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A coupled multi-domain approach for soil salinization

Vishal Jambhekar

Karen Schmid, Rainer Helmig

Department of Hydromechanics and Hydrosystemmodeling

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Wageningen University
Universiteit Utrecht
Universitetet i Bergen
Universität Stuttgart
TU Delft
Delft University of Technology
TU/e Technische Universiteit Eindhoven University of Technology

Overview

- Motivation
- Model Concept
- Results
- Outlook

Motivation

Qatar desert

Punjab, India

Jammu and Kashmir, India

Motivation

Soil salinization problem across the world

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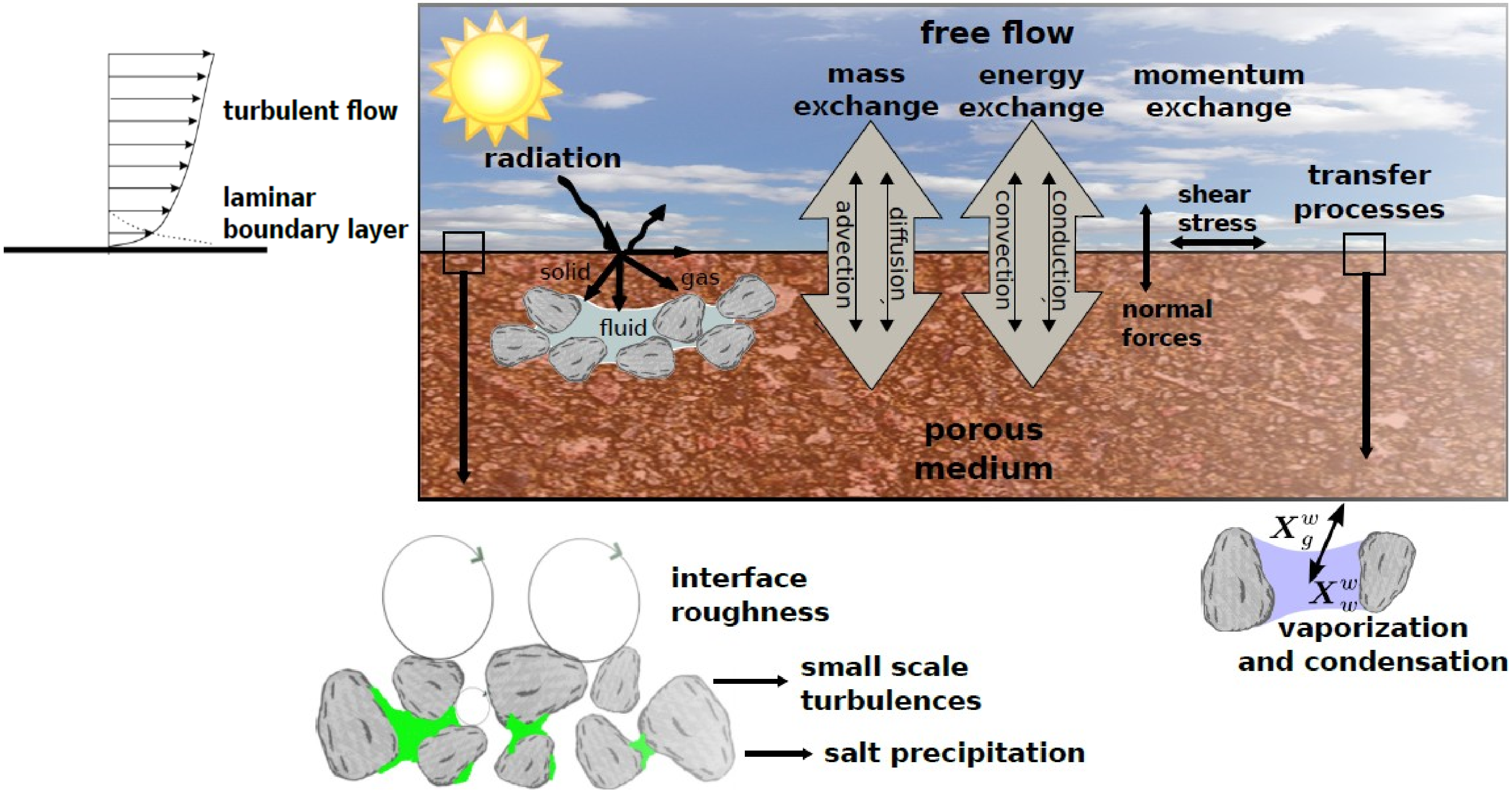
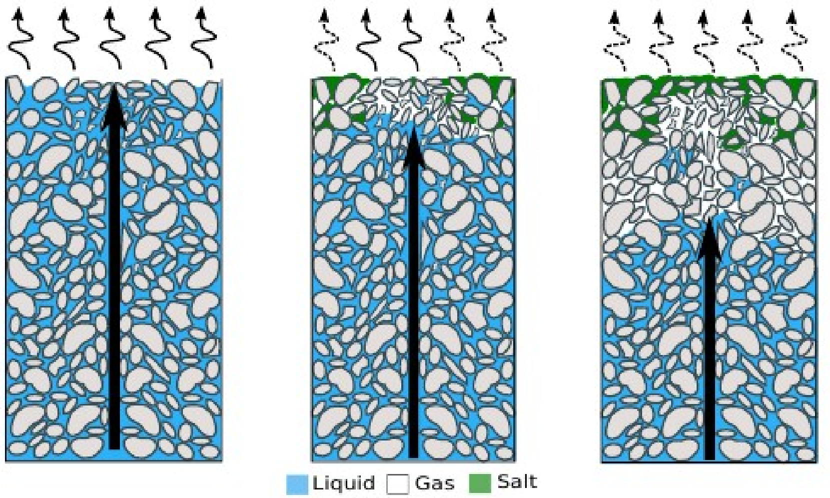
Motivation

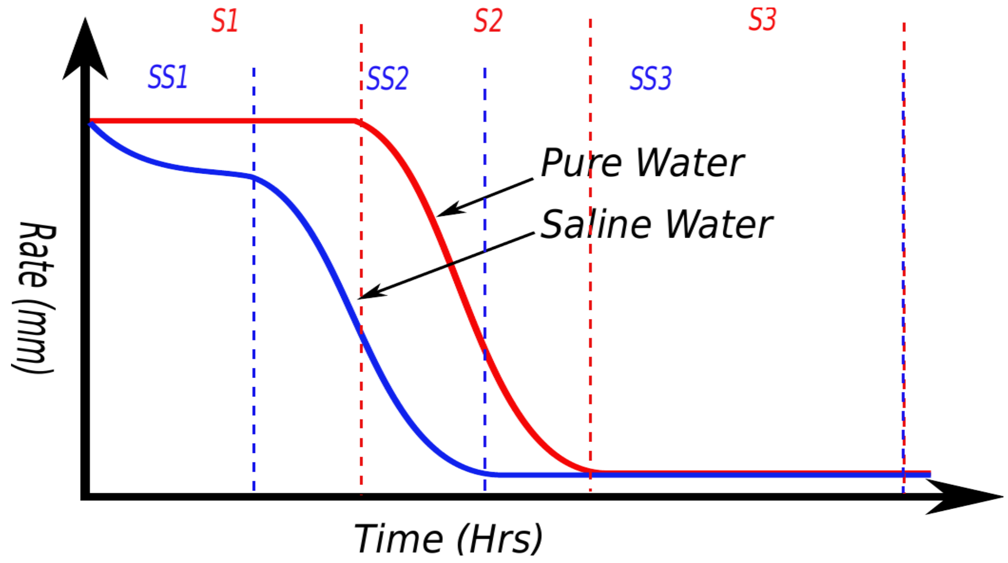


“A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow”, *Mosthaf et al., 2011*

Stages of saline water evaporation



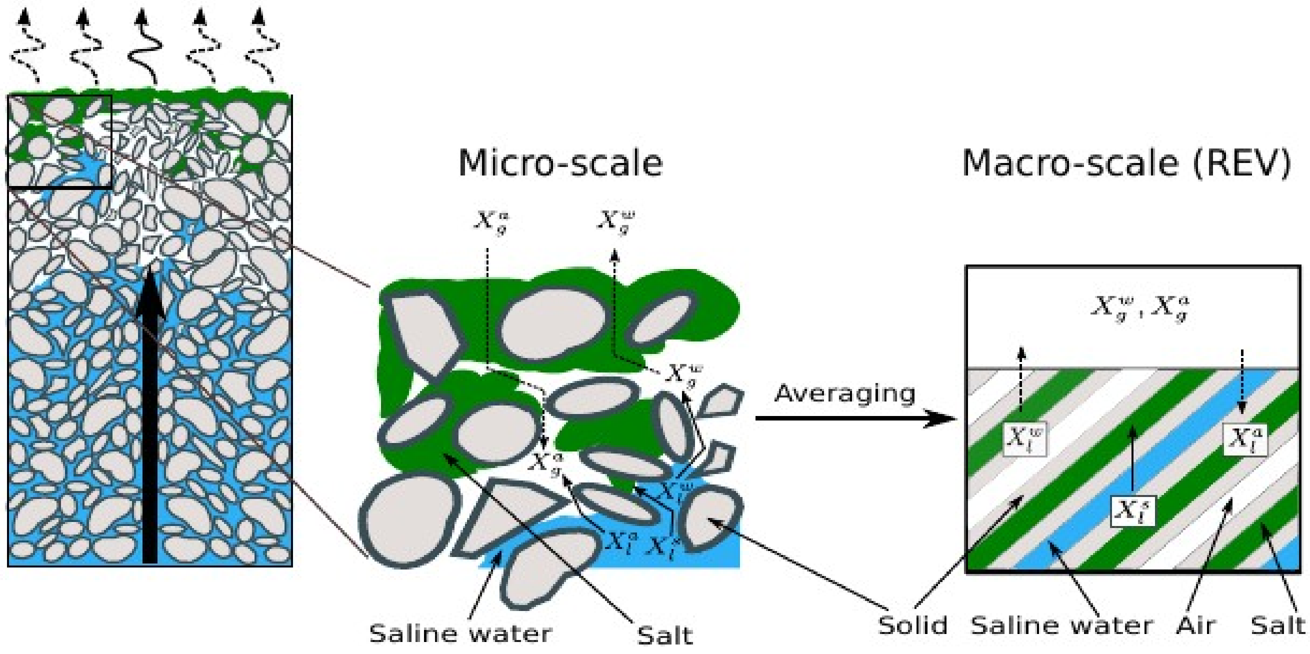
(a) SS1 (b) SS2 (c) SS3



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

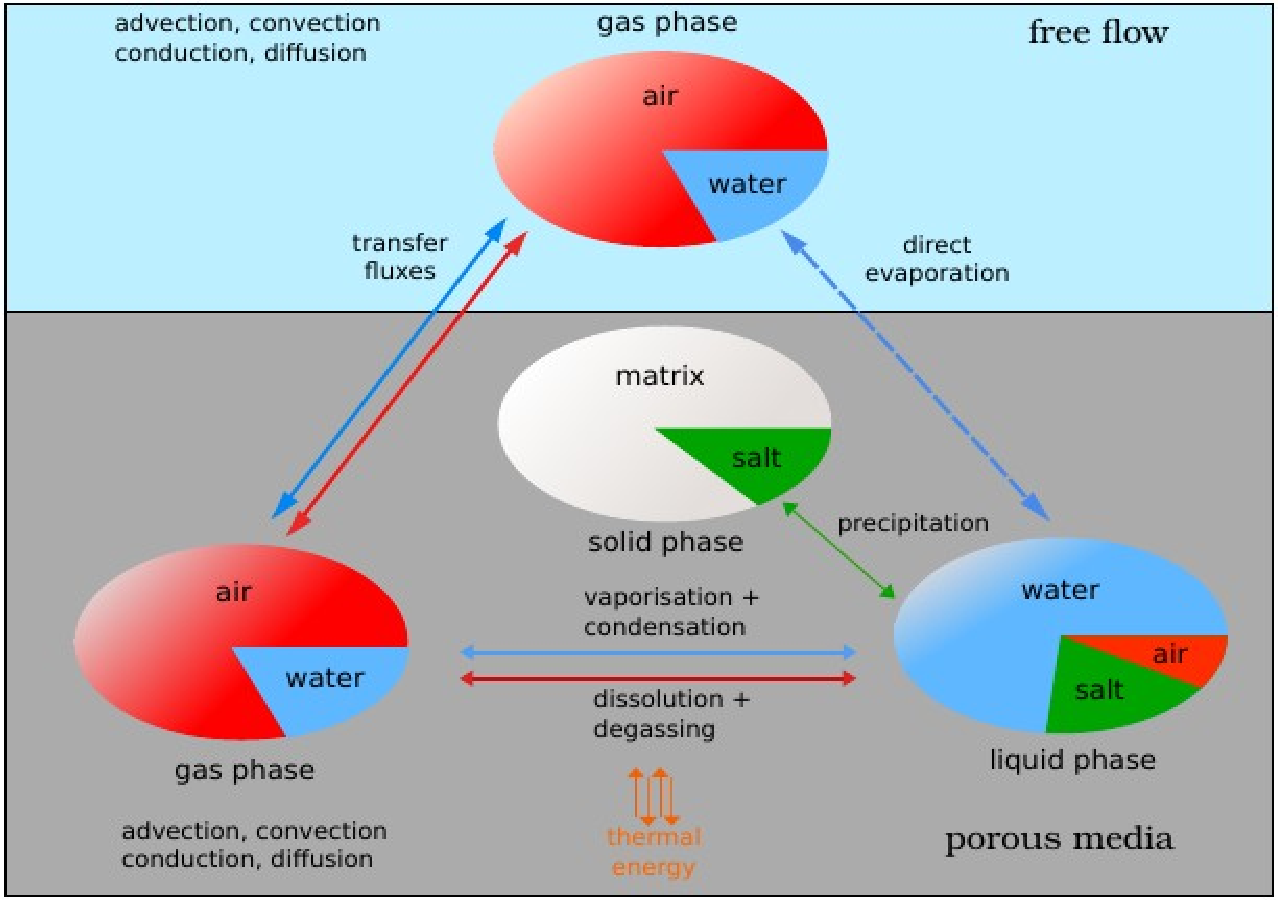
Salinization: Interplay between salt transport, evaporation dynamics and salt precipitation

Macro-scale (REV)



Micro-scale to macro-scale transition

Model Concept



Objectives

Developent of the model concept:

- Three-phase-n-component model for porous media flow
- Description of dissolved salt transport and precipitation
- Changes in the porous media properties
- Accounting for osmosis
- Single-phase-n-component model for free-flow
- Free-flow-porous-meida interaction physics
- Comparitive studies for effects of atmospheric processes and porous media properties

Porous-media Equations : ($p_{g,}$ $s_{w,}$ x_l^{NaCl})

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

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

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

- Salt precipitation:

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

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

Porous-media Equations: (Φ, K)

– Conservation of precipitated salt:

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

– Porosity change:

$$\phi = \phi_0 - \phi_s^{NaCl}$$

– Porosity-permeability relations:

- Kozeny-Carman

$$\frac{K}{K_0} = \left(\frac{\phi}{\phi_0}\right)^3 \left(\frac{1-\phi_0}{1-\phi}\right)^2$$

- Verma-Pruess

$$\frac{K}{K_0} = \left(\frac{\phi - 0.9\phi_0}{\phi_0 - 0.9\phi_0}\right)^2$$

- Tsypkin-Woods

$$\frac{K}{K_0} = \frac{1 - e^{(\omega\phi(1-(\phi_s^{NaCl})))}}{1 - e^{(\omega\phi)}}$$

- Timur

$$K = 0.136\phi^{4.4} S_w^2$$

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:

$$p_g = \sum_\kappa p_g^\kappa \qquad p_g^\kappa = x_g^\kappa p_{\text{sat}}^\kappa \qquad p_g^\kappa = x_w^\kappa H_w^\kappa \qquad f_l^\kappa = f_g^\kappa$$

  - 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:

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

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

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 Behavior of rocks Associated with Geothermal Type Reservoirs”, *Somerton et al., 1974*

Porous-media Equations: (S_g, P_w, x^k_α)

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 sum of mole fractions of all components in each phase is one:

$$\mathrm{x}_\alpha^w + x_\alpha^a + x_\alpha^{\mathrm{NaCl}} = 1$$

- The fugacity for each component is equal each phase:

$$f_l^\kappa = f_g^\kappa$$

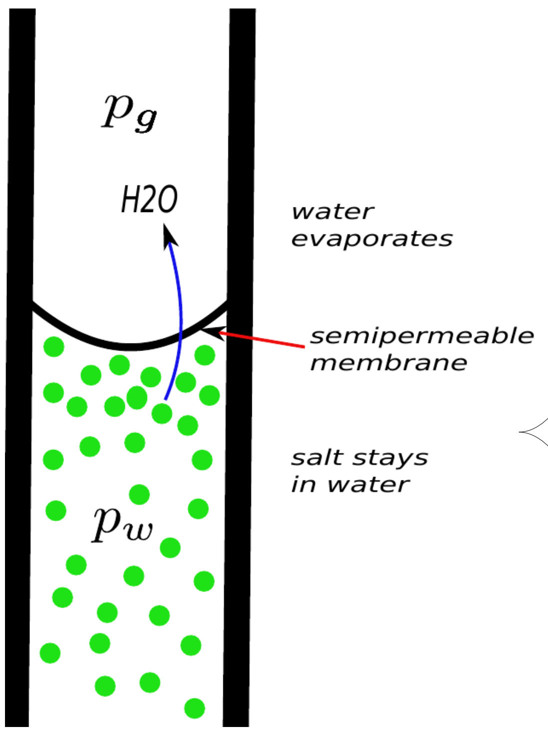
Fluid Properties:

$$\varrho_g(p_g, T) \qquad \mu_l(p_l, T, X_l^{NaCl}) \qquad \varrho_l(p_l, T, X_l^{NaCl})$$

$$h_g(p_g, T) \qquad h_l(p_l, T, X_l^{NaCl}, h_{NaCl})$$

Batzle, M. L. and Wang, Z. (1992). Seismic properties of pore fluids. Geophysics, 57:1396–1408.

Osmosis: Effect on vapour Pressure



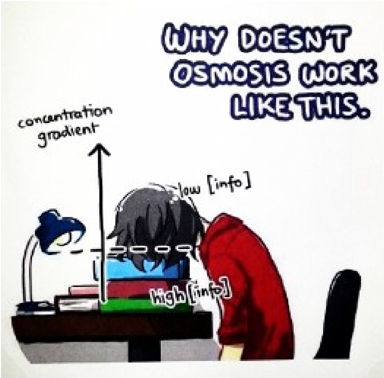
- Water-gas interface acts as a semipermeable membrane.
- Chemical equilibrium needed

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

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

$$p_{sat} = \bar{p}_{sat} \exp\left(\frac{\pi \overline{V}_w}{\mathrm{RT}}\right)$$

$$\pi = \frac{\mathrm{RT}\ \ln x_A}{\overline{V}_w}$$



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

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

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

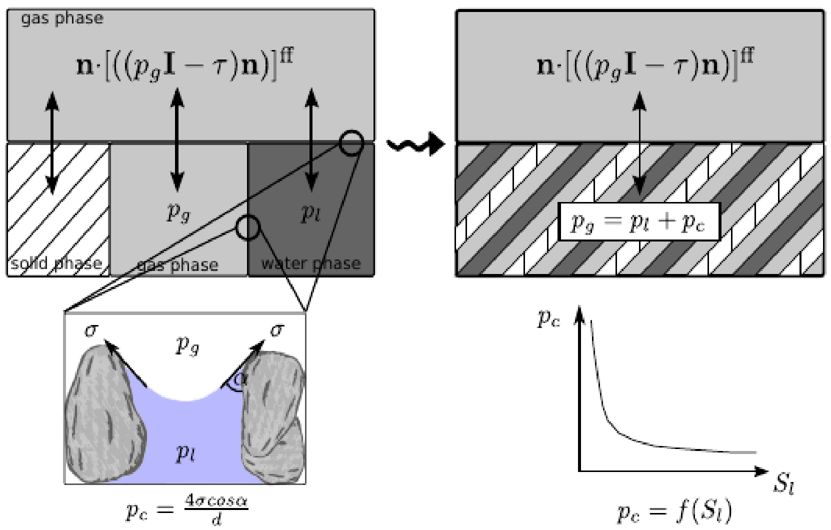
- Energy balance equation:

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

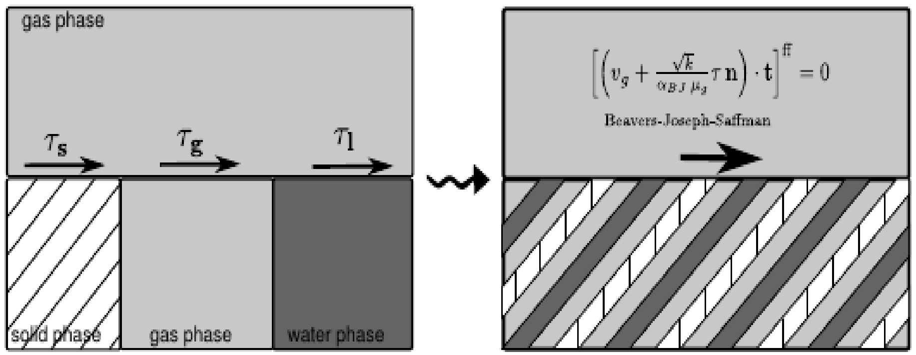
Interface

– Mechanical equilibrium:

Normal



Tangential



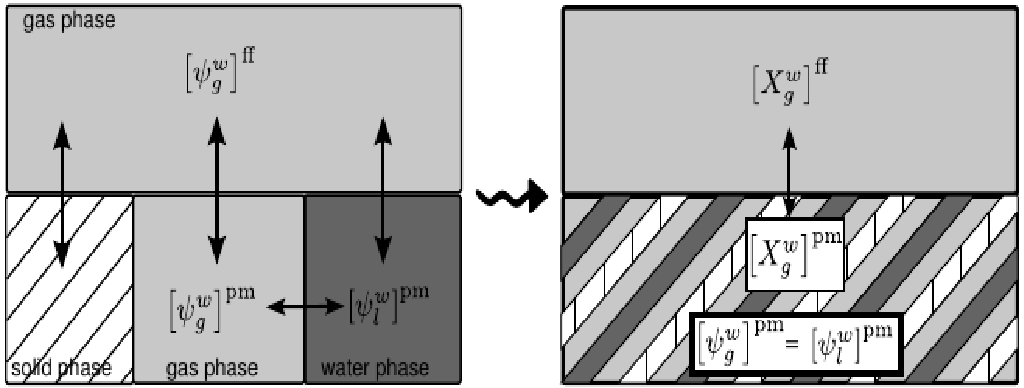
– Continuity of phase and componemt fluxes:

$$[\varrho_g \mathbf{v}_g \cdot \mathbf{n}]^{ff} = -[(\varrho_g \mathbf{v}_g + \varrho_l \mathbf{v}_l) \cdot \mathbf{n}]^{pm}$$

$$[(\varrho_{mol,g} \mathbf{v}_g x_g^k - D_g \varrho_{mol,g} \nabla x_g^k) \cdot \mathbf{n}]^{ff} = -[(\varrho_{mol,g} \mathbf{v}_g x_g^k - D_{g,pm} \varrho_{mol,g} \nabla x_g^k + \varrho_{mol,l} \mathbf{v}_l x_l^k - D_{l,pm} \varrho_{mol,l} \nabla x_l^k) \cdot \mathbf{n}]^{pm}$$

Interface

– Chemical equilibrium:



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

– Thermal equilibrium:

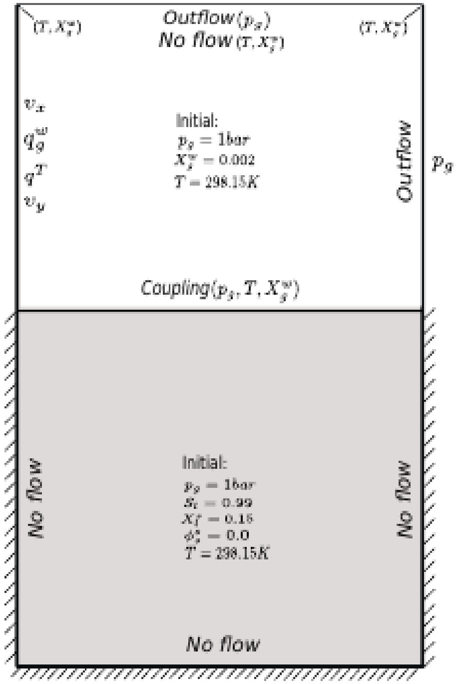
- local thermal equilibrium:

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

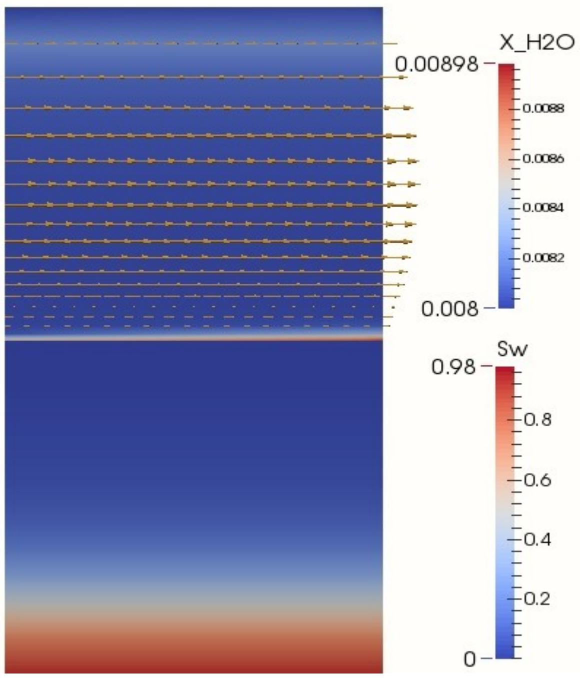
- Continuity of heat flux:

$$[(\varrho_g h_g \mathbf{v}_g - \lambda_g \nabla T) \cdot \mathbf{n}]^{ff} = -[(\varrho_g h_g \mathbf{v}_g + \varrho_l h_l \mathbf{v}_l - \lambda_{pm} \nabla T) \cdot \mathbf{n}]^{pm}$$

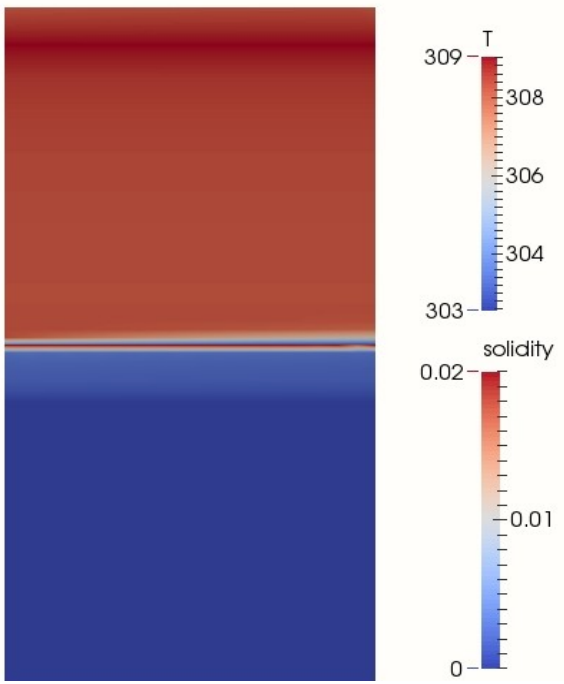
Mulit-domain problem



Numerical example



Drying



Salinization

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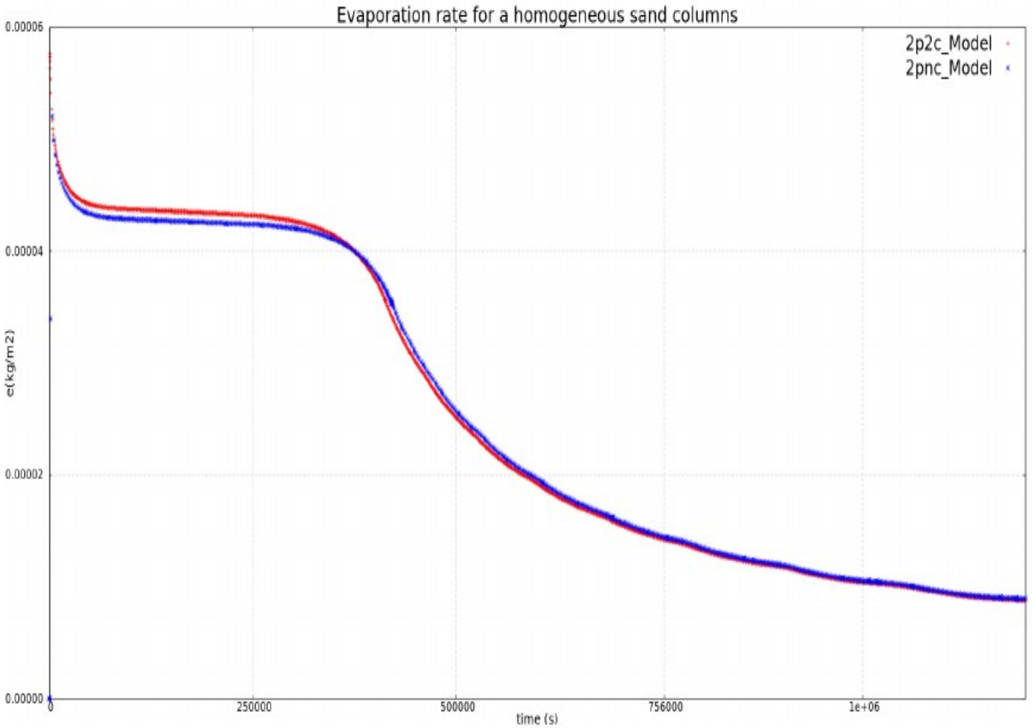
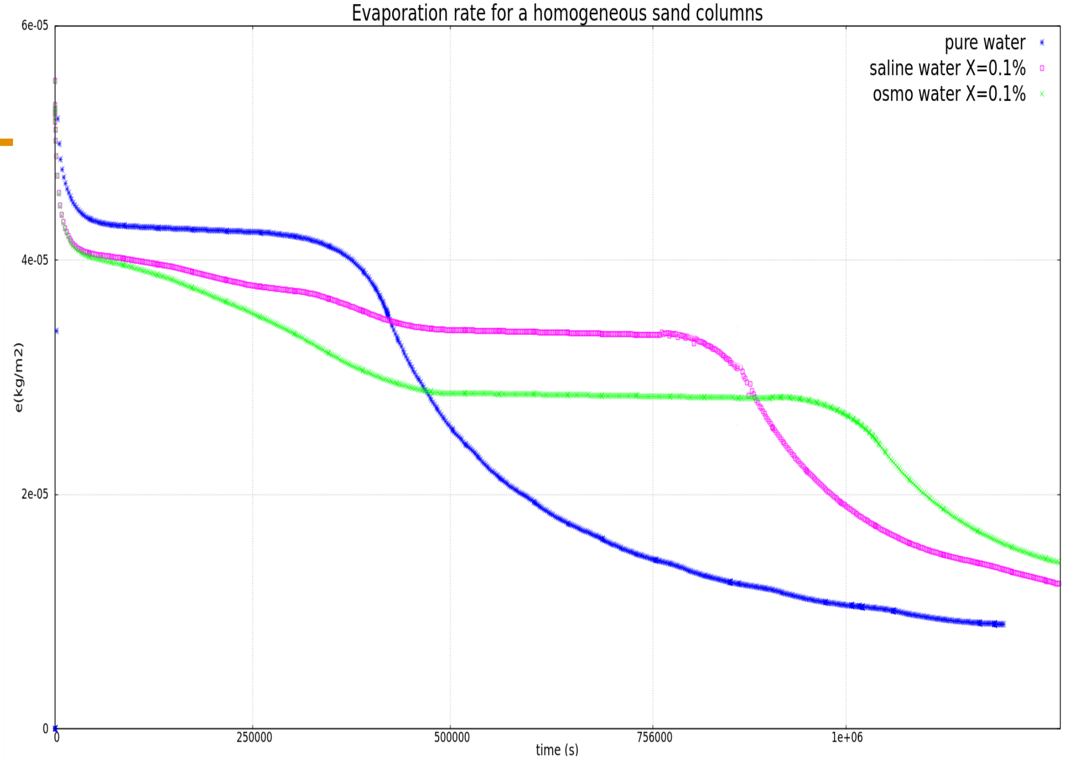
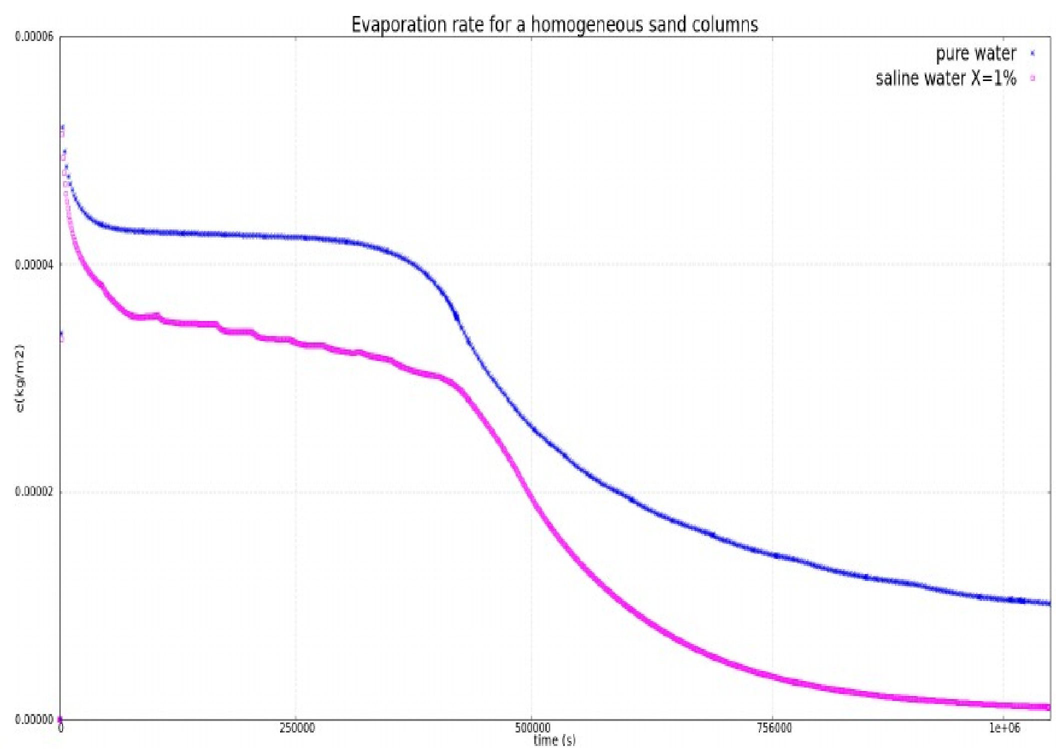
Evaporation rates







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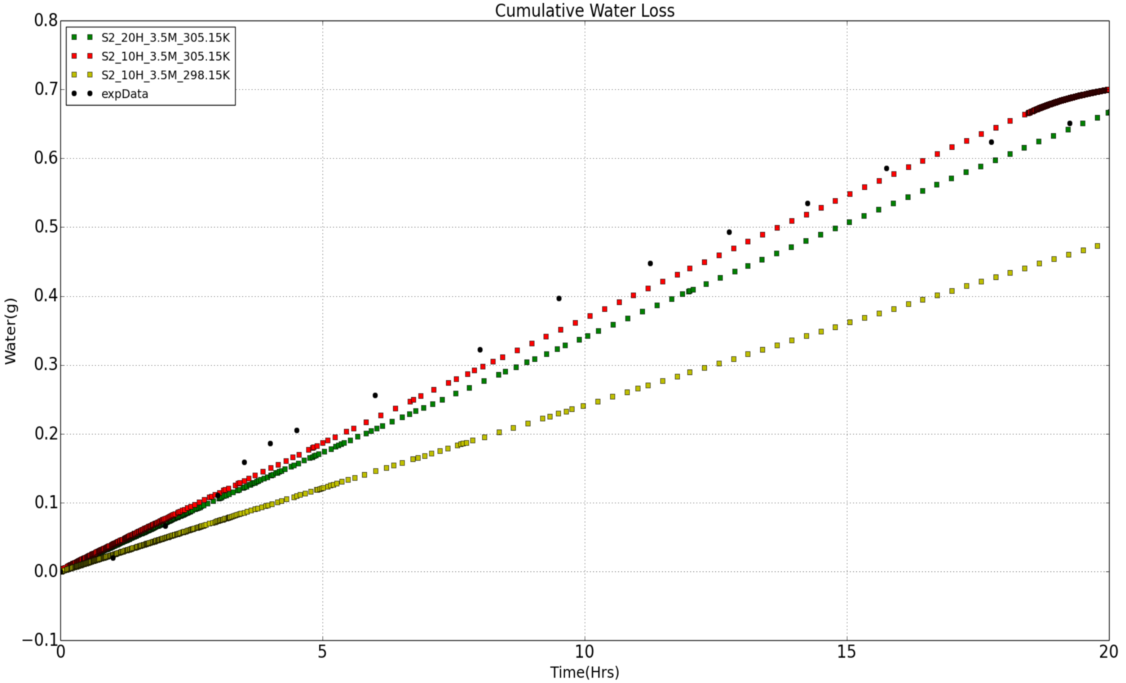
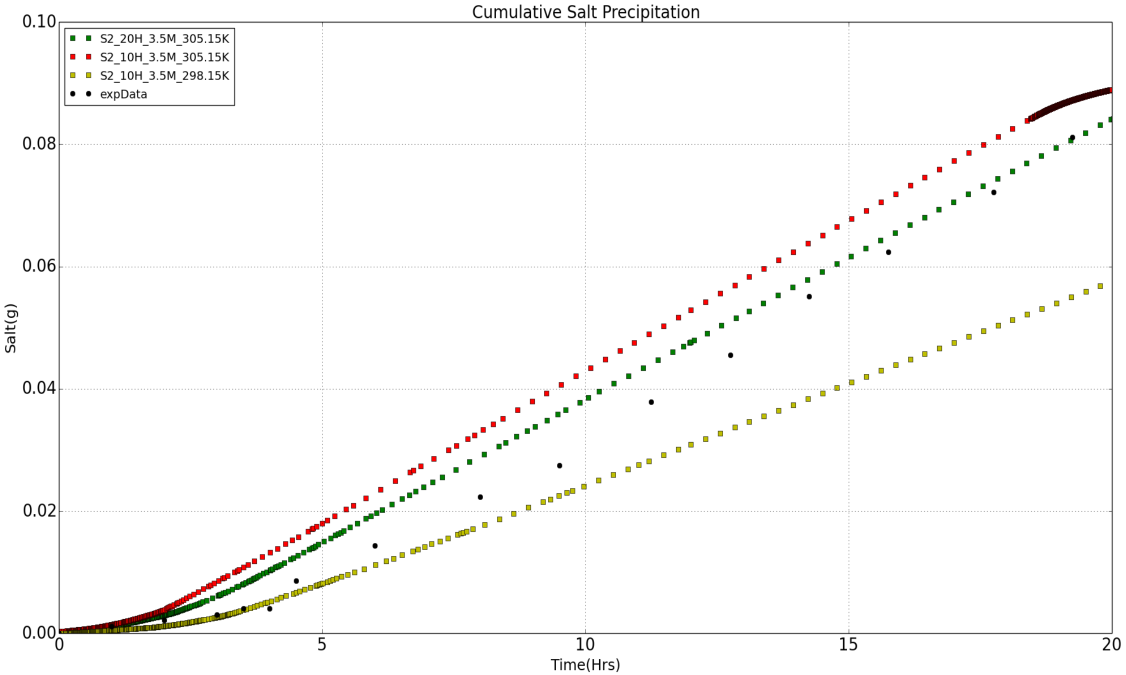
Validation





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

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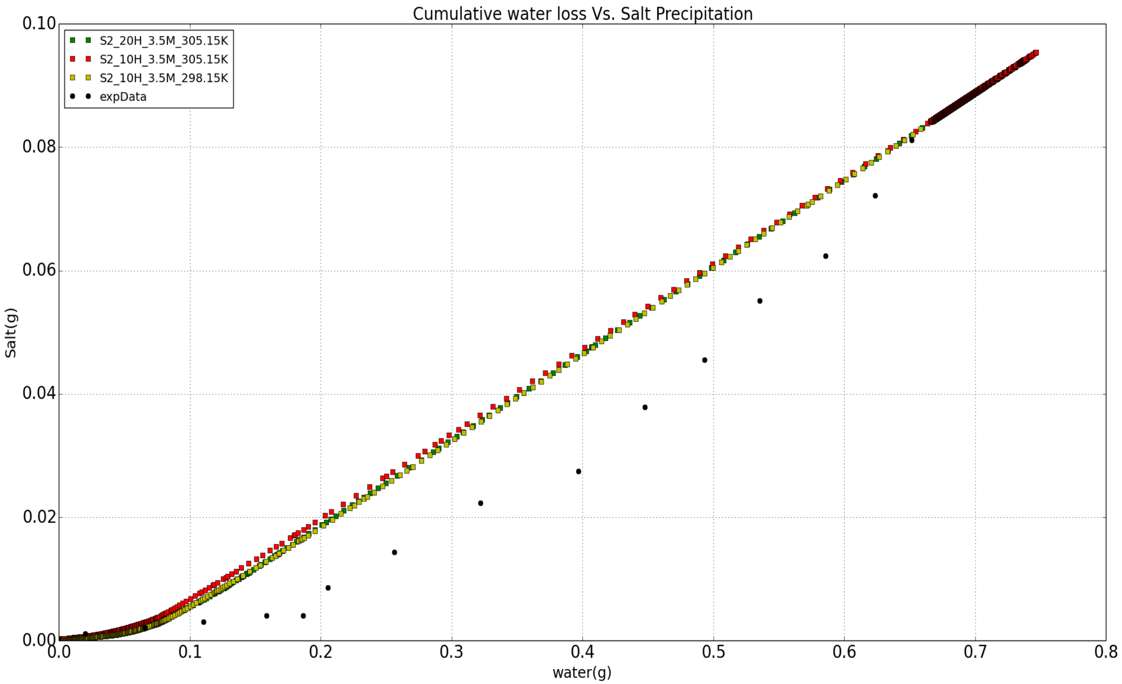

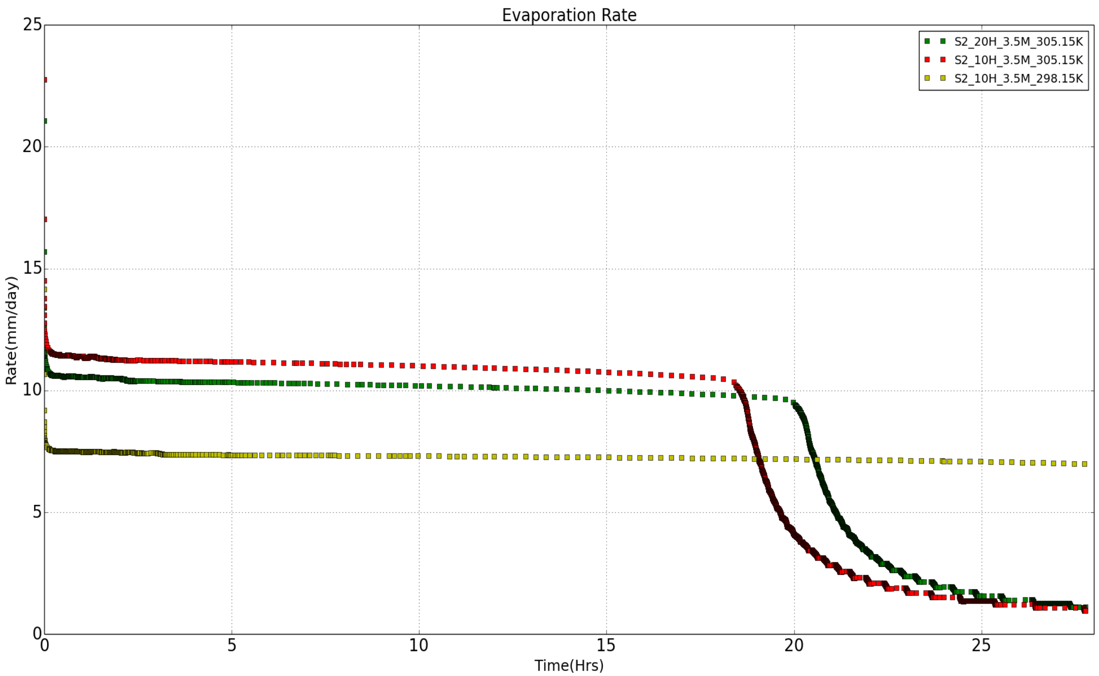

"Pore-scale dynamics of salt precipitation in drying porous media", Rad *et al., 2013*

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Outlook

Future Work:

- Reactive precipitation approach implemented and being tested
- Precipitation analysis for different salts (NaCl and NaI)
- Prarmeter analysis for free-flow and porous media