\partial t} + \nabla \cdot (C_{li} \boldsymbol{v}_{li}) = 0 \qquad \text{i=1,2}$$

$$\rho_l = cste \qquad \nabla \cdot \boldsymbol{v_l} = 0$$

$$\rho_l = \sum_{i=1}^{3} M_i C_{li} \quad \text{and,} \quad \boldsymbol{v}_l = \frac{1}{\rho_l} \sum_{i=1}^{3} M_i C_{li} \boldsymbol{v}_{li}$$

- Energy

$$T_{li} = T_l$$

$$\rho_l C_{P_l} (\frac{\partial T}{\partial t} + (\boldsymbol{v}_l \cdot \nabla) T) - \nabla \cdot \lambda_l \nabla T_l = 0$$

- Charge

$$\sum_{i=1}^{2} z_i C_{li} = 0 \qquad \text{(Electroneutrality)}$$

Current intensity is assumed to be null : $\boldsymbol{i} = F \sum_{i=1}^{2} z_i \boldsymbol{J}_i = \boldsymbol{0}$

Model

Conservation laws - liquid phase

- Momentum $$\rho_l\left(\frac{\partial \boldsymbol{v}_l}{\partial t}+(\boldsymbol{v}_l\cdot\nabla)\boldsymbol{v}_l\right)=\rho_l\boldsymbol{g}-\nabla P_l+\mu_l\Delta\boldsymbol{v}_l$$

$$\boldsymbol{J}_i=C_{li}(\boldsymbol{v}_{li}-\boldsymbol{v}_l)=-D_i\left(\boldsymbol{\nabla}C_{li}+C_{li}z_i\frac{F}{RT}\boldsymbol{\nabla}\Phi\right)\qquad \text{i=1,2}$$

$$\sum_{\mathrm{i}=1}^{3}M_i\boldsymbol{J}_i=0$$

Under the null current hypothesis we have :

$$\boldsymbol{\nabla}\Phi=-\frac{RT}{F}\frac{\sum_{i=1}^{2}D_i\boldsymbol{\nabla}(z_iC_{li})}{\sum_{i=1}^{2}D_iC_{li}z_i^2}$$

We can then express an effective diffusion coefficient :

$$D_{eff}=\frac{2D_1D_2}{D_1+D_2}\qquad \text{and,}\qquad \boldsymbol{J}_i=-D_{eff}\boldsymbol{\nabla}C_{li}\qquad \text{i=1,2}$$

Model

Conservation laws - solid phases

	Solid	Pipe
Mass (Homogeneous phase)	$\rho_s = cste$	$\rho_p = cste$
Momentum (Non-deformable and fixed solid)	$\boldsymbol{v}_s = 0$	$\boldsymbol{v}_p = 0$
Energy (No body sources of heat)	$\frac{\partial}{\partial t}(\rho_s h_s) = \nabla \cdot \lambda_s \nabla T_s$ $h_s = h_s(T_s)$	$\frac{\partial}{\partial t}(\rho_p h_p) = \nabla \cdot \lambda_p \nabla T_p$ $h_p = h_p(T_p)$

Model

Boundary conditions

- Liquid-deposit interface Σ :

$$Ba^{2+} + SO_4^{2-} \rightarrow BaSO_{4(s)}$$

- Solid flux: $\rho_s \boldsymbol{w} \cdot \boldsymbol{n}_l = -M_s R_s^{\Sigma}$ (**w** : *interface's speed*)
- Flux of reacting species: $C_{li}(\boldsymbol{v}_{li} - \boldsymbol{w}) \cdot \boldsymbol{n}_l = -R_s^{\Sigma}$ i = 1,2
- Flux of the water: $C_{lH_2O}(\boldsymbol{v}_{lH_2O} - \boldsymbol{w}) \cdot \boldsymbol{n}_l = 0$
- Kinetics (ideal mixture) : $R_s^{\Sigma} = k_r \left(\frac{C_{l1} C_{l2}}{C_s^{sat}(T^{\Sigma})^2} - 1 \right)$ *(from Naillon et al. 2017)*
- Momentum: $\begin{cases} \boldsymbol{v}_l \cdot \boldsymbol{n}_l = \boldsymbol{w} \cdot \boldsymbol{n}_l \left(1 - \frac{\rho_s}{\rho_l}\right) \\ \boldsymbol{v}_l . \boldsymbol{t}_l = 0 \end{cases}$
- Temperature continuity : $T_l = T_s$
- Heat flux continuity : $R_s^{\Sigma} \Delta_c h_s + \boldsymbol{q}_l \cdot \boldsymbol{n}_l + \boldsymbol{q}_s \cdot \boldsymbol{n}_s = 0$

- For all other boundaries

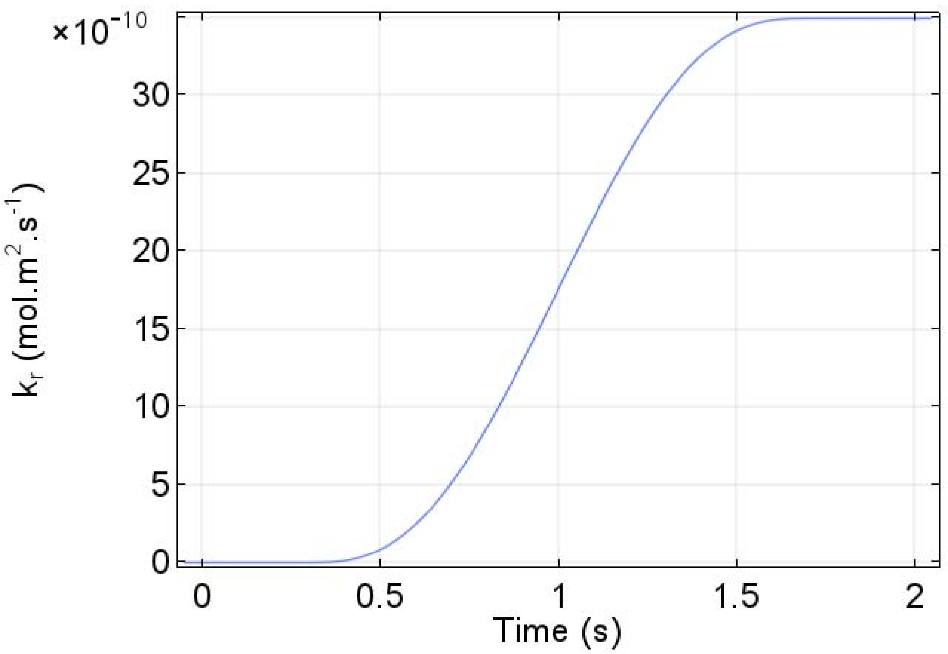
Model

Initial values

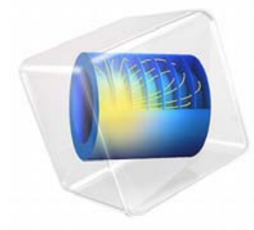
- ➢ Initial values for the relevant variables
- ➢ Use of a step for the kinetic coefficient : from 0 to its value.

- Calculation at t=0 to match the initial values to the boundary conditions is made without crystallization and deformed geometry

- In the results it allows to have the real initial value of the concentration plotted at t=0.



Simulation



Geometry

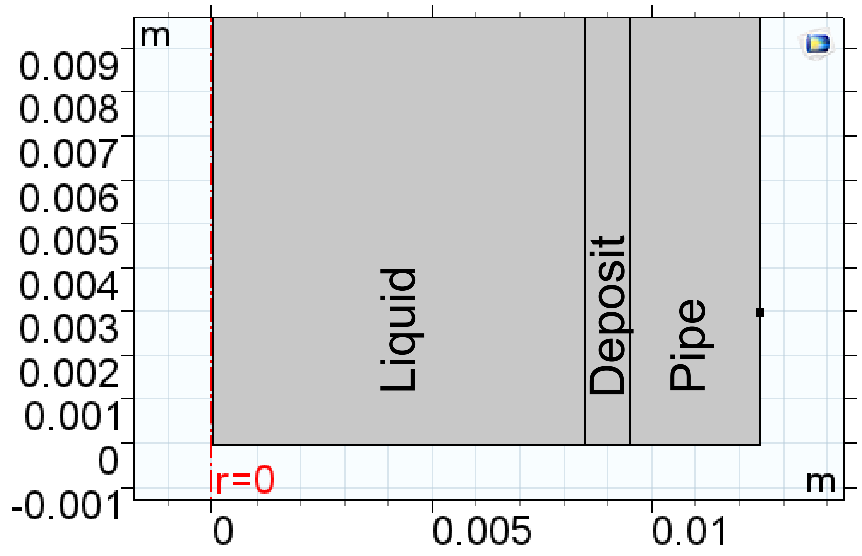
- 2D Axisymmetric
- 2 m * 12,5 mm

Components :

- Heat Transfer
- Laminar Flow
- Transport of diluted species
- Deformed Geometry

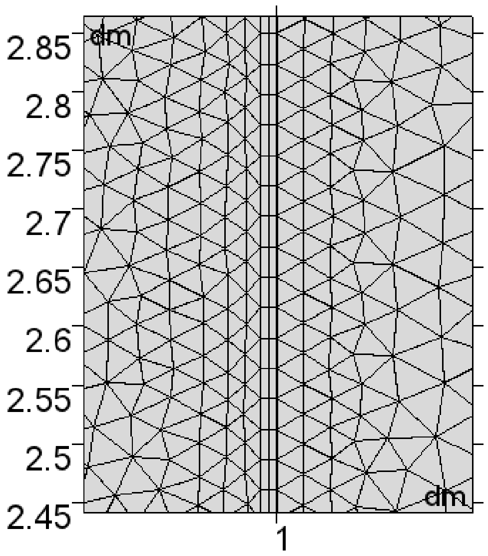
Multiphysics :

- Nonisothermal flow

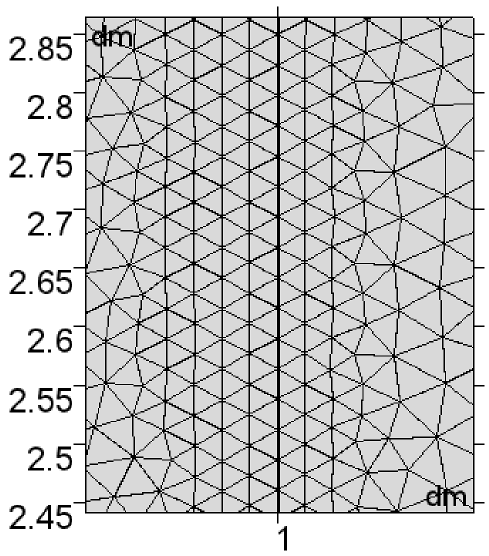


Simulation

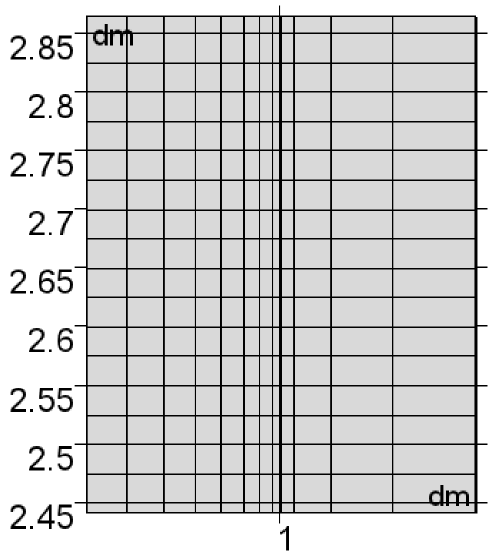
Study of the impact of meshing and controlling the time step taken by the solver



M1 : Boundary layer



M2 : Free triangles

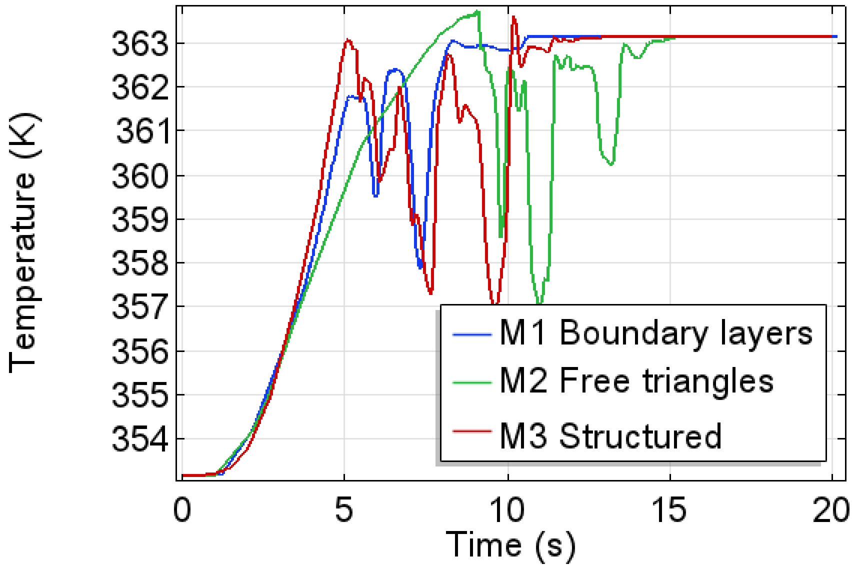


M3 : Structured

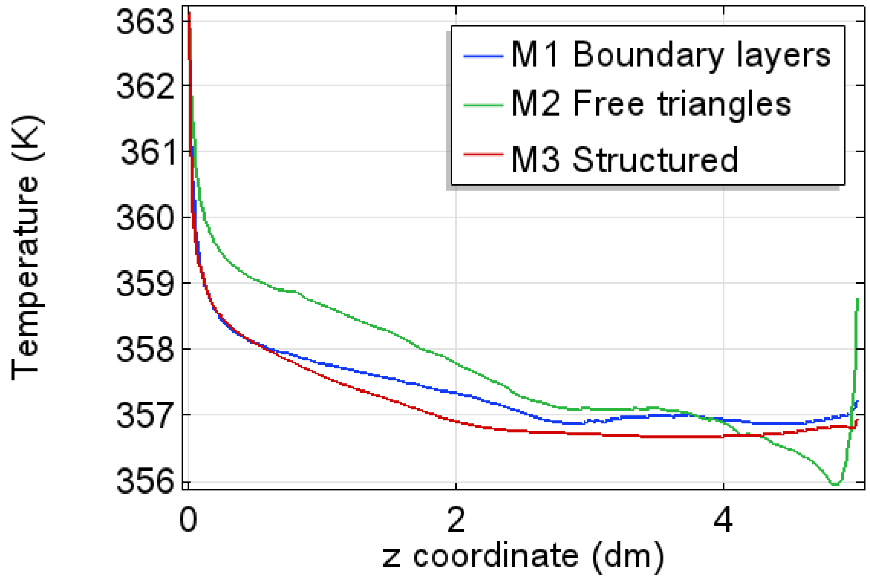
Simulation

Study of the impact of meshing and controlling the time step taken by the solver

Temperature evolution of one point in the fluid (close to the exit)



Temperature evolution over the liquid/solid interface (t=30 s)

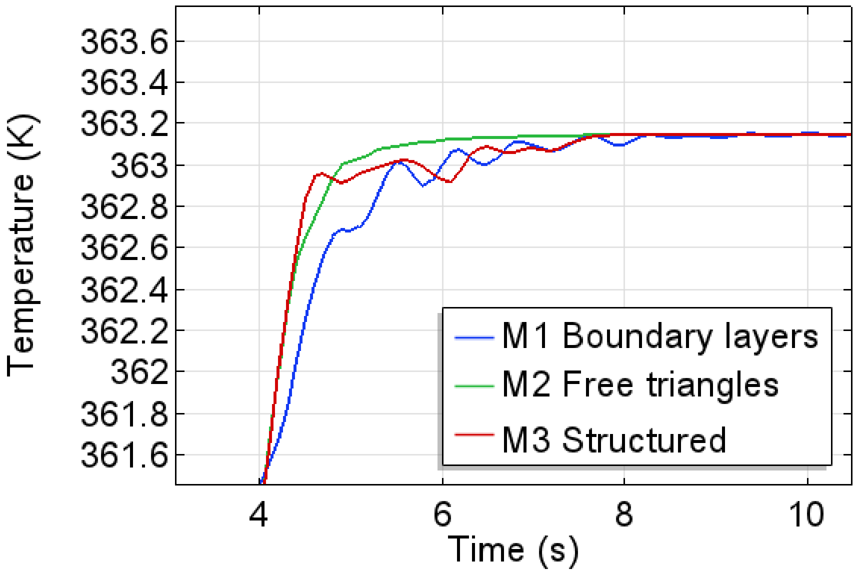


→ Free time steps taken by the solver

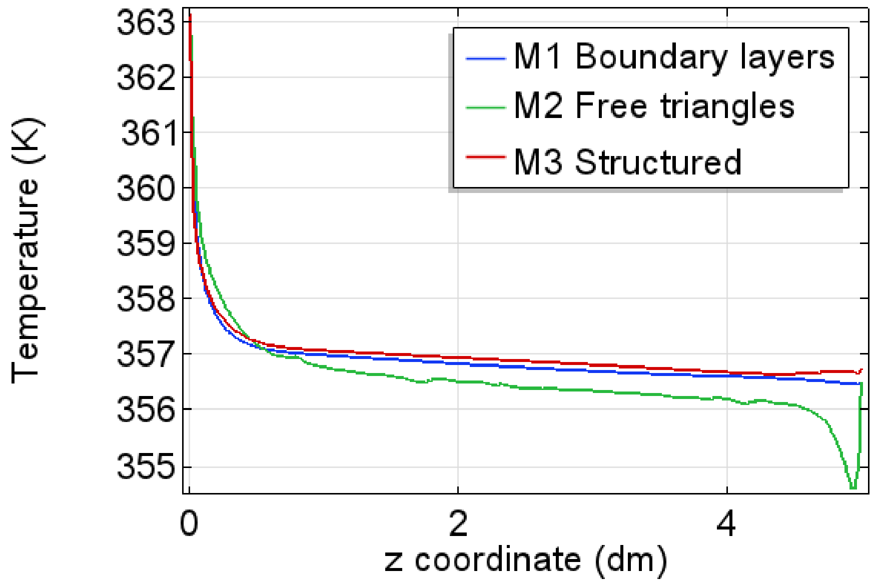
Simulation

Study of the impact of meshing and controlling the time step taken by the solver

Temperature evolution of one point in the fluid (close to the exit)



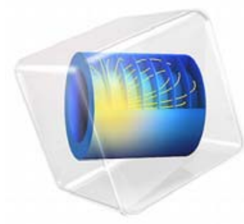
Temperature evolution over the liquid/solid interface (t=30 s)



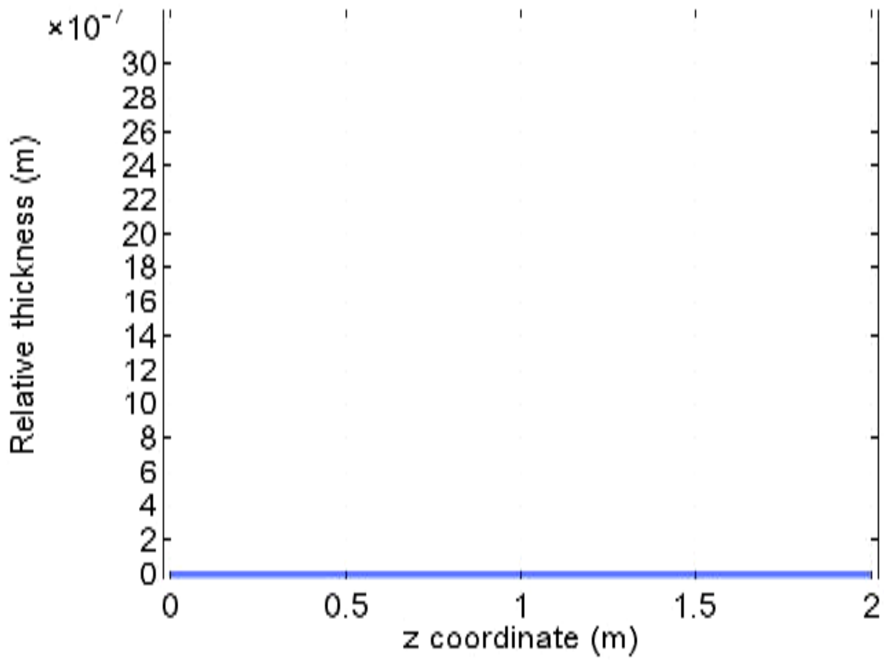
→ Time steps taken by the solver limited to 0,1 s

Simulation

→ A boundary layer mesh (M1) is used at the moving boundary
→ The time step taken by the solver is limited

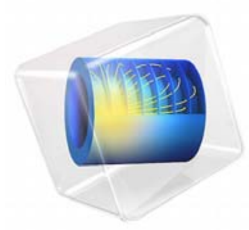


Temporal evolution over one year
of the deposit along the pipe

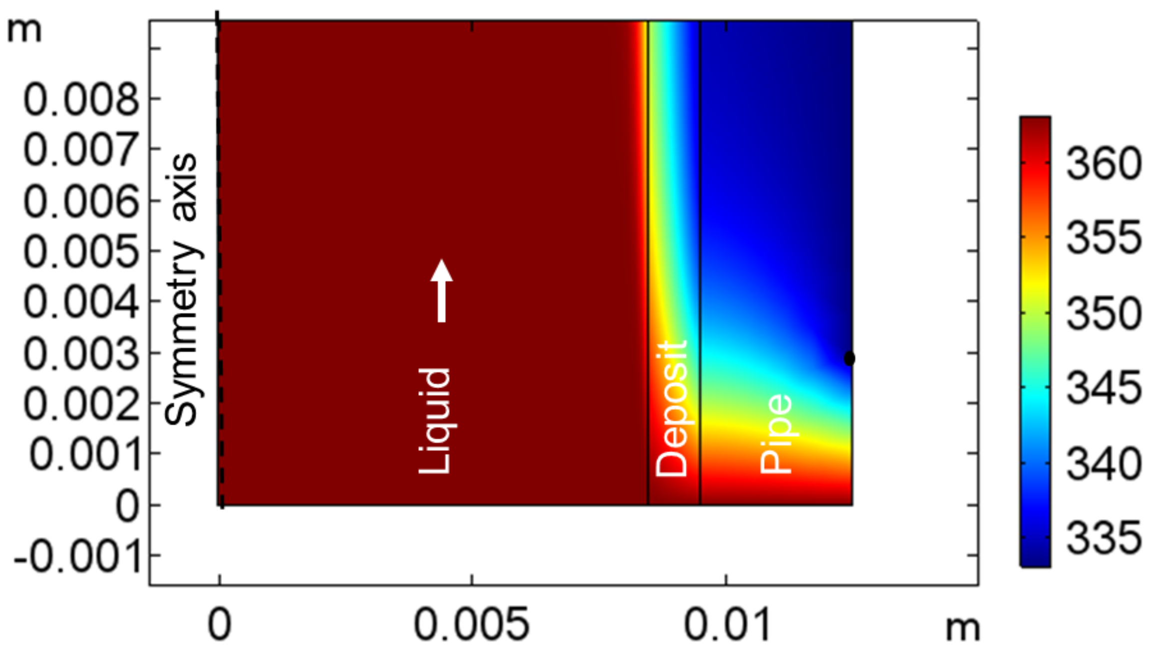


Simulation parameters	
P_{out}	20 bar
V_{in}	0,1 m.s^{-1}
T_{in}	90 °C
T_{cold}	20 °C
$C^{in}_{Ba^{2+}}$	2.10^{-5} mol.L^{-1}
$C^{in}_{SO_4^{2-}}$	2.10^{-5} mol.L^{-1}
E_{pipe}	3 mm
$E^0_{deposit}$	1 mm
R^i_{pipe}	10 mm
K_r	3,49.10^{-9} mol.m^{-2}.s^{-1}
D_{eff}	0,944.10^{-9} m^2.s^{-1}

Simulation



Temperature profile close to the entrance



Simulation parameters	
P_{out}	20 bar
v_{in}	0,1 m.s^{-1}
T_{in}	90 °C
T_{cold}	60 °C
$C^{in}_{Ba^{2+}}$	2.10^{-5} mol.L^{-1}
$C^{in}_{SO_4^{2-}}$	2.10^{-5} mol.L^{-1}
e_{pipe}	3 mm
$e^0_{deposit}$	1 mm
r^i_{pipe}	10 mm
k_r	$3{,}49.10^{-9}$ mol.m^{-2}.s^{-1}
D_{eff}	$0{,}944.10^{-9}$ m^2.s^{-1}

Conclusions and prospects

Conclusions :

- Using a step for some variables is a good way to improve initialization
- Investigating the effect of the mesh on the results is important and the conclusions will be different for every problem
- Controlling the time steps taken by the solver is crucial

Prospects :

- Working with turbulent flow (in progress)
- Add more species to the fluid composition
- Solving Nernst-Planck equations

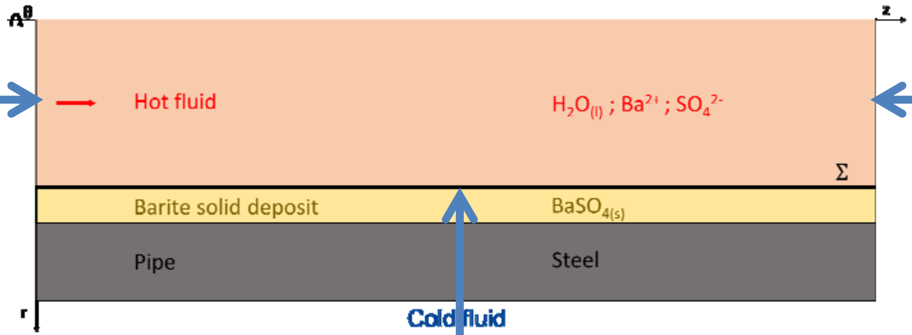
Conclusions and prospects

Nernst-Planck equations

$$\begin{cases} \frac{\partial C_{li}}{\partial t} + \boldsymbol{\nabla} \cdot \Big[C_{li}\boldsymbol{v_l} - \underbrace{D_i\left(\boldsymbol{\nabla} C_{li} + C_{li} z_i \frac{F}{RT} \boldsymbol{\nabla}\Phi\right)}_{\boldsymbol{J}_i}\Big] = 0 \\ \sum_{i=1}^{2} z_i C_{li} = 0 \\ \boldsymbol{\nabla} \cdot \boldsymbol{i} = 0 \end{cases}$$

i=1,2

$$\Phi = 0\ V$$
$$C_{l1} = C_{l1}^{in}$$



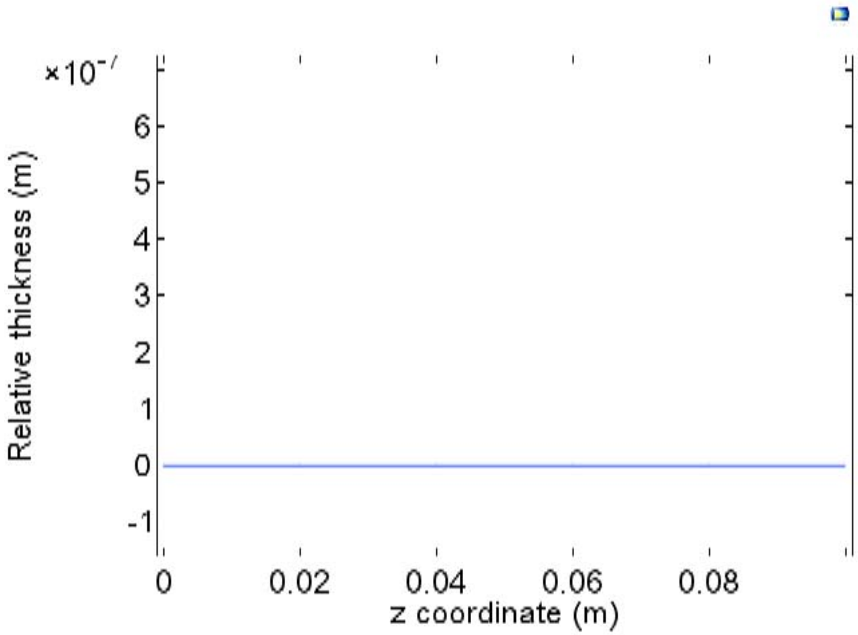
$$\boldsymbol{\nabla}\Phi \cdot \boldsymbol{n_l} = \boldsymbol{0}$$
$$D_i \boldsymbol{\nabla} C_{li} \cdot \boldsymbol{n_l} = \boldsymbol{0}$$

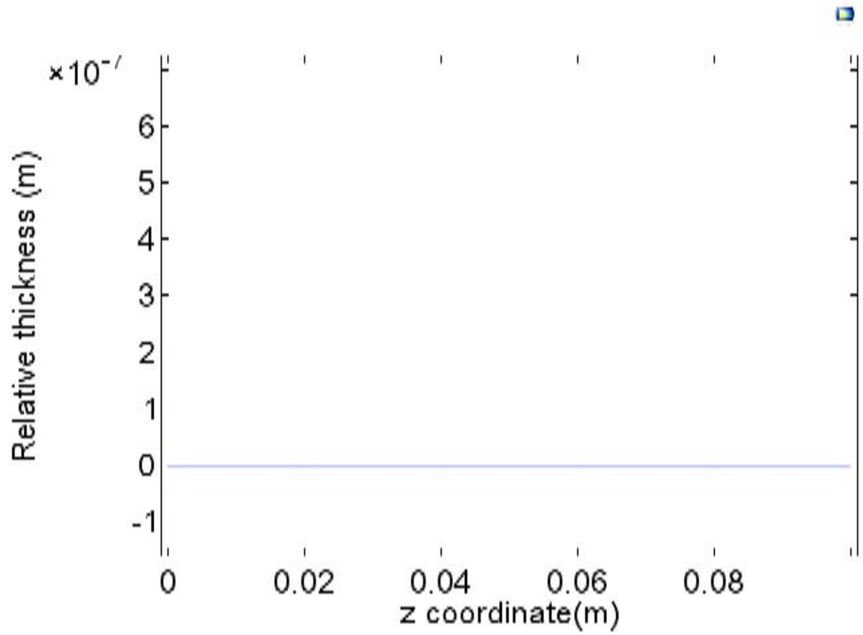
$$\boldsymbol{i} \cdot \boldsymbol{n_l} = 0$$
$$N_{l1} = R_s^{\Sigma} + C_{l1} \boldsymbol{w} \cdot \boldsymbol{n_l}$$

Conclusions and prospects

Nernst-Planck equations

Refining →





Temporal evolution of the deposit
along the pipe (1 day)

Thank you

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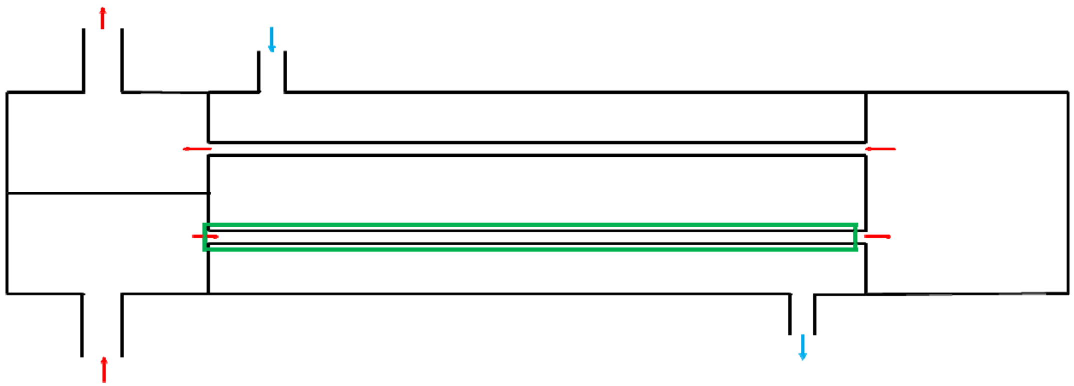
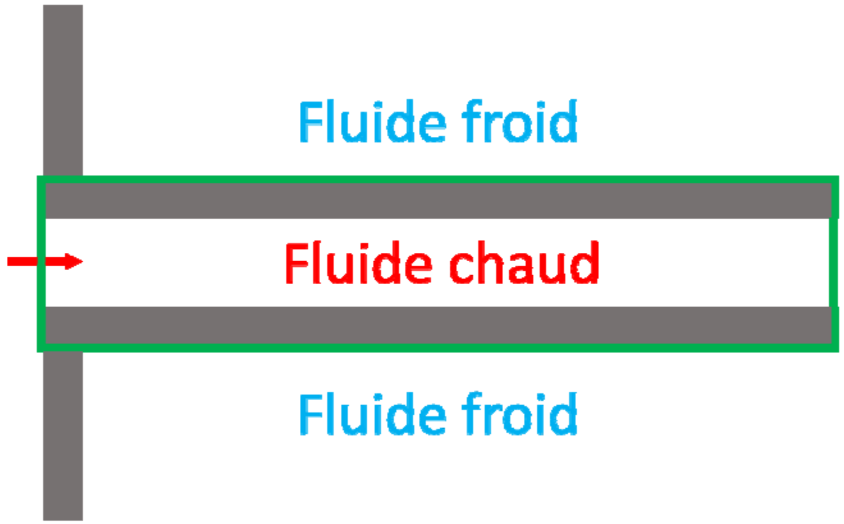
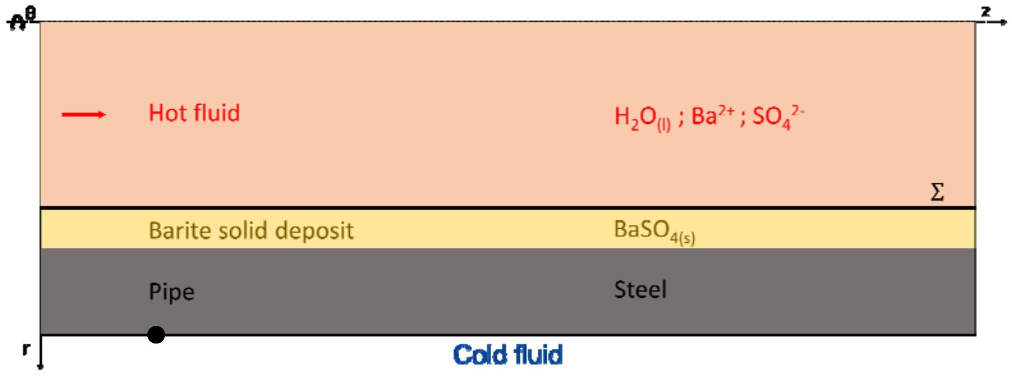
Appendix





Appendix

Boundary conditions



Liquid inlet
- Constant speed
- Temperature
- Composition

Liquid outlet
- Defined pressure
- Established flow

Solid boundary (Inlet side)
- Inlet temperature of the hot fluid

Solid boundary (Outlet side)
- Thermal insolation

Pipe-cold fluid interface
- Temperature

Exchanger's wall
- Linear thermal gradient

Pipe-deposit interface
- Temperature continuity
- Heat flux continuity