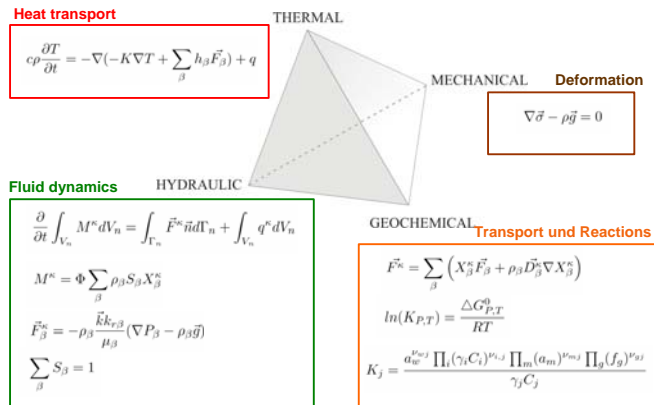


Coupled numerical THMC simulation of governing processes for CO₂ storage in saline formations



Sebastian Bauer
 Institute of Geosciences
 Christian-Albrechts-University Kiel
sebastian.bauer@gpi.uni-kiel.de

Acknowledgements

CO₂-MoPa



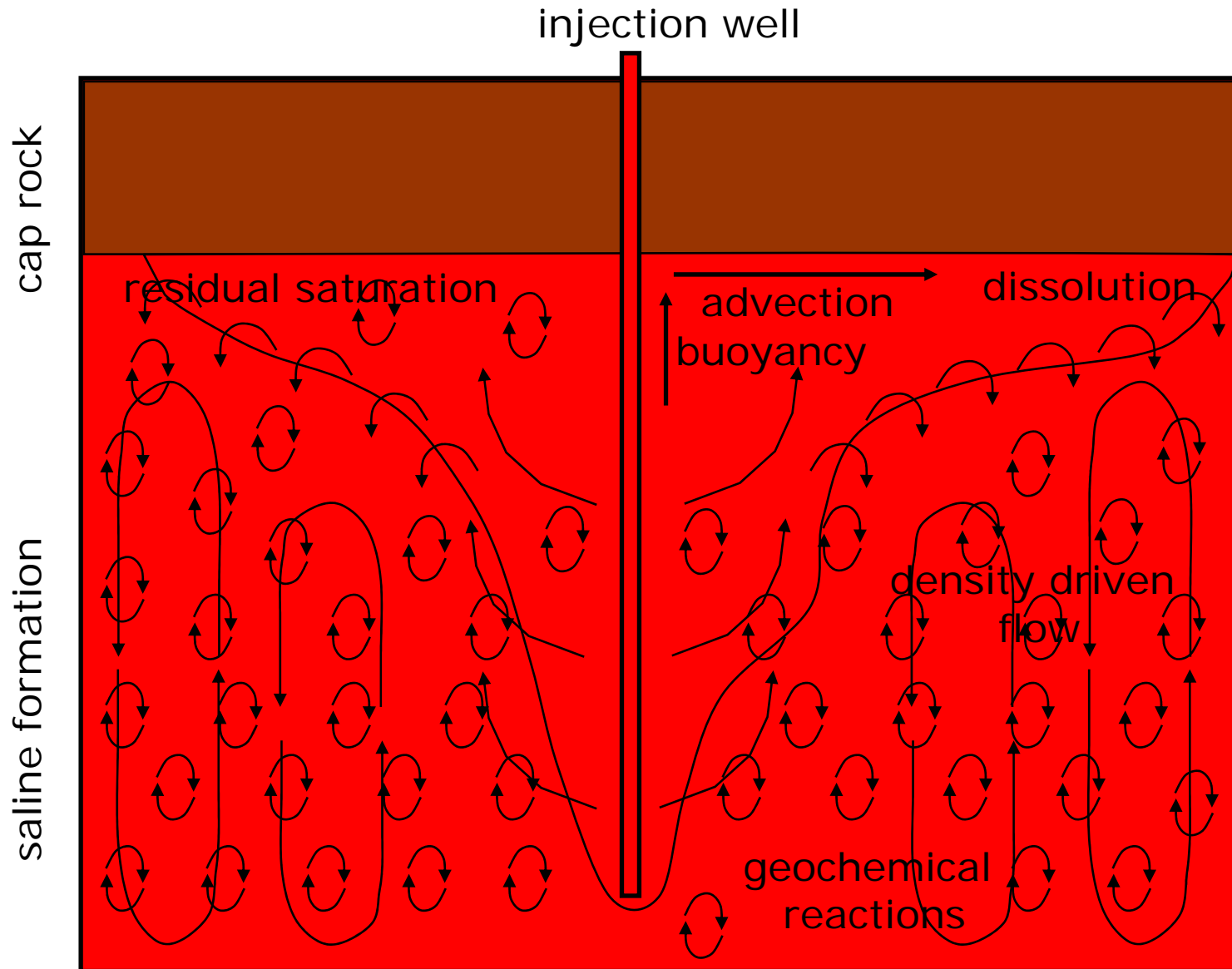
CLEAN



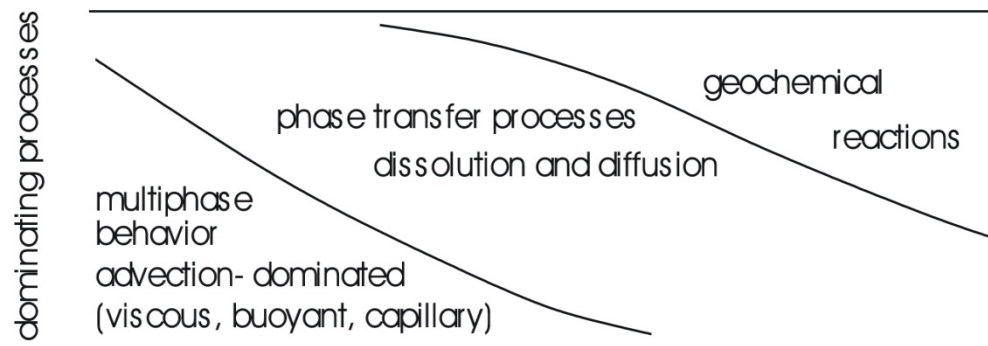
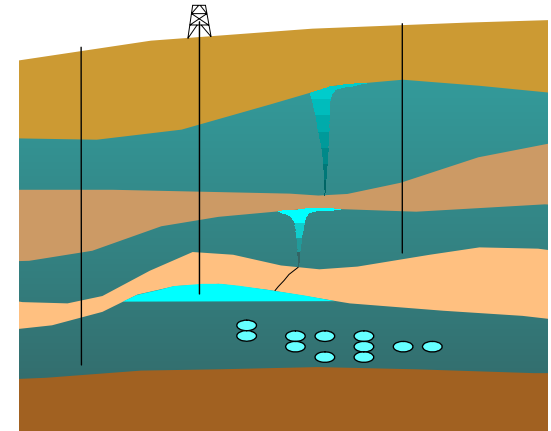
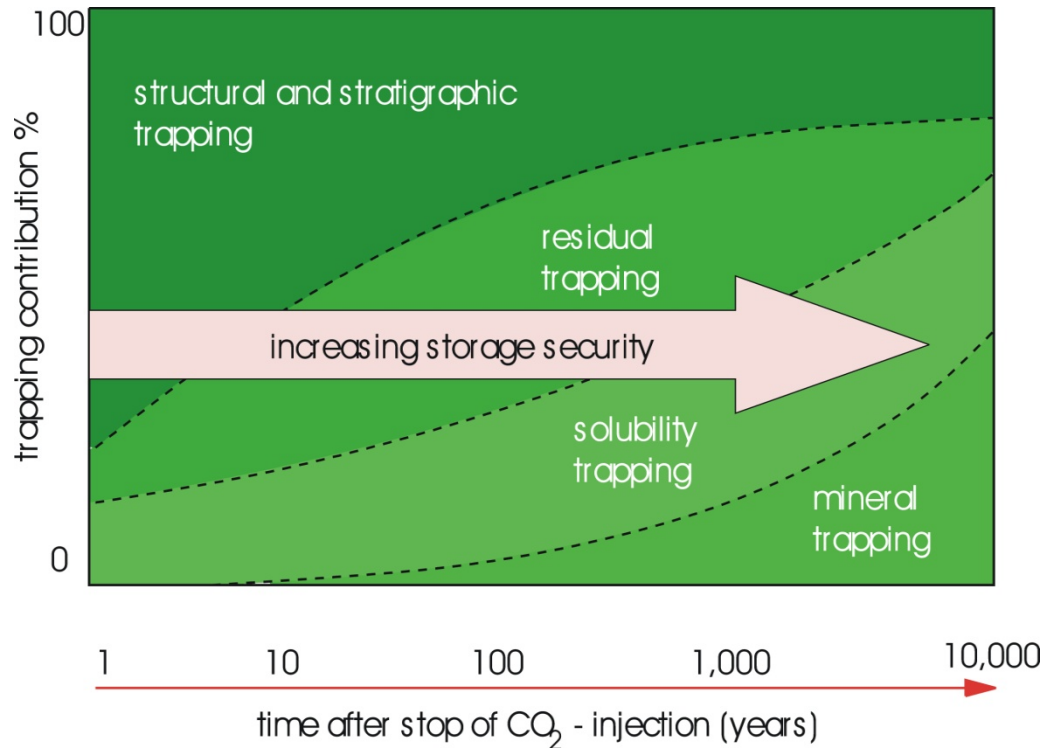
Work group contributors:

Katharina Benisch, Dedong Li, Bastian Graupner

- **Characterisation** of the reservoirs / saliniferous aquifers:
storage volume, cap rock, pressure - temperature –
geochemical parameter ranges
- **Risk analyses** Is CO₂-storage save ?
Will the environment be affected? If yes, how?
Migration out of the reservoir, geochemical change,
transport of trace elements,
lokal pH-changes, ...
- **Identification** and characterisation
of the governing processes and their interactions
- **Management** of the reservoir
sustainable development and optimal use
- **Dimensioning** and parameterisation

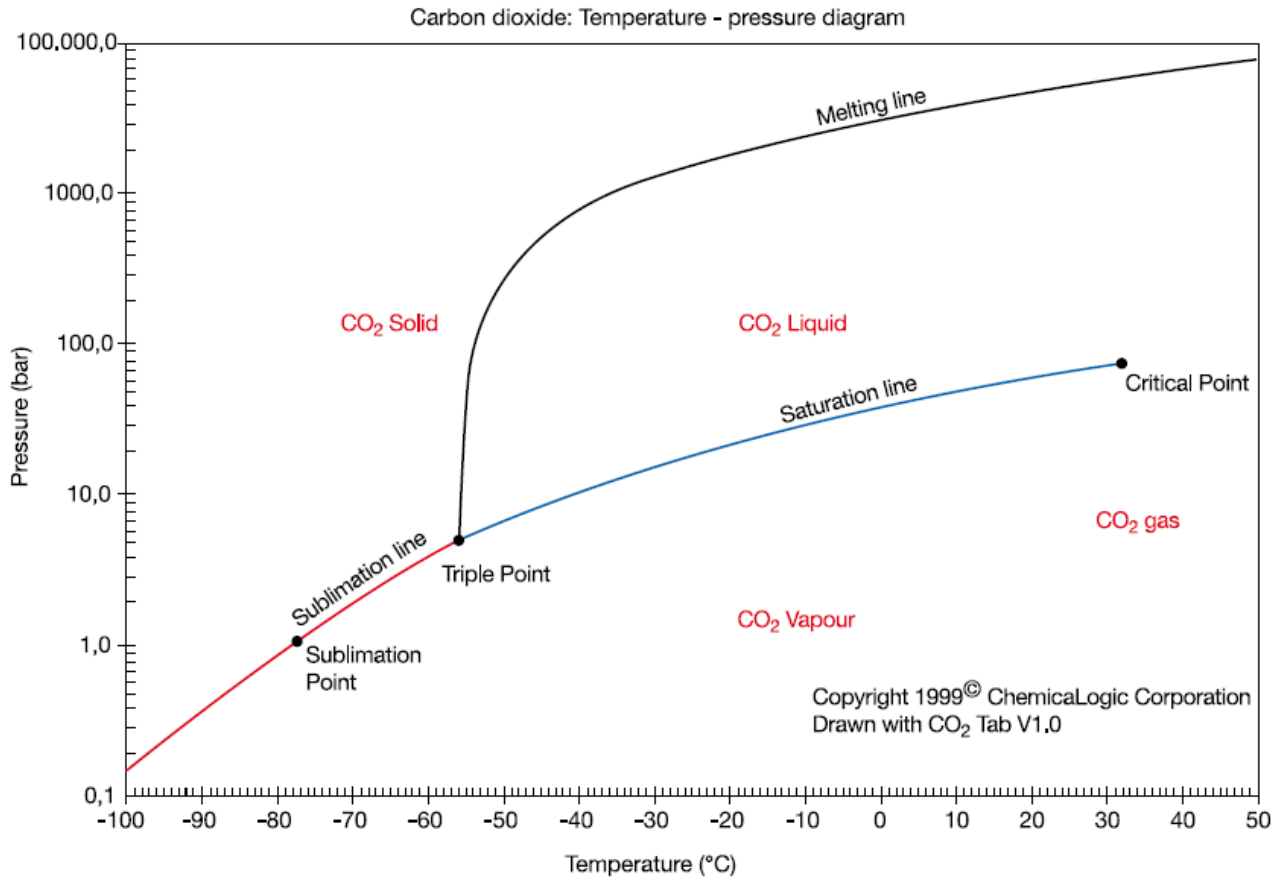


Time scales



IPCC - Report 2006,
H. Class, pers. Mitt.

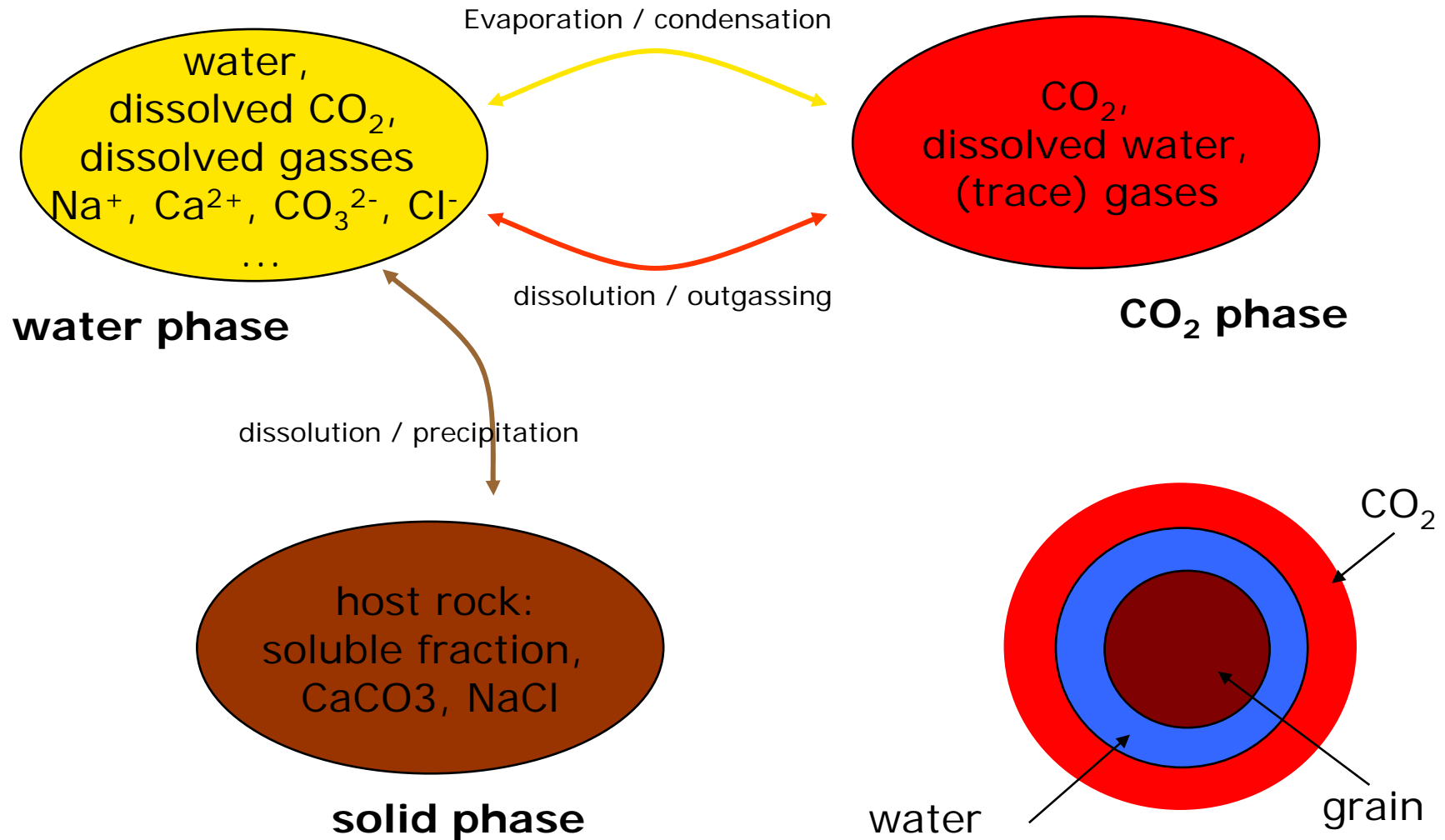
Properties of CO₂

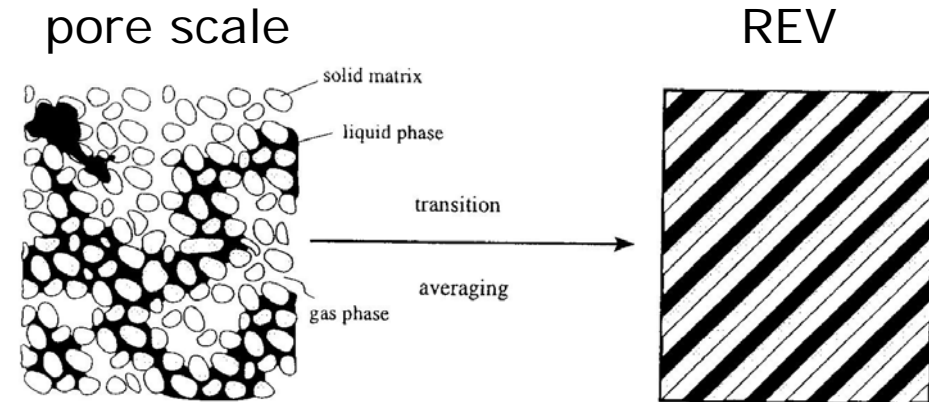
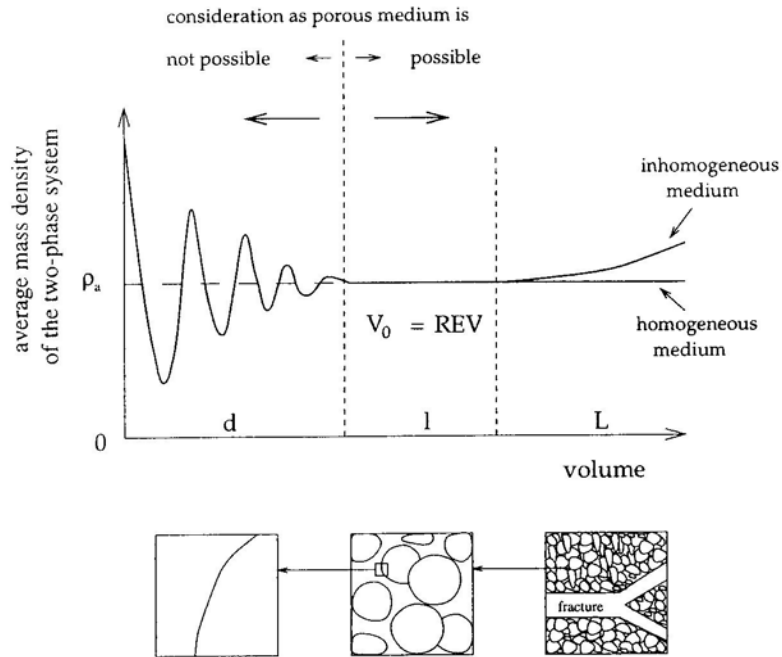


Critical Point:
73.8 bar, 30.95 °C

IPCC 2005

Multi-phase – multi-component approach





Helmig, 1997

Assumption:
Porous media

=> equivalent parameters
exist (n , k , ...)

Defininition of phase saturations:

$$S_{\text{CO}_2}, S_{\text{Water}}, S_{\text{solid}}$$

$$\sum S_i = 1$$

$$S_{\text{CO}_2} + S_{\text{Water}} = n = \text{porosity}$$

Liquid phase momentum conservation:

Generalized Darcy's law

$$\mathbf{v}_\alpha = -\frac{k_{r\alpha}k}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g)$$

Momentum + Mass conservation = phase balance equation

$$\frac{\partial(\rho_\alpha n S_\alpha)}{\partial t} - \nabla \cdot \left(\rho_\alpha \frac{k_{r\alpha}k}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g) \right) - q_\alpha \rho_\alpha = 0$$

$$\sum_{\alpha=1}^{\alpha=n_{phase}} S_\alpha = 1 \quad p_{c\alpha\beta} = p_\alpha - p_\beta = f(S_1, \dots, S_{n_{phase}})$$

Solid phase momentum conservation:

$$\nabla \vec{\sigma} - \rho \vec{g} = 0$$

Energy balance:

$$\frac{\partial(u\rho)}{\partial t} + \nabla \cdot (u\rho\mathbf{v}) + \nabla \cdot (p\mathbf{v}) - \nabla \cdot (\lambda\nabla T) = 0$$

u = internal energy
h = specific enthalpy
T = temperature

Mass balance of a component in a phase:

$$\frac{\partial(nS_\alpha\rho_\alpha X_\alpha^\kappa)}{\partial t} + \nabla \cdot (v_\alpha\rho_\alpha X_\alpha^\kappa - nS_\alpha D_{DD,\alpha}^\kappa \nabla(\rho_\alpha X_\alpha^\kappa)) - q_\alpha^\kappa = 0$$

X = mass fraction
 D_{DD} = dispersion

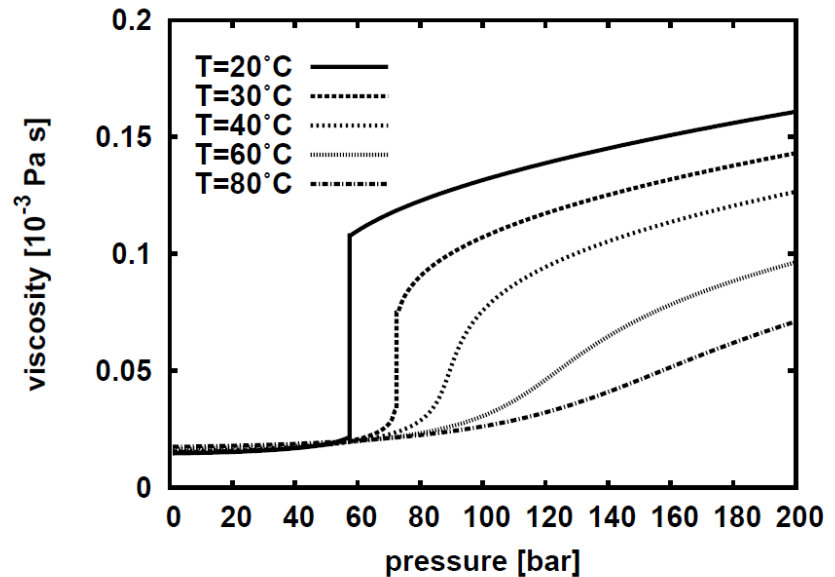
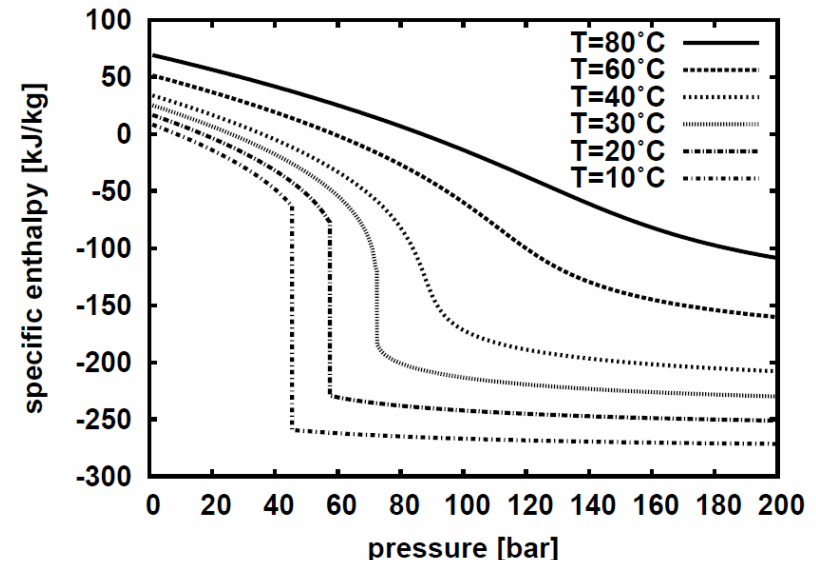
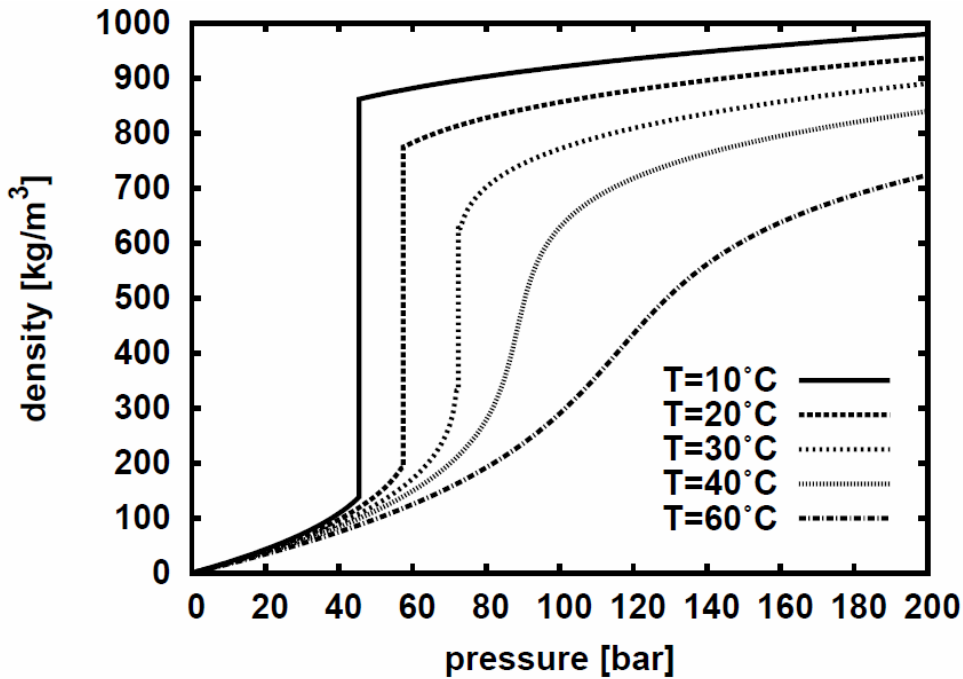
↑
reactions

Phase transfer of a component:

$$x_\alpha^\kappa = H_\alpha^\kappa p_g^\kappa \quad \text{equilibrium (Raoult, Henry)}$$

$$q_{\alpha\beta}^\kappa = k_{\alpha\beta}^\kappa (C_{\alpha,eq}^\kappa - C_\alpha^\kappa) \quad \text{kinetic}$$

Properties of CO₂

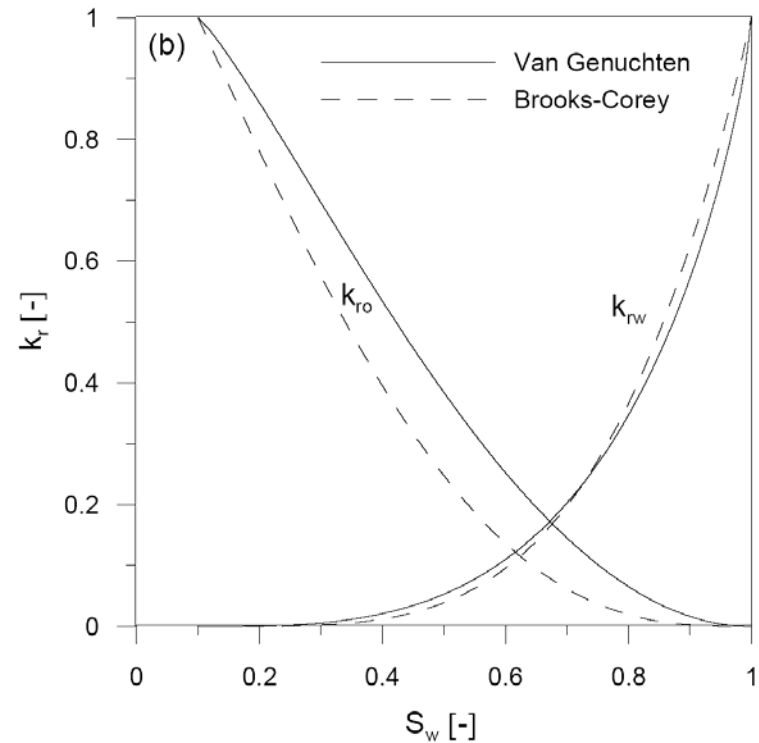
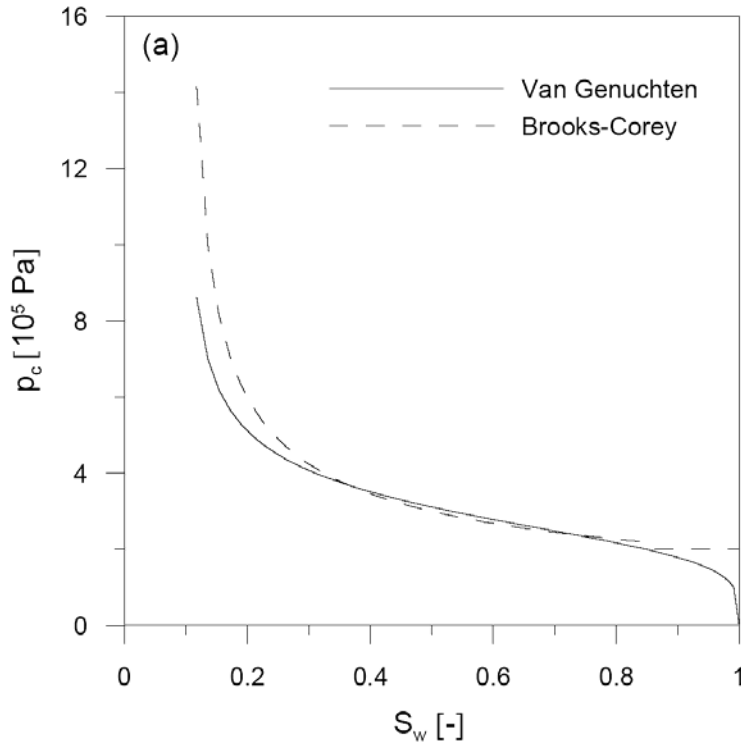


fluid properties as function
of reservoir conditions:
 $f = (P, T, S)$

Bielinski, 2007; Span und Wagner 1996;
Fenghour et al. 1998

Relative permeability k_r :

$$K_f = k_{r\alpha} k \frac{\rho_\alpha g}{\mu_\alpha}$$



p_c - S and k_r - S relationships according to Brooks-Corey and Van Genuchten versus saturation of the wetting phase

Helmig, 1997

Heat transport

$$\frac{\partial(u\rho)}{\partial t} + \nabla \cdot (u\rho\mathbf{v}) + \nabla \cdot (p\mathbf{v}) - \nabla \cdot (\lambda\nabla T)$$

THERMAL

MECHANICAL

Deformation

$$\nabla \vec{\sigma} - \rho \vec{g} = 0$$

HYDRAULIC

GEOCHEMICAL

Transport und Reactions

Fluid dynamics

$$\frac{\partial(\rho_\alpha n S_\alpha)}{\partial t} - \nabla \cdot \left(\rho_\alpha \frac{k_{r\alpha} k}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g) \right) - q_\alpha \rho_\alpha = 0$$

$$\sum_{\alpha=1}^{\alpha=n_{phase}} S_\alpha = 1$$

$$p_{c\alpha\beta} = p_\alpha - p_\beta = f(S_1, \dots, S_{n_{phase}})$$

$$\frac{\partial(n S_\alpha \rho_\alpha X_\alpha^\kappa)}{\partial t} + \nabla \cdot (v_\alpha \rho_\alpha X_\alpha^\kappa - n S_\alpha D_{DD, \alpha}^\kappa \nabla(\rho_\alpha X_\alpha^\kappa))$$

$$x_\alpha^\kappa = H_\alpha^\kappa p_g \quad - q_\alpha^\kappa = 0$$

$$K_m = \prod_i a_i^{\nu_i} = \exp\left(\frac{-\Delta G_0}{RT}\right)$$

$$r_m = k_{m, T_0} \left(\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right) A_m \left[1 - \frac{Q_m}{K_m} \right]$$

Fluid-phase balance

$$\begin{aligned}
 & n X_k^g \left(S^g \frac{\partial \rho^g}{\partial p^g} + S^l \frac{\partial \rho^l}{\partial p^l} \right) \frac{\partial p^g}{\partial t} \\
 & - \nabla \cdot \left(\rho^g X_k^g \frac{k_{rel}^g \mathbf{k}}{\mu^g} \nabla p^g \right) - \nabla \cdot \left(\rho^l X_k^l \frac{k_{rel}^l \mathbf{k}}{\mu^l} \nabla p^g \right) \\
 & + n \left(-\rho^g X_k^g + \rho^l X_k^l \right) \frac{\partial S^l}{\partial t} \\
 & + \underbrace{\left(S^g \rho^g + S^l \rho^l \right) \mathbf{m}^T \mathbf{L}}_{\text{MH coupling term}} \frac{\partial \mathbf{u}^s}{\partial t} \\
 & = Q_k \\
 & + \left(n S^l X_k^l \frac{\partial \rho^l}{\partial p^l} \right) \frac{\partial p_c}{\partial t} - \nabla \cdot \left(\rho^l X_k^l \frac{k_{rel}^l \mathbf{k}}{\mu^l} \nabla p_c \right) \\
 & - \nabla \cdot \left(\rho^g X_k^g \frac{k_{rel}^g \mathbf{k}}{\mu^g} \rho^g \mathbf{g} \right) + \nabla \cdot \left(\rho^l X_k^l \frac{k_{rel}^l \mathbf{k}}{\mu^l} \rho^l \mathbf{g} \right)
 \end{aligned}$$

Coupling via

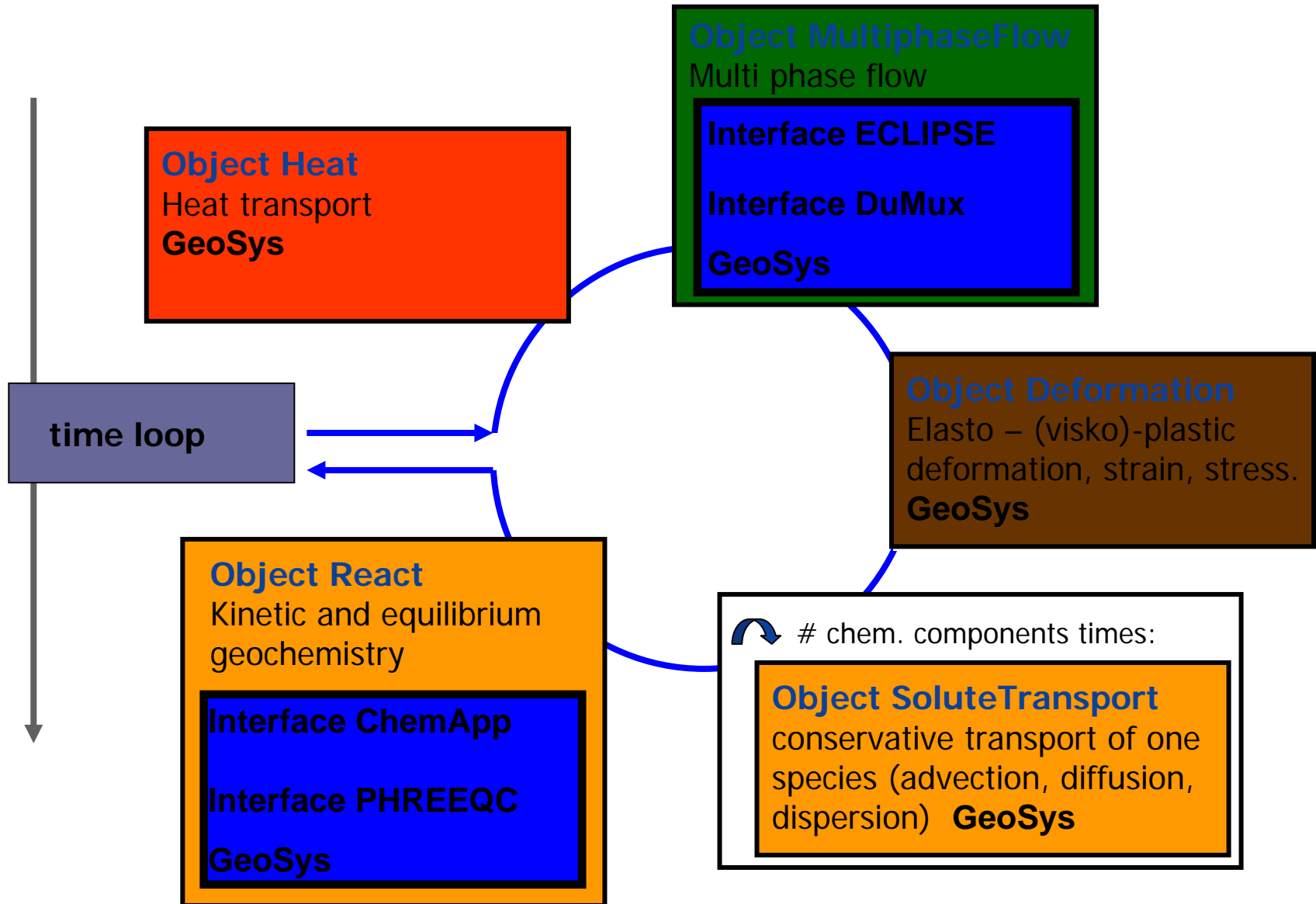
- coupling terms

- material parameters

Solid-phase balance

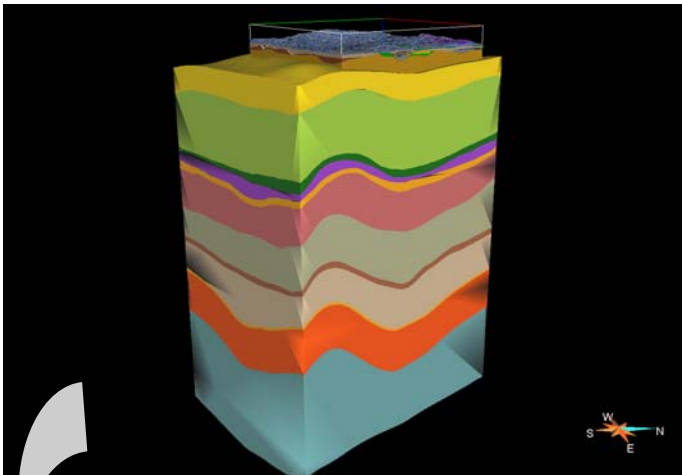
$$\nabla \cdot \left(\boldsymbol{\sigma} - \underbrace{\left(S^l p^l + S^g p^g \right) \mathbf{I}}_{\text{HM coupling term}} - \underbrace{\beta_T (T - T_0) \mathbf{I}}_{\text{TM coupling term}} \right) + \rho \mathbf{g} = 0$$

Coupled processes: Code structure

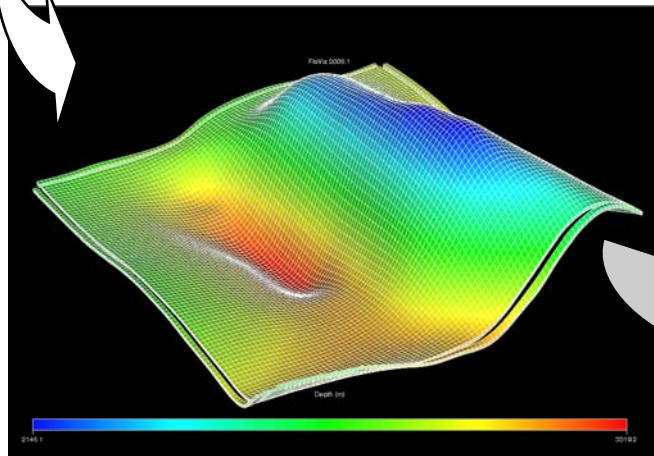


CO₂ storage simulation

Geological model



Heese et al (2010)



Heat transport THERMAL

$$\rho c_p \frac{\partial T}{\partial t} = -\nabla \cdot (-K \nabla T + \sum_i h_i \vec{F}_i) + q$$

Fluid dynamics HYDRAULIC

$$\frac{\partial}{\partial t} \int_{V_c} M^* dV_c = \int_{V_c} \vec{F}^* \cdot d\vec{T}_* + \int_{V_c} q^* dV_c$$

$$M^* = \phi \sum_i \rho_i S_i X_i^*$$

$$\vec{F}_i^* = -\rho_i \frac{k_{rel,i}}{\mu_i} (\nabla P_i - \rho_i \vec{g})$$

$$\sum_i S_i = 1$$

GEOCHEMICAL Transport und Reactions

$$\vec{F}^* = \sum_i (X_i^* \vec{F}_i^* + \rho_i \mu_i^* \nabla X_i^*)$$

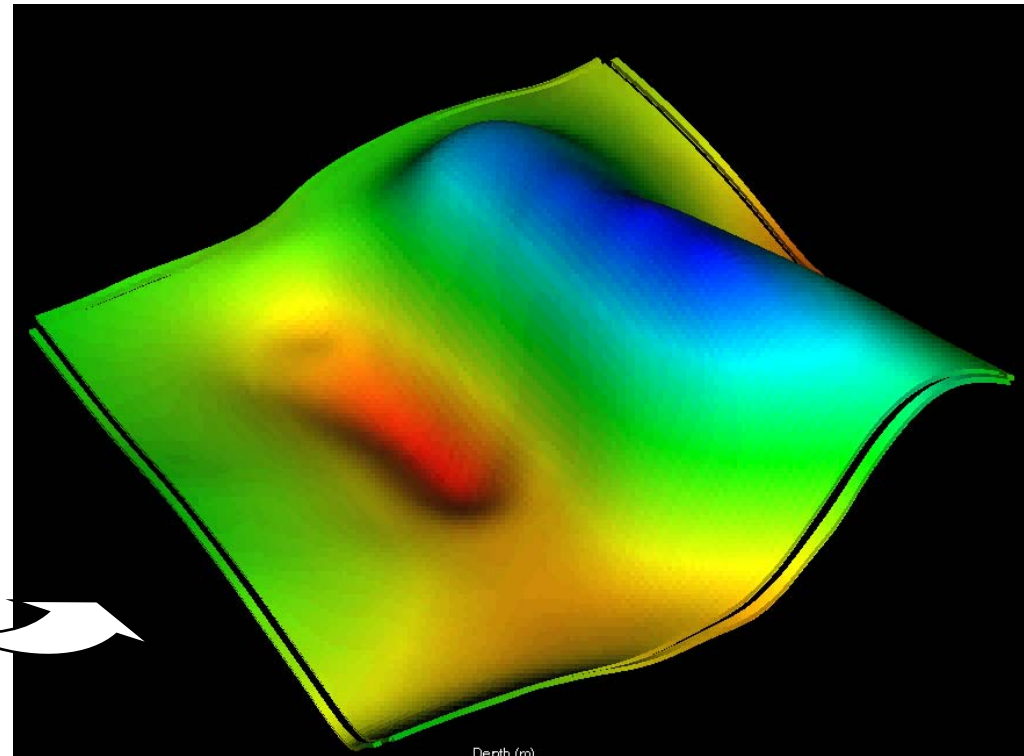
$$\ln(K_{rx}) = \frac{\Delta G_{rx}^*}{RT}$$

$$K_j = \frac{a_{Ca}^{2+} \prod_i (\gamma_i C_i)^{\nu_i} \prod_m (a_m)^{\nu_m} \prod_l (f_l)^{\nu_l}}{\gamma_j C_j}$$

MECHANICAL Deformation

$$\nabla \cdot \vec{\sigma} - \rho \vec{g} = 0$$

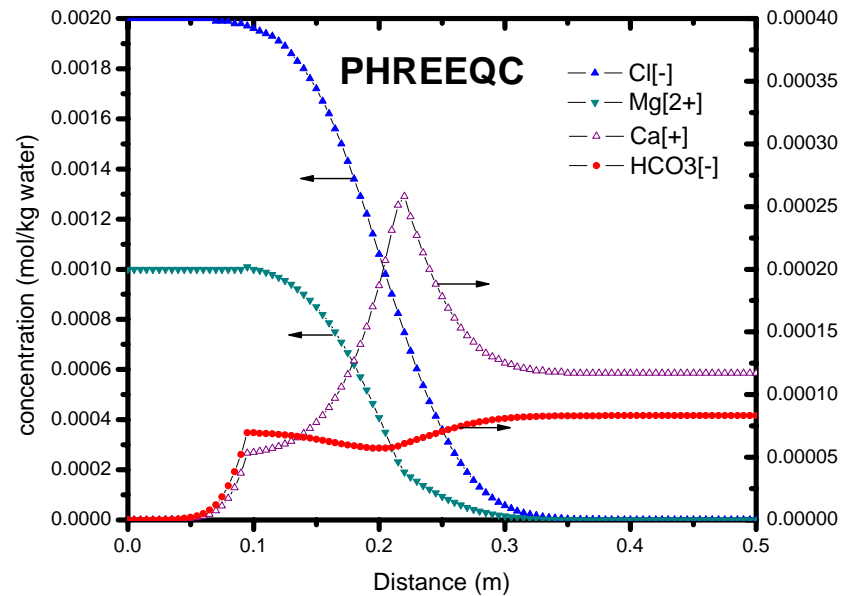
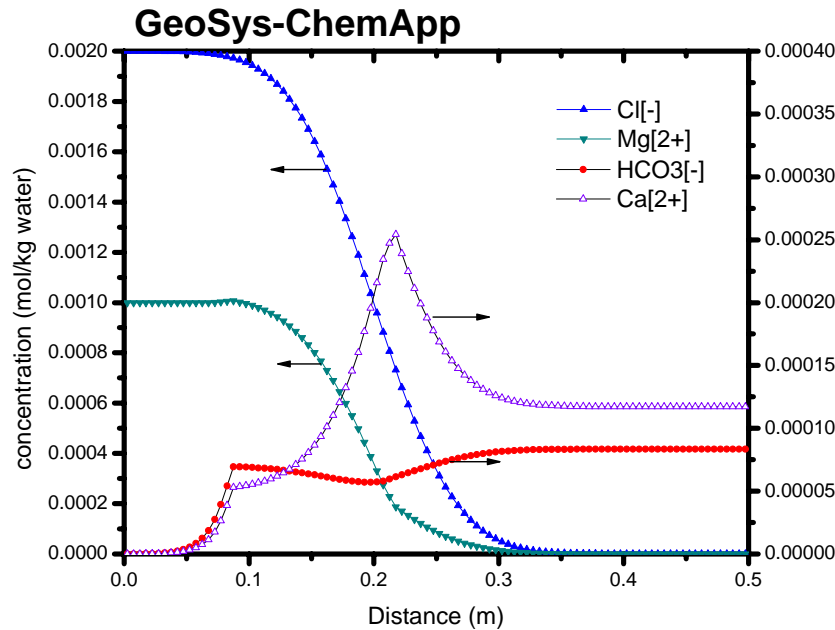
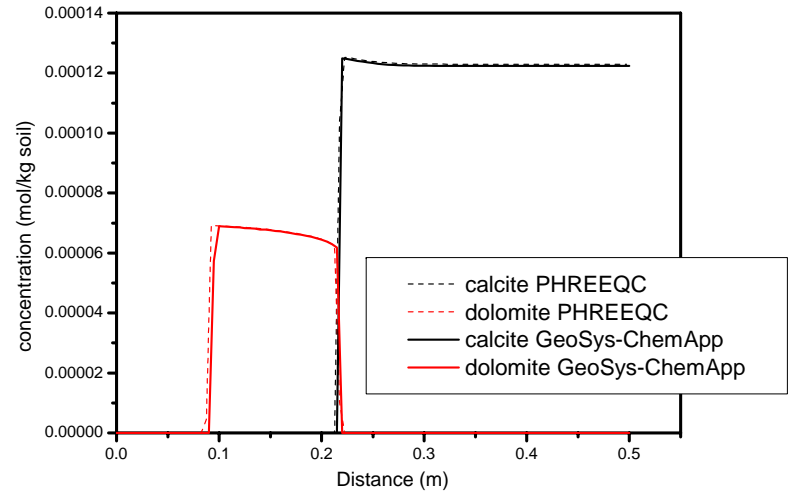
Numerical process model



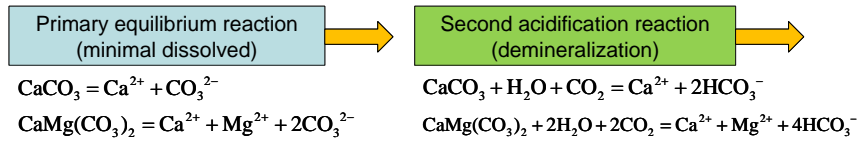
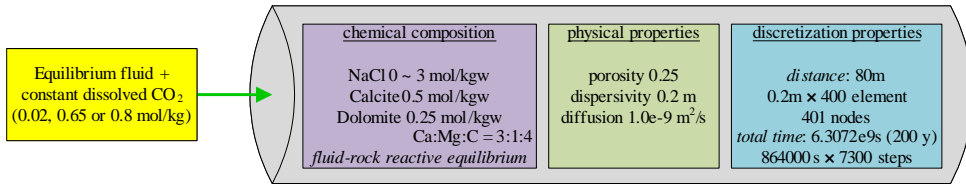
Verification: 1D reactive transport model

GeoSys/ChemApp
versus
PHREEQC

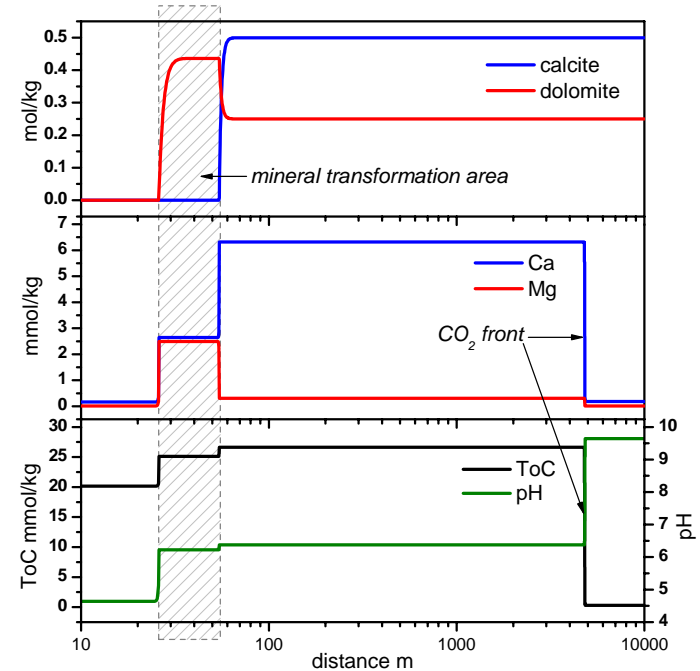
Benchmarking!



1D transport simulation



Component profiles



Geochemical feedback: Porosity change

25% -> 25.2% -> 25.87%

Carbonate fraction solid phase: 1.15%

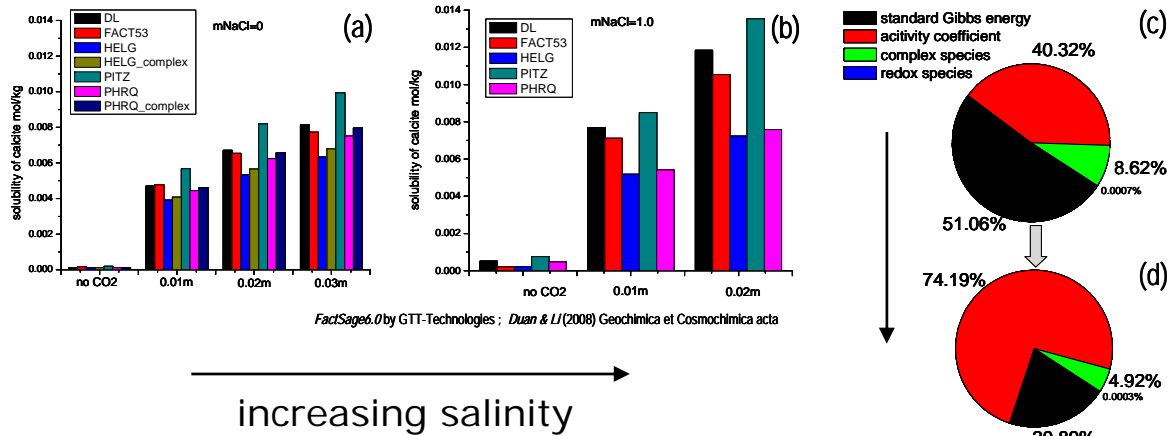
Carbonate fractions of 5 / 10% would yield porosity increases to 28.5 / 32.5%

Porosity dependent permeability: $k(n)$ (e.g. Kozeny-Carman, Fair-Hatch)

Geochemical parameters and uncertainty

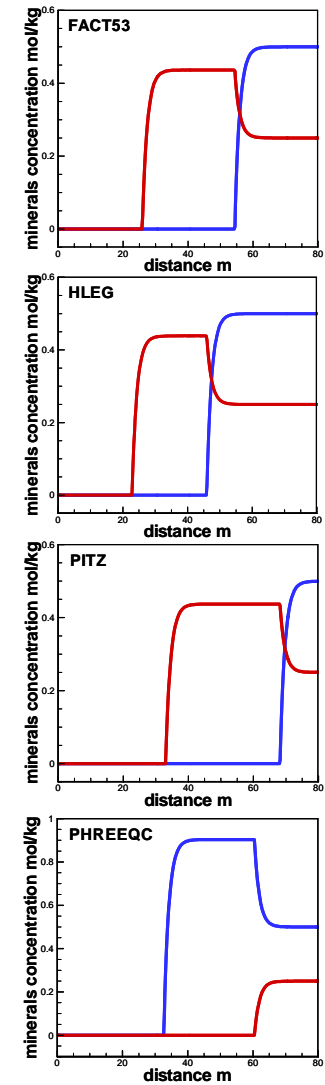
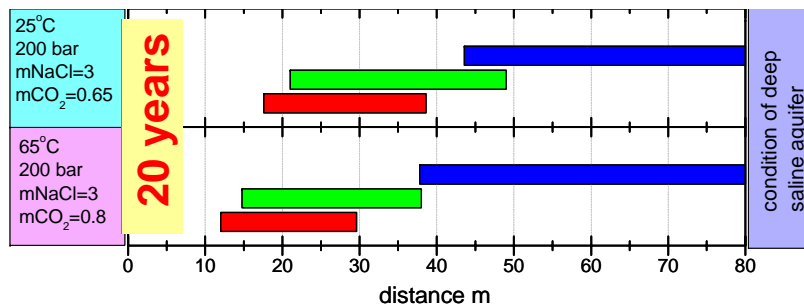
Equilibrium constant $K = K(P, T, S)$

Calcite solubility for different data bases



increasing salinity

Mineral transformation zone variability



- Need for coupled (numerical) simulations for investigating effects of CO₂ injection in the subsurface
- Parameters need to cover the P-T-S range given by the reservoir conditions
- Specifically adapted mathematical methods required
- Numerical modelling tool have to be improved, and benchmarked
- Interaction of coupled processes and material parameters needs to be investigated
- Integration of scales of individual processes – mm to km

Thank you for your attention

