Reliability of numerical models for simulating CO_2 storage in deep geological formations

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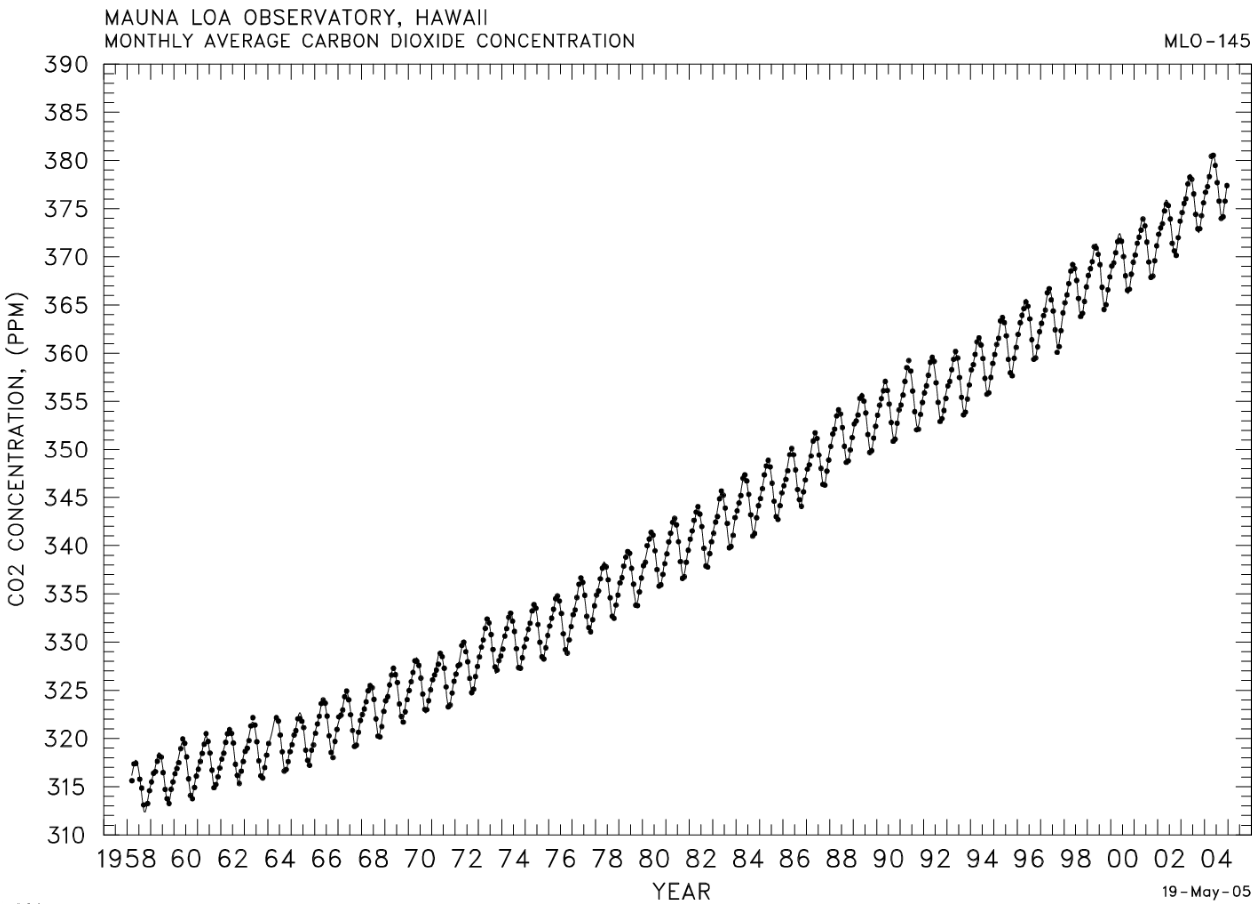
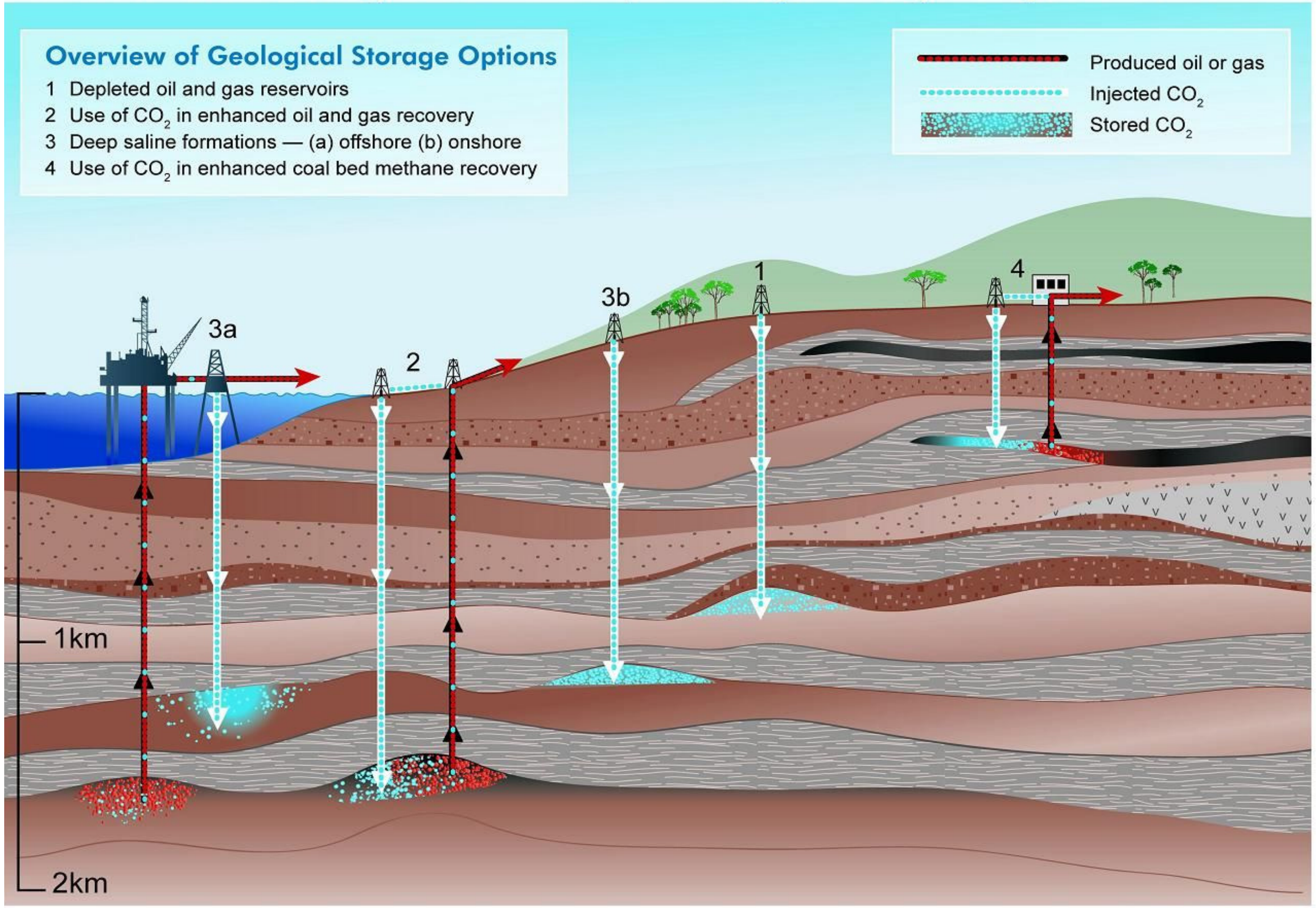
Atmospheric CO_2 Concentration

Increase in atmospheric CO_2 concentration is causing global climate change since CO_2 is a greenhouse gas.

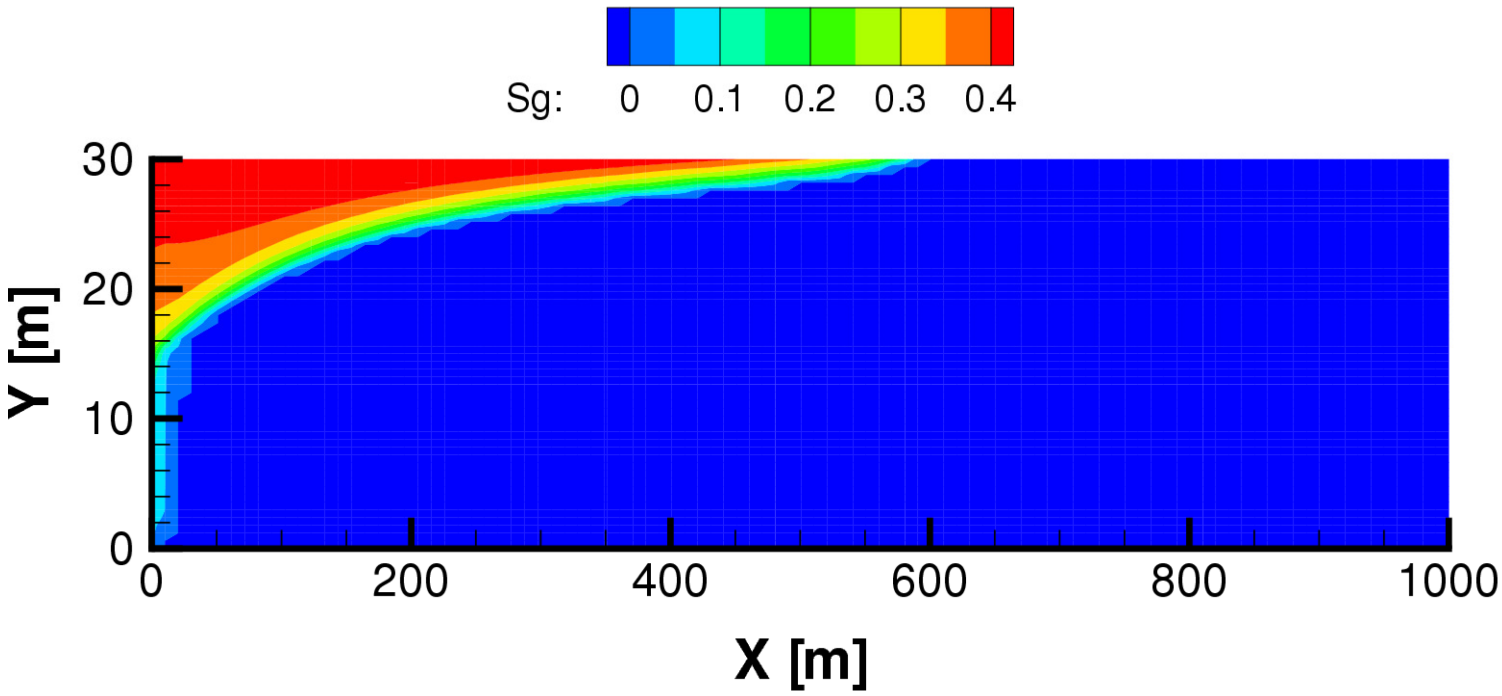


Keeling & Whorf, 2005

Geological Storage Options



CO2-injection



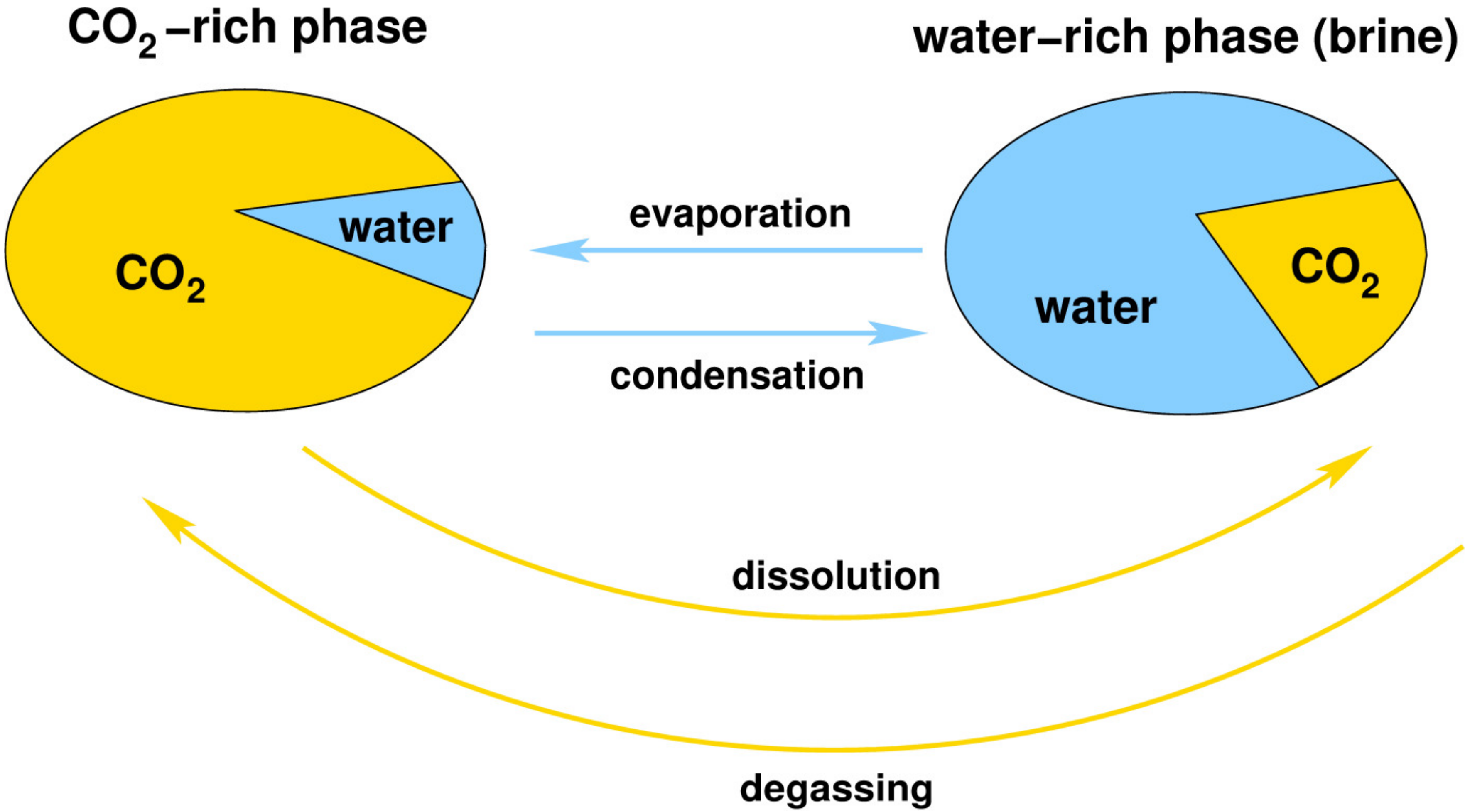
- Interface depends on injection rate, aquifer structure and fluid properties (viscosities, densities).

Model: Main Assumptions

General assumptions

- Slow velocities (Reynolds number < 1)
- Local thermodynamical equilibrium
  - thermal
  - mechanical
  - chemical
- Rock matrix is rigid
  - porosity $\phi = f(\mathbf{x}),\ \phi \neq f(t)$
  - permeability $\mathbf{K} = f(\mathbf{x}),\ \mathbf{K} \neq f(t)$

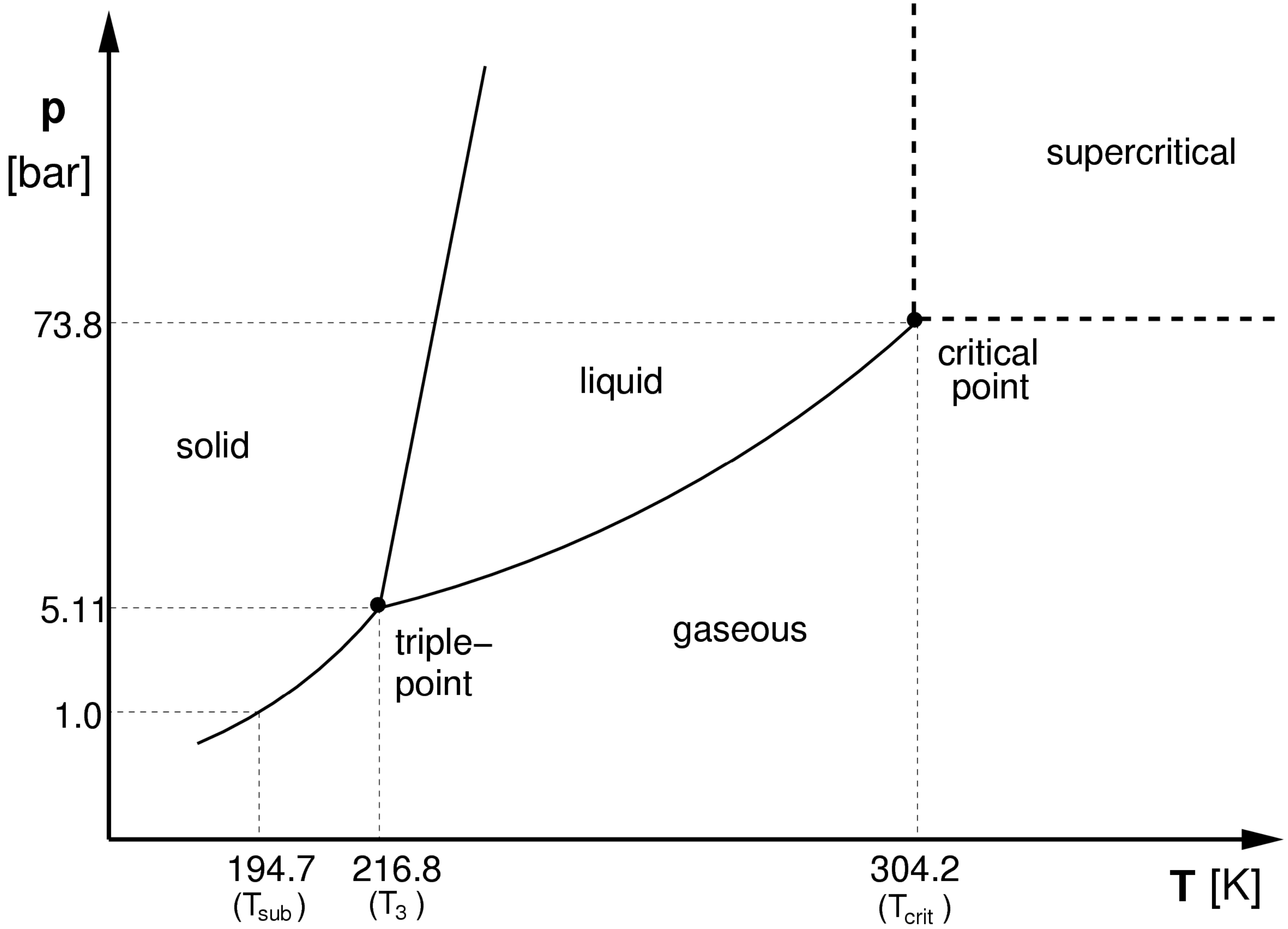
Model Concept: Two-Phase Two-Component



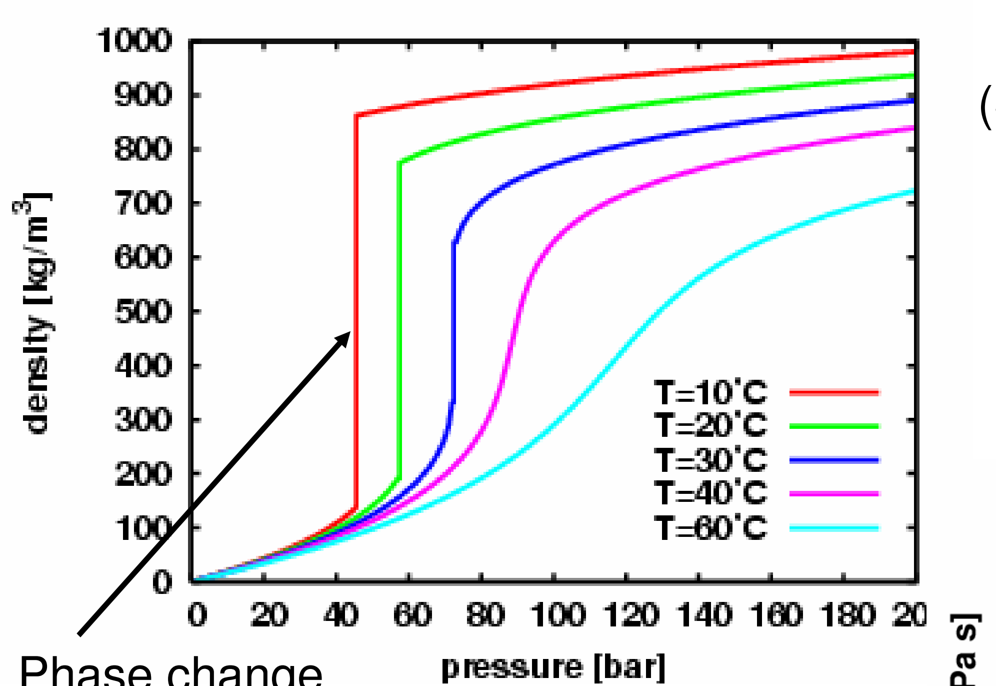
Model Assumptions

- Two fluid phases in a rigid rock matrix: CO_2 and brine
- Salinity influences brine fluid properties but does not change with time $S = f(\mathbf{x}),\ S \neq f(t)$
- Diffusion only in the brine phase
- Multi-phase behavior is taken into account by
  - Capillary pressure-saturation relationships $p_c = f(S_\alpha, \mathbf{x})$
  - Relative permeability-saturation relationship $k_{r\alpha} = f(S_\alpha, \mathbf{x})$
- No chemical reactions with rock matrix and no geomechanical effects

CO_2 Phase Diagram

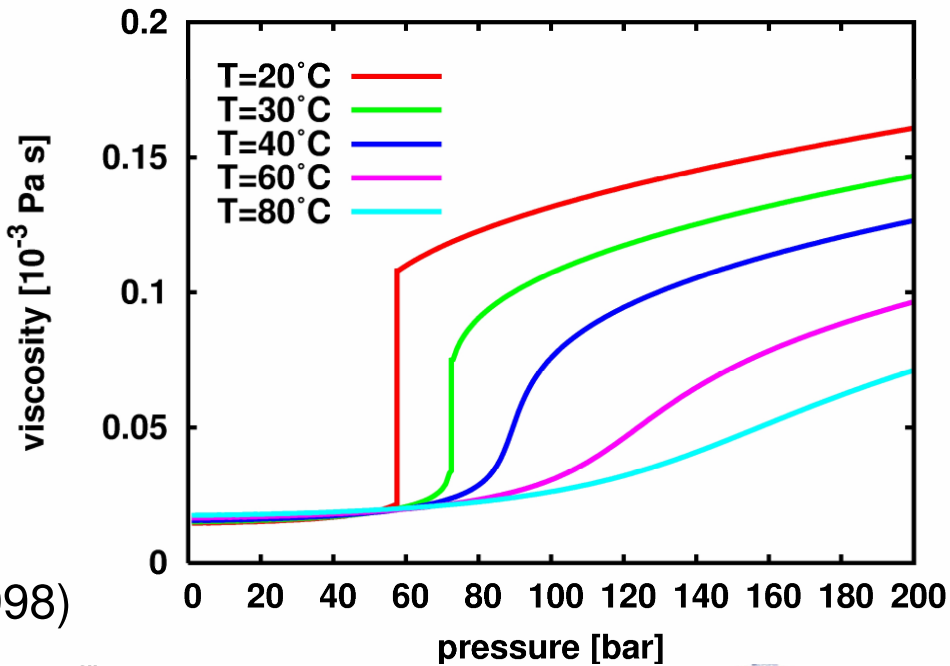


Density and viscosity of CO_2



Phase change

(Span & Wagner, 1996)



(Fenghour et al, 1998)

Model: Mass Balance Equations

$$\underbrace{\phi \frac{\partial(\sum_\alpha \rho_\alpha X_\alpha^C S_\alpha)}{\partial t}}_{\text{storage}}$$

$$-\underbrace{\sum_\alpha \nabla \cdot \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \rho_\alpha X_\alpha^C \mathbf{K} (\nabla p_\alpha - \rho_\alpha \mathbf{g}) \right\}}_{\text{advective transport}}$$

$$-\underbrace{\nabla \cdot \left\{ D_{pm}^C \rho_b \nabla X_b^C \right\}}_{\text{diffusive transport}}$$

$$-\underbrace{q^C}_{\text{source/sink}} = 0 \qquad C \in \{w, CO2\},\ \alpha \in \{b, CO2\}$$

Two mass balance equations

for components CO_2 and water

Model: Energy Balance Equation

$$\underbrace{\phi \frac{\partial \left(\sum_\alpha \rho_\alpha u_\alpha S_\alpha\right)}{\partial t} + (1-\phi)\frac{\partial \rho_s c_s T}{\partial t}}_{\text{storage}}$$

$$-\underbrace{\nabla \cdot \left(\lambda_{\text{pm}} \nabla T\right)}_{\text{heat conduction}}$$

$$-\underbrace{\sum_\alpha \nabla \cdot \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \rho_\alpha h_\alpha \mathbf{K} \left(\nabla p_\alpha - \rho_\alpha \mathbf{g}\right) \right\}}_{\text{heat transport due to advection}}$$

$$-\underbrace{\sum_C \nabla \cdot \left\{ D^C_{\text{pm}} \rho_b h^C_b \nabla X^C_b \right\}}_{\text{heat transport due to diffusion}} - \underbrace{q^h}_{\text{source/sink}} = 0$$

One energy balance equation,

assumption: local thermal equilibrium

Numerical Model

- Time discretization: fully implicit Euler scheme
- Space discretization: BOX-method, node-centered finite volume method (locally mass conservative, unstructured grid)
- Linearization: Newton-Raphson method
- Several linear solvers available (e.g. Multigrid)
- Model runs parallel

Model testing – validation/verification

The model is running – what‘s next??

Apply it to the field-scale, solve the problems and produce colorful pictures ← *the self-confident way*

or

the self-critical way → Develop a strategy to improve the confidence in the model and then go to the field-scale

Model testing – validation/verification

Why should there be doubts concerning reliability?

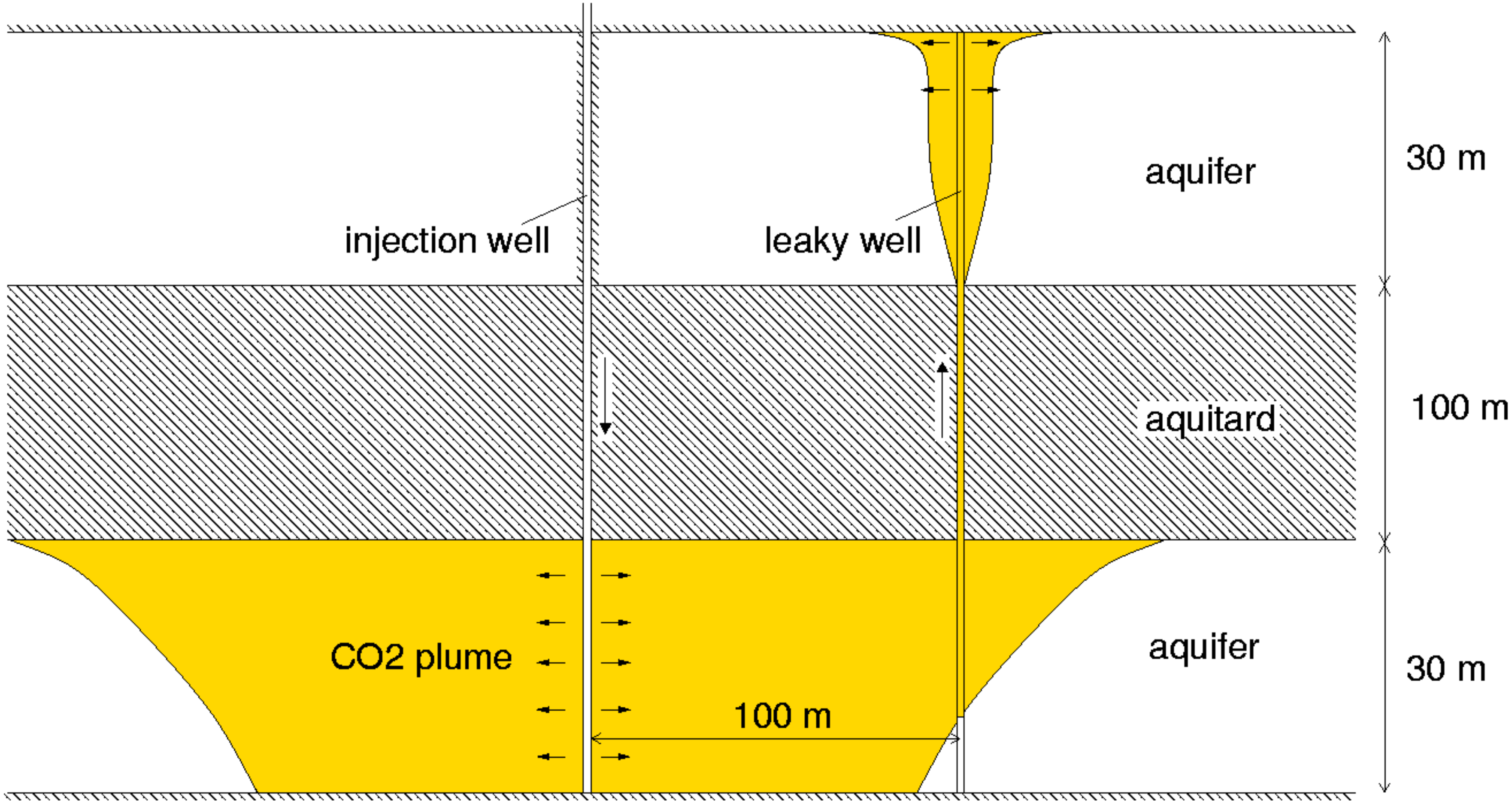
- Capillary pressure and relative permeabilities
- Fluid properties (density, viscosity, enthalpy)
- Phase behavior (dissolution, evaporation)
- Influence of other components (e.g. salt, non-pure CO2, etc.)
- Justification of the model assumptions

- Mathematical and numerical solution methods (discretization, meshing, etc.)
- …?

Benchmark Example

- CO_2 injection into an aquifer,
- subsequent plume evolution and
- leakage through an abandoned/leaky well.

Benchmark Example



Leakage scenario from *Nordbotten et al. 2005*

Simulation(1)

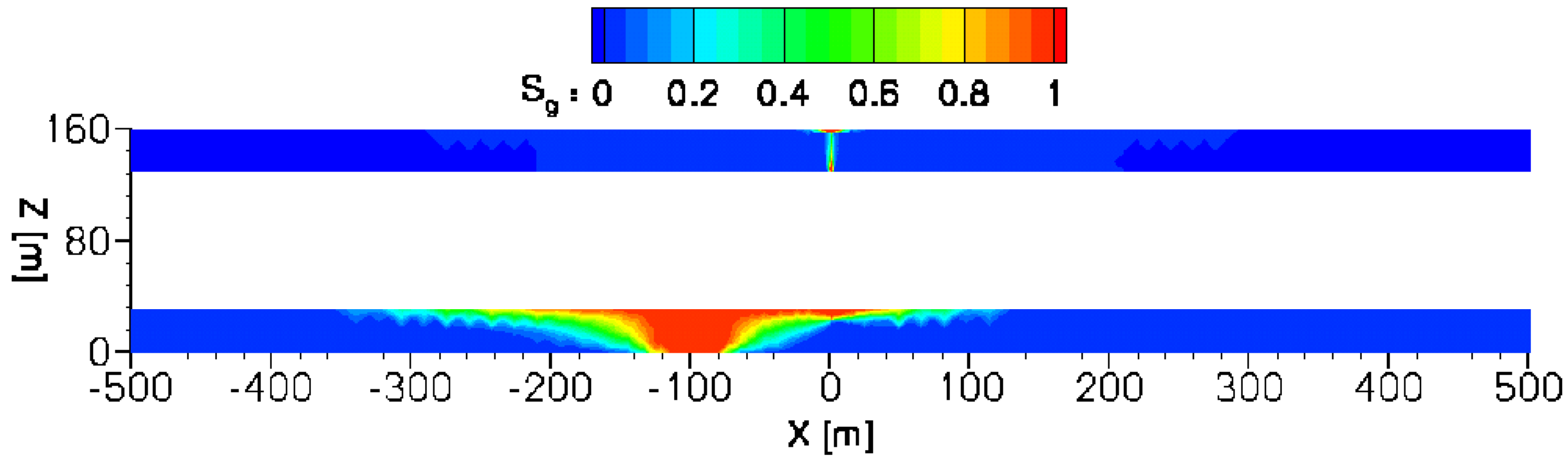
Comparison of numerical simulation
with semi-analytical solution (by *Nordbotten et al. 2005*)

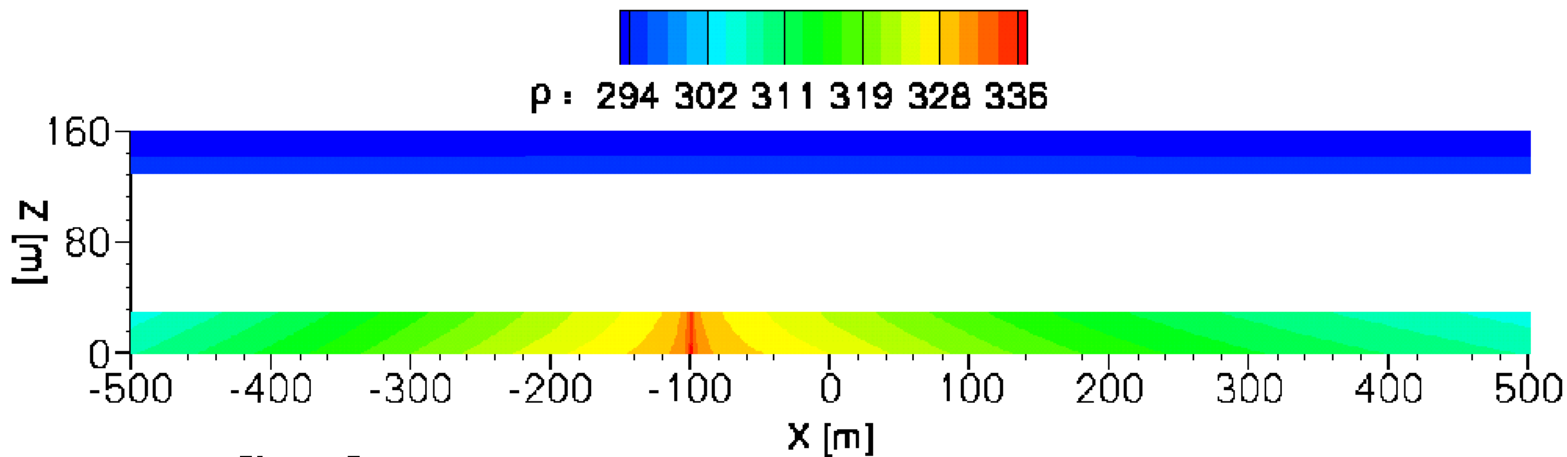
- Domain dimensions: 1000 m x 1000 m x 160 m
- Aquifer permeability: 20 mD
- CO_2 injection rate: 8.87 kg/s
- Distance between wells: 100 m

- ***Aquifer depth: Between 2840 m and 3000 m***
- ***Constant fluid properties; isothermal; no dissolution***

Simulation(1) : Results

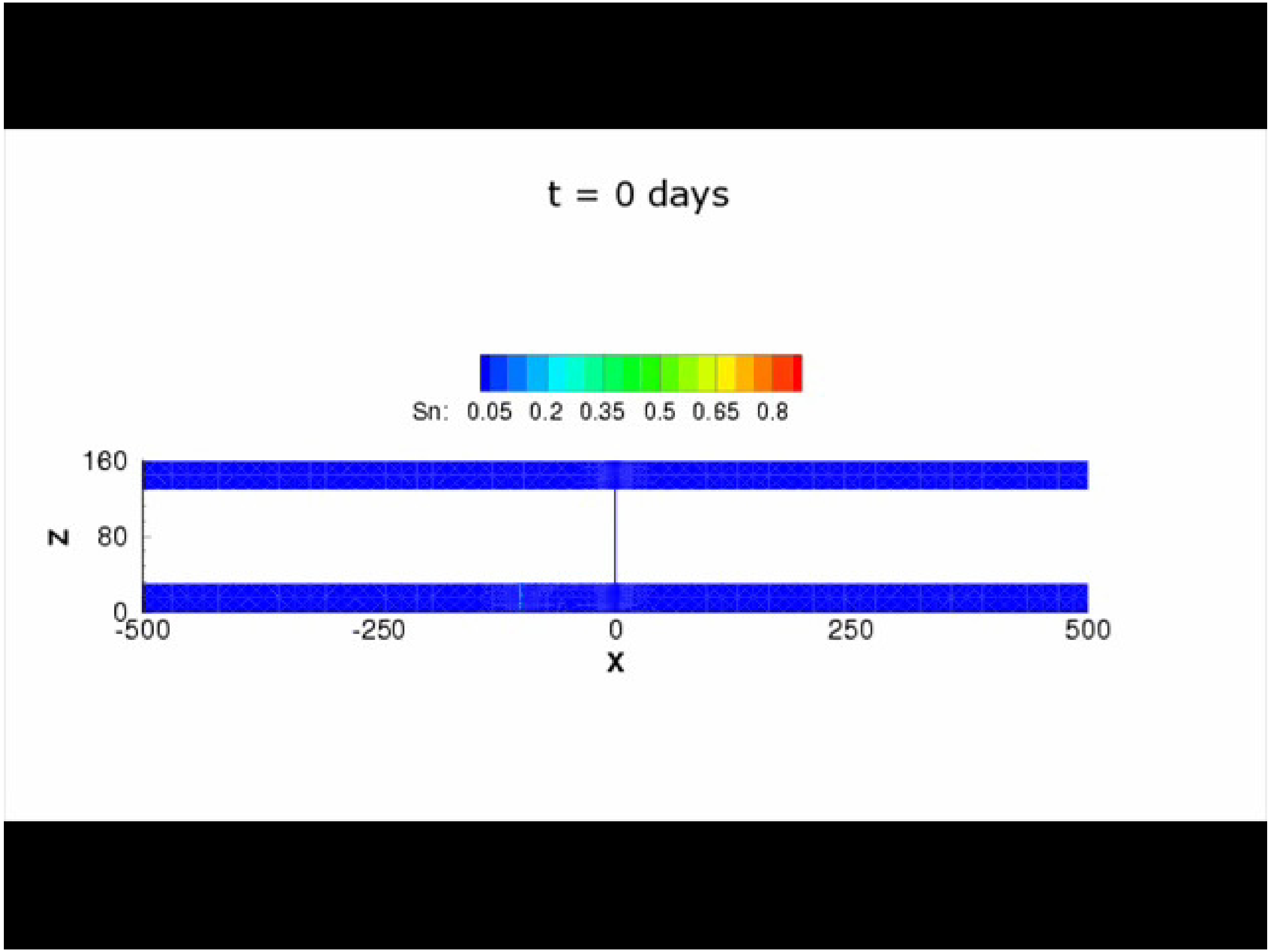
Saturation





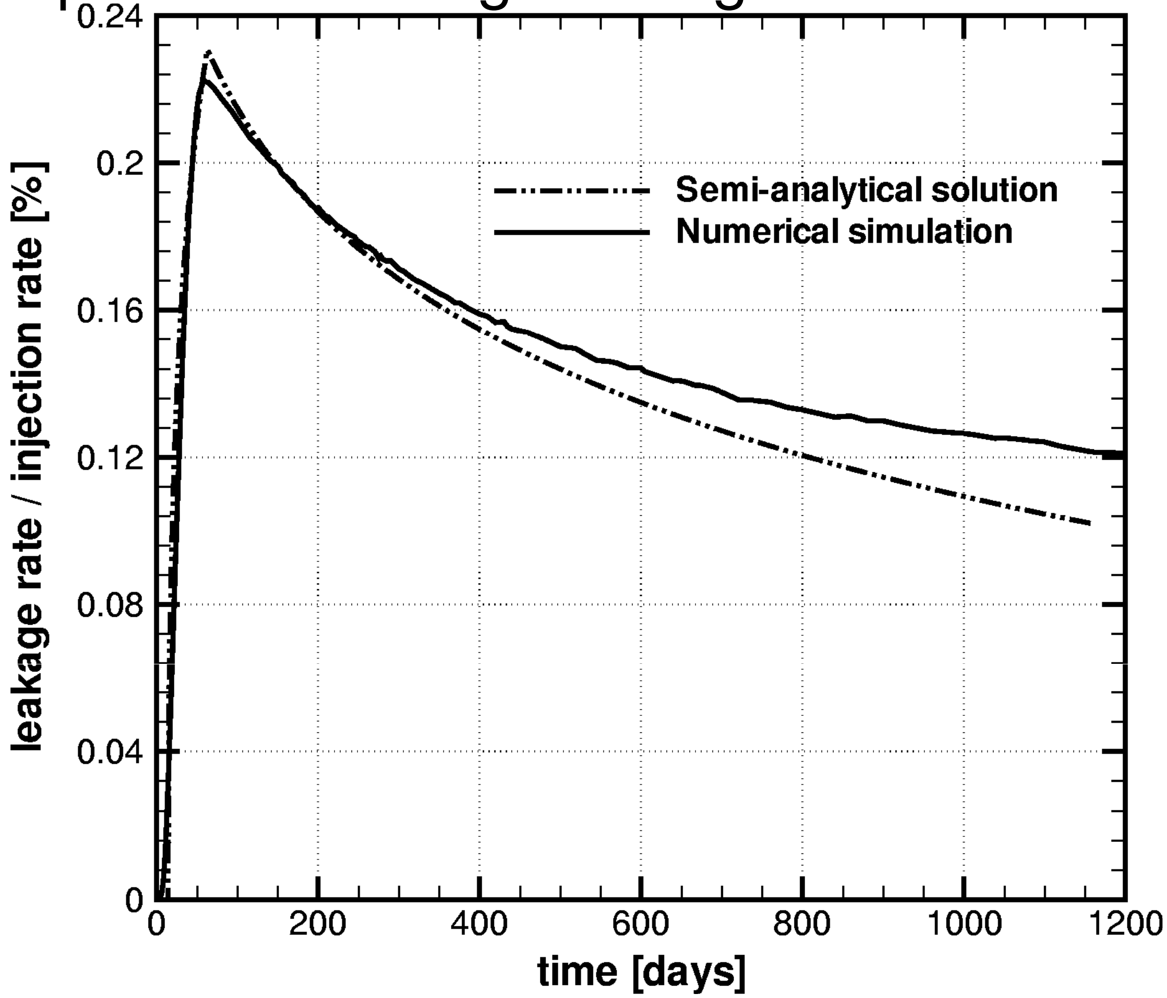
Pressure [bar]

Simulation (1): Results



Simulation(1): Results

Comparison: Leakage through abandoned well



Ebigbo et al., 2006 (Computational Geosciences)

Simulation(2)

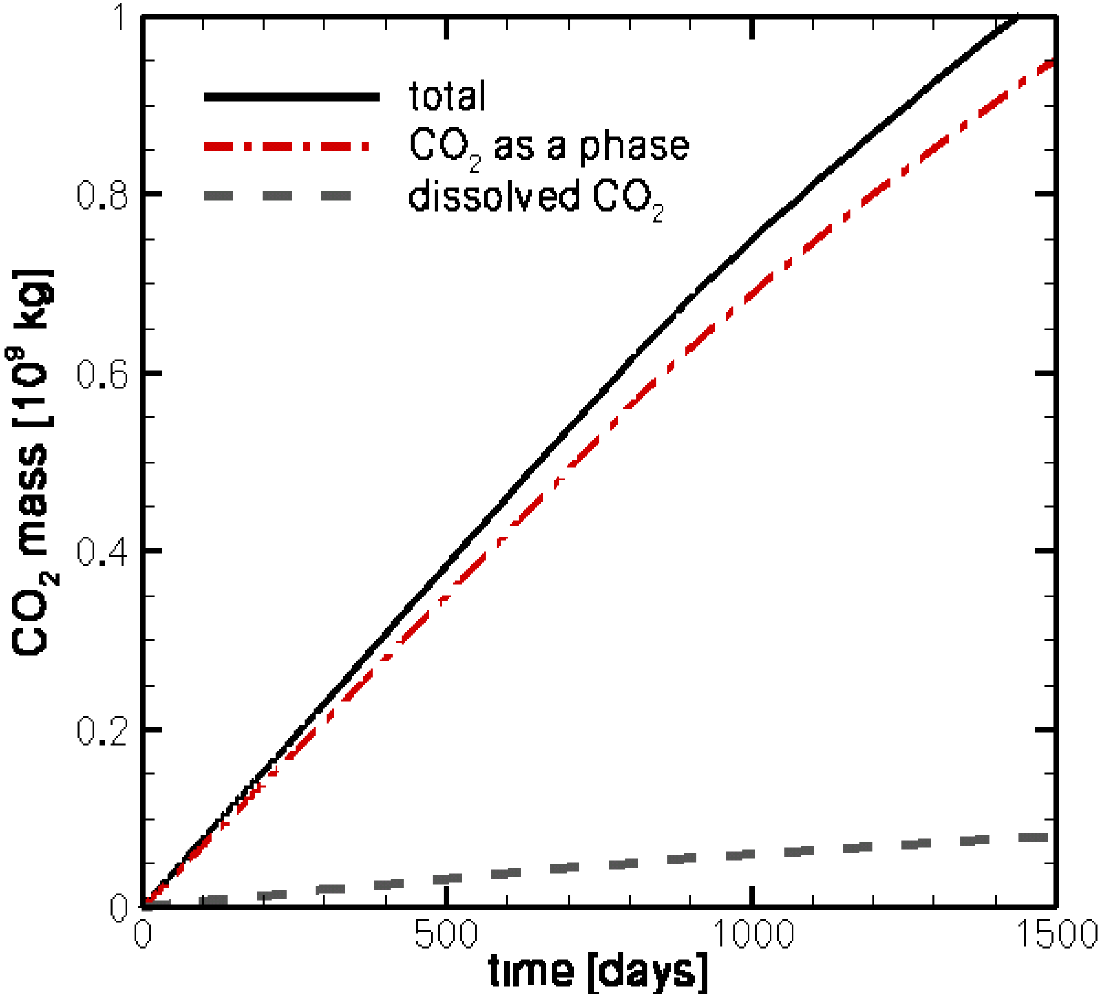
Including dissolution and thermal effects

- Domain dimensions: 1000 m x 1000 m x 160 m
- CO_2 injection rate: 8.87 kg/s
- Distance between wells: 100 m

- **Aquifer depth: Between 640 m and 800 m**
- **Fluid properties depend on *T, p* and phase composition; non-isothermal; CO_2 can dissolve in brine**

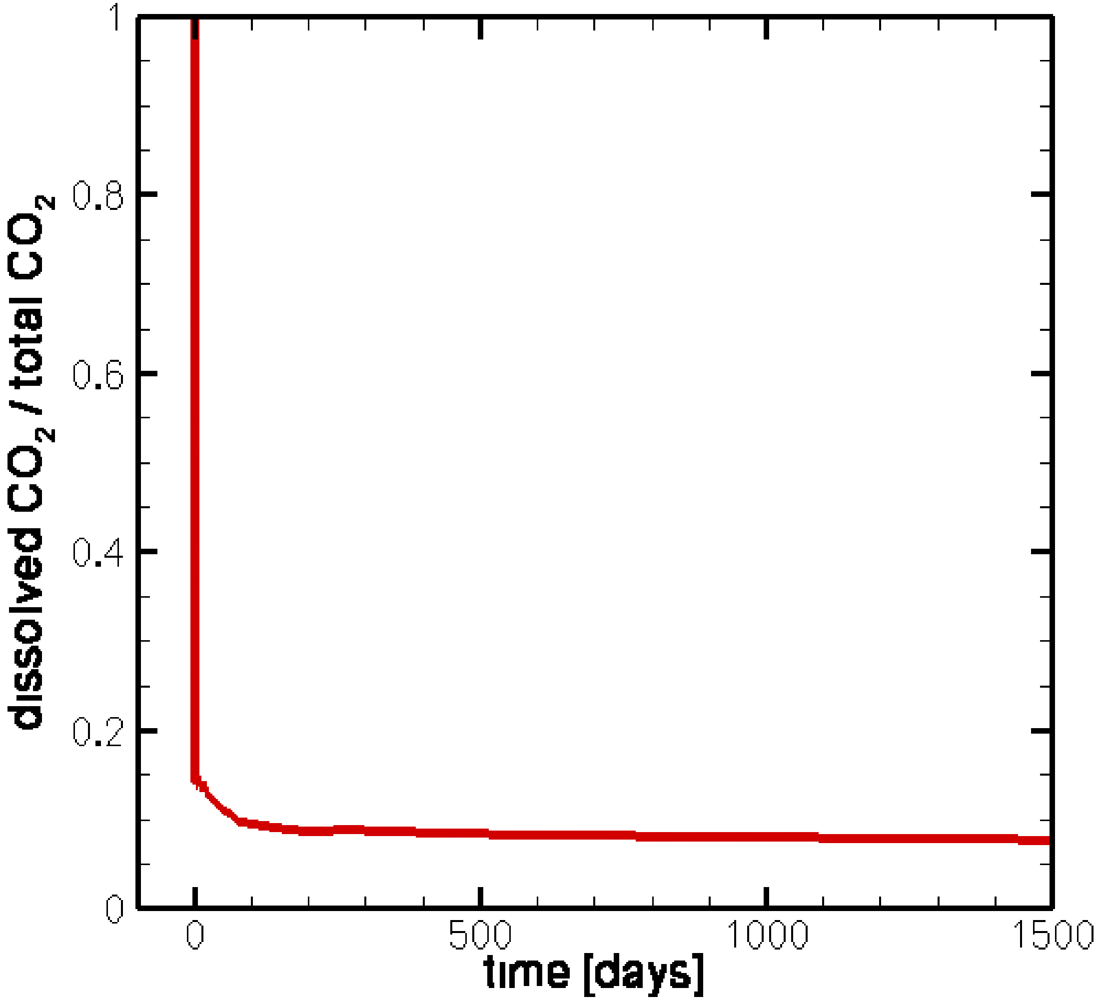
Simulation(2): Results

Mass of injected CO_2 in domain

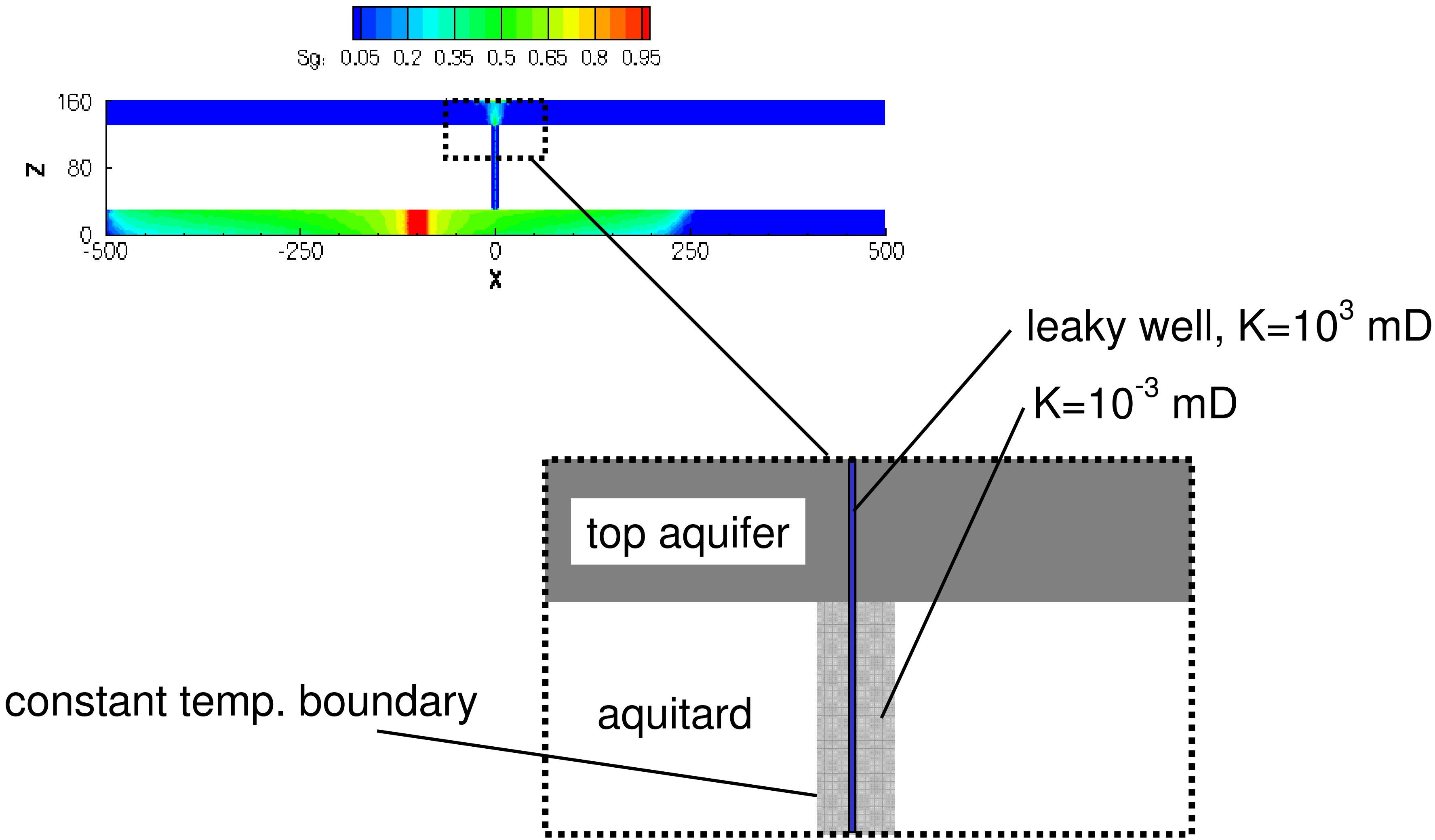


Simulation(2): Results

Fraction of the total mass of CO_2 dissolved in brine

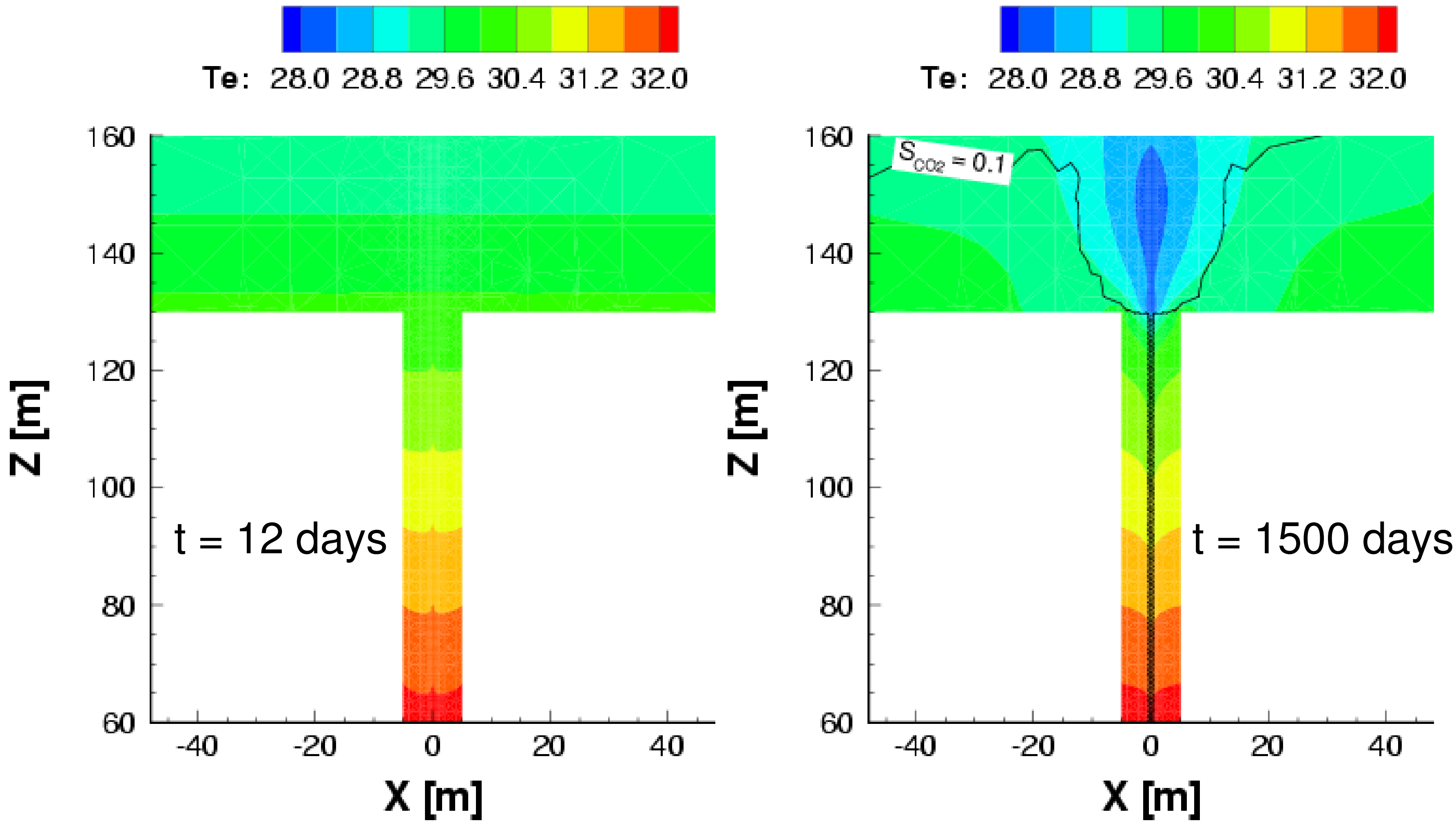


Simulation(2): Results



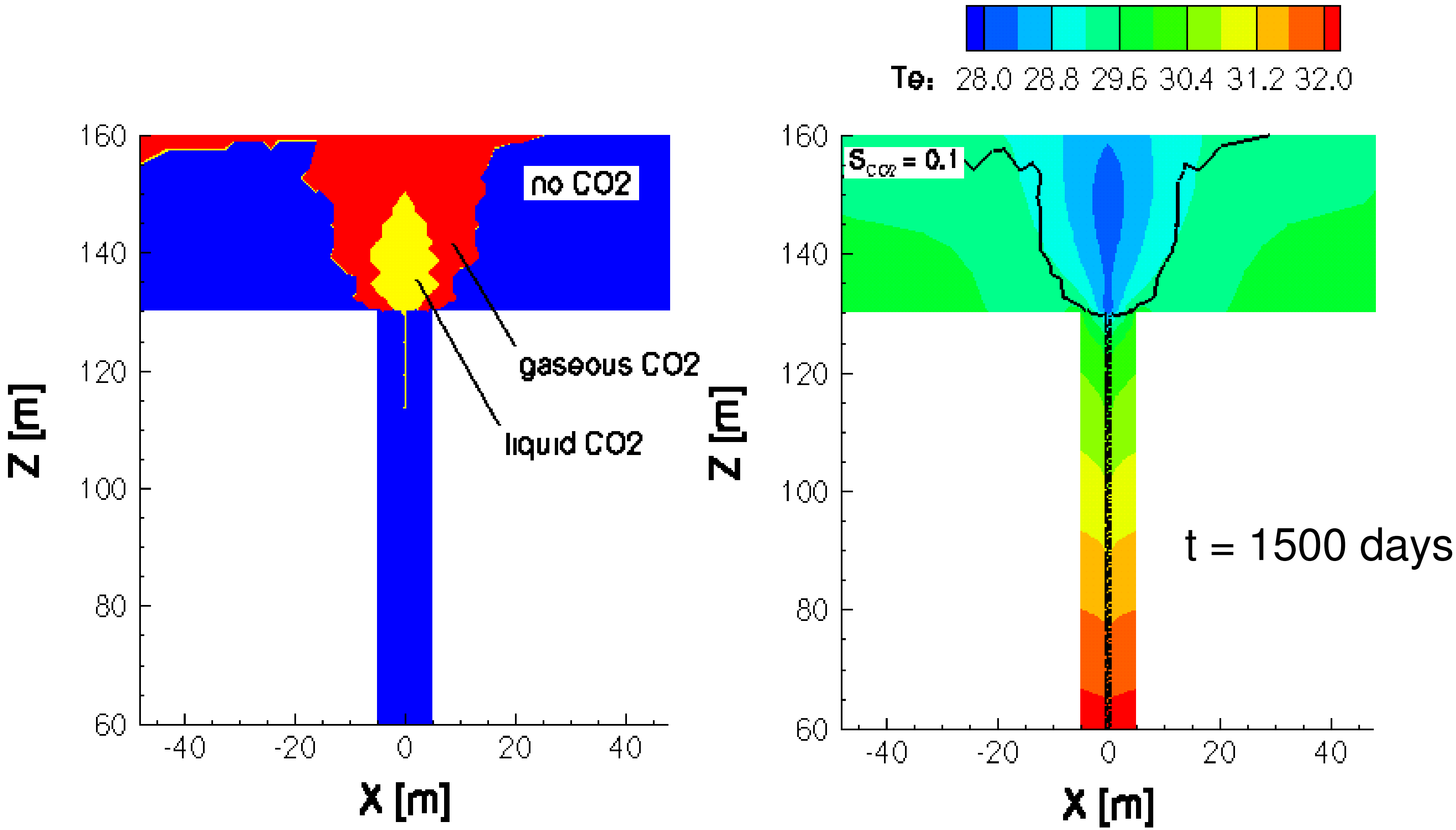
Simulation(2): Results

Temperature [℃] at the top of the leaky well



Simulation(2): Results

Temperature [℃] at the top of the leaky well and state of CO_2



Summary & Outlook

Reliability of a numerical model for CO_2 injection and storage in deep geological formations depends on

- Validity of the simplifying assumptions (are the governing processes sufficiently reproduced?)
- Accuracy of the mathematical and numerical model

Gaining confidence in the model requires a validation/verification

- Possible for simple problems by comparison with (semi-)analytical solutions
- Hardly feasible for complex problems due to a lack of well-controlled experimental or field data

Strategy for improving the confidence in complex models

- Application of the models for the simulation of field-scale projects, e.g. Ketzin (CO2SINK) with detailed monitoring and measurement campaigns.
- Code intercomparison with benchmark problems

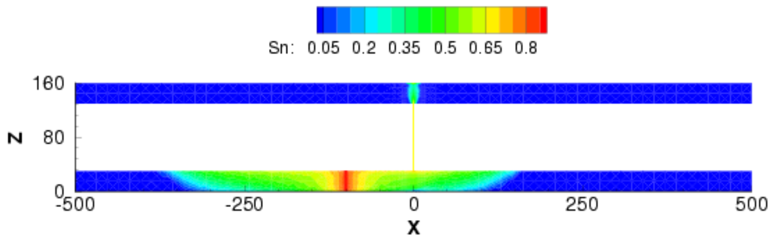
International Workshop on CO_2-Modelling

www.iws.uni-stuttgart.de/co2-workshop

Numerical Models for CO_2 Storage in Geological Formations

Aims:

- presenting the current capabilities of mathematical and numerical models for CO2 storage in geological formations
- discussing the future developments and application of numerical models for large-scale CO2 storage projects
- model intercomparison study: benchmarks will be anounced by August 2007



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Stuttgart, April 2.- 4., 2008