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Evaporation-driven transport and precipitation of salt in porous media: A multi-domain approach

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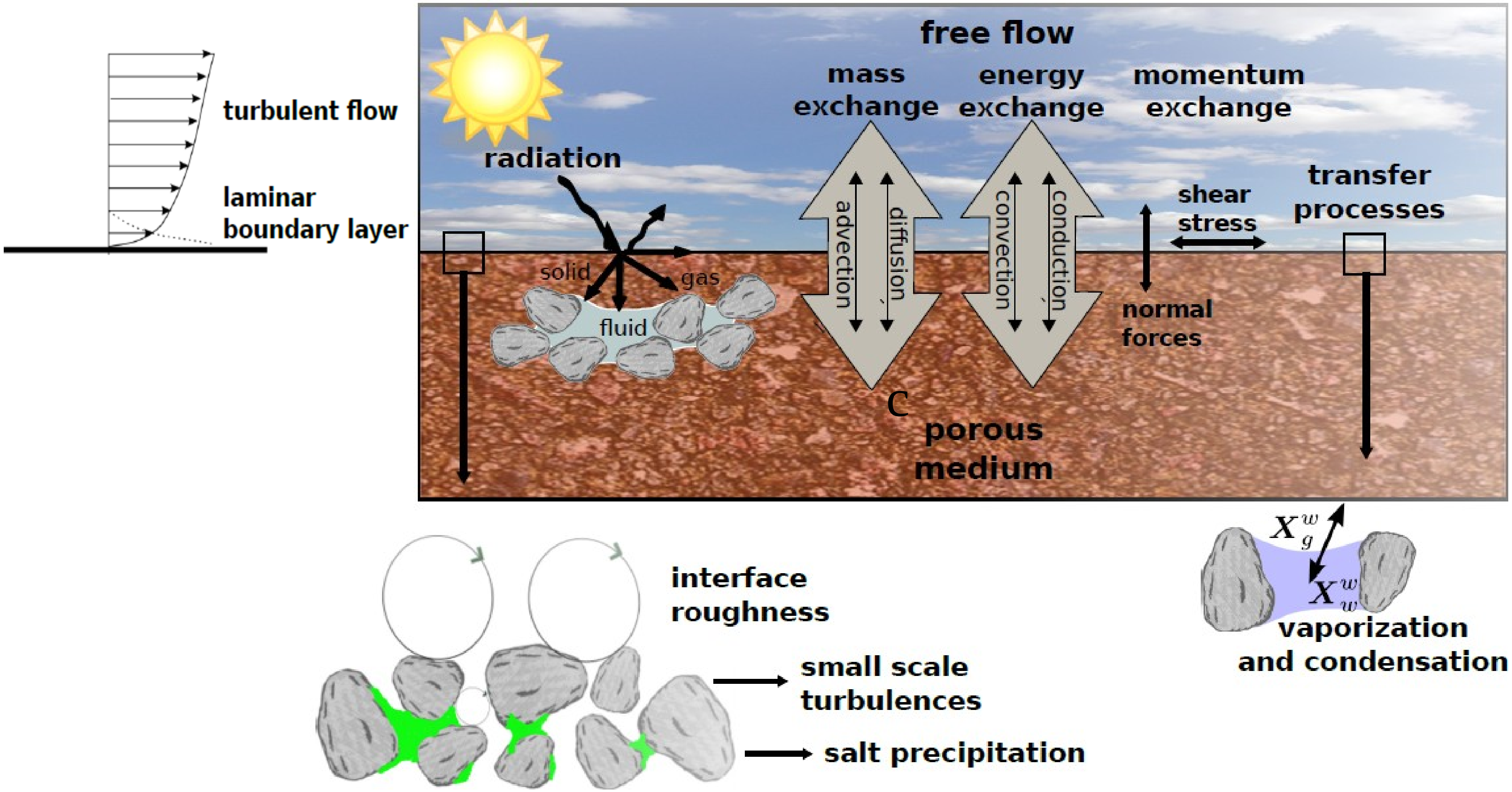
Overview

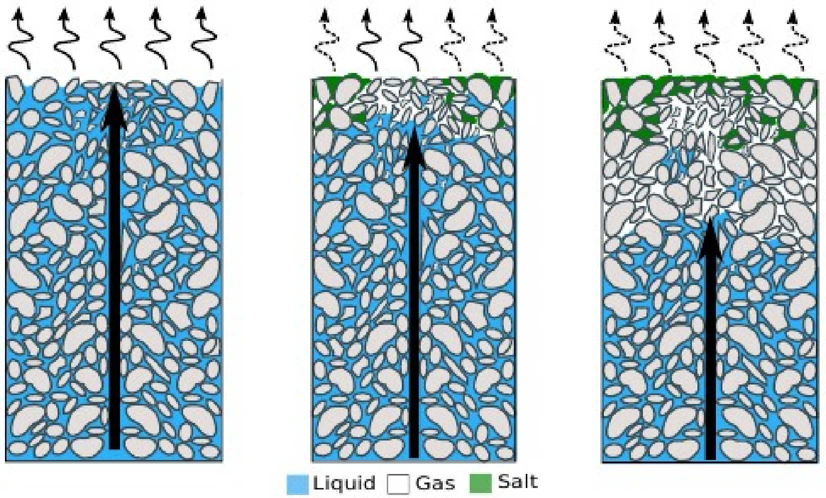
- Motivation
- Model Concept
- Results
- Outlook

Motivation

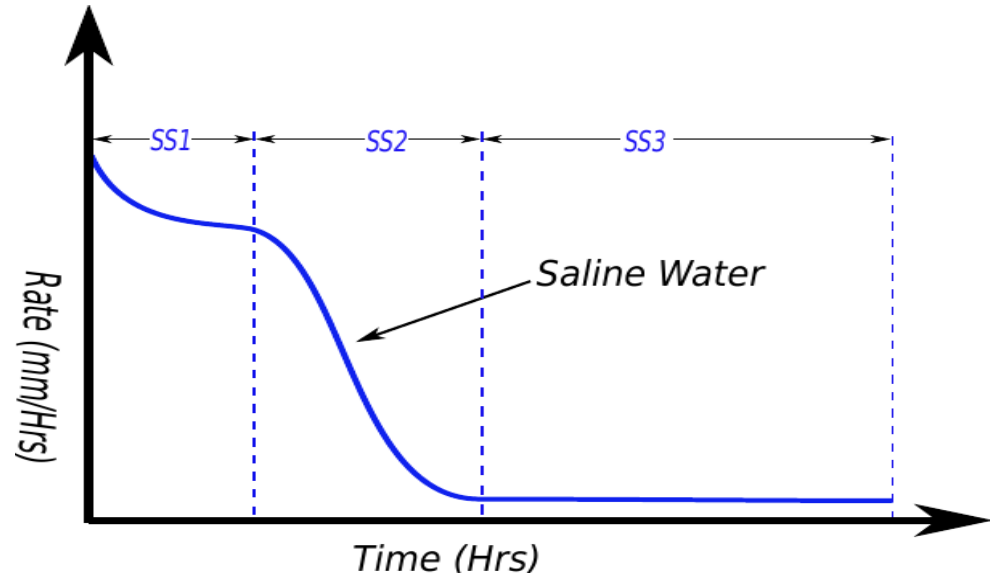


“A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow”, *Mosthaf et al., 2011*

Stages of saline water evaporation



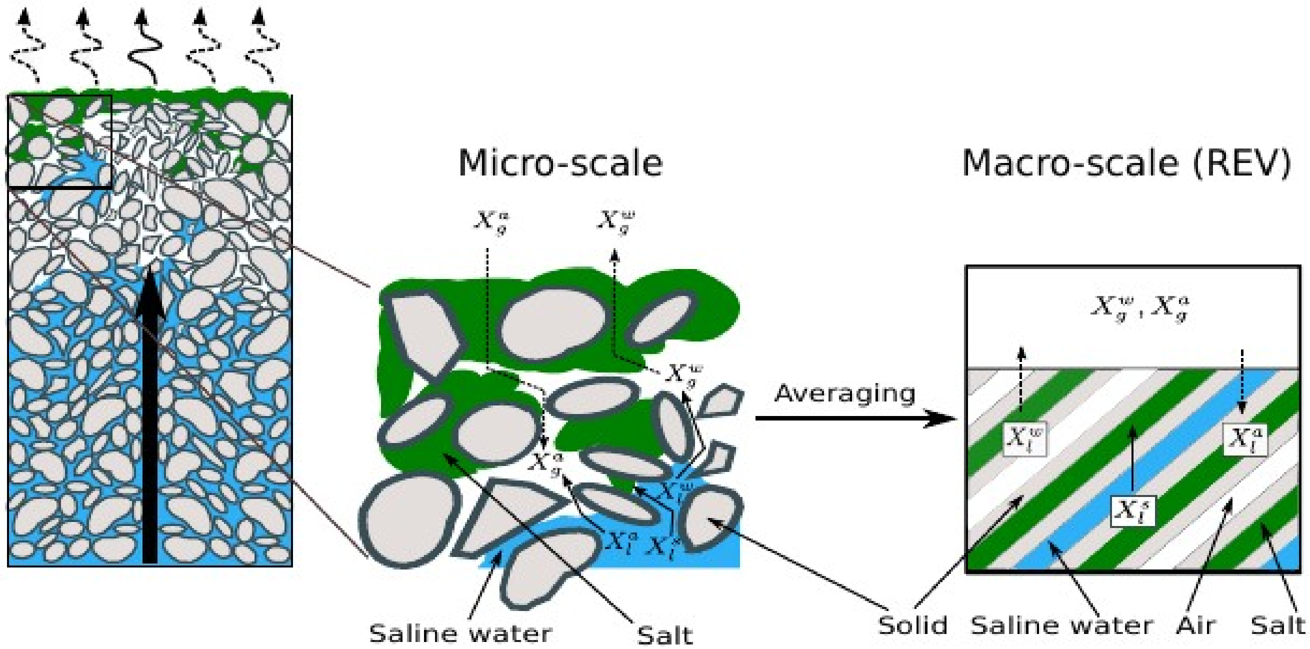
(a) SS1 (b) SS2 (c) SS3



- Stages of evaporation:
  - SS1: High evaporation rate
  - SS2: Evaporation rate falls subsequently
  - SS3: Constant low evaporation rate

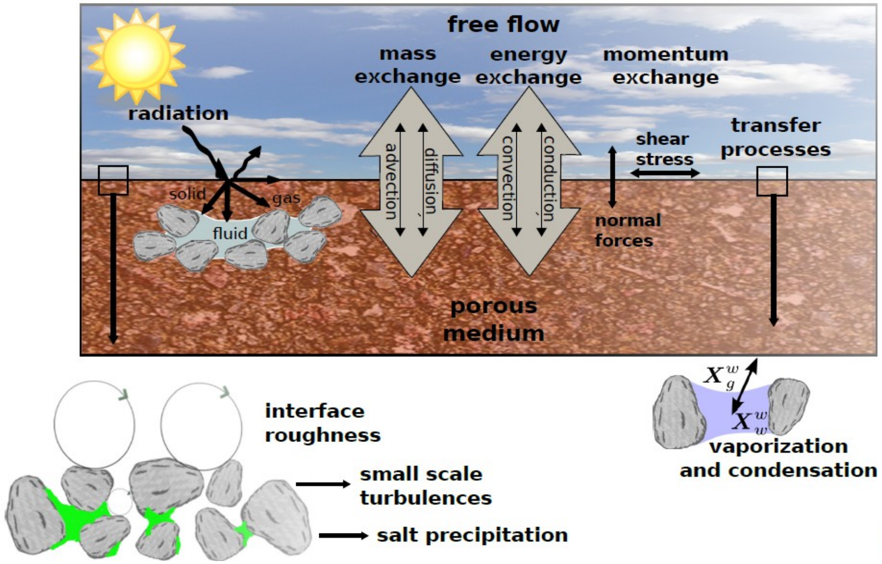
Salinization: Interplay between salt transport, evaporation dynamics and salt precipitation

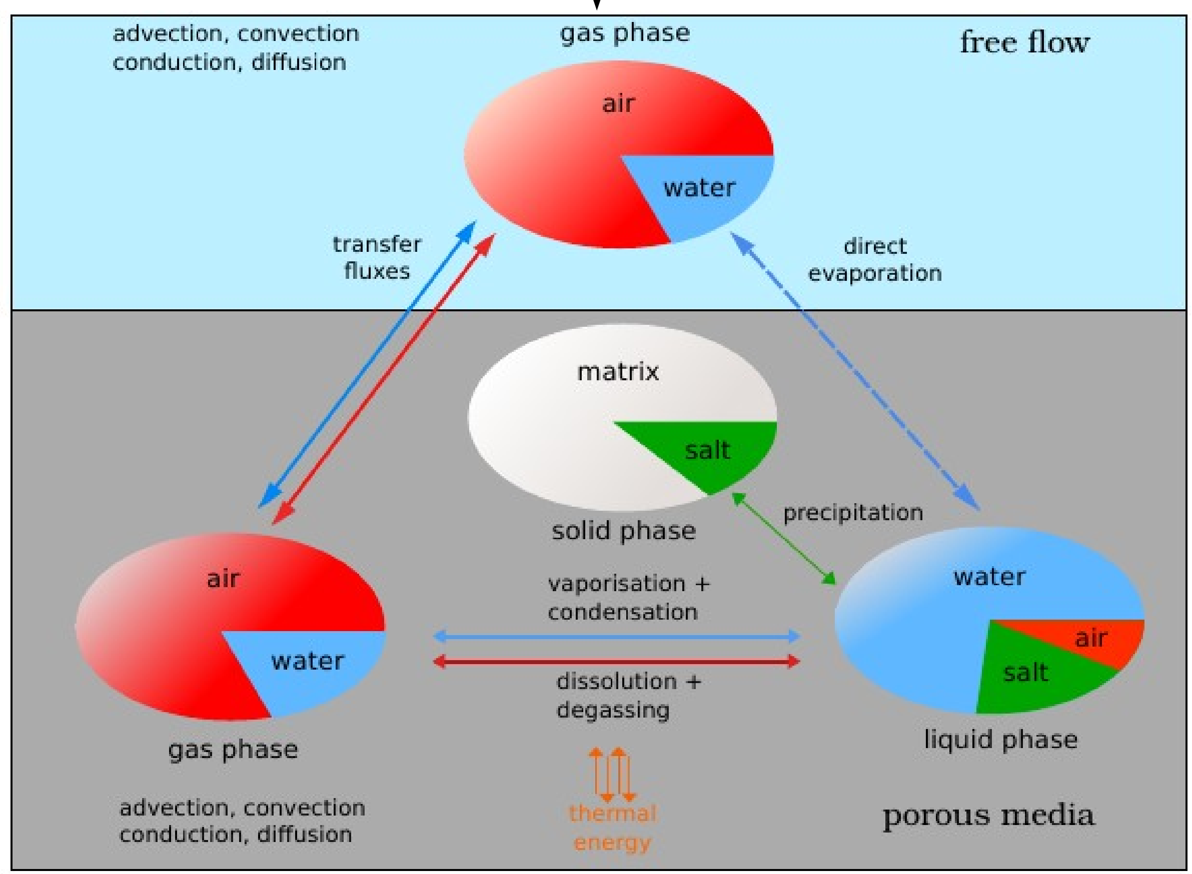
Macro-scale (REV)



Micro-scale to macro-scale transition

Model Concept





“A mathematical/numerical model requires an idealization of the physical processes in a natural system in such a way that their characteristic properties are maintained .”

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Porous-media Equations : (p_g, s_w, x_l^{NaCl})

- Multi-phase-multi-component Darcy flow
- Mass conservation for each component :

$$\sum_\alpha \underbrace{\frac{\partial(\phi \varrho_{mol,\alpha} S_\alpha x_\alpha^\kappa)}{\partial t}}_{\text{storage}} - \sum_\alpha \underbrace{\nabla. \left[\frac{k_{r\alpha}}{\mu_\alpha} \varrho_{mol,\alpha} x_\alpha^\kappa K (p_\alpha - \varrho_\alpha g)\right]}_{\text{advection}}$$

$$- \sum_\alpha \underbrace{\nabla. \left[D_{pm,\alpha}^\kappa \varrho_{mol,\alpha} \nabla x_\alpha^\kappa\right]}_{\text{diffusion}} = \sum_\alpha \underbrace{q_\alpha^\kappa}_{\text{source/sink}}$$

- Salt precipitation:

$$q_\alpha^\kappa = \begin{cases} \frac{\partial(\phi \varrho_{mol,l} S_l (x_l^{\text{NaCl}} - x_{l,max}^{\text{NaCl}}))}{\partial t} & \text{for } \kappa = \text{NaCl},\ \alpha = l \\ 0 & \text{else} \end{cases}$$

$$\frac{\partial(\phi_s^{\text{NaCl}} \varrho_{mol,s}^{\text{NaCl}})}{\partial t} + q_l^{\text{NaCl}} = 0$$

"Analytical solution to evaluate salt precipitation during CO2 injection in saline aquifers", *Zeidouni et al., 2009*

Porous-media Equations

- Local thermodynamic equilibrium:
  - Local thermal equilibrium:

$$T_l = T_g = T_s = T$$

  - Chemical equilibrium accounts for the mass transfer across different phases:

$$p_g = \sum_{\kappa} p_g^\kappa \qquad p_g^\kappa = x_g^\kappa p_{\mathrm{sat}}^\kappa \qquad p_g^\kappa = x_w^\kappa H_w^\kappa$$

  - Mechanical equilibrium is valid locally. Discontinuities in pressure exists across fluid-fluid-solid interface:

$$p_c = p_g - p_l$$

Porous-media Equations:(T)

– One energy balance equation:

$$\sum_\alpha \underbrace{\frac{\partial(\phi\varrho_\alpha u_\alpha S_\alpha)}{\partial t}}_{\text{storage I}} + \sum_\alpha \underbrace{\frac{\partial(\phi_s^{\mathrm{NaCl}}\varrho_s^{\mathrm{NaCl}}c_s^{\mathrm{NaCl}}T)}{\partial t}}_{\text{storage II}} + \sum_\alpha \underbrace{(1-\phi_0)\frac{\partial(\varrho_s c_s T)}{\partial t}}_{\text{storage III}}$$

$$+\sum_\alpha \underbrace{\nabla\cdot(\varrho_\alpha h_\alpha \mathbf{v}_\alpha)}_{\text{convection}} - \underbrace{\nabla\cdot(\lambda_{pm}T)}_{\text{conduction}} = 0$$

Where heat conductivity :

$$\lambda_{pm} = \lambda_{\mathrm{eff},g} + \sqrt{S_l}(\lambda_{\mathrm{eff},l} - \lambda_{\mathrm{eff},g})$$

Effective heat conductivity :

$$\frac{\lambda_{\mathrm{eff},\alpha}}{\lambda_\alpha} = \left(\frac{\lambda_s}{\lambda_\alpha}\right)^{0.28-0.757\log\phi-0.057\log(\lambda_s/\lambda_\alpha)}$$

“High Temperature Behaviour of rocks Associated with Geothermal Type Reservoirs”, *Somerton et al., 1974*

Porous-media Equations

Supplementary constraints:

- Total void-space within the porous matrix is occupied by liquid and gas phases:

$$\mathrm{S}_g = 1 - S_l$$

- The secondary phase pressure is determined using capillary-pressure:

$$\mathrm{p}_c(S_l) = p_g - p_l$$

- The mass and mole fractions of all components in each phase sums up to one:

$$\mathrm{X}_l^w + X_l^a + X_l^{\mathrm{NaCl}} = x_l^w + x_l^a + x_l^{\mathrm{NaCl}} = 1$$

Fluid Properties:

$$\mu_l = 0.1 + 0.333 X_l^{\mathrm{NaCl}} + (1.65 + 91.9 X_l^{\mathrm{NaCl}^3}) + exp\{-[0.42(X_l^{\mathrm{NaCl}^{0.8}} - 0.17)^2 + 0.045] T^{0.8}\}$$

$$\varrho_l = \varrho_w + 1000 X_l^{\mathrm{NaCl}}\{0.668 + 0.44 X_l^{\mathrm{NaCl}} + [300p - 2400 p X_l^{\mathrm{NaCl}}$$
$$+ T(80 + 3T - 3300 X_l^{\mathrm{NaCl}} - 13p + 47 p X_l^{\mathrm{NaCl}})] \times 10^{-6}\}$$

Free-flow Equations: (v_x, v_y, P_g, T, x_g^w)

- Stokes equation: (no turbulence - 1Phase)

$$\underbrace{\frac{\partial(\varrho_g \mathbf{v}_g)}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot \left[p_g \mathbf{I} - \mu_g(\nabla \mathbf{v}_g + \nabla \mathbf{v}_g^T)\right]}_{\text{flux}} = \underbrace{\varrho_g \mathbf{g}}_{\text{body force}}$$

- Phase conservation:

$$\underbrace{\frac{\partial \varrho_g}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot (\varrho_g v_g)}_{\text{advection}} = \underbrace{q_g}_{\text{source/sink}}$$

- Component conservation

$$\underbrace{\frac{\partial(\varrho_{mol,g} x_g^\kappa)}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot \left(\varrho_{mol,g} x_g^\kappa v_g\right)}_{\text{advection}} - \underbrace{\nabla \cdot \left(D_{pm,g}^\kappa \varrho_{mol,g} \nabla x_g^\kappa\right)}_{\text{diffusion}} = \underbrace{q_g^\kappa}_{\text{source/sink}}$$

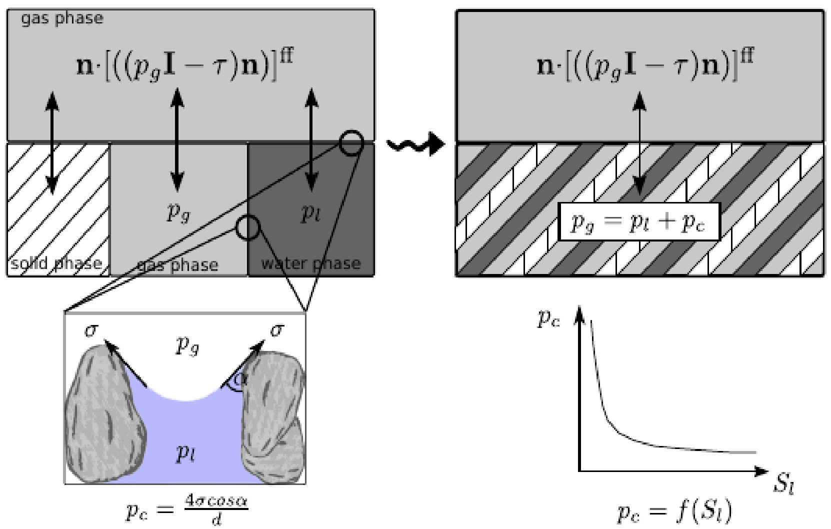
- Energy balance equation:

$$\underbrace{\frac{\partial(\varrho_g u_g)}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot (\varrho_g h_g \mathbf{v}_g)}_{\text{convection}} - \underbrace{\nabla \cdot (\lambda_g \nabla T)}_{\text{conduction}} = \underbrace{q_T}_{\text{source/sink}}$$

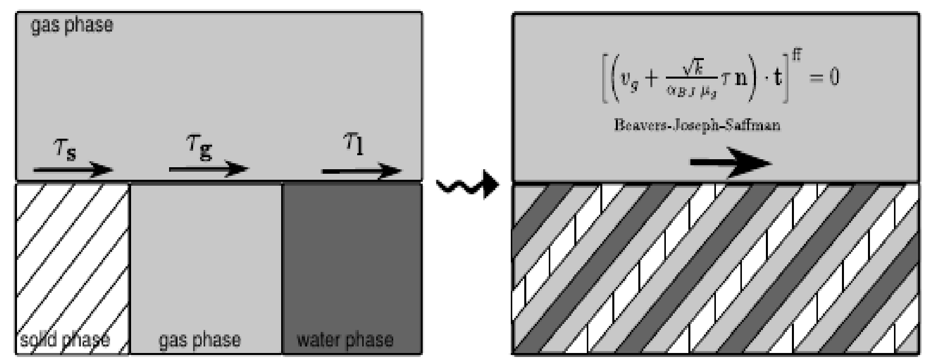
Coupling at the ff-pm interface

– Mechanical equilibrium:

Normal



Tangential

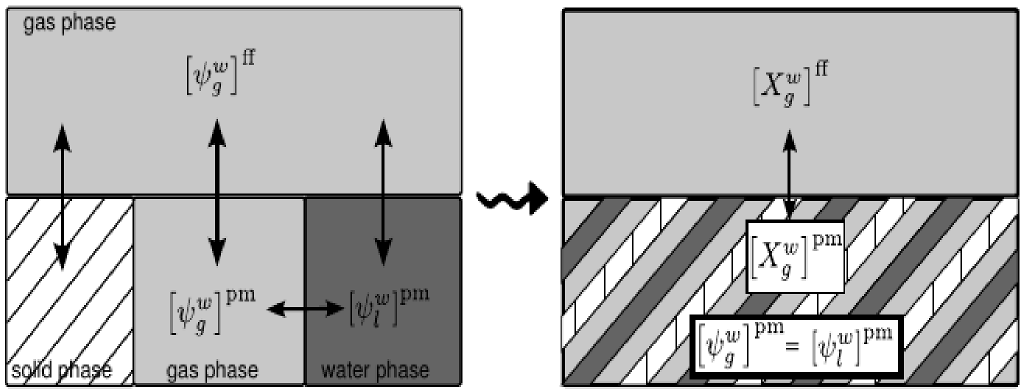


– Continuity of phase and component fluxes:

$$\underbrace{[\varrho_g \mathbf{v}_g \cdot \mathbf{n}]^{ff}}_{\text{Gas flux}} = -\underbrace{[(\varrho_g \mathbf{v}_g + \varrho_l \mathbf{v}_l)\cdot \mathbf{n}]^{pm}}_{\text{Total mass flux}}$$

Coupling at the ff-pm interface

– Chemical equilibrium:



- Continuity of chemical potential between phases inside the porous medium
- Continuity of mass or mole fraction at the interface

– Thermal equilibrium:

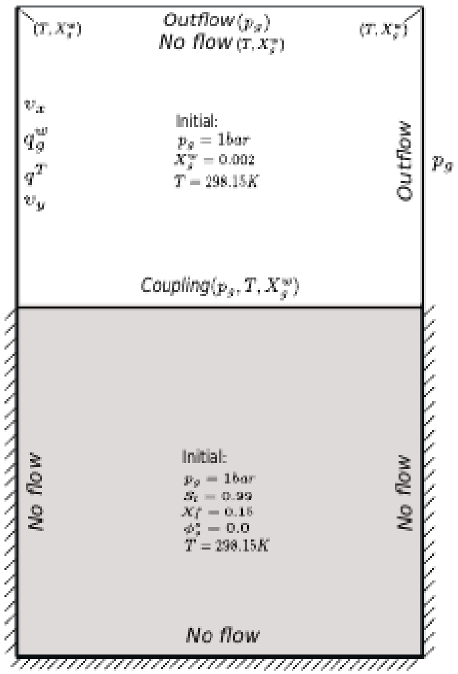
- local thermal equilibrium:

$$[T]^{ff} = [T]^{pm}$$

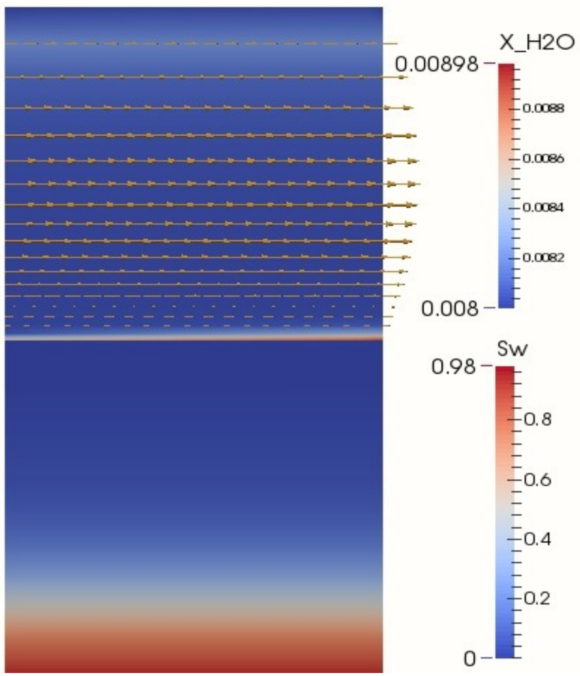
- Continuity of heat flux:

$$\underbrace{[(\varrho_g h_g \mathbf{v}_g - \lambda_g \nabla T) \cdot \mathbf{n}]^{ff}}_{\text{heat flux gas phase}} = \underbrace{-[(\varrho_g h_g \mathbf{v}_g + \varrho_l h_l \mathbf{v}_l - \lambda_{pm} \nabla T) \cdot \mathbf{n}]^{pm}}_{\text{Total heat flux}}$$

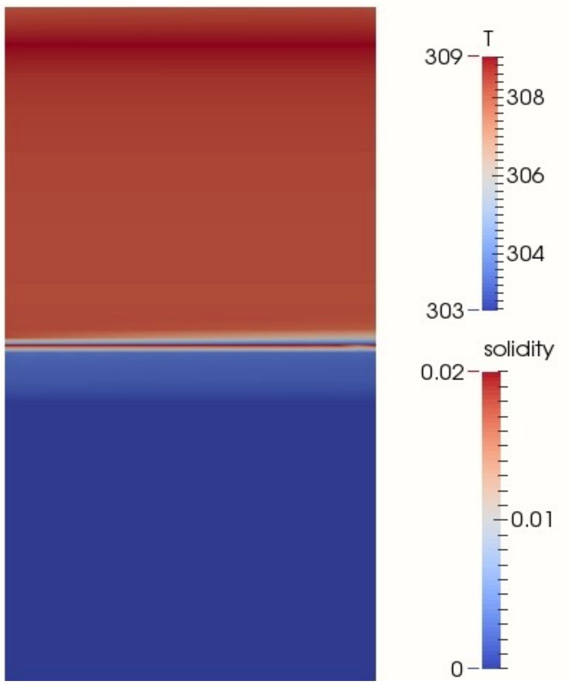
Mulit-domain: Coupled problem



Numerical example

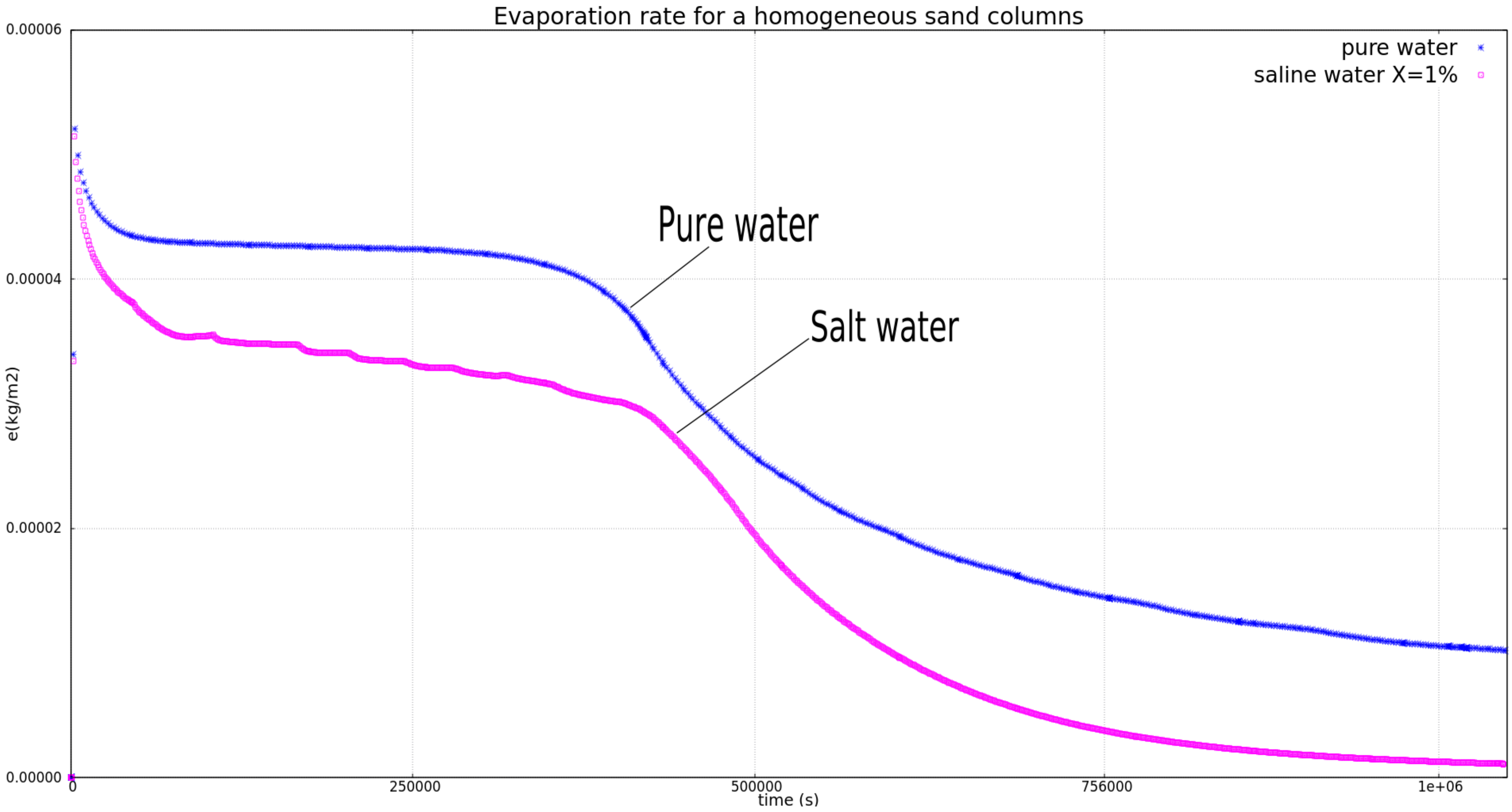


Drying



Salinization

Effect of salt: Case II



- Osmotic potential combined with pore clogging reduce vapour pressure

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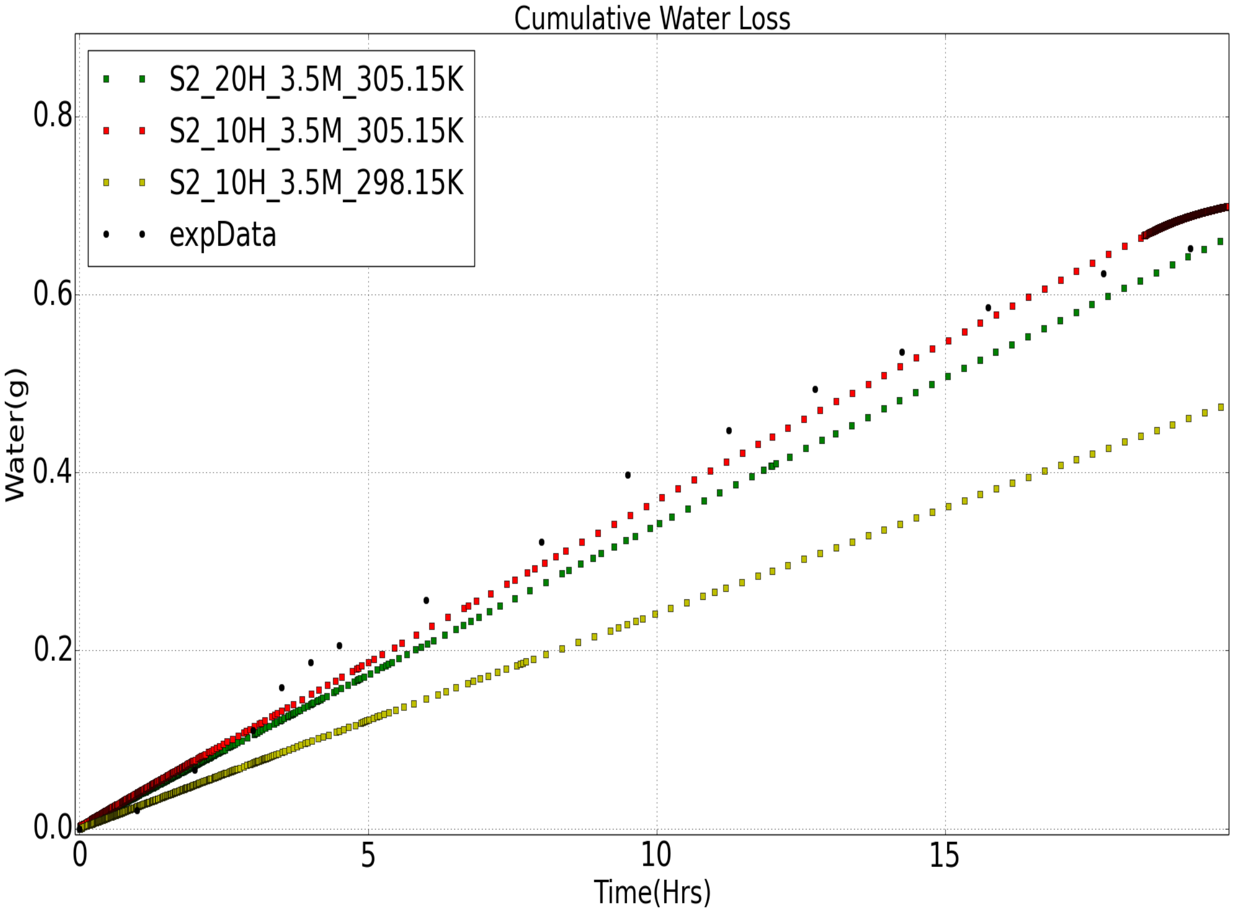
Validation



$$K = 2.65e-10[m^2]$$

$$\phi = 0.37$$

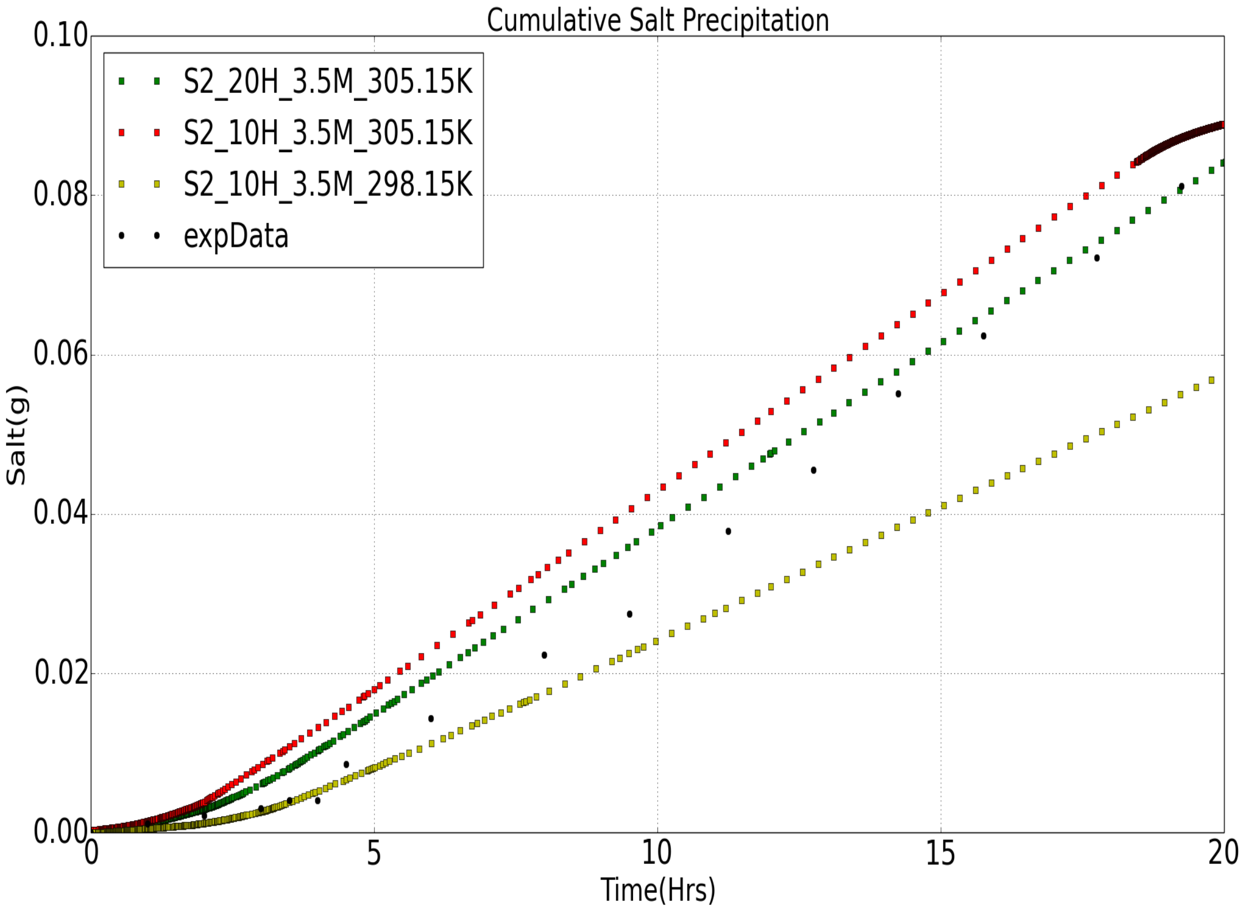
$$\alpha_{vg} = 6.02371e-4$$

$$n_{vg} = 12.18$$

$$X_w^{NaCl} = 0.20454(3.5M)$$

"Pore-scale dynamics of salt precipitation in drying porous media", Rad *et al., 2013*

Validation



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Conclusion

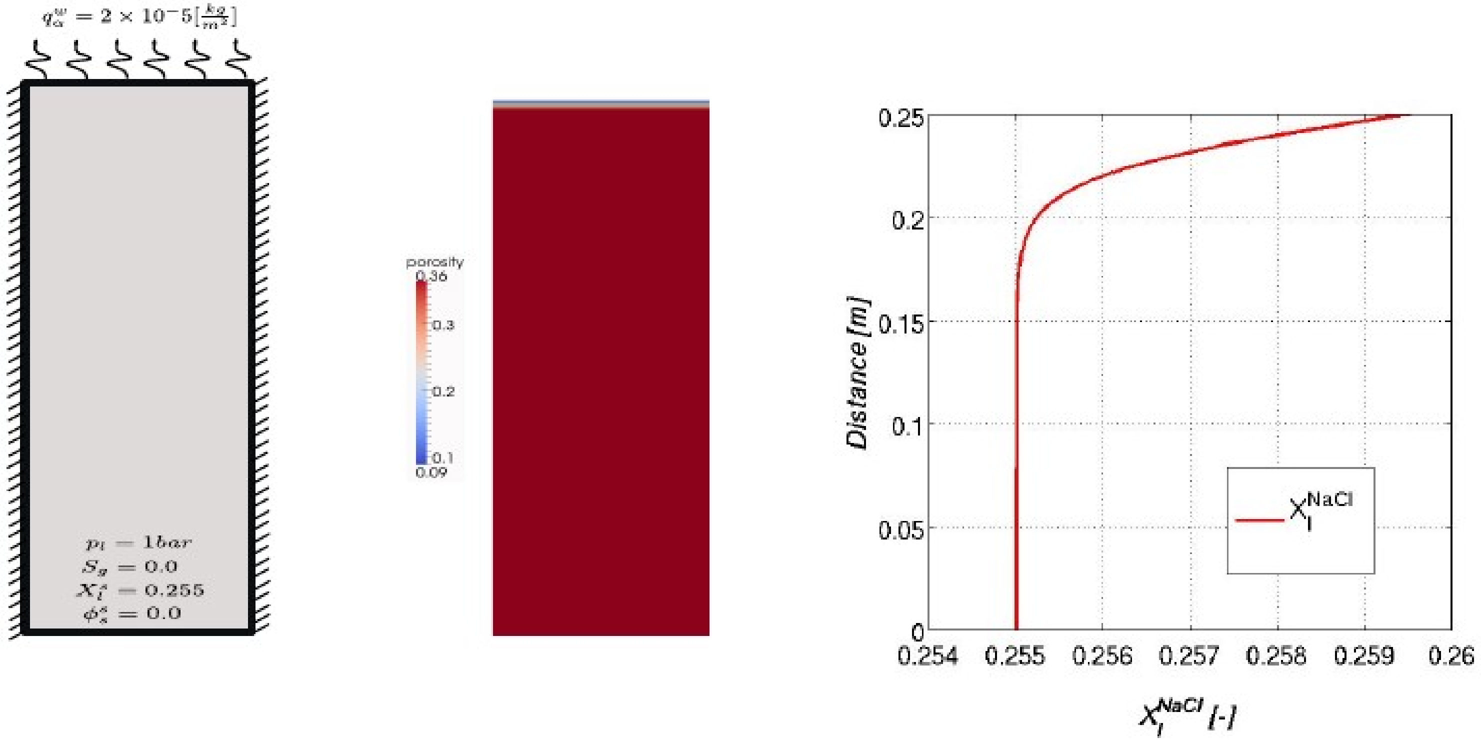
- The model is capable to predict evaporation dynamics for non-saline, saline and hyper-saline scenarios.
- One can analyse the influence of variation in free-flow and porous-media parameters on evaporation dynamics and salinization.
- Validation cases clearly shows that the numerical simulations are in good agreement with the experimental data.

Outlook

Future Work:

- Reactive precipitation approach (under testing)
- Precipitation analysis for different salts (e.g. NaCl and NaI)
- Parameter analysis for free-flow and porous media
- Effect of random heterogeneities

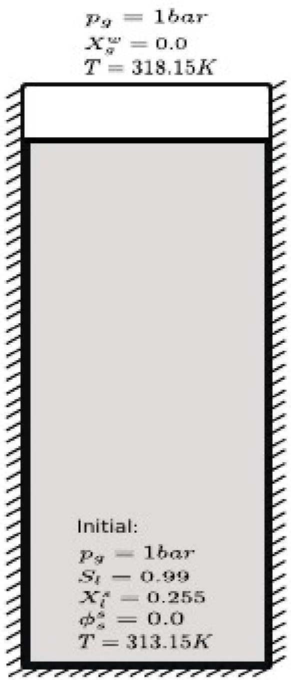
Single-domain PM problem: Case I

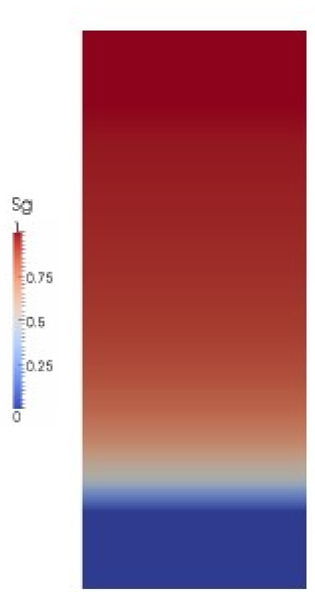


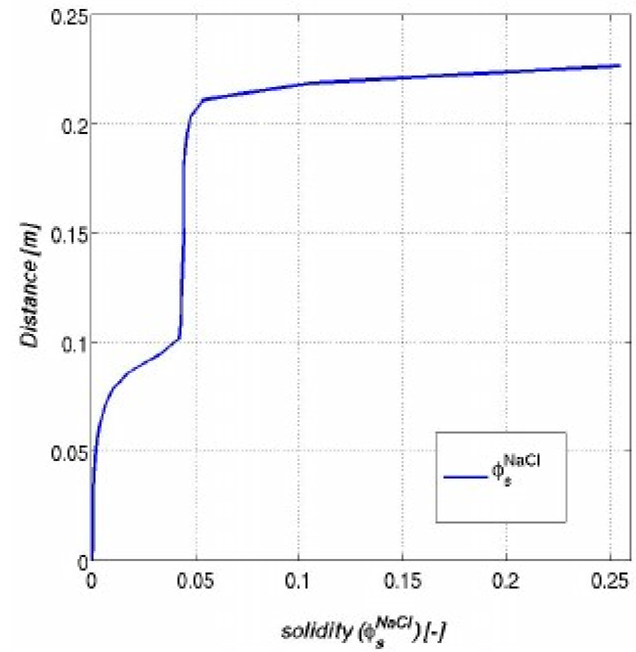
Dissolved NaCl distribution in a fully saturated homogeneous sand column

- Dirichlet BC at the bottom ensures the domain to be fully saturated.
- Fixed flux BC on top.

Single-domain PM problem: Case II



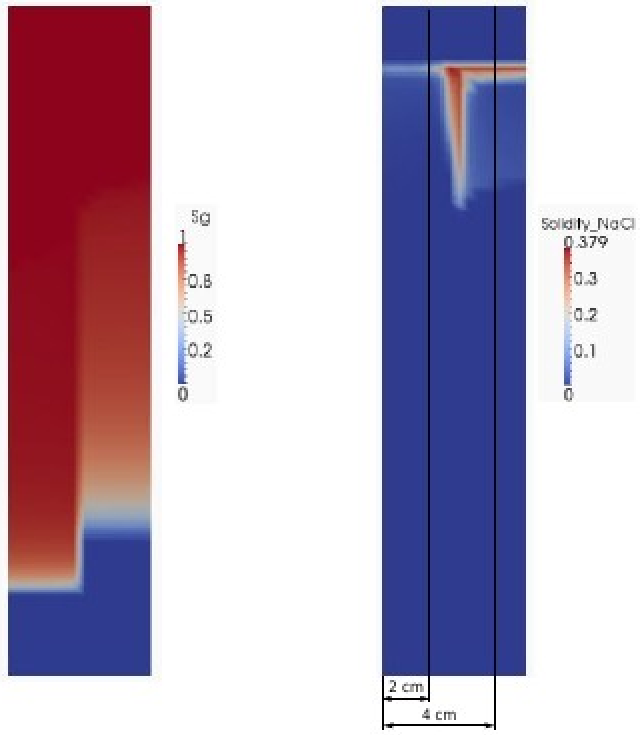




Evaporation driven NaCl precipitation in an unsaturated homogeneous sand column

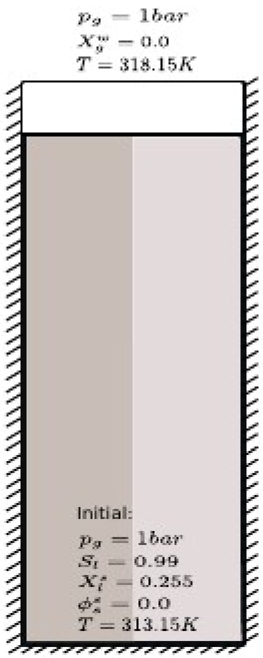
- No flow BC allows the domain to dry out with evaporation.
- Far-filed dirichlet BC are used at top boundary.

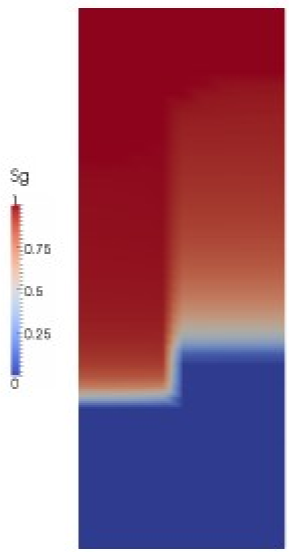
Single-domain PM problem: Case III

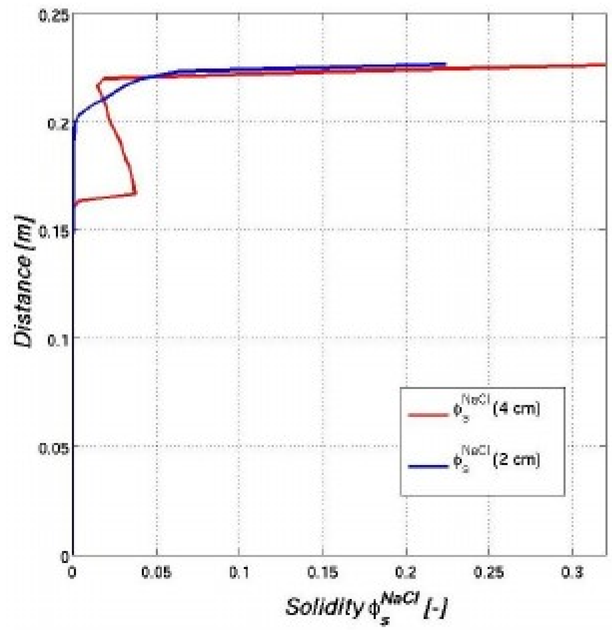


Movie: Evaporation driven NaCl precipitation in an unsaturated heterogeneous sand column

Single-domain PM problem: Case III

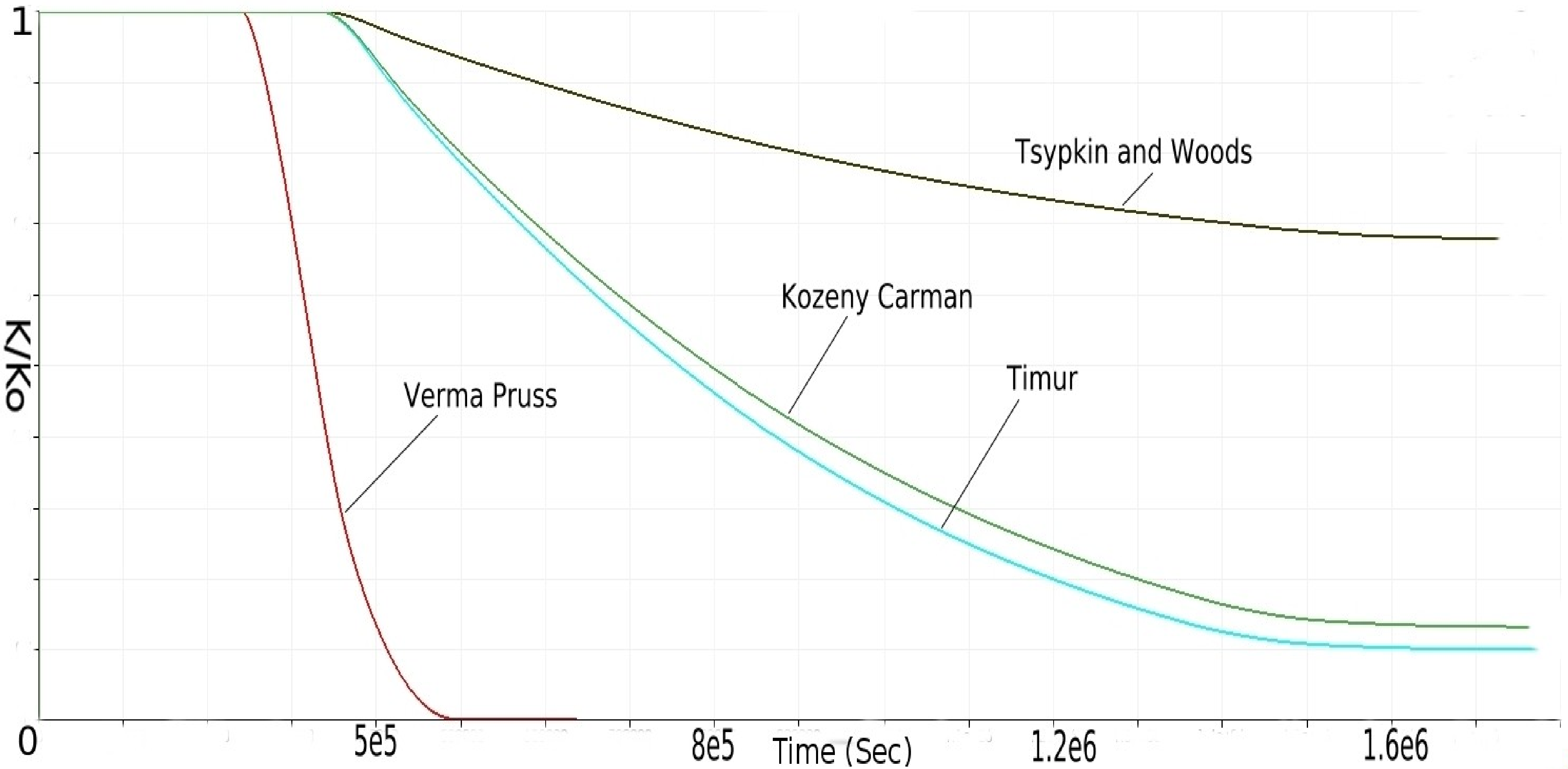






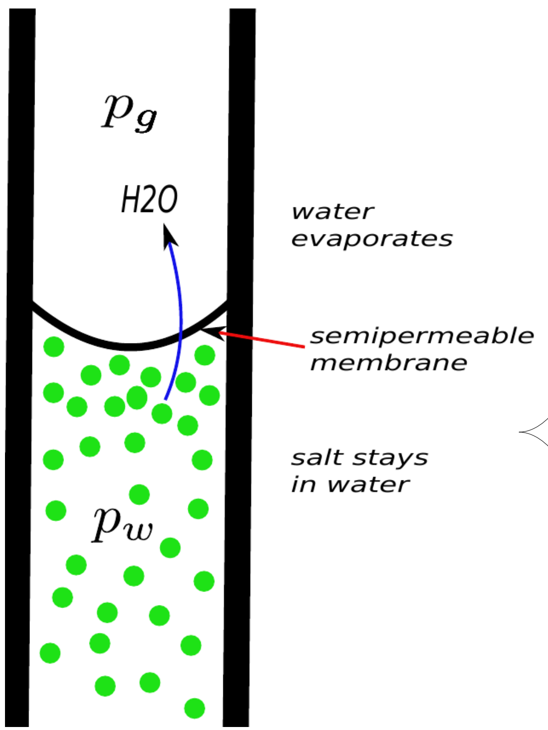
Evaporation driven NaCl precipitation in an unsaturated heterogeneous sand column

Single-domain PM problem: Case IV



- Different models need to be validated against the experimental data.
- For further calculations Kozeny-Carman relationship is used.

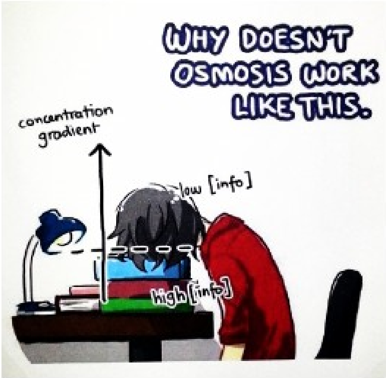
Osmotic potential & Vapour pressure



- Water-gas interface acts as a semi-permeable membrane
- Chemical equilibrium needed

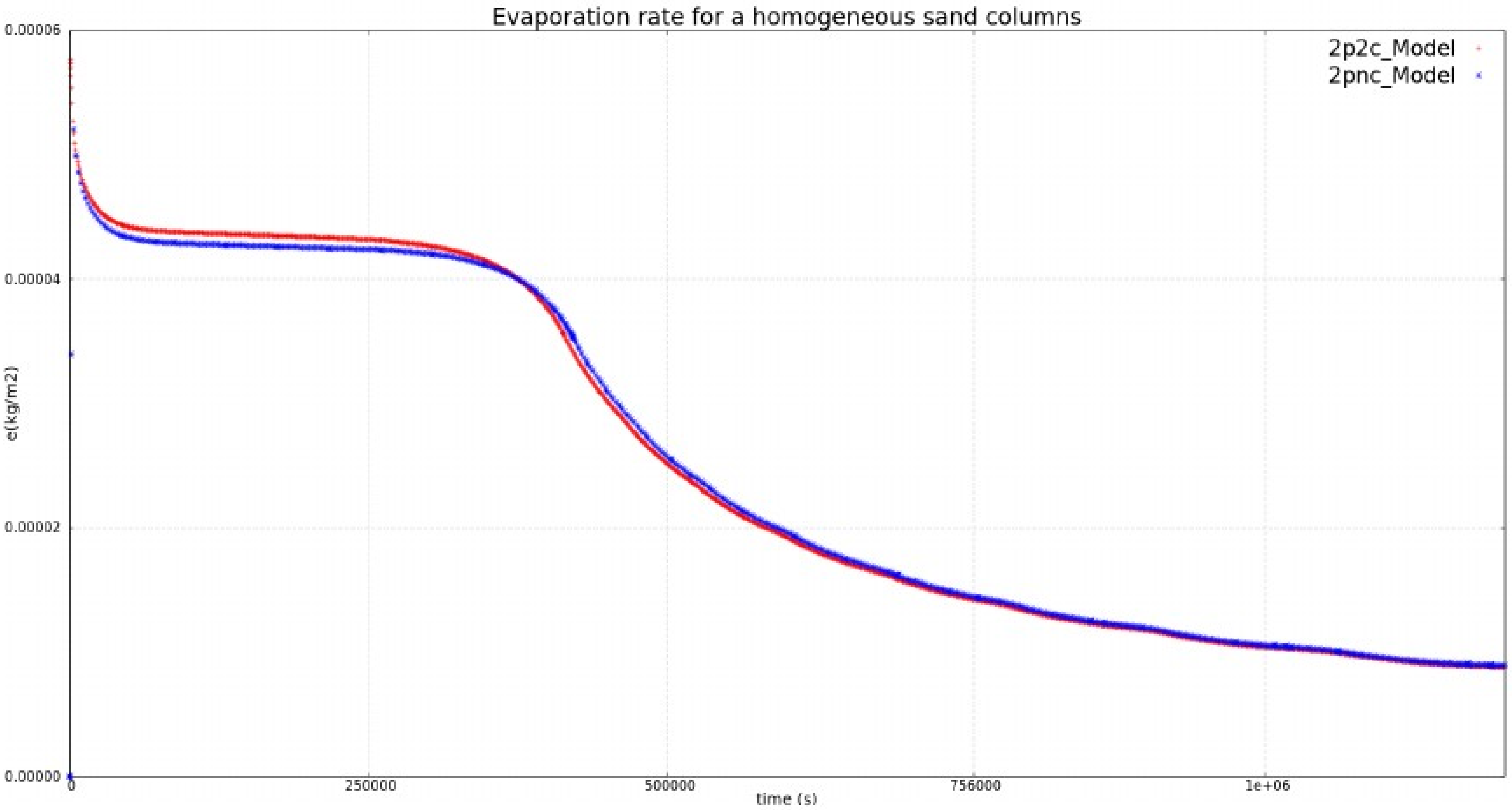
$$\psi_w(T, p_l, x_l^{NaCl}) = \psi_g(T, p_g, x_g^{NaCl} = 0)$$

$$f_l^{H2O} = f_g^{H2O} \Longrightarrow p_{sat}\, x_l^{H2O} = p_g x_g^{H2O}$$



“Osmotically Driven Water Vapour transport in Unsaturated Soils”, Kelly et.al., 2001

Evaporation: Pure water



- Comparison for pure water evaporation with the model presented by Mosthaf et.al (2011).