Safe Storage Parameters During CO₂ Injection Using Coupled Reservoir-Geomechanical Analysis

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Abstract: Safe short term storage of CO₂ depends mainly on structural trapping; migration of injected CO₂ is blocked by impermeable cap rock, and solubility trapping; CO₂ dissolves in pore water. On longer term, mineral trapping is also contributing to the trapping of CO₂.

To be able to investigate the importance of these different storage mechanisms, a finite element model for simulation of CO₂ injection has been developed in COMSOL Multiphysics. The model describes and solves for two-phase flow (including dissolution of CO₂ in water) and fully coupled two-way interaction between the fluid flow and the solid displacement using elastic linear Biot poroelasticity theory.

A rudimentary model is presented here to illustrate the practical use of the model by determining the flow regime (considering dissolution of CO₂) and the stress distribution due to CO₂ injection into a formation.

The most important mechanisms for CO₂ storage seems to be residual and solubility trapping. Good storage conditions can be reservoirs with high air entry pressure values, since this tends to diffuse the CO₂ phase very efficiently.

Keywords: Two-phase flow, poroelasticity, porous media, CO₂

1. Introduction

Almost all produced hydrocarbon is, and will be, used as fuel and therefore produce CO₂ that eventually will be released into the atmosphere. In this perspective, plans for long-term storage of CO₂ are a good and sustainable idea for reducing climate effect of the atmospheric emission of CO₂. One of the most promising ideas is injecting CO₂ into a reservoir where it is stored indefinitely. Good potential geological formations to store captured CO₂ are depleted and disused oil and gas fields, deep saline aquifers and unminable coal seams [#1].

One ideal scenario is to inject CO₂ into a permeable aquifer underneath a very low-permeable caprock. When injected, CO₂ will dissolve in the reservoir water, increasing the density. After hundreds to thousands of years the injected CO₂ will react to form carbonates and precipitate and this is the safest storage mechanism. However, migration of the CO₂ beyond the natural reservoir seals could become problematic. Thus, modelling of CO₂ injection can help to better understand cause of leakage and its mechanisms and make CO₂ storage safer.

The trapping contributions of the various storage mechanisms as function of time is indicated in figure 1.

![Figure 1. The trapping contributions of the various mechanisms as function of time. (Illustration from the IPPC Special report, 2005).](image)

Storage of CO₂ depends mainly on the four trapping mechanisms (illustrated in figure 1):
1. Structural trapping; migration of injected CO₂ is blocked by impermeable cap rock
2. Residual trapping; capillary forces and adsorption onto the surfaces of mineral grains within the rock matrix immobilize (residual) parts of the injected CO₂
3. Solubility trapping; CO₂ dissolves and become trapped in the pore water. Dissolving CO₂ in water increases the density; hence the water with CO₂ will descend
4. Mineral trapping; Dissolved CO₂ forms carbonic acid, in time the surrounding
mineral dissolves and reacts with the CO$_2$ to form solid carbonates.

The timescales on which these processes operate need to be taken into account in CO$_2$ storage capacity assessment. Mineral trapping reactions that induce carbonate precipitation will play little part in creating additional space during CO$_2$ injection because they act too slowly. The kinetics of mineral trapping is so slow that they will only have a significant effect over hundreds to thousands of years. In practice, mineral trapping commonly can be ignored as a significant storage mechanism on a hundred-year timescale. To be able to investigate the importance of the other storage mechanisms a finite element model for simulation of CO$_2$ injection will be defined. The model describes and solves for two-phase flow (including dissolution of CO$_2$ in water) and fully coupled two-way interaction between the fluid flow and the solid displacement using elastic linear Biot poroelasticity theory.

2. Use of COMSOL Multiphysics

The system equations consists of two mass balances; one for each phase in the two-phase flow system, a mass balance for the dissolved CO$_2$ in water and a stress-strain application mode for modeling the geo-mechanics. The mass balances are all defined in PDE general form application mode.

3. Equations

In the following section, the various systems of partial differential equations that define the model are described.

3.1. Equations; two-phase flow

The two-phase flow formulation used in this paper is often referred to as fractional flow formulation. The background for the two-phase flow equations are the general mass balance equations. This approach treats the two-phase flow problem as a total fluid flow of a single mixed fluid, and then describes the individual phases as fractions of the total flow.

The general mass balance equation is defined as:

$$\frac{\partial (\phi \rho_a S_a)}{\partial t} + \nabla (\rho_a u_a) = \rho_a g$$  \hspace{1cm} \text{Eq. 1}

In addition, auxiliary equations apply:

$$S_w + S_e = 1$$ \hspace{1cm} \text{Eq. 2}

$$p_e(S_a) = p_a - p_e$$ \hspace{1cm} \text{Eq. 3}

The Darcy velocity is defined as:

$$u_a = -\frac{k_{ra}}{\mu_a} (\nabla p_a - \rho_a g)$$ \hspace{1cm} \text{Eq. 4}

Doing some equation manipulations on equations 1-4 (for both wetting and non-wetting phase) results in an equation for the global pressure (total pressure) and an equation for the saturation of one of the phases (here for the wetting phase; $S_w$).

Note: There are many variations of the capillary pressure function and relative permeabilities, they can be expressed by for instance Van Genuchten or Brooks-Corey, in the Example model Van Genuchten is used, see appendix B for the expressions.

3.2 Equations; Biot linear poroelasticity

Linear Biot poroelasticity theory is used to account for elastic response of fluid saturated porous solid. The formulation is restricted to linear elastic solids undergoing quasistatic small deformations and is here based on Naviers equation for the study of displacements, stresses, and strains in an in-plane, or axial symmetric, loaded body. The formulation can also account for thermal strain using a thermal expansion coefficient.

Similar to thermal expansion, where change in temperature relative to a reference temperature can cause a solid to deform, poroelasticity combines the theory of fluid flow with constitutive equations that couple the stress in the porous solid and pore pressure due to fluid flow. An increase in fluid pressure will cause the porous solid to swell.

For more information on the theory background of small, linear and elastic deformations the reader is referred to Structural Mechanics Module User’s guide manual in COMSOL Multiphysics [#2].
The equation for linear Biot poroelasticity:

\[
\nabla \cdot (\sigma) = -F \quad \text{Eq. 5}
\]
\[
\sigma = D \varepsilon - \alpha_{biotel} p I \quad \text{Eq. 6}
\]

The coupling between geomechanics and flow is: Deformation of a porous media affects the porosity:

\[
\phi^* = (1 - \varepsilon_c) \phi \quad \text{Eq. 7}
\]

Additional source/sink terms to the mass balances (eq. 1) due to deformation:

\[
q_w = q_n = -\alpha_{biotel} \frac{\partial \varepsilon_c}{\partial t} \quad \text{Eq. 8}
\]

Permeability is affected by porosity change according to [3]:

\[
K = K_0 \left( \frac{\phi^*}{\phi} \right)^{20} \quad \text{Eq. 9}
\]

(The exponent in eq. 9 can vary from case to case)

### 3.3 Equations; CO\textsubscript{2} mass balance

The chemical-part is implemented as strictly dissolution of super-critical (liquid) CO\textsubscript{2} in reservoir water. CO\textsubscript{2} solubility in water depends on pressure, temperature and salinity of the system. With the constant temperature profile, constant zero salinity of the water and the hydrostatic pressure used in the model, the saturation concentration of CO\textsubscript{2} in water varies very little and is therefore considered constant in the model [4]. For a more detailed model, though, density variations in the water should be taken into consideration.

The general mass balance for the dissolved amount of CO\textsubscript{2} in water is given by:

\[
\frac{\partial (\phi^* C_{CO2})}{\partial t} + \nabla \cdot (-D_{CO2} \phi^* \nabla C_{CO2}) = F \quad \text{Eq. 10}
\]

The natural source term \( F \) is defined as the dissolution \( T_d \), described below.

Assuming that the dissolution of CO\textsubscript{2} in water is mass transfer controlled, a mass balance for the dissolved CO\textsubscript{2} in water is added to the system of equations. Dissolution of CO\textsubscript{2} in water is almost instantaneous is implemented as a sink in the non-wetting phase mass balance equation source term. Since CO\textsubscript{2} is miscible with water, it is not implemented as a source term to the wetting phase mass balance. The sink is defined as:

\[
T_d = k_s (min(C_{sat,CO2} S_w, C_{CO2} S_n) - C_{CO2}) \quad \text{Eq. 11}
\]

Dissolution rate \( k_s \) of CO\textsubscript{2} in water is considered almost instantaneous. The value is unknown, here a rate of \( 0.5 \times 10^{-4} \text{[s}^{-1}\text{]} \) is used and meaning that after approximately \( \sim 5.6 \) hours dissolution of CO\textsubscript{2} in water has reached equilibrium.

Dissolved CO\textsubscript{2} and water is miscible and therefore has the same volume fraction as water, here the wetting phase; \( S_w \).

\( min \) in eq. 11 is a function returning the minimum value of the two input arguments. This makes sure that dissolved CO\textsubscript{2} can never be more than available CO\textsubscript{2} in the non-wetting phase (liquid CO\textsubscript{2}) or maximum saturation concentration of CO\textsubscript{2} in the wetting phase.

### 3.4 Equations; calculating \( p\text{H} \)

When the concentration of dissolved CO\textsubscript{2} in water is calculated, the \( p\text{H} \) can be evaluated. CO\textsubscript{2} dissolves in water according to the following equilibrium reactions:

I \quad CO_2^{(sc)} \rightleftharpoons CO_2^{(aq)}

II \quad CO_2^{(aq)} + H_2O(l) \rightleftharpoons H_2CO_3^{(aq)}

Treating CO\textsubscript{2}\textsuperscript{(aq)} and H\textsubscript{2}CO\textsubscript{3}\textsuperscript{(aq)} as one entity, CO\textsubscript{2}\textsuperscript{*}:

III \quad CO\textsubscript{2}* + H\textsubscript{2}O \rightleftharpoons HCO\textsubscript{3}^{−}(aq) + H\textsubscript{3}O^{+}(aq)

IV \quad HCO\textsubscript{3}^{−}(aq) \rightleftharpoons CO\textsubscript{3}^{2−}(aq) + H\textsubscript{3}O^{+}(aq)

Using the protolysis constants from III and IV, \( K_{w} \) and \( K_{w3} \), respectively, the stechiometric relation for initial concentration of carbonic acid, the water constant, \( K_w \) and applying electroneutrality, an expression for the \( p\text{H} \) is approximated to:

\[
p\text{H} = - \log_{10} \left( \sqrt{K_{w} C_{CO2} + K_{w3} C_{CO2} + K_w} \right) \quad \text{Eq. 12}
\]
For the details of this derivation and values for the various constants \( K_w, K_{a1}, \) and \( K_{a2}, \) see appropriate section in appendices. In real life, the pore water will have certain salinity and these constants can also depend on the salinity. Also, carbonates can act as buffers on the \( pH \) so in a more realistic model, more mass balances needs to be considered in order to get the “real” value, or more correct value, of the \( pH \).

4. Model example: geometry

The geometry of the model is given in figure 2. It is a 300x300 m\(^2\) domain consisting of a sand reservoir with a high permeability and porosity and two shale lenses with lower permeability and porosity, see table 1. The model is solved axial symmetric so the real size of the reservoir is 600x300 m\(^2\).

![Figure 2](image)

**Figure 2.** Illustration of geometry used in the model, note that the figure is not to scale. See text for explanation of boundary conditions.

<table>
<thead>
<tr>
<th></th>
<th>( \phi ) [-]</th>
<th>( K_0 ) [D]</th>
<th>( p_d ) [kPa]</th>
<th>( E ) [GPa]</th>
<th>( v ) [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td>0.4</td>
<td>3</td>
<td>20</td>
<td>2</td>
<td>0.3</td>
</tr>
<tr>
<td>Shale</td>
<td>0.1</td>
<td>0.01</td>
<td>20</td>
<td>2</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 1. Material properties used in model, refer to figure 2.

Boundary A is constrained to move in the horizontal direction because of axial symmetry conditions, boundary B is constrained from moving at all, boundary D can move vertically only and boundary C is free to move.

Injection point is located in the centre of the domain, 170 meters below the top boundary, on the axial symmetry line A. The injection rate is equivalent to 30 kg/s (app. 1 mill ton/year) \( CO_2 \) being injected, and consists of 30 % water and 70 % \( CO_2 \). Dissolved \( CO_2 \) is assumed to be in equilibrium at the injection point.

5. Model example: results and discussion

Following are some discussions on the contributions of the various storage mechanisms.

5.1 Structural trapping

Migration of injected \( CO_2 \) is blocked by impermeable cap rock, if the permeability is low enough (close to impermeable), the fluid will not penetrate.

5.2 Residual trapping

Capillary forces and adsorption onto the surfaces of mineral grains within the rock matrix immobilize (residual) parts of the injected \( CO_2 \).

![Figure 3](image)

**Figure 3.** Residual trapping. The figure shows the non-wetting saturation (\( CO_2 \)) for various times (from top left to lower right); 0.1, 0.5, 100 and 100 years. The plot shows how the injected \( CO_2 \) continue to rise, leaving a trail of undissolved \( CO_2 \) (equivalent to a residual saturation of 5%).
In this case the injection of CO₂ into the reservoir is stopped after 0.1 year. CO₂ is lighter than water and will continue to rise. When the saturation of CO₂ reaches the saturation level, here defined at 5\%, the effective non-wetting saturation and the Van Genuchten relative permeability approaches zero, hence immobilizing and stabilizing the CO₂.

5.3 Solubility trapping

CO₂ dissolves and become trapped in the pore water.

![Figure 4. Solubility trapping. The colours show the saturation of non-wetting phase (here CO₂). The columns show the spreading of CO₂ phase for two times; 0.03 years and 0.15 years after injection. When including dissolution of CO₂ in water it is observed that some of the injected CO₂ is dissolved and trapped in the wetting (water) phase, slightly retarding the movement of the front of intruding CO₂.](image)

Two models were solved; one where dissolution of CO₂ in water was taken into account and one where it was not taken into account. Comparing the two solutions show how CO₂ is dissolved and stabilized in the water; the CO₂ injection front moves slightly slower, see figure 4.

5.4 pH

Using equation 12, the pH can be evaluated in the model. In Figure 5 the pH is shown after two time steps: 0.03 and 0.1 years of injection. The pH-front follows exactly the CO₂ front (compare with figure 4).

![Figure 5. pH value in the reservoir after 0.03 years and 0.1 years of injection. The green color is approximately 4.4 and the blue color is app. 3.2.](image)

5.5 Deformation

The increased pressure due to injection of CO₂ causes the reservoir to deform. Figure 6 shows a time series of the deformation due to injection.

![Figure 6. Deformation at various times; here exaggerated 5000 times.](image)

In figure 7 deformations in selected points in the model is shown. The results show that the maximum deformation is achieved directly, on boundary C in figure 2 and is app. 14 mm.

![Figure 7. Deformation in selected points (indicated with the colors blue, green and red in the left figure) of the reservoir due to injection of CO₂. A close-up of the shaded area in the middle figure is given in the right figure.](image)
6. Conclusion

A robust model for CO\textsubscript{2} storage and injection modelling, considering two-phase flow, simple chemistry considering dissolution of CO\textsubscript{2} in water and linear elastic poroelasticity has been developed using COMSOL Multiphysics. The most important mechanisms for CO\textsubscript{2} storage seems to be residual and solubility trapping. Good storage conditions can be reservoirs with high air entry pressure values, since this tends to diffuse the CO\textsubscript{2} phase very efficiently. The large variations in pH indicate that pH measurements can be a very good detection method in monitoring. Proper boundary conditions need more attention. It can be seen at longer times that the right boundary affects the dissolved CO\textsubscript{2} concentration, extracting the non-wetting phase and thereby lowering the concentration and increasing the pH.

To make the model more complete, more advanced material models for the soil can be used and/or implemented. Also, more chemical reactions can be added to more accurate description of the spreading of CO\textsubscript{2} and pH calculation. Geomechanical modelling can in general say something about cause of fracturing, faulting and induced brittle deformation. This can be done using failure criteria such as the Drucker-Prager, the Lade, and the Coulomb failure criteria. These criteria provide different relationship between rock failure and the principal stresses, but no failure criterion is evaluated in this study. Also, brittle failure criteria can estimate slip tendency of faults and estimate maximum fluid pressure that can be attained during injection.

7. References

2. COMSOL Multiphysics User manual, Structural Mechanics Module, v.3.5a
4. Diamond, Larryn W., Akinfiev, Nikolay N., "Solubility of CO\textsubscript{2} in water from −1.5 to 100 C and from 0.1 to 100 MPa: evaluation of literature data and thermodynamic modeling", Fluid Phase Equilibria 208 (2003) 265–290

8. Acknowledgements

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Appendix A. Nomenclature

Table 1: Symbols used in this paper

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi$</td>
<td>Effective reservoir porosity, [-]</td>
</tr>
<tr>
<td>$\phi^*$</td>
<td>Intrinsic reservoir porosity, [-]</td>
</tr>
<tr>
<td>$\rho_a$</td>
<td>Density, [kg/m$^3$]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Phase index, $\alpha$ can be w - wetting phase, or n - non-wetting phase, [-]</td>
</tr>
<tr>
<td>$S_a$</td>
<td>Saturation, [-]</td>
</tr>
<tr>
<td>$S_{ew}$</td>
<td>Effective saturation for phase $\alpha$, [-]</td>
</tr>
<tr>
<td>$S_{er}$</td>
<td>Residual wetting sat. phase, [-]</td>
</tr>
<tr>
<td>$S_{en}$</td>
<td>Residual non-wetting sat. phase, [-]</td>
</tr>
<tr>
<td>$t$</td>
<td>Time, [s]</td>
</tr>
<tr>
<td>$p_c$</td>
<td>Capillary pressure function, from Van Genuchten relations, [Pa]</td>
</tr>
<tr>
<td>$q_a$</td>
<td>Partial pressure, [Pa]</td>
</tr>
<tr>
<td>$k_{eq}$</td>
<td>Relative permeability coefficient, [-]</td>
</tr>
<tr>
<td>$k_{eq}$</td>
<td>Relative permeability coefficient, from Van Genuchten relations, [-]</td>
</tr>
<tr>
<td>$\mu_a$</td>
<td>Dynamic viscosity, [kg/ms]</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Global fluid pressure, [Pa]</td>
</tr>
<tr>
<td>$K_d$</td>
<td>Intrinsic permeability tensor, [m$^2$]</td>
</tr>
<tr>
<td>$K$</td>
<td>Effective permeability tensor, [m$^2$]</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravity coefficient vector, [m/s$^2$]</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress tensor, [Pa]</td>
</tr>
<tr>
<td>$F$</td>
<td>Body force vector, [N]</td>
</tr>
<tr>
<td>$D_{el}$</td>
<td>Elasticity matrix, [Pa]</td>
</tr>
<tr>
<td>$E$</td>
<td>Youngs modulus, [Pa]</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson ratio, [-]</td>
</tr>
<tr>
<td>$e_d$</td>
<td>Volumetric strain, [m/m]</td>
</tr>
<tr>
<td>$\lambda_{bio}$</td>
<td>Biot coefficient, [-]</td>
</tr>
<tr>
<td>$I$</td>
<td>Identity matrix, [-]</td>
</tr>
<tr>
<td>$C_{CO2}$</td>
<td>Concentration dissolved CO$_2$, [mol/m$^3$]</td>
</tr>
<tr>
<td>$T_d$</td>
<td>Dissolution rate CO$_2$, [mol/(m$^3$/s)]</td>
</tr>
<tr>
<td>$k_d$</td>
<td>Mass transfer rate, [1/s]</td>
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<tr>
<td>$C_{sat,CO2}$</td>
<td>Saturation concentration CO$_2$, [mol/m$^3$]</td>
</tr>
<tr>
<td>$C_{0,CO2}$</td>
<td>Molar density of CO$_2$, [mol/m$^3$]</td>
</tr>
<tr>
<td>$K_{d1}$</td>
<td>Carbonic acid dissociation constant, first dissociation reaction, [-]</td>
</tr>
<tr>
<td>$K_{d2}$</td>
<td>Carbonic acid dissociation constant, second dissociation reaction, [-]</td>
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<tr>
<td>$K_n$</td>
<td>Water dissociation constant, [-]</td>
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<td>$m$</td>
<td>Model parameter, [-]</td>
</tr>
<tr>
<td>$n$</td>
<td>Model parameter, [-]</td>
</tr>
<tr>
<td>$p_d$</td>
<td>Air entry pressure, [Pa]</td>
</tr>
<tr>
<td>$\lambda_n, \lambda_{ew}$</td>
<td>Total mobility, mobility for phase $\alpha$, [m$^2$/kg]</td>
</tr>
<tr>
<td>$f_a$</td>
<td>Mobility fraction phase $\alpha$, [-]</td>
</tr>
</tbody>
</table>

Appendix B. Van Genuchten relations

The advantage of using van Genuchten vs. Brooks-Corey functions is that the derivatives are continuous, improving numerical stability.

Capillary pressure vs. saturation function:

$$p_c(S_w) = \frac{1}{\alpha} \left( \frac{S_w - 1}{S_m - 1} \right)^{\frac{1}{\alpha}}$$ (B.1)

The effective wetting saturation, $S_{ew}$, is given by:

$$S_{ew} = \frac{S_w - S_{en}}{1 - S_{en} - S_{er}}$$ (B.2)

where $S_{ew} \in [0, 1]$.

The derivative is analytically derived:

$$\frac{dp_c}{dS_{ew}} = -\frac{1}{\alpha} \frac{n}{m} \left( \frac{1}{S_w - 1} \right)^{\frac{n-1}{m}} \frac{1}{m} S_{ew}^{\frac{1}{m} - 1}$$ (B.3)

Relative permeability functions to the van Genuchten model:

$$k_{ew}(S_{ew}) = S_{ew}^{\frac{1}{m}} \left( 1 - \left( \frac{1}{S_m} \right)^{\frac{1}{m}} \right)^{2n}$$ (B.4)

$$k_{en}(S_{en}) = \left( 1 - S_{ew} \right)^{\frac{1}{m}} \left( 1 - \left( \frac{1}{S_m} \right)^{\frac{1}{m}} \right)^{2n}$$ (B.5)

Note: The relation between the air entry pressure and the fitting parameter $\alpha$ is given by $[\#5]$:

$$\frac{1}{\alpha} = P_d \frac{2x(x-1)}{x+3} 147.8 + 8.1x + 0.092x^2$$ (B.6)

Where $x = 1 + 2/m$

Appendix C. Velocity vectors

The velocity expressions for the two phases:

$$u_w = f_w u + \lambda_w f_w (\nabla p_w + (\rho_w - \rho_g)g)$$ (C.1)

$$u_n = f_n u - \lambda_n f_n (\nabla p_n + (\rho_n + \rho_g)g)$$ (C.2)

The total velocity expression:

$$u = -K(\nabla p - (\lambda_n \rho_n + \lambda_w \rho_w)g)$$ (C.3)

Mobility (wetting/non-wetting phase/total):

$$\lambda = \lambda_n \mu_n + \lambda_w \mu_w$$ (C.4-6)

Mobility fraction (wetting/non-wetting):

$$f_w = \lambda_w / \lambda, \ f_n = \lambda_n / \lambda$$ (C.7-8)

Capillary pressure gradient:

$$\nabla p_c = \frac{dp_c}{dS_w} \nabla S_w$$ (C.9)