Evaporation Driven Soil Salinization

International Research Training Group nupus

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Motivation

- Focus: modeling and interpretation of evaporative salinization under the influence of atmospheric processes
- At hand: REV-scale model concept, coupling of single-phase compositional laminar free-flow and a multi-phase compositional porous-media flow
- Project: describe transport and precipitation of dissolved salts
- Goal: Determine the limits of state-of-the-art models and improve the predictability of evaporative salinization

Figure: Salinized Abandoned land

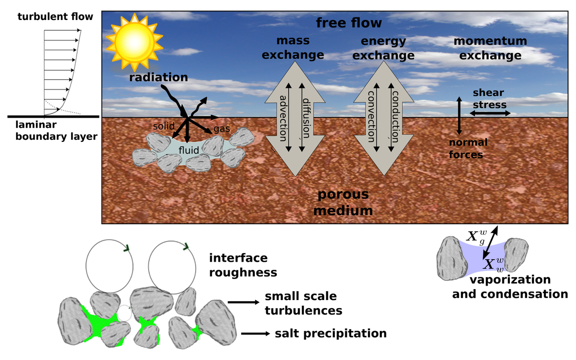

Figure: Relevant interface processes [1]

Model concept

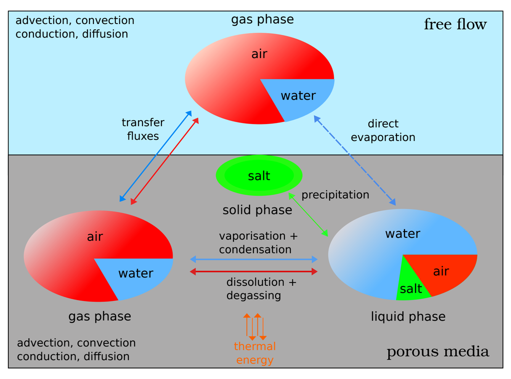

Figure: Overview of the model concept

- Non-isothermal porous-medium flow (salt transport)
- Non-isothermal laminar (Stokes) free-flow
- Implementation within the modeling framework of DuMu^x

Porous media

For each component a mass balance equation is solved:

$$\sum_{\alpha\in\{l,g\}}\frac{\partial(\phi\varrho_{mol,\alpha}S_\alpha x_\alpha^\kappa)}{\partial t}-\sum_{\alpha\in\{l,g\}}\nabla\cdot\left\{\frac{k_{r\alpha}}{\mu_\alpha}\varrho_{mol,\alpha}x_\alpha^\kappa\mathbf{K}(\nabla p_\alpha-\varrho_\alpha\mathbf{g})\right\}$$
$$-\sum_{\alpha\in\{l,g\}}\nabla\cdot(D_{pm,\alpha}^\kappa\varrho_{mol,\alpha}\nabla x_\alpha^\kappa)-\sum_{\alpha\in\{l,g\}}q_\alpha^\kappa=0\qquad\forall\,\kappa\in\{w,a,s\}$$

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

One energy balance equation (Local thermal equilibrium):

$$\sum_{\alpha\in\{l,g\}}\frac{\partial(\phi\varrho_\alpha u_\alpha S_\alpha)}{\partial t}+\frac{\partial(\phi_S^s\varrho_S^s c_S^s T)}{\partial t}+(1-\phi_0)\frac{\partial(\varrho_S c_S T)}{\partial t}$$
$$+\sum_{\alpha\in\{l,g\}}\nabla\cdot(\varrho_\alpha h_\alpha\mathbf{v}_\alpha)-\nabla\cdot(\lambda_{\text{pm}}\nabla T)-q_T=0$$

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

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

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

Free flow

Component mass balance:

$$\frac{\partial(\varrho_{mol,g}x_g^\kappa)}{\partial t}+\nabla\cdot(\varrho_{mol,g}x_g^\kappa\mathbf{v}_g)-\nabla\cdot(D_g^\kappa\varrho_{mol,g}\nabla x_g^\kappa)-q_g^\kappa=0\qquad\forall\,\kappa\in\{w,a\}$$

Phase mass balance:

$$\frac{\partial\varrho_g}{\partial t}+\nabla\cdot(\varrho_g\mathbf{v}_g)-q_g=0$$

Stokes equation for momentum balance [1]:

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

Energy balance:

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

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Interface

- Normal and tangential traction contribution [1]:

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

- Continuity of fluxes:

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

- Local thermal equilibrium:

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

- Local chemical equilibrium:

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

Results

Decoupled model:

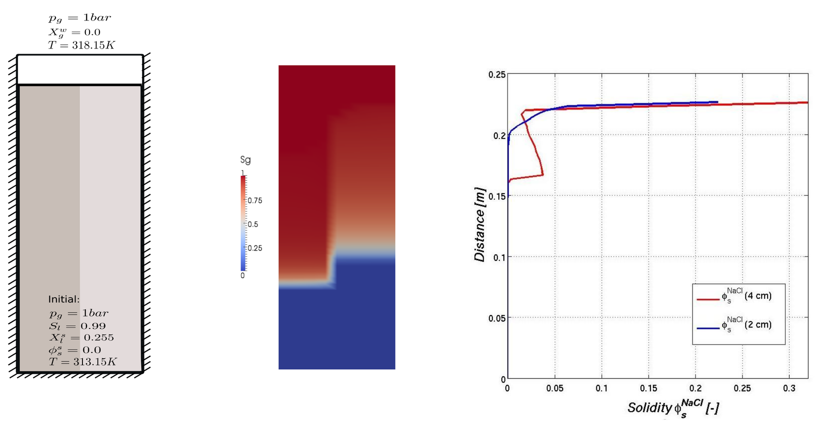


Figure: Evaporative drying

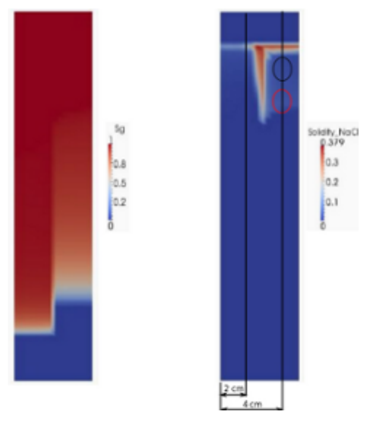
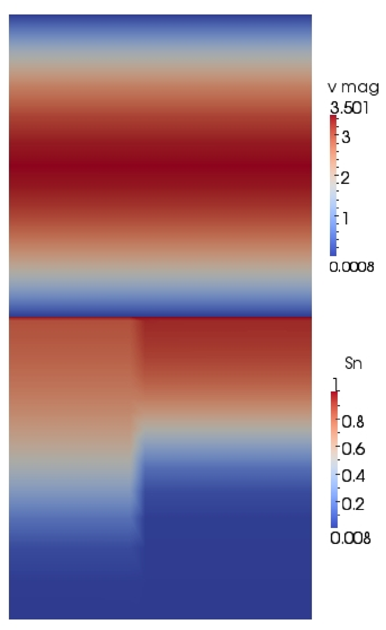


Figure: Salinization

- Non- isothermal porous-media flow
- Salt transport, accumulation and precipitation, mainly at the top surface and the heterogeneity interface

- Change in porosity and permeability resulted from salt precipitation

Coupled model:



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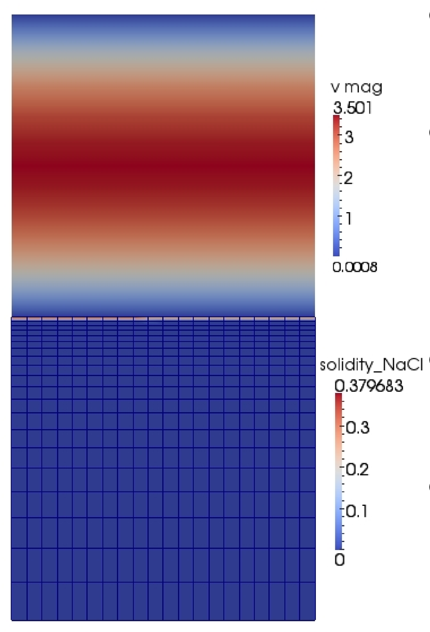

Figure: Salinization

- Isothermal porous-media flow
- Salt transport, accumulation and precipitation at the top surface
- Change in porosity and permeability
- So far, no precipitation is observed along vertical heterogeneity interface

Outlook

Following issues need to be addressed in detail:

- Extension of the coupled model to handle non-isothermal scenario
- Test alternative models to describe change in porosity and permeability
- Transport for dissolved salt species (e.g. Na^+ and Cl^-) and reactive precipitation
- Validity of chemical equilibrium at the interface
- Effects of turbulence and solar radiation on salinization

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).