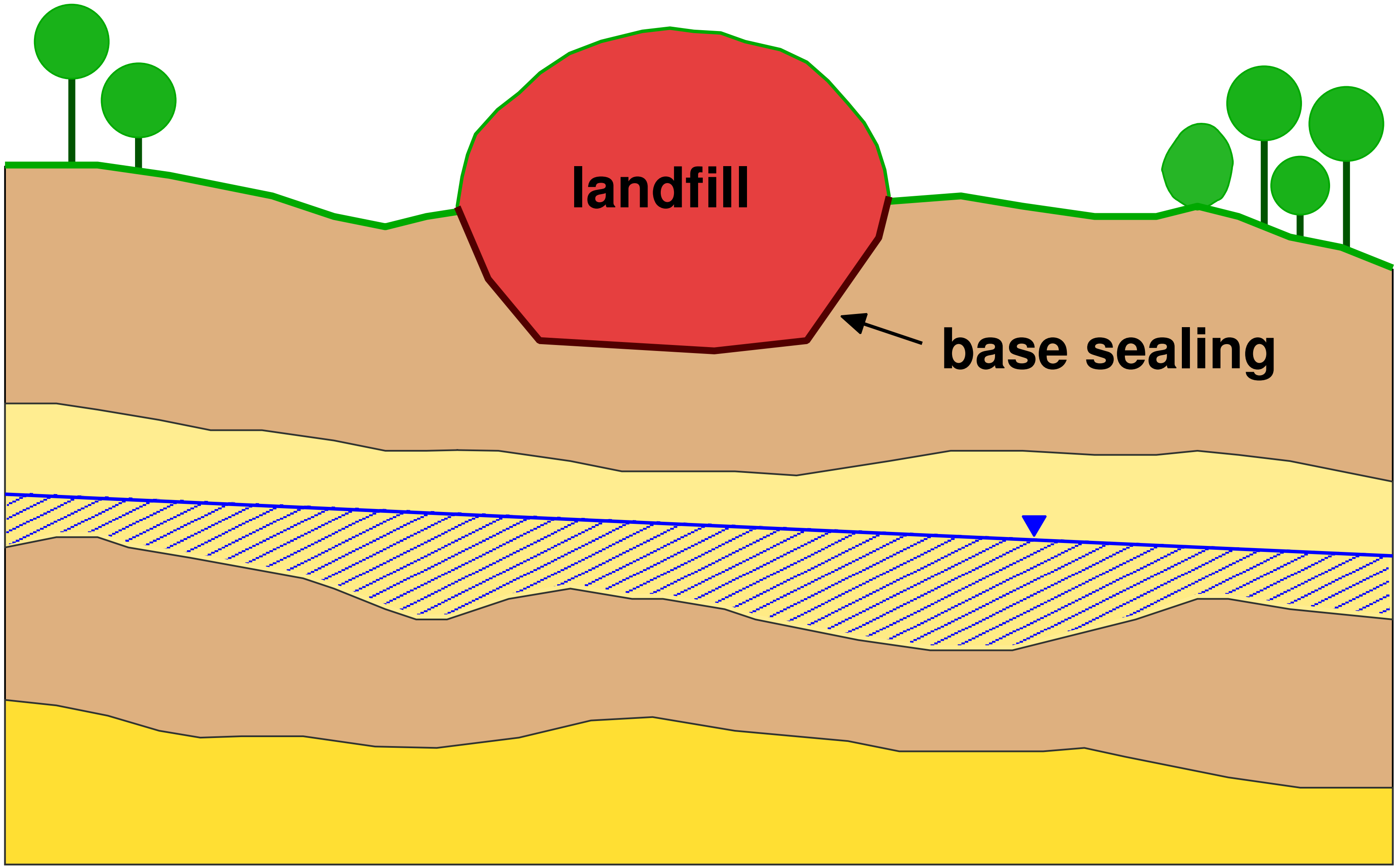
A Phenomenological Model Concept for the Numerical Simulation of Two-Phase Two-Component Processes in Cohesive Soils

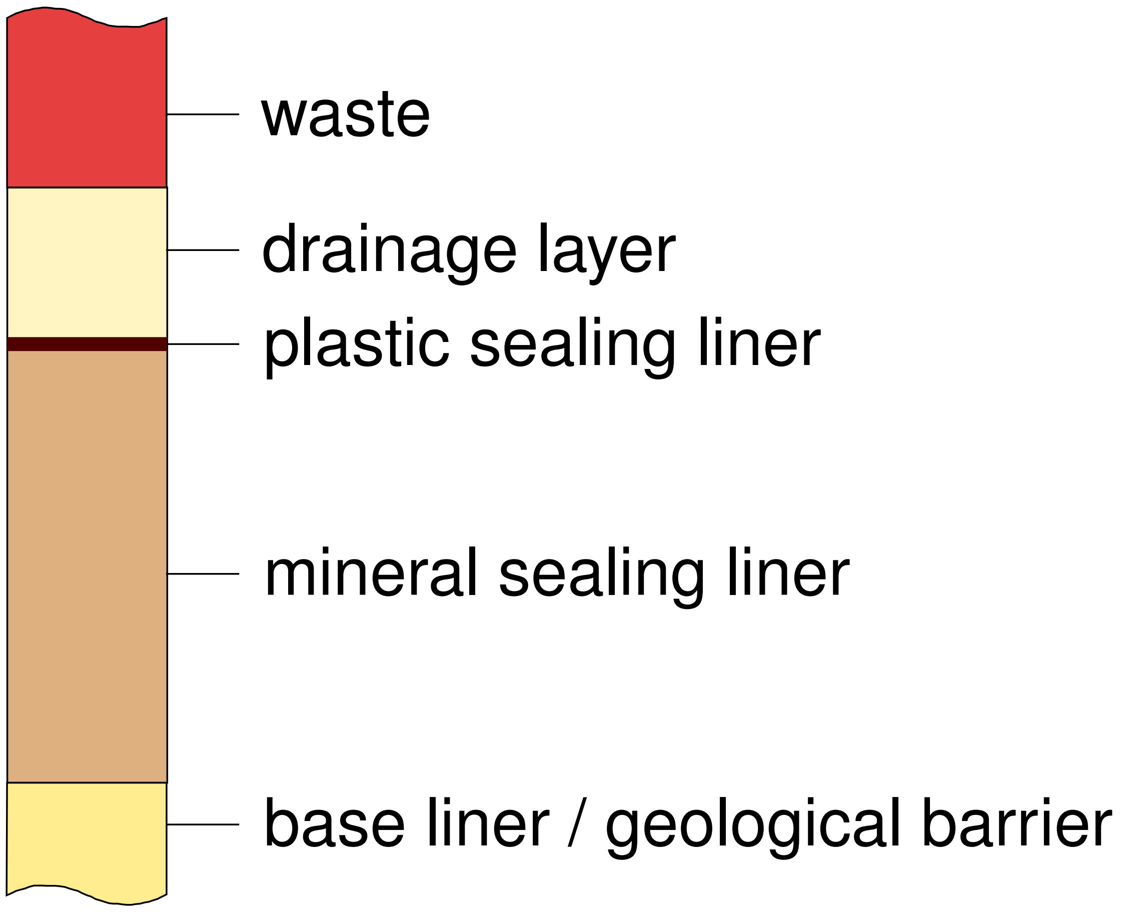
Sandra Freiboth, Holger Class, Rainer Helmig

Lehrstuhl für Hydromechanik und Hydrosystemmodellierung
Institut für Wasserbau, Universität Stuttgart

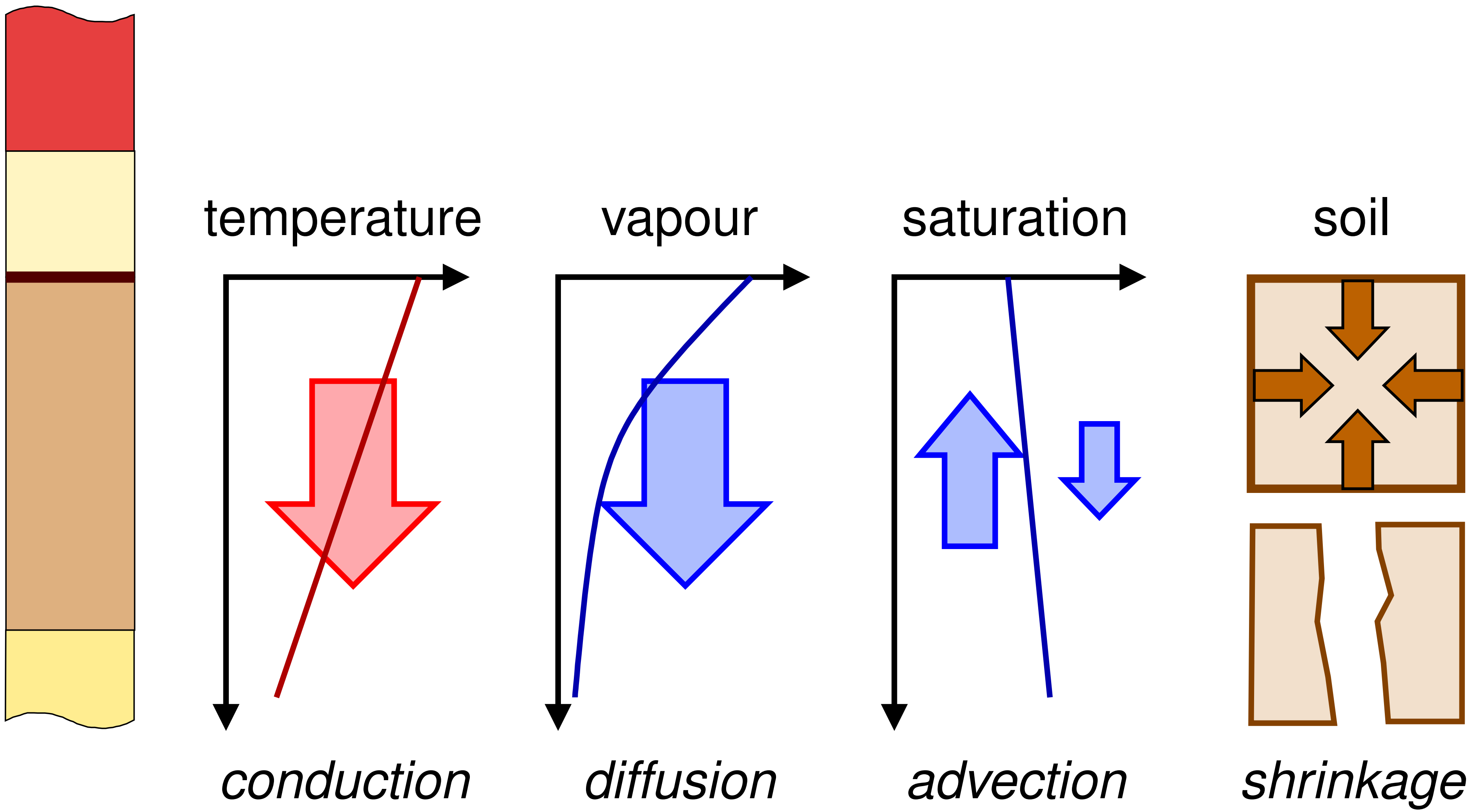
Motivation



Structure of a Base Liner

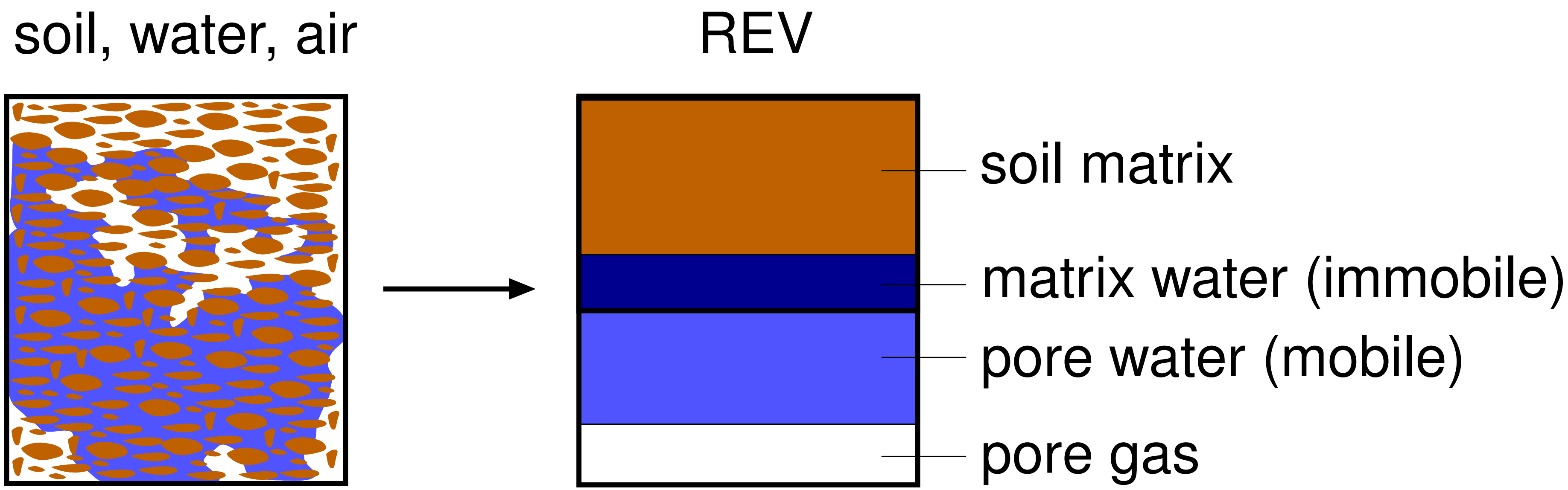


Processes in a Base Liner



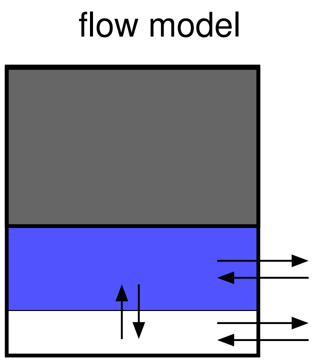
Conceptual Model (1)

constituents

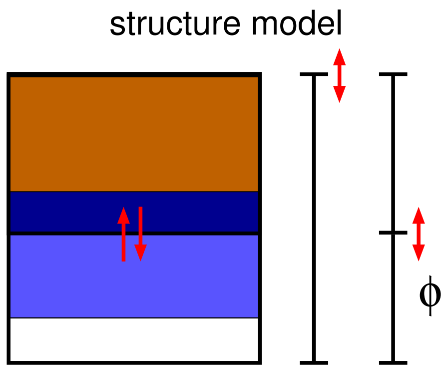


Conceptual Model (2)

flow and transport



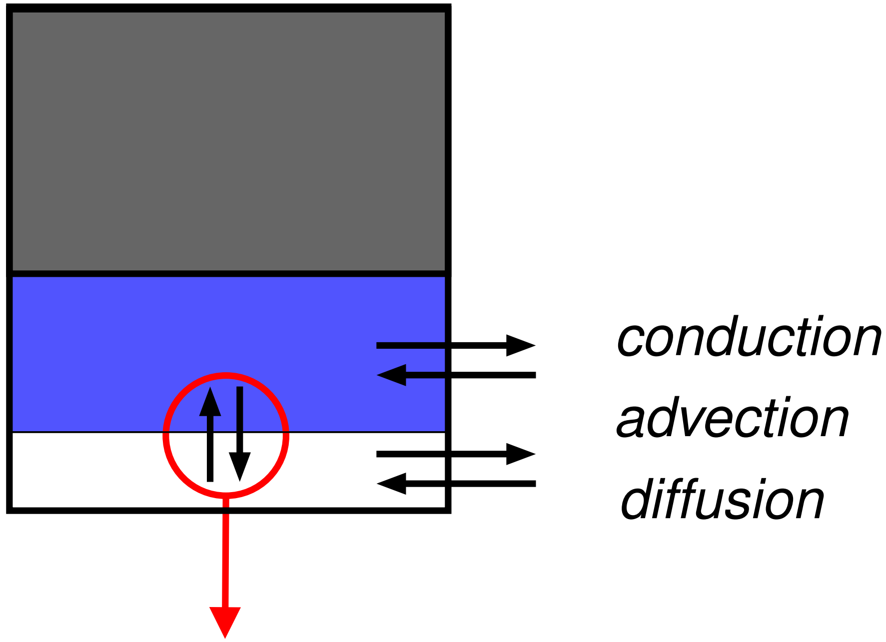
structural alterations



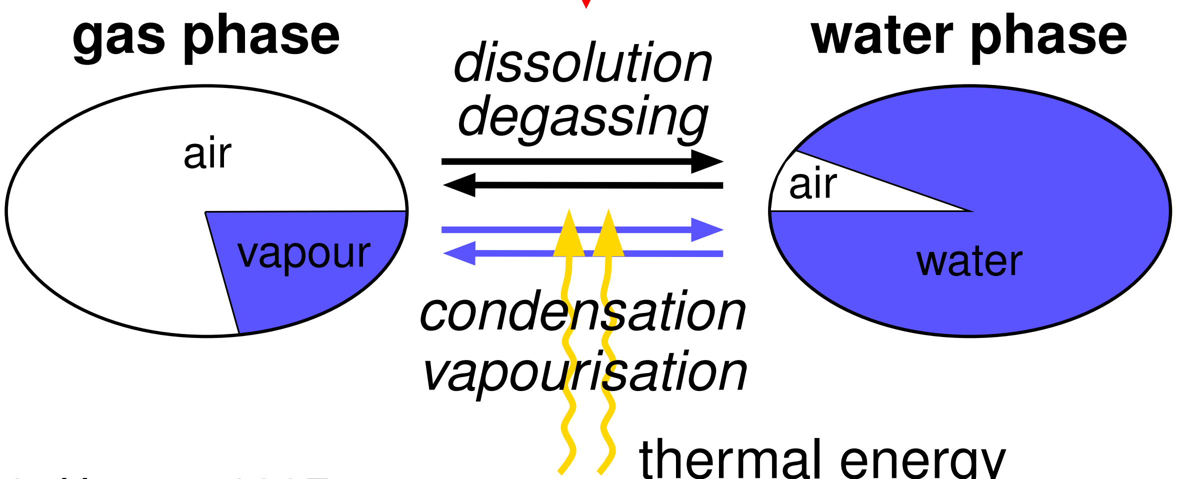
considering flow / transport and structural alterations as two separate, decoupled steps

Flow and Transport Model (1)

flow and transport

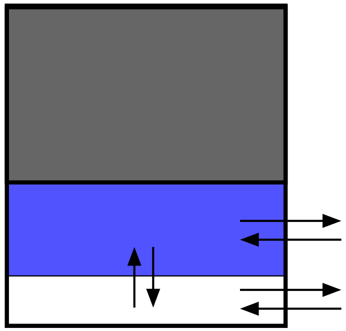


transfer between the phases



CLASS, HELMIG, BASTIAN 2002; HELMIG 1997

Flow and Transport Model (2)



Assumptions:

- local thermal equilibrium
- chemical equilibrium
- stiff skeleton

Mass Balance Equations

$K \in \{w, a\}$
$\alpha \in \{w, g\}$

formulation for each component
$\rightarrow$ 2 balance equations

constraints:

$S_w + S_g = 1$
$p_g = p_w + p_c(S_w)$

$$\underbrace{\frac{\partial(\sum_\alpha \phi \varrho_\alpha^{mol} x_\alpha^K S_\alpha)}{\partial t}}_{\text{storage}}$$

$$- \underbrace{\sum_\alpha \operatorname{div} \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \varrho_\alpha^{mol} x_\alpha^K \mathbf{K} (\,\mathbf{grad}\, p_\alpha - \varrho_{mass,\alpha} \mathbf{g}) \right\}}_{\text{advective transport}}$$

$$- \underbrace{\operatorname{div} \left\{ D_{pm}^K \varrho_g^{mol} \,\mathbf{grad}\, x_g^K \right\}}_{\text{diffusive transport in gas phase}}$$

$$- \underbrace{q^K}_{\text{sink/source}} = 0$$

Balance Equation for Thermal Energy

$K \in \{w, a\}$

$\alpha \in \{w, g\}$

assumption of local thermal equilibrium

$\longrightarrow$ 1 balance equation for the entire fluid-filled, porous medium

$$\underbrace{\frac{\partial \left(\sum_\alpha \phi \varrho_{mass,\alpha} u_\alpha S_\alpha\right)}{\partial t} + \frac{\partial \left(1-\phi\right) \varrho_s c_s T}{\partial t}}_{\textbf{storage}}$$

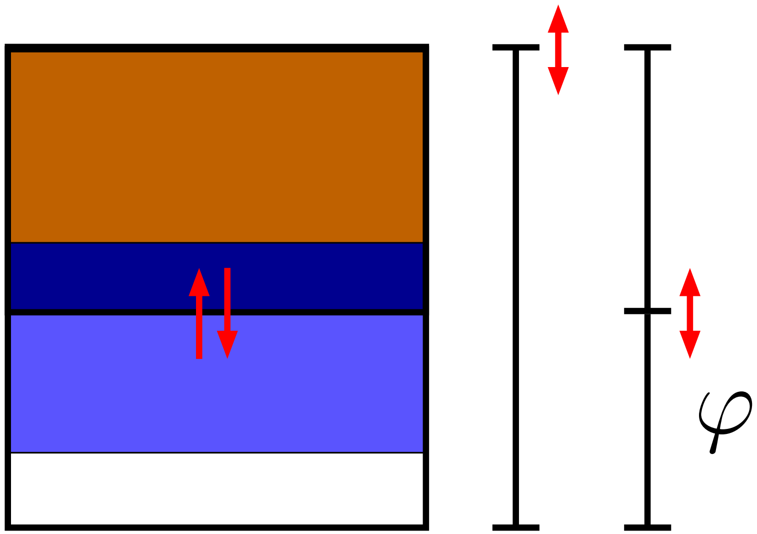
$$- \underbrace{\operatorname{div}\left(\lambda_{pm}\,\mathbf{grad}\,T\right)}_{\textbf{thermal conduction}}$$

$$\underbrace{-\sum_\alpha \operatorname{div}\left\{\frac{k_{r\alpha}}{\mu_\alpha}\varrho_{mass,\alpha} h_\alpha \mathbf{K}\left(\mathbf{grad}\,p_\alpha - \varrho_{mass,\alpha}\mathbf{g}\right)\right\}}_{\textbf{convective transport}}$$

$$\underbrace{-\sum_K \operatorname{div}\left\{D_{pm}^K \varrho_{mol,g} h_g^K M^K\,\mathbf{grad}\,x_g^K\right\}}_{\textbf{thermal transport due to diffusion}}$$

$$- \underbrace{q^h}_{\textbf{sink/source}} = 0$$

Structural Alterations (1)



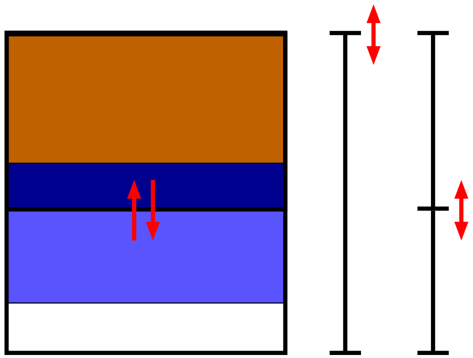
immobilisation / mobilisation

changes in volume + porosity

↓

adaptation of hydraulic parameters

Structural Alterations (2)



key points:

- influence of structural alterations on flow and transport processes ...
- ... by means of adapted hydraulic properties
- ... using constitutive relationships
- rigid soil skeleton
- exclusive of crack formation

Structure Parameter

- swelling / shrinking factor

$$\varepsilon = \frac{V}{V_o}$$

- (computationally) effective porosity

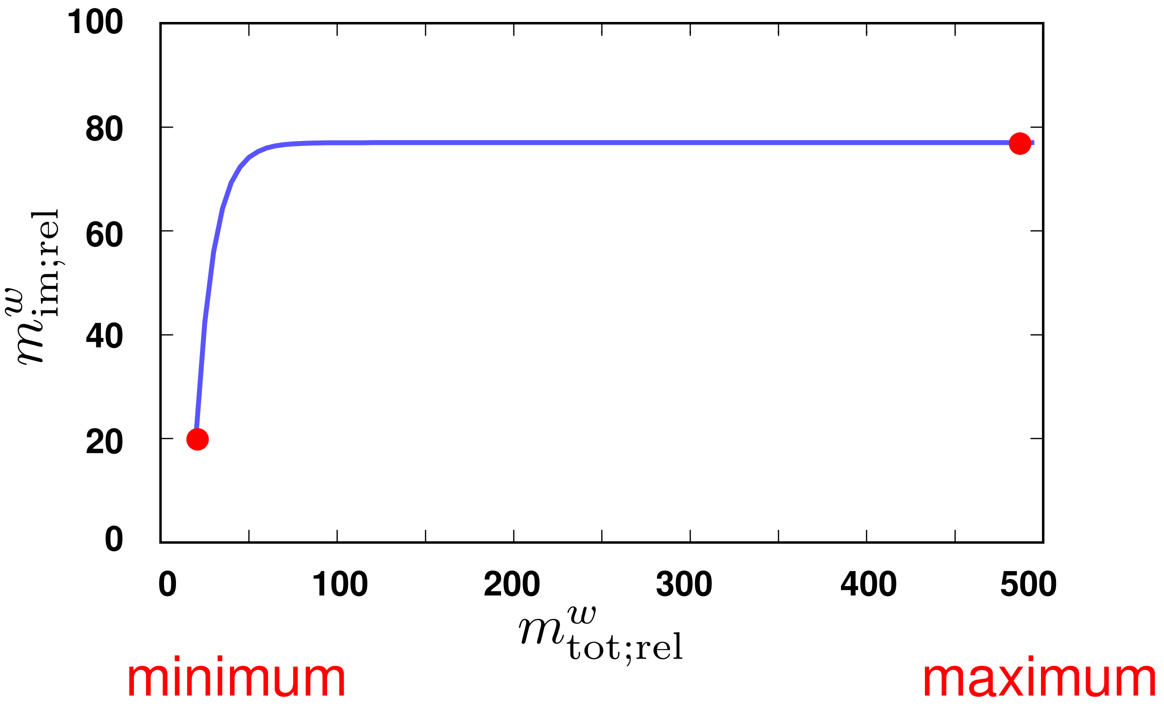
$$\varphi_{\text{eff}} = \frac{V_{\text{pore}}}{V_o} = \varphi\, \varepsilon$$

- relative total mass of water

$$m^w_{\text{tot;rel}} = \frac{\left(n^w_{\text{im}} + n^w_w + n^w_g\right)\, M^w}{V}$$

Immobile Matrix Water

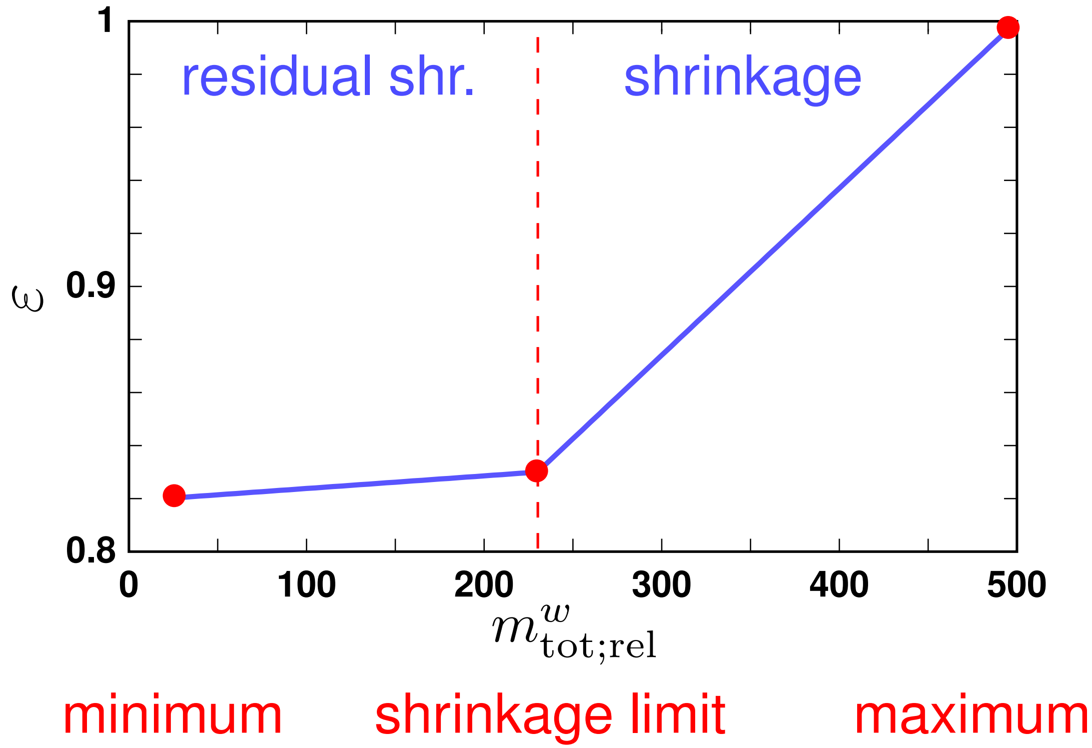
$$m^{w}_{\mathrm{im;rel}} = f_{\mathrm{sat.}}(m^{w}_{\mathrm{tot;rel}})$$



(MEISSNER, DOBROWOLSKY 2003)

Shrinking Factor

$$\varepsilon = f_{\text{linear; residu}}(m^w_{\text{tot;rel}}) \qquad \varepsilon = f_{\text{linear; schrumpf}}(m^w_{\text{tot;rel}})$$

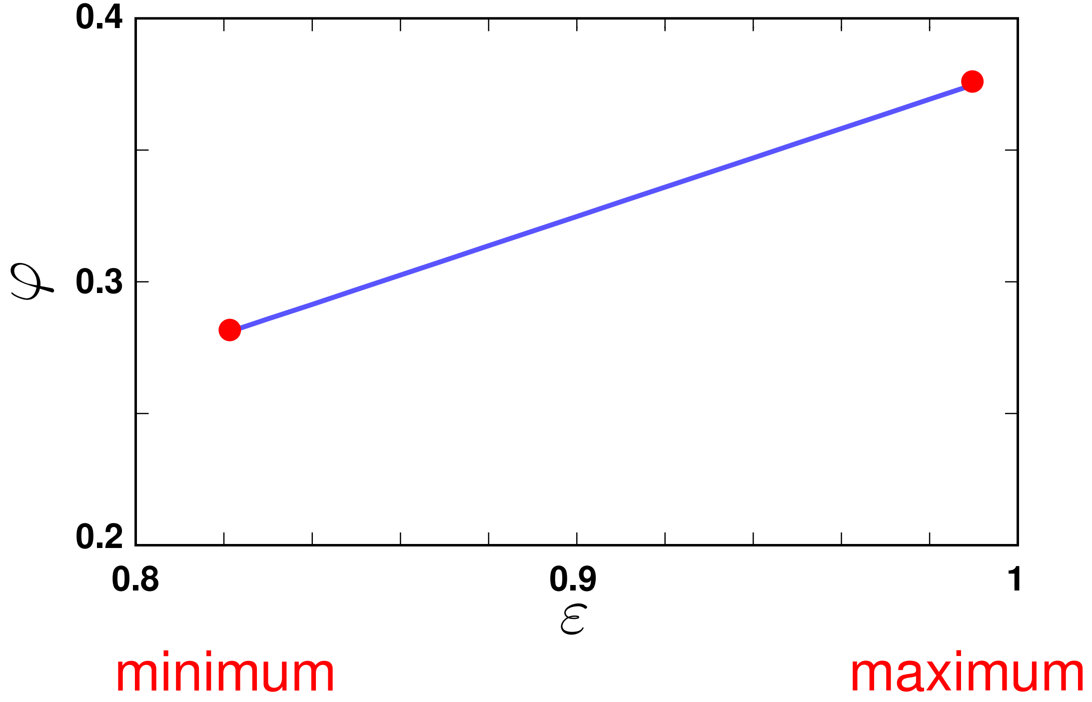


(e.g. BRAUNS, SCHNEIDER, GOTTHEIL 2000)

Porosity

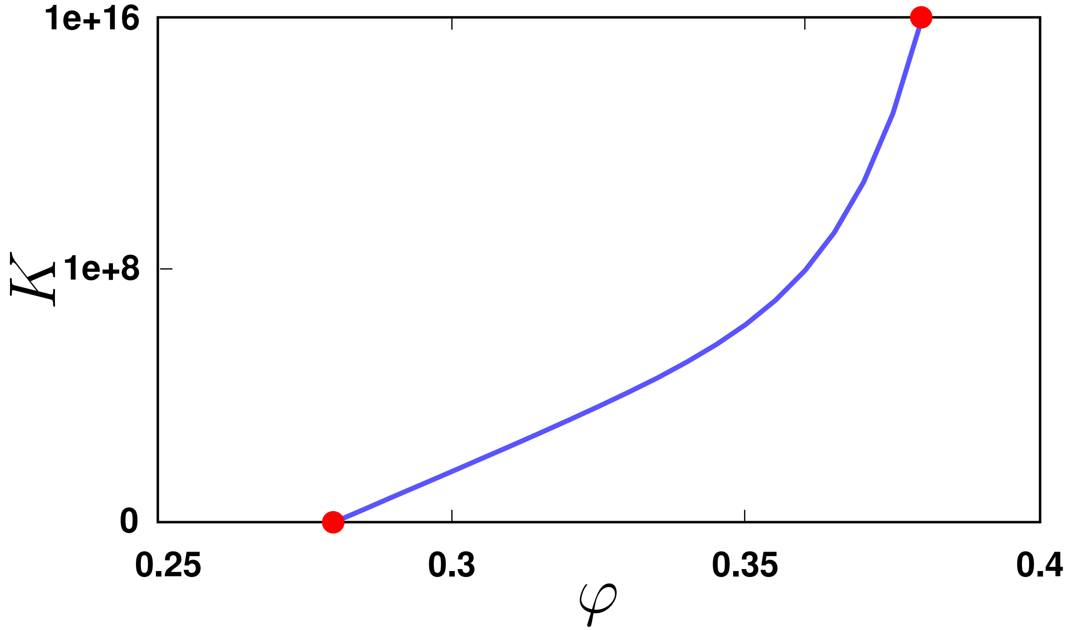
a) $\varphi = f(m^w_{\text{tot;rel}})$

b) $\varphi = f_{\text{linear}}(\varepsilon)$



Permeability

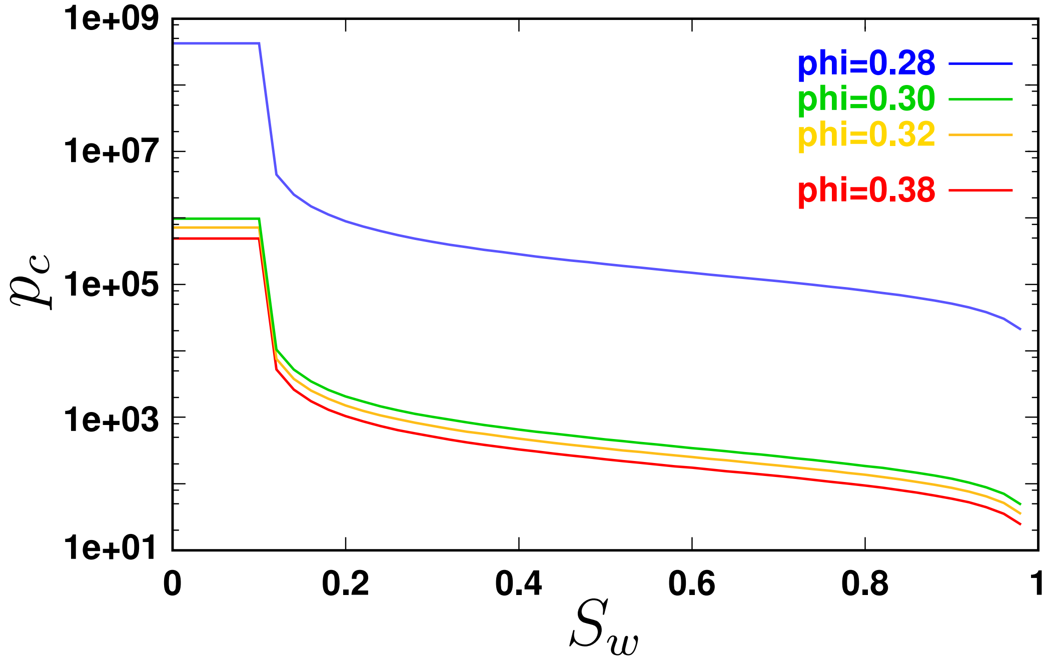
$$K = f(\varphi)$$



(e.g. CLAUSER 2003)

Capillary Pressure

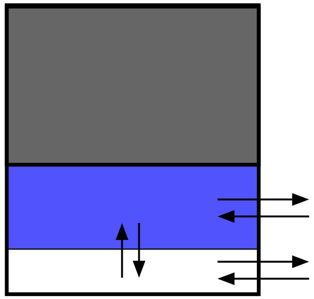
$$p_c(S_w) = p_{c;\mathrm{ref}}(S_w)\ \sqrt{\frac{K_{\mathrm{ref}}}{\varphi_{\mathrm{ref}}}\ \frac{\varphi}{K}}$$



(LEVERETT 1941)

Coupling Flow + Structural Alterations

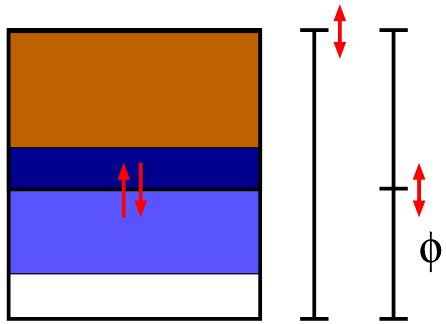
flow and transport



1st step within one time step

- compute flow and transport
- compute mass of water, mass of air and energy

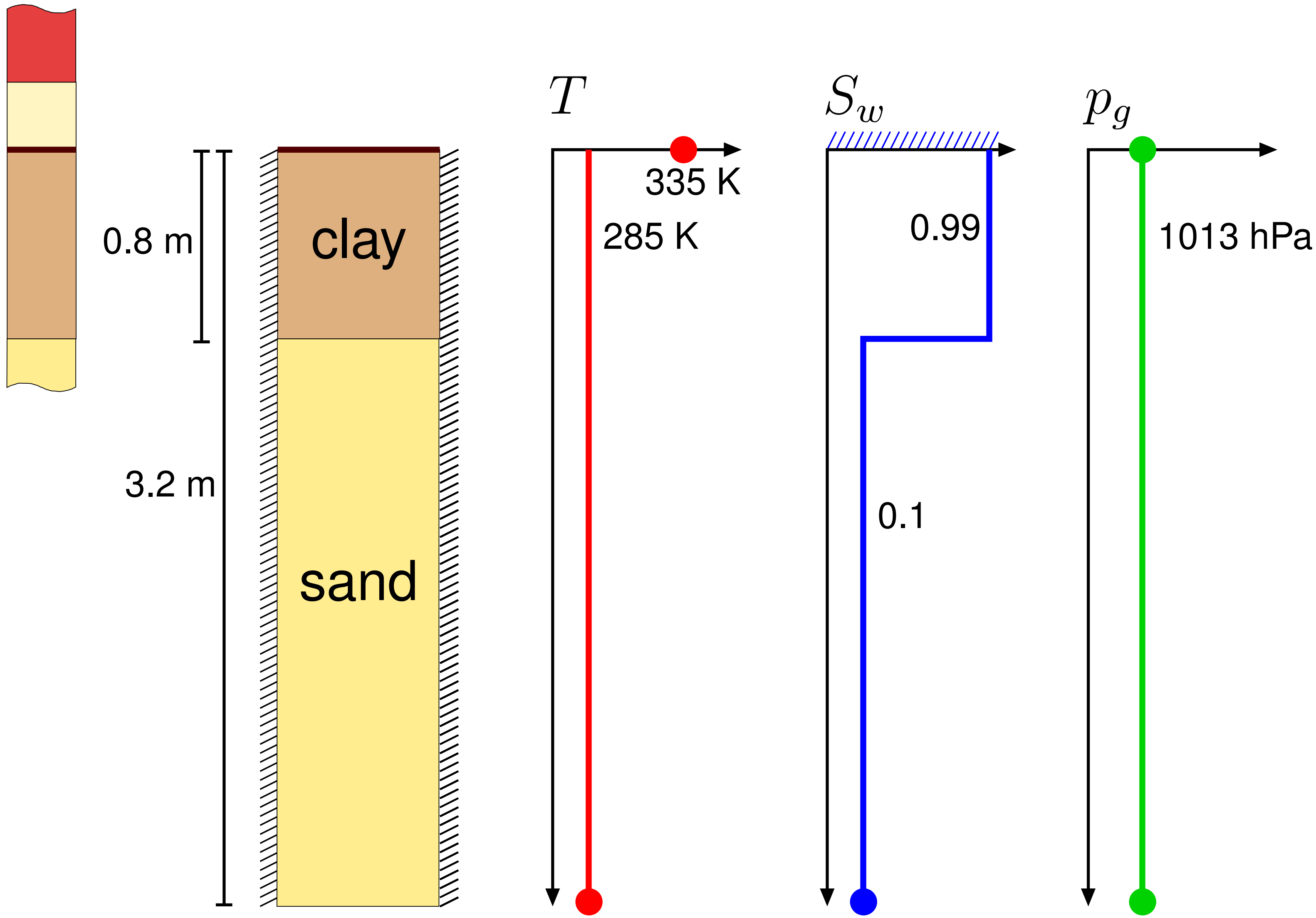
structural alterations



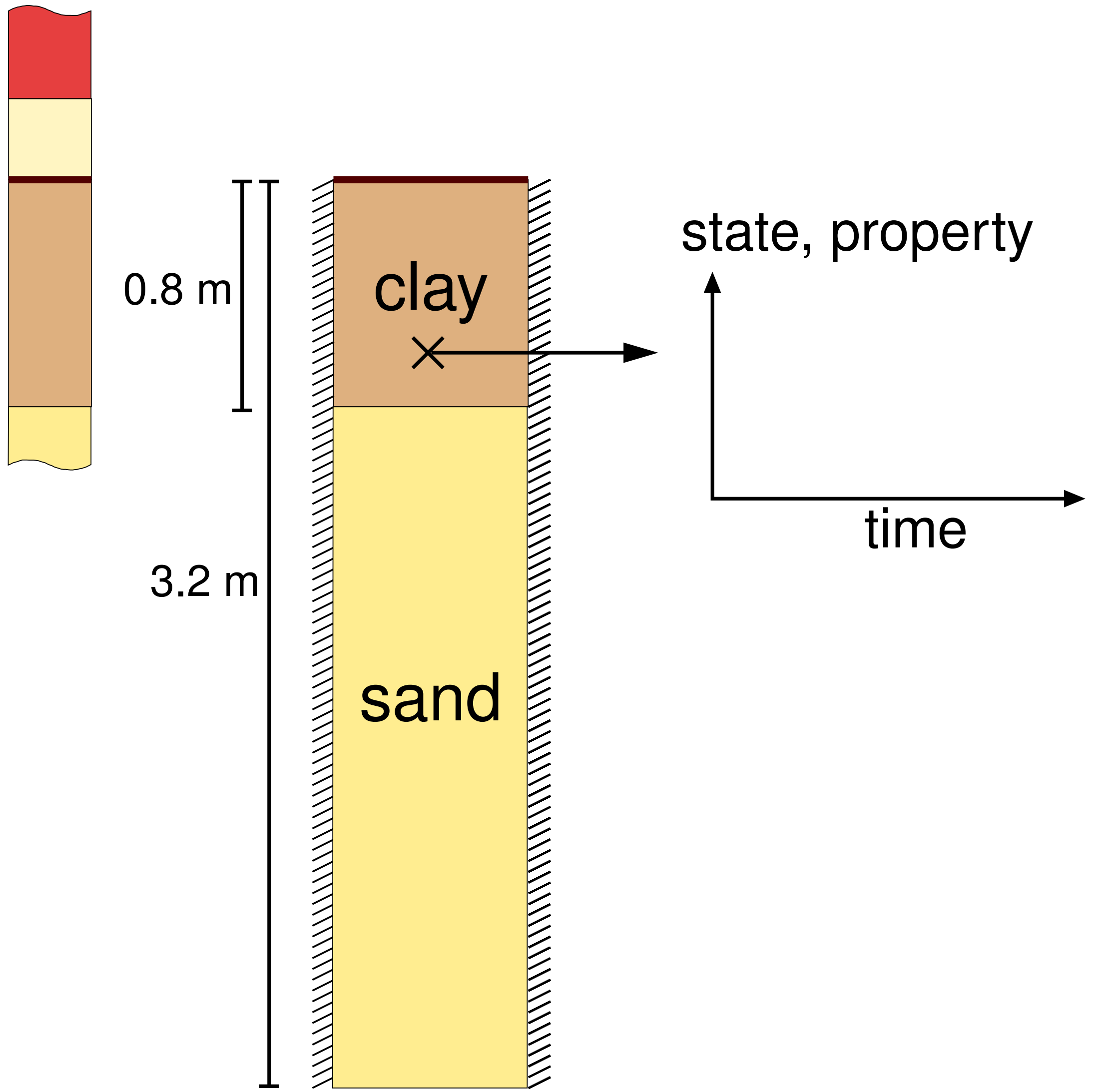
2nd step within one time step

- update structure parameters
- compute new state variables while maintaining mass and energy conservation and thermodynamic equilibrium

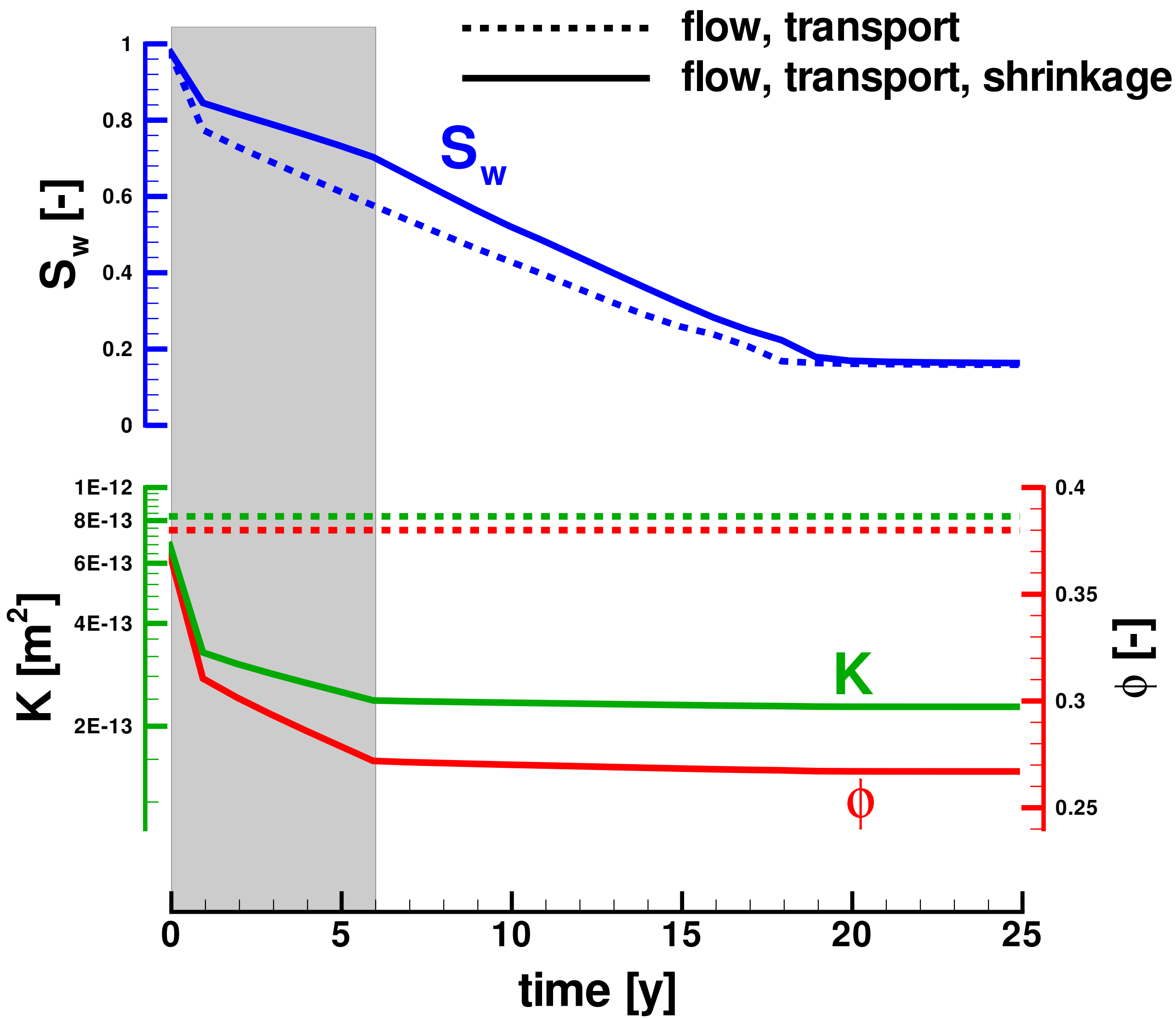
Model Comparison (1)



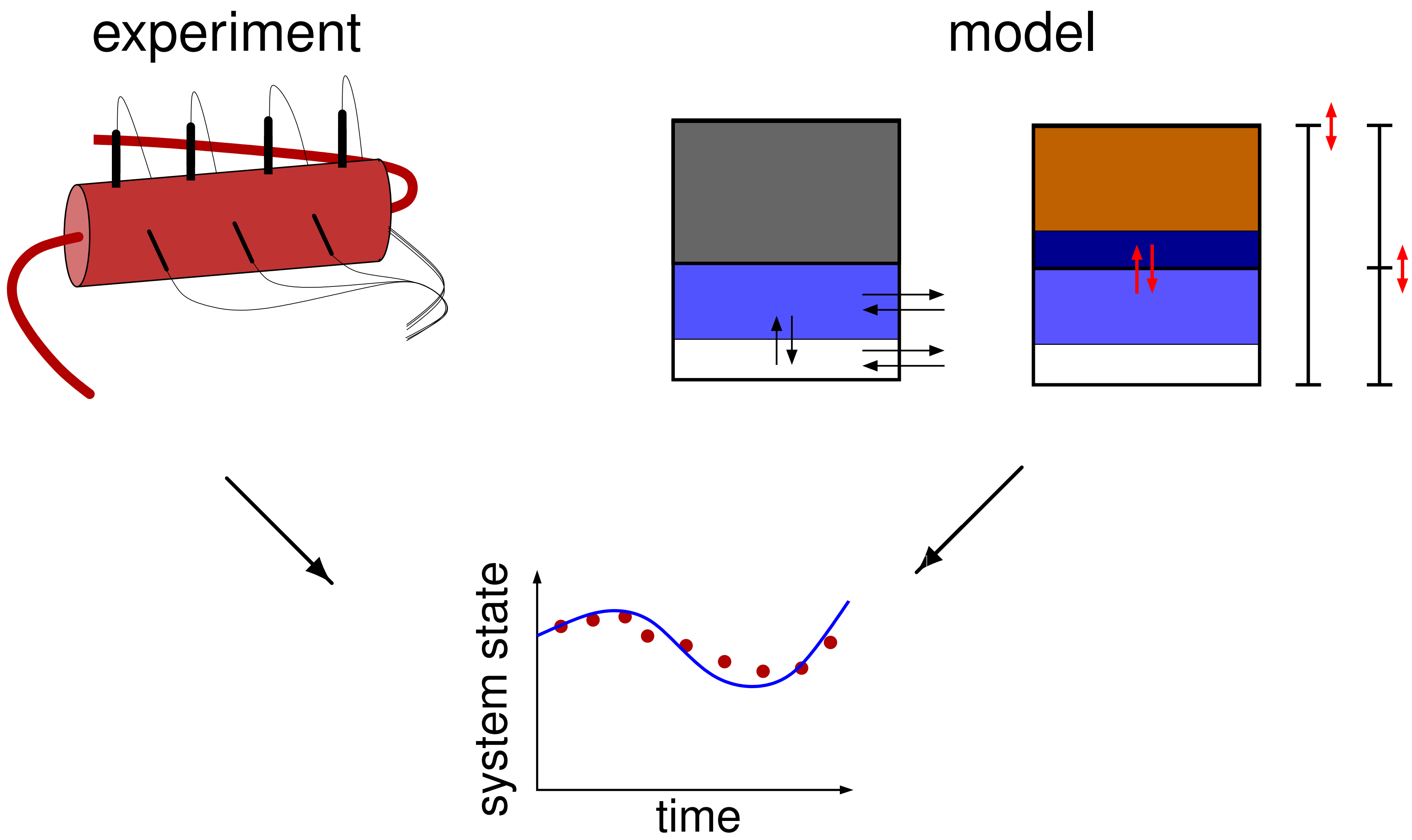
Model Comparison (1)



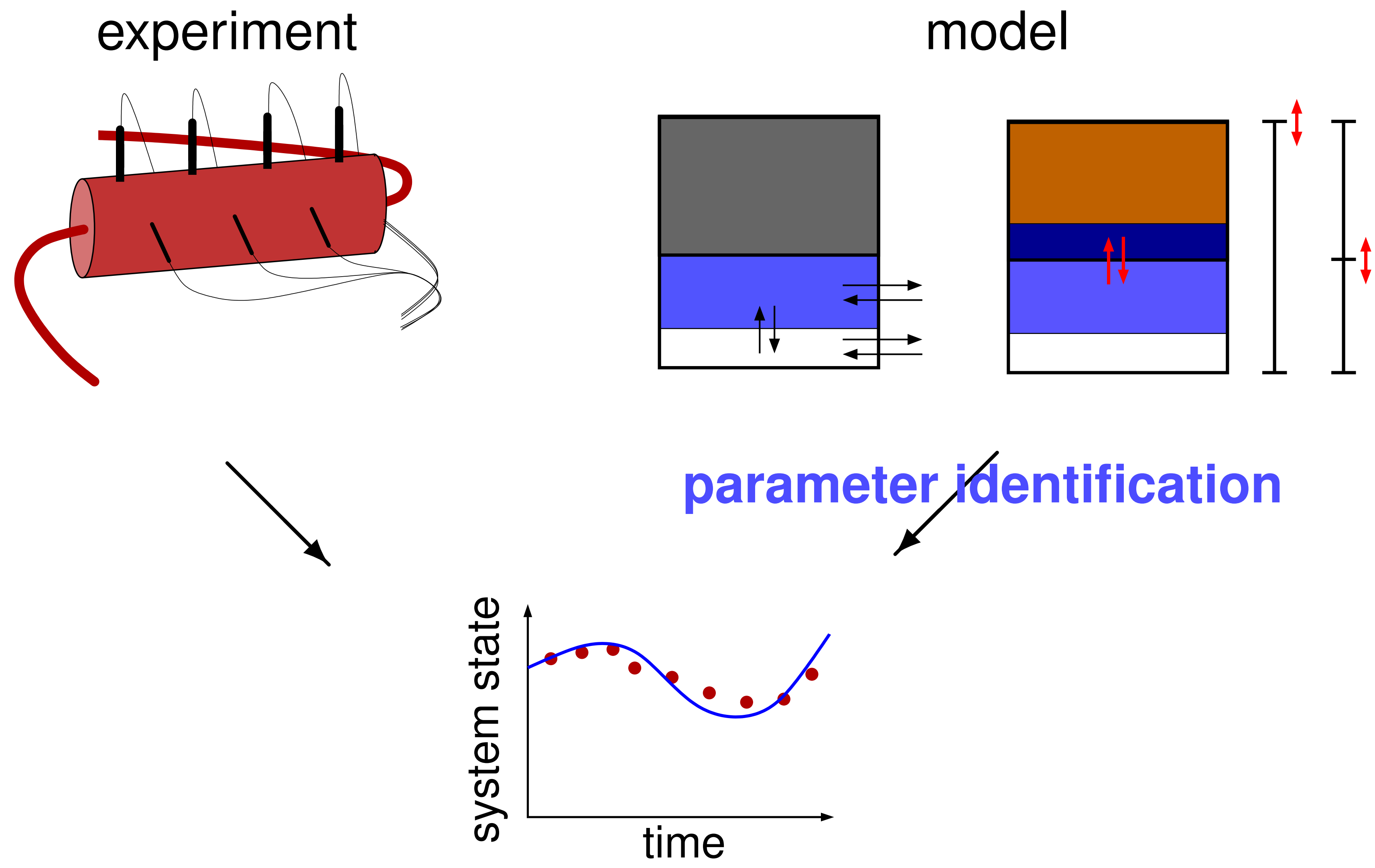
Model Comparison (2)



Model Calibration and Validation



Model Calibration and Validation



Final Remarks

- model concept that includes – on a phenomenological basis (rigid porous matrix) – the effects of swelling/shrinking within a non-isothermal multiphase multicomponent flow and transport model
- integration of additional constitutive relationships into existing model
- application example shows reasonable results
- comparison with experimental data in preparation
- parameter-identification strategy requires further development