Numerical modeling of evaporation-driven salinization in porous-media with focus on the free-flow porous-media coupling

International Research Training Group nupus

Vishal A. Jambhekar[1], Karen S. Schmid[1], Rainer Helmig[1], Nima Shokri[2]

1. Dept. of Hydromechanics and Modelling of Hydrosystems, University of Stuttgart
2. School of Chemical Engineering and Analytical Science, University of Manchester

LH² University of Stuttgart Germany

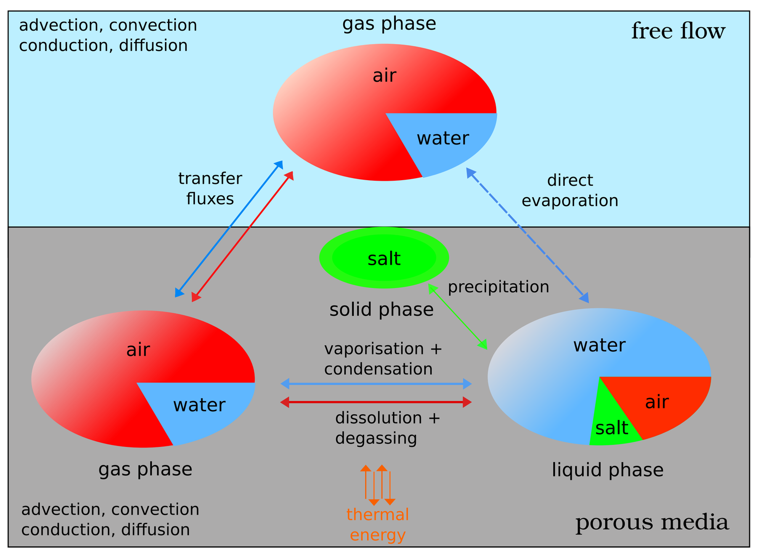
Motivation

- Focus: Modeling atmospheric processes for evaporative salinization
- State-of-the-art: Free-flow porous-media coupled REV-scale model concept

Figure: Irrigated agricultural lands

Figure: Salinized abandoned land

Model concept



- Non-isothermal porous-medium flow and transport (phases: solid, liquid and gas)
- Non-isothermal Stokes free-flow (gas phase)
- Implementation within the modeling framework of DuMu^x

Porous-media

For each component conservation equation is solved:

$$\sum_{\alpha\in\{l,g\}} \frac{\partial(\phi \varrho_{mol,\alpha} S_\alpha x_\alpha^\kappa)}{\partial t} - \sum_{\alpha\in\{l,g\}} \nabla\cdot\left\{\frac{k_{r\alpha}}{\mu_\alpha}\varrho_{mol,\alpha} x_\alpha^\kappa \mathbf{K}(\nabla p_\alpha - \varrho_\alpha \mathbf{g})\right\}$$

$$-\sum_{\alpha\in\{l,g\}} \nabla\cdot(D_{pm,\alpha}^\kappa \varrho_{mol,\alpha}\nabla x_\alpha^\kappa) - \sum_{\alpha\in\{l,g\}} = q^\kappa \;\forall\, \kappa \in \{w,a,s\}$$

$$q^\kappa = \begin{cases} k_p \phi \varrho_{mol,l} S_l (x_l^s - x_{l,max}^s) & \forall\, \kappa = s \\ 0 & \text{else} \end{cases}$$

One energy balance equation (Local thermal equilibrium)

Conservation of the precipitated salt and porosity and permeability change [2] :

$$\frac{\partial(\phi_S^s \varrho_{mol,S}^s)}{\partial t} = q^s \quad \left(\phi = \phi_0 - \phi_S^s,\; \frac{K}{K_0} = \left(\frac{\phi}{\phi_0}\right)^3 \left(\frac{1-\phi_0}{1-\phi}\right)^2,\; \frac{p_c}{p_{c0}} = \sqrt{\frac{K}{K_0}}\right)$$

Free-flow

Stokes equation for momentum balance [1]:

$$\frac{\partial(\varrho_g \mathbf{v}_g)}{\partial t} + \nabla\cdot[p_g \mathbf{I} - \mu_g(\nabla \mathbf{v}_g + \nabla \mathbf{v}_g^T)] - \varrho_g \mathbf{g} = 0$$

Energy balance:

$$\frac{\partial(\varrho_g u_g)}{\partial t} + \nabla\cdot(\varrho_g h_g \mathbf{v}_g) - \nabla\cdot(\lambda_g \nabla T) - q_T = 0$$

Interface

- Normal and tangential traction contribution [1]:

$$\mathbf{n}\cdot[(p_g\mathbf{I} - \tau)\mathbf{n}]^{\text{ff}} = [p_g]^{\text{pm}} \qquad \left[\left(\mathbf{v}_g + \frac{\sqrt{k_i}}{\alpha_{\text{BJ}}\mu_g}\tau\mathbf{n}\right)\cdot\mathbf{t}\right]^{\text{ff}} = 0$$

- Continuity of fluxes:

$$[\mathbf{q}\cdot\mathbf{n}]^{\text{ff}} = [\mathbf{q}\cdot\mathbf{n}]^{\text{pm}}$$

- Local thermal equilibrium:

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

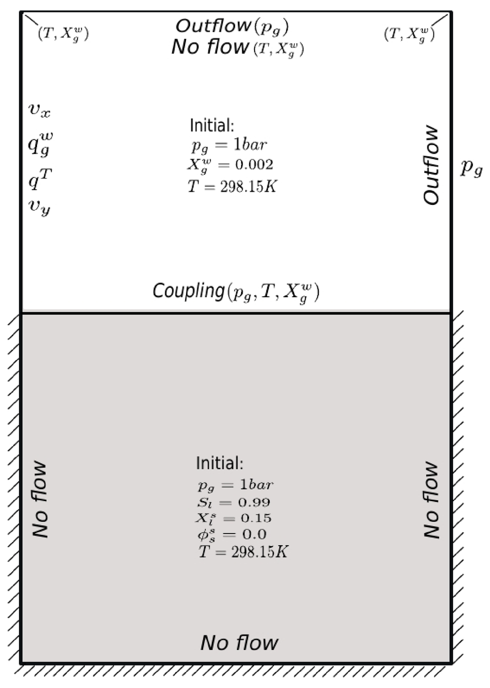
- Local chemical equilibrium:

$$[x_g^\kappa]^{\text{ff}} = [x_g^\kappa]^{\text{pm}} \qquad \forall\,\kappa \in \{w,a\}$$

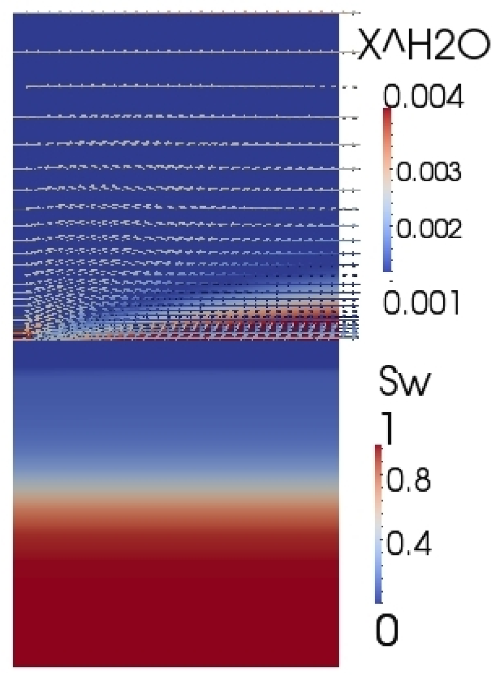
DFG Support of the German Research Foundation is gratefully acknowledged.

Numerical experiments

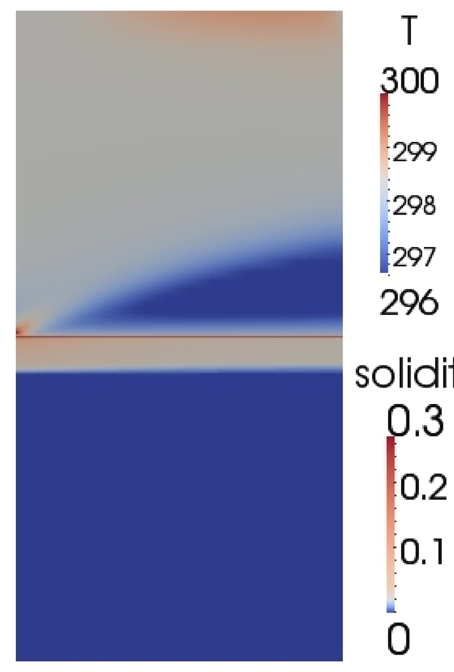
Validation (Homogeneous case):



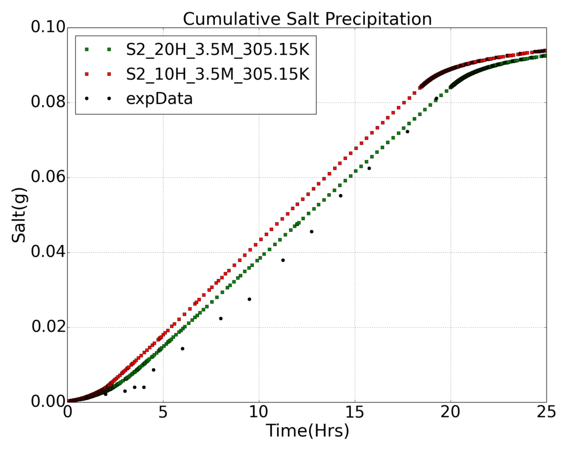
Numerical setup



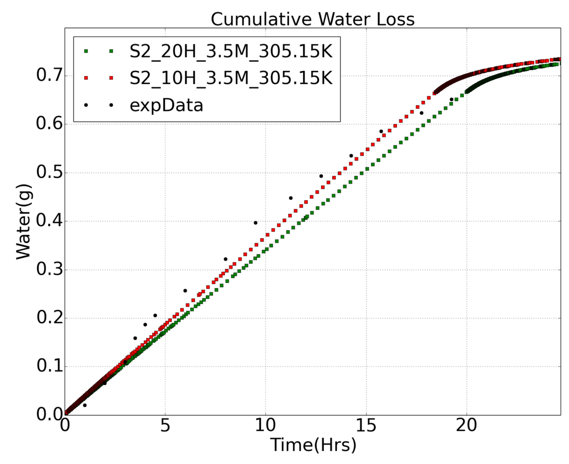
Drying



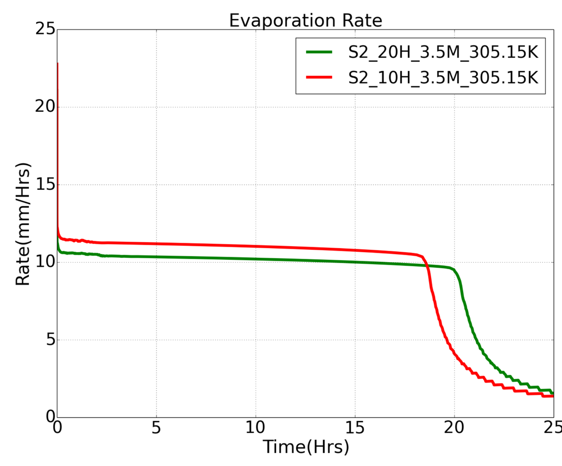
Salinization



Salt precipitation

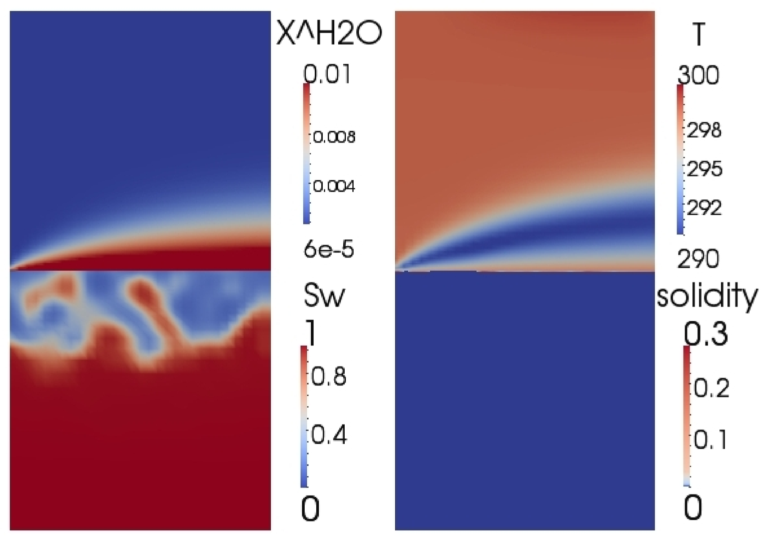


Water loss

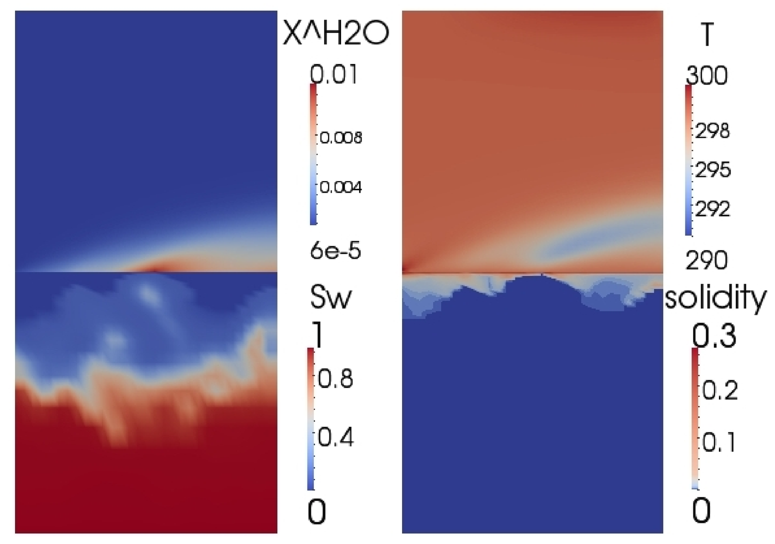


Evaporation rate

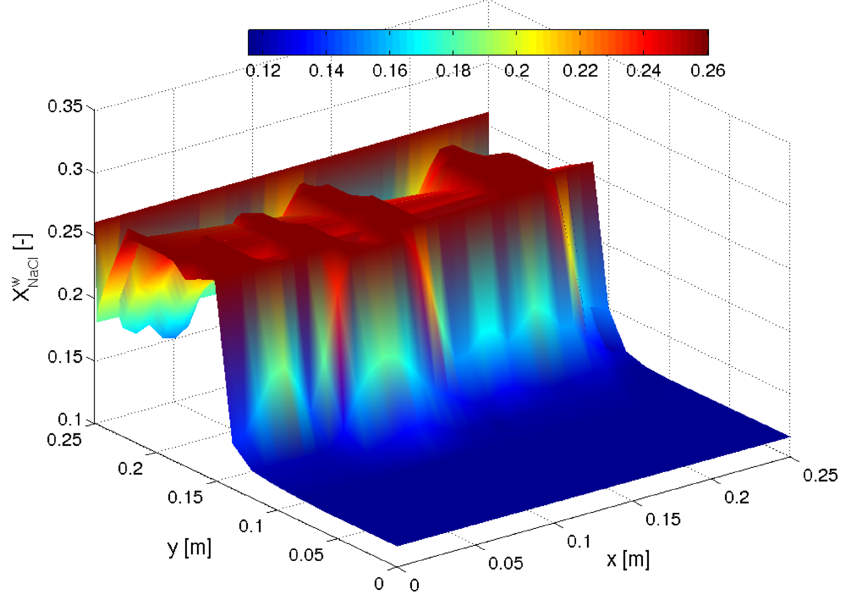
Heterogeneous case:



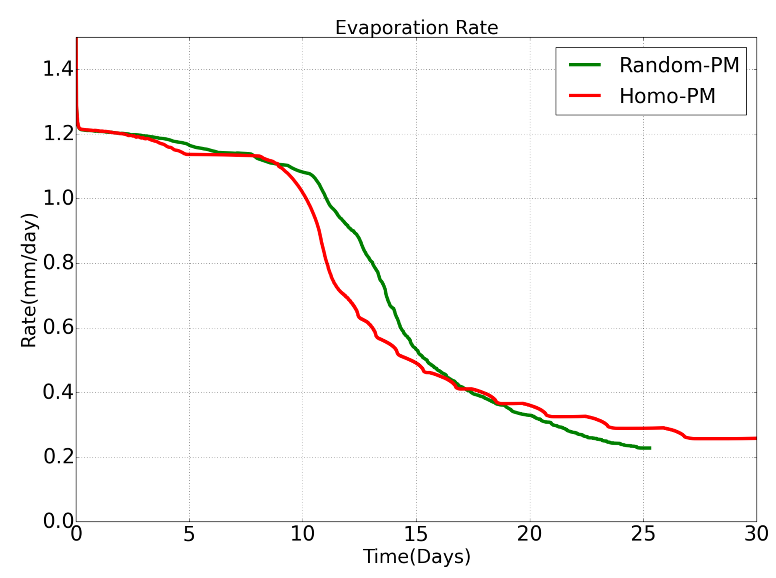
Drying after 5 days



Drying after 20 Days



Salinity after 15 Days



Evaporation rate

Outlook

Ongoing work:

- Validation for all stages of salinization
- Reactive precipitation approach for mixed salts (e.g. Na^+, Cl^- and I^+)

Future work:

- Effects of processes such as radiation and turbulence
- Effects of variation in the porous media parameters at the interface

Literature

[1] K. Mosthaf, K. Baber, B. Flemisch, R. Helmig, A. Leijnse, I. Rybak, and B. Wohlmuth. A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow. *Water Resources Research*, 47, 2011.

[2] M. Zeidouni, M. Pooladi-Darvish and D. Keith. Analytical solution to evaluate salt precipitation during CO2 injection in saline aquifers. *International Journal of Greenhouse Gas Control*, 3:600-611 (2009).

[3] Rad et al. Pore-scale dynamics of salt precipitation in drying porous media. *Physical Review E*, 88(3)(2013).

DuMu^x The simulations are preformed using DuMu^X.