CO_2-injection modelling

Two-phase flow, poroelasticity, dissolution of CO_2

Deep Saline Aquifers for Geological Storage of CO2 and Energy – IFP, Paris 27. – 29. May 2009

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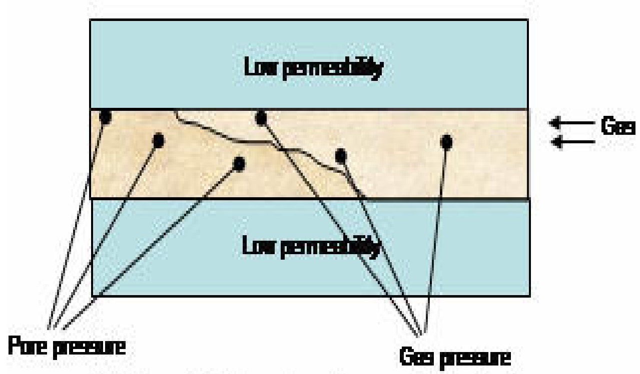
Agenda

- Background and motivation
- Short on CO_2 storage mechanisms
- Model review: equations and physics
- Examples, storage mechanisms:
  1. Comparing two viscosity ratios: 1. $\mu_w > \mu_n$, 2. $\mu_n > \mu_w$
  2. Solubility trapping: Comparing dissolution of CO_2 vs. no-dissolution
  3. Residual trapping
  4. Poroelasticity (including dissolution of CO_2)
  5. Calculating pH

Background and motivation

Two main areas of interest:

1. CO_2 Storage: focus on short term storage and the injection process
2. Gas flow into and out of a well; shallow gas seepage

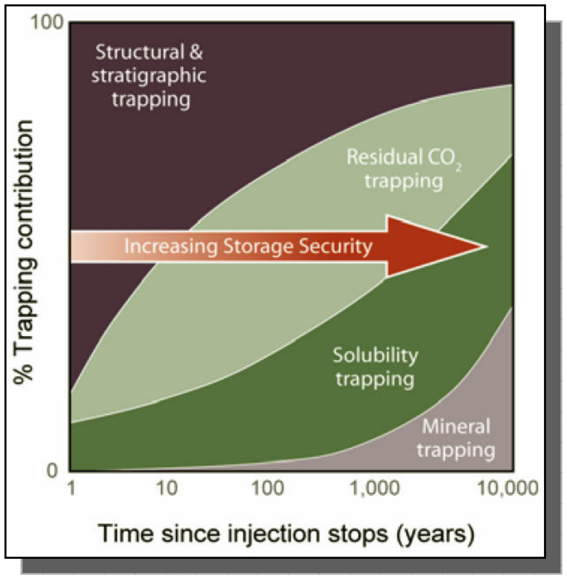


Capillary effects: Lower bound pressure for gas front movement.

Low permeability = impermeable for 1st approx.

CO_2 storage mechanisms

- Storage idea: Inject CO_2 into a **suitable** porous formation below an intact cap rock so that it will not **leak**
- Types of storage mechanism of CO_2:
  1. Structural trapping: Migration blocked by impermeable cap rock
  2. Residual trapping: CO_2 stabilized by capillary pressure
  3. Solubility trapping: In time CO_2 will dissolve in salt pore water (heavy, descends)
  4. Mineral trapping: In time CO_2 will chemically react with rock to form carbonates and precipitate



(From: IPPC Special report, 2005)

Modelling challenges

1. How does the CO_2 migrate in the formation, considering perforated/poorly plugged wells, faults, fractures, etc.
   - Two-phase flow (maybe even more phases)
2. How does CO_2 injection affect the rock
   - Poroelasticity
3. Chemical reactions and borehole integrity
   - Solubility of CO_2 in water

   (Other effects are: chemical reaction with rock formation, corrosion, erosion, degradation of bore hole)

Model review

Equations and physics

Two-phase flow equations

$$\left.\begin{array}{l}\frac{\partial}{\partial t}(\phi\rho_\alpha S_\alpha) - \nabla\cdot[\rho_\alpha\lambda_\alpha\mathbf{K}(\nabla p_\alpha + \gamma_\alpha\nabla z)] = \rho_\alpha q_\alpha \\ \sum S_\alpha = 1, \quad p_c = p_n - p_w, \quad S_{e\alpha} = f(p_c)\end{array}\right\}$$

General mass balances and auxiliary equations

Two-phase flow equations

$$\frac{\partial}{\partial t}(\phi\rho_\alpha S_\alpha) - \nabla\cdot[\rho_\alpha\lambda_\alpha \mathbf{K}(\nabla p_\alpha + \gamma_\alpha \nabla z)] = \rho_\alpha q_\alpha$$

$$\sum S_\alpha = 1, \quad p_c = p_n - p_w, \quad S_{e\alpha} = f(p_c)$$

} General mass balances and auxiliary equations

$\Downarrow$

Do some equation manipulation: Fractional flow formulation

(The fractional flow approach treats the multiphase flow problem as a total fluid flow of a single mixed fluid, and then describes the individual phases as fractions of the total flow)

Two-phase flow equations

$$\frac{\partial}{\partial t}(\phi\rho_\alpha S_\alpha) - \nabla\cdot[\rho_\alpha\lambda_\alpha\mathbf{K}(\nabla p_\alpha + \gamma_\alpha\nabla z)] = \rho_\alpha q_\alpha$$

$$\sum S_\alpha = 1, \quad p_c = p_n - p_w, \quad S_{e\alpha} = f(p_c)$$

General mass balances and auxiliary equations

$$\Downarrow$$

$$\nabla\cdot\mathbf{u} = q_w + q_n - \frac{1}{\rho_w}\frac{\partial\rho_w}{\partial p}\left(\frac{\partial p}{\partial x}u_{w,x} + \frac{\partial p}{\partial y}u_{w,y} - \frac{\partial p}{\partial t}\phi S_w\right) - \frac{1}{\rho_n}\frac{\partial\rho_n}{\partial p}\left(\frac{\partial p}{\partial x}u_{n,x} + \frac{\partial p}{\partial y}u_{n,y} - \frac{\partial p}{\partial t}\phi S_n\right) - \frac{\partial\phi}{\partial t}$$

$$\phi\rho_w\frac{\partial S_w}{\partial t} + \nabla\cdot(\rho_w\mathbf{u}_w) = \rho_w q_w - \phi S_w\frac{\partial\rho_w}{\partial p}\frac{\partial p}{\partial t} - \rho_w S_w\frac{\partial\phi}{\partial t}$$

$$\mathbf{u} = -\mathbf{K}(\lambda\nabla p - (\lambda_w\rho_w + \lambda_n\rho_n)\mathbf{g})$$

$$\mathbf{u}_w = f_w\mathbf{u} + \lambda_n f_w K(\nabla p_c + (\rho_w - \rho_n)\mathbf{g})$$

$$\mathbf{u}_n = f_n\mathbf{u} - \lambda_n f_w K(\nabla p_c + (\rho_w - \rho_n)\mathbf{g})$$

Biot linear poroelasticity equation

Flow coupled to geomechanics

$$\nabla \cdot [\boldsymbol{\sigma}] = -\mathbf{F}$$

$$\boldsymbol{\sigma} = \mathbf{D}_{el}\boldsymbol{\varepsilon} - \alpha_{biot}\, p\mathbf{I}$$

Geomechanics coupled to flow:

$$\phi^{*} = (1 - \varepsilon_{v})\phi$$

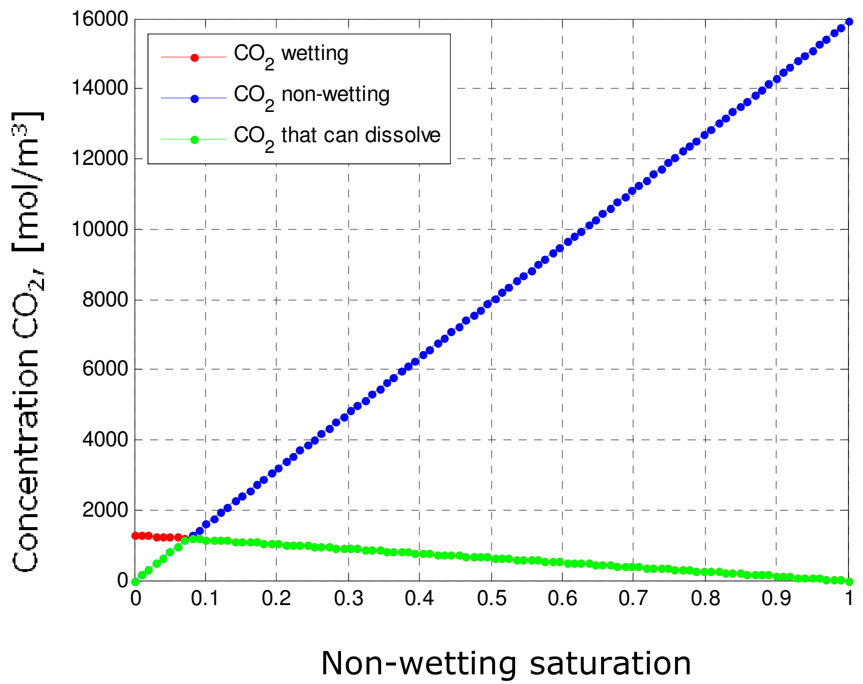
$$K = K_{0}\left(\frac{\phi^{*}}{\phi}\right)^{3.4}$$

(vary from case to case)

Mass balance equation, $CO_2(aq)$

$$\frac{\partial C_{CO_2}}{\partial t} + \nabla \cdot \left(-D \nabla C_{CO_2} \right) = F$$

$$F = k_s \left(min\left(C_{sat,CO_2} S_w , C_{0,CO_2} S_n \right) - C_{CO_2} \right)$$



$C_{sat,CO2}$ – saturated concentration of CO_2 in water; $CO_2(aq)$ [mol/m^3]
C_0 – concentration of pure CO_2 [mol/m^3]

pH calculation

$CO_2(sc) \rightleftharpoons CO_2(aq)$, dissolution (sc – super critical)
$CO_2(aq) + H_2O(l) \rightleftharpoons H_2CO_3(aq)$, hydration

Treating $CO_2(aq)$ and $H_2CO_3(aq)$ as one entity, CO_2*:

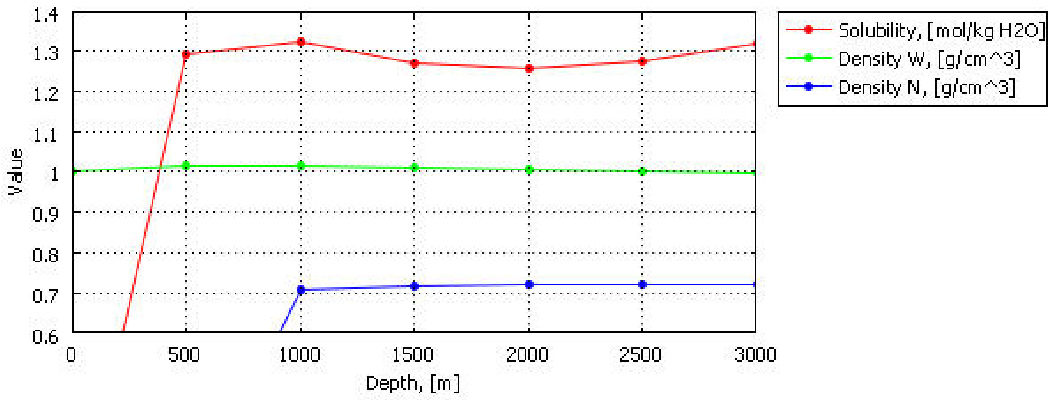
$CO_2^* + H_2O \rightleftharpoons HCO_3^-(aq) + H_3O^+(aq)$, first dissociation, p$Ka_1$
$HCO_3^-(aq) \rightleftharpoons CO_3^{2-}(aq) + H_3O^+(aq)$, second dissociation, p$Ka_2$

Using:
- Protolysis constants, K_{a1} and K_{a2}
- Steuchiometric relation for initial concentration c of carbonic acid
- Water constant, K_w
- Electro neutrality

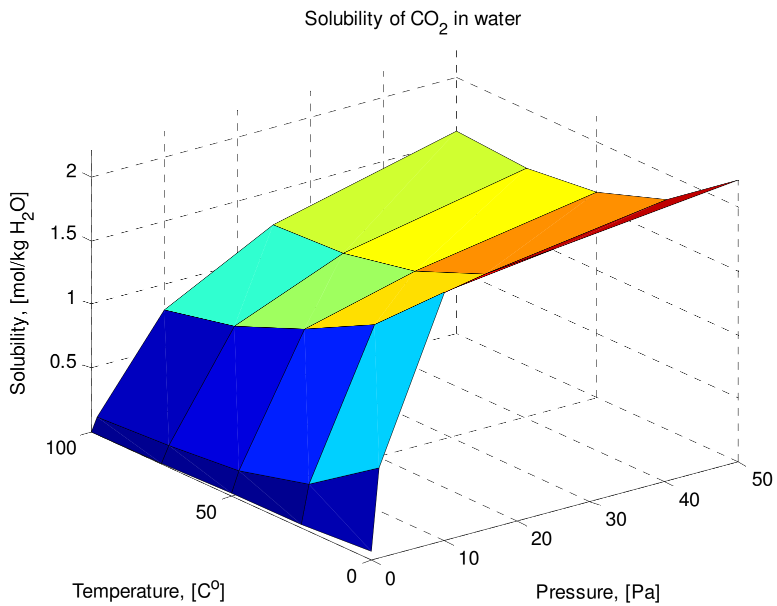
$\Rightarrow$ Four equation, four unknowns: $pH = -log_{10}(\sqrt{K_{a1}c + K_{a2}c + K_w})$

CO_2 density and solubility

Symbol	Value	Unit	Description
ρ_{H2O}	1000	[kg/m^3]	Density of water-phase
ρ_{CO2}	700	[kg/m^3]	Density of CO_2-phase
c_{sat}	1300	[mol/m^3]	Saturation concentration of CO_2 in water

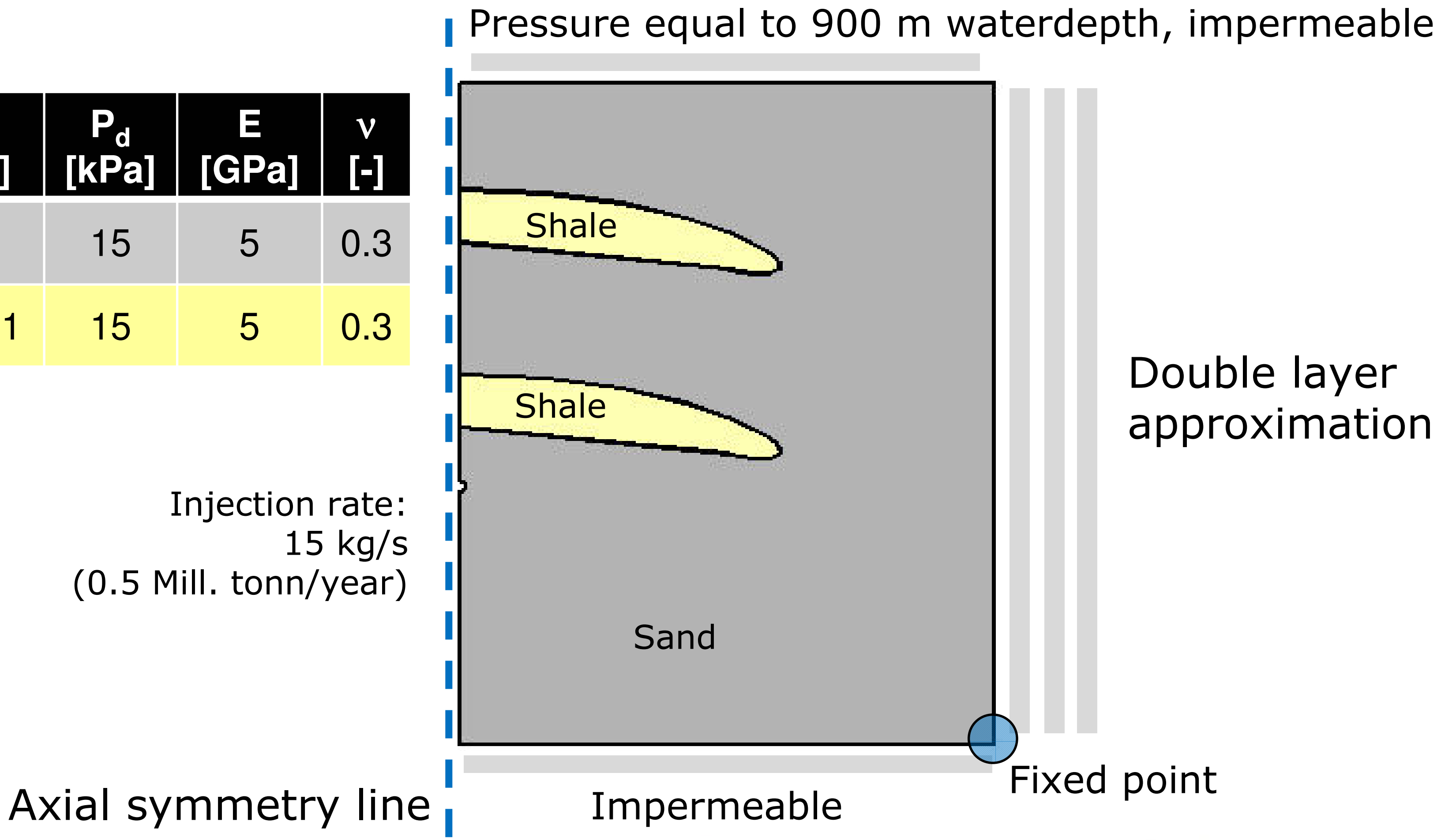


(Temperature gradient used: 28K/km)



Model (200 x 250 m^2), axial symmetry

ϕ [-]	K [D]	P_d [kPa]	E [GPa]	ν [-]
0.42	1	15	5	0.3
0.1	0.01	15	5	0.3



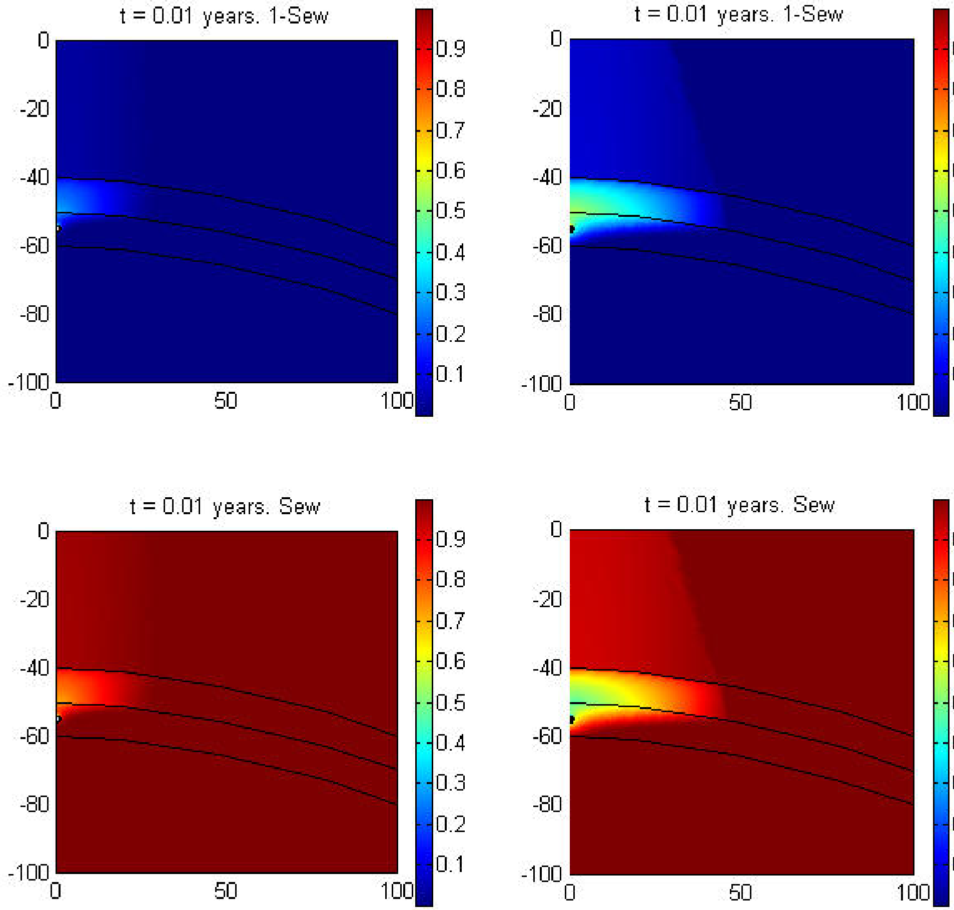
Examples

Storage mechanisms

Example 1: Viscosity ratios

High value:
0.5 mPa·s

Low value:
0.05 mPa·s



Example 1: Viscosity ratios, version 2

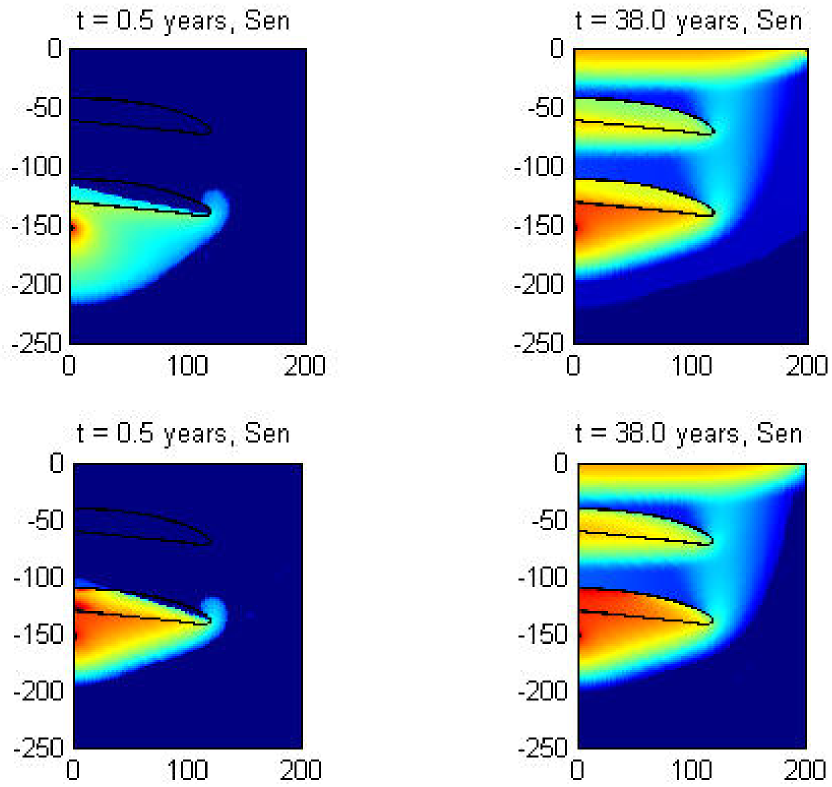
Water high:
5 mPa·s

CO_2 low:
0.5 mPa·s

CO_2 constant

Water Low:
0.05 mPa·s

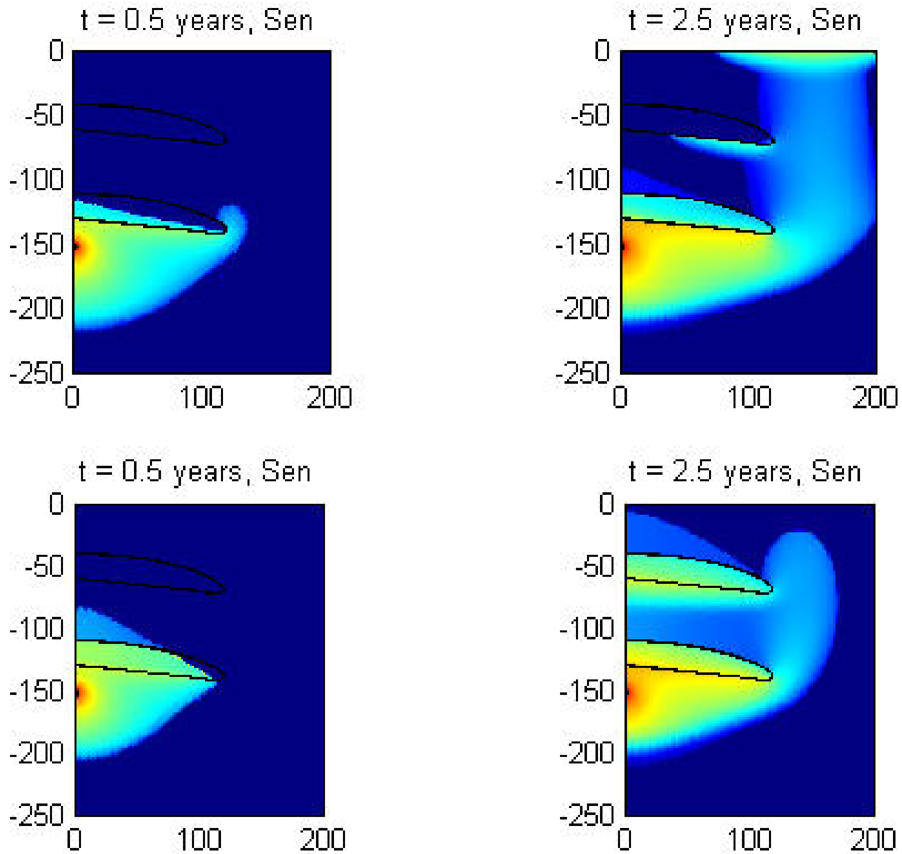
CO_2 high:
0.5 mPa·s



Example 2: Solubility trapping

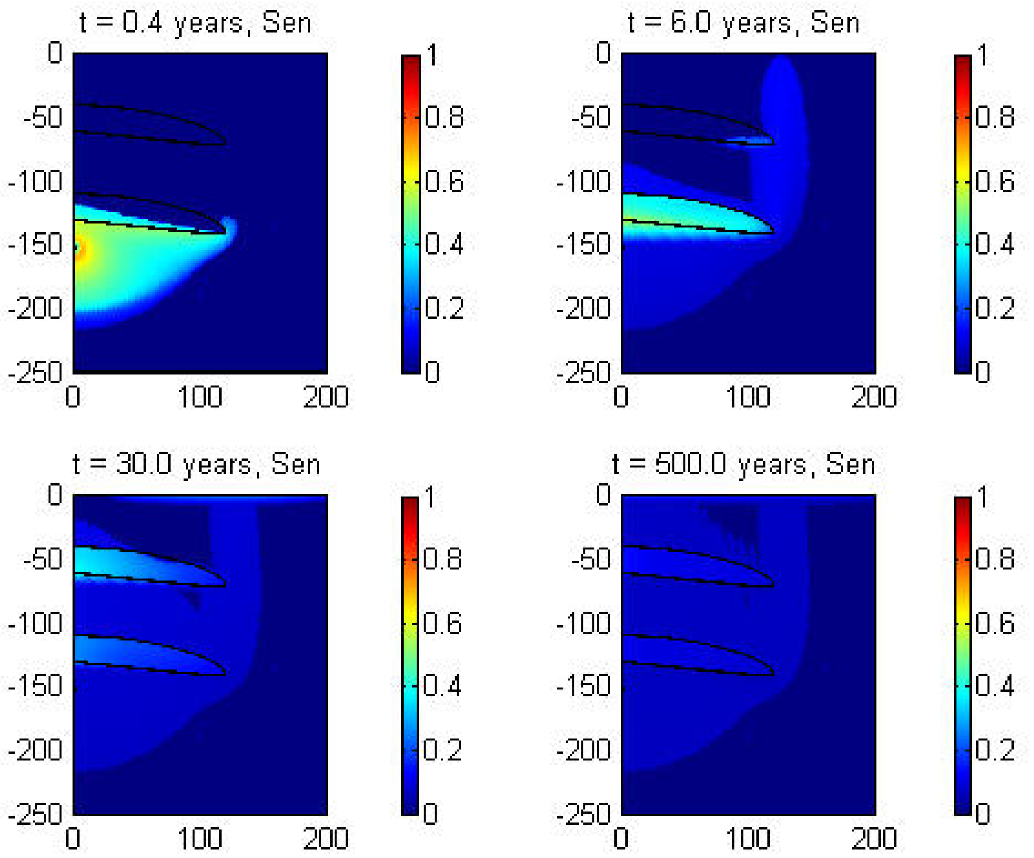
No-dissolution

Dissolution

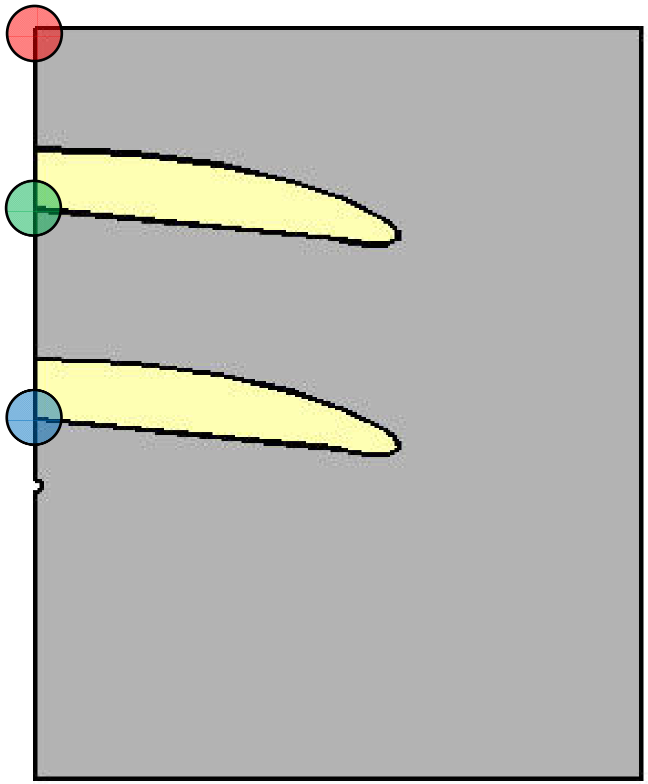


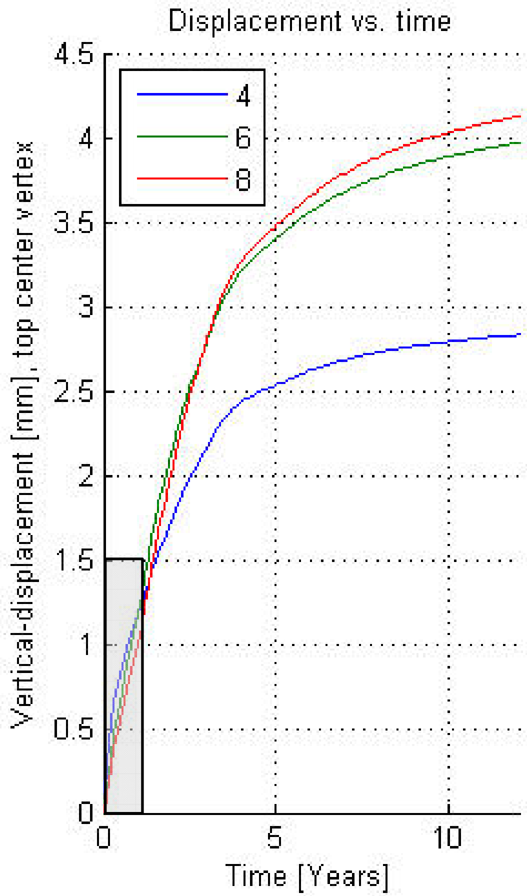
Example 3: Residual trapping

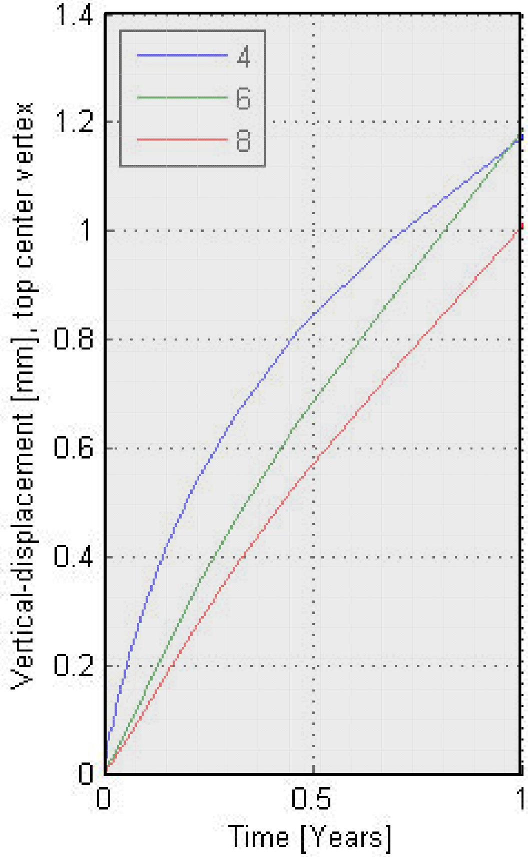
$(S_{r,CO2} = 0.05)$



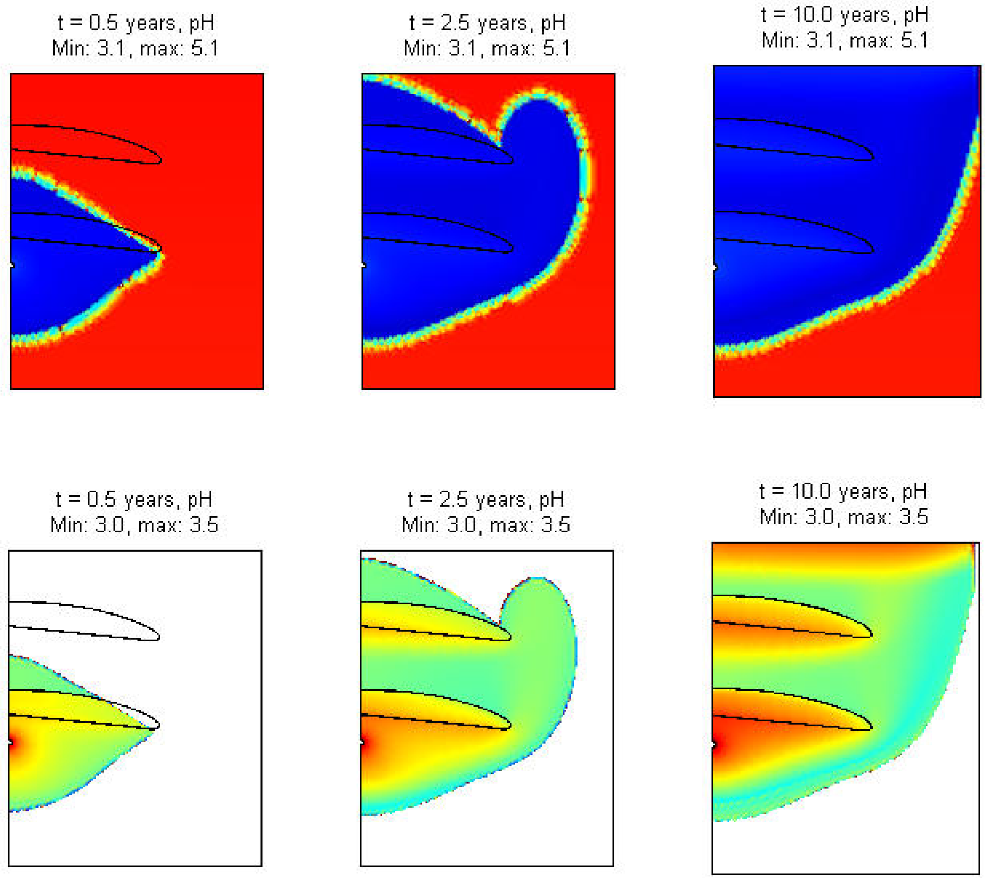
Example 4: Poroelasticity







Example 5: Calculating pH



Acknowledgements: Financial support from the Research Council of Norway and NGI is gratefully acknowledged

Conclusion

- A robust model (2D and axial symmetric) that considers many main features related to CO_2 injection
  - More chemical reactions to be added
  - More realistic material models (poroelasticity)
- Most important storage mechanisms:
  - Residual and solubility trapping
- Remaining tasks:
  - Verification (planned lab-experiment summer/fall 2009)
  - Simulation of "real-life" cases
- Thank you for you attention!

CO_2 solubility and pK_w

```
% X-data and Y-data, pressure [Pa], temperature [degC]
 0.1 1.0 10.0 25.0 50.0
 0.0 25.0 50.0 75.0 100.0
% Interpolation data, solubility [mol/kg H20]
 0.08         0.72          1.95          2.06          2.21
 0.03         0.33          1.45          1.61          1.81
 0.02         0.19          1.16          1.38          1.61
 0.01         0.13          0.93          1.27          1.55
 0.0010       0.1           0.8           1.24          1.58
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```
Function data:
% X-data and Y-data, temperature [degC], pressure [MPa]
 0.0 25.0 50.0 75.0 100.0 150.0 200.0 250.0 300.0
 0.1 25.0 50.0 75.0 100.0 150.0 200.0 250.0 300.0 350.0 400.0 500.0 600.0 700.0 800.0 900.0 1000.0
% Interpolation data
 14.946      13.995       13.264       12.696       12.252       11.641       11.31        11.205       11.339
 14.848      13.908       13.181       12.613       12.165       11.543       11.189       11.05        11.125
 14.754      13.824       13.102       12.533       12.084       11.45        11.076       10.898       10.893
 14.665      13.745       13.026       12.458       12.006       11.364       10.974       10.769       10.715
 14.58       13.668       12.953       12.385       11.933       11.283       10.88        10.655       10.568
 14.422      13.524       12.815       12.249       11.795       11.135       10.713       10.458       10.327
 14.278      13.39        12.687       12.123       11.668       11           10.564       10.289       10.131
 14.145      13.265       12.567       12.004       11.549       10.876       10.43        10.14        9.963
 14.021      13.148       12.453       11.892       11.437       10.76        10.306       10.005       9.814
 13.906      13.037       12.346       11.786       11.331       10.651       10.191       9.881        9.679
 13.797      12.932       12.243       11.685       11.23        10.548       10.083       9.766        9.555
 13.595      12.736       12.052       11.496       11.042       10.356       9.884        9.557        9.332
 13.411      12.556       11.875       11.322       10.868       10.181       9.703        9.369        9.135
 13.24       12.389       11.71        11.159       10.705       10.018       9.537        9.197        8.956
 13.08       12.233       11.556       11.006       10.553       9.865        9.381        9.037        8.791
 12.93       12.085       11.41        10.861       10.41        9.721        9.236        8.888        8.638
 12.788      11.946       11.272       10.725       10.273       9.585        9.098        8.748        8.495
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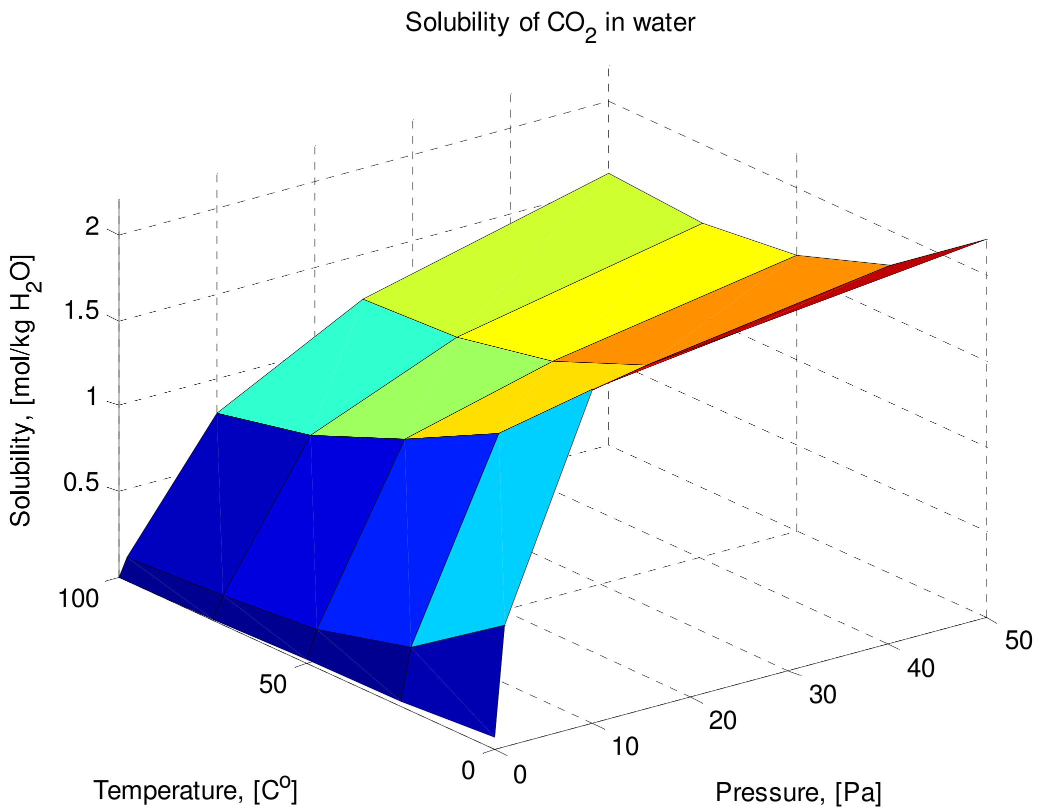
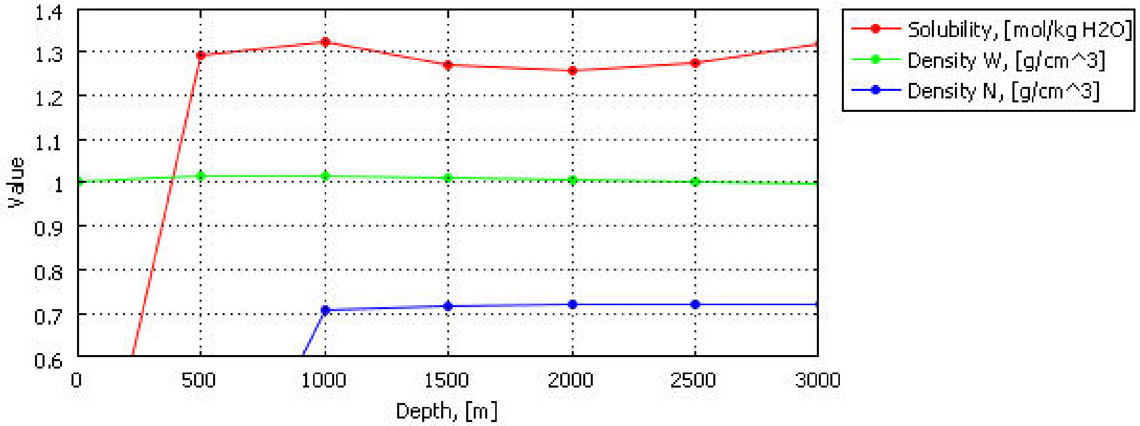


Solubility of CO_2 in water as function of temperature (°C) and pressure (MPa)



Plots of solubility of CO_2 in water and density of CO_2 and water plotted as a function of depth (taking pressure and temperature variations into account). Pressure gradient is app. 10000 [Pa/m] and the temperature gradient is 28 [K/km].