The coupled multiphase flow and reactive transport simulator
OGS-Eclipse for CO2 storage simulations

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Abstract The long-term prognosis of the behaviour of CO2 injected into the subsurface is of relevance for
risk assessment and reservoir management. Due to the coupled multiphase flow and reactive transport
processes interacting in the subsurface, adequate numerical methods are required for a reliable simulation.
This work presents the scientific open source software OpenGeoSys, which was coupled to the standard
multiphase flow simulator Eclipse. Eclipse provides a fast and reliable numerical solution to the multiphase
flow problem, whereas OpenGeoSys is used for simulating component transport and geochemical reactions.
This paper shows the code structure and verifies the coupled code by a number of benchmark simulations.
The applicability to real site conditions is shown using data for a typical site in the North German Basin.

Key words multi phase flow; reactive transport; CO2 storage, saline aquifer

INTRODUCTION
Carbon capture and storage (CCS) is generally considered a potential option for the campaign
against global warming. A major topic for CCS research is to investigate and characterize possible
sites where CO2 could be stored for a long time. Due to their common occurrence in many
countries and the large available volumes, saline aquifers are one of the main targets sites for
carbon dioxide geological sequestration (Metz et al., 2005). During CO2 injection, a number of
processes are involved that influence storage efficiency and storage safety within the reservoir
(e.g. Metz et al., 2005). Multiphase flow is the dominating process that describes the movement of
the injected CO2 phase and of the formation brine. Main parameters influencing the movement of
CO2 are buoyancy, due to the lower density of CO2 compared to that of the resident brine, and the
pressure gradient caused by the injection. Furthermore, dissolution of CO2 in brine has to be
considered, as it changes the CO2 density and may initiate convective mixing. Dissolved CO2 in
brine changes the geochemical conditions reducing the pH value significantly. This disturbs
the initial equilibrium between the brine and the rock minerals. This rising weathering potential may
lead to the dissolution of minerals, e.g. calcite or feldspars. In the vicinity of the injection well,
high saturations of the injected CO2 phase lead to the vaporization of the residual brine phase
at the prevailing pressure and temperature conditions. Due to the large amount of solvents within the
brine, this may induce salt precipitation. Dissolution as well as precipitation of minerals changes
the porosity and thus also the permeability of the formation rocks, which feeds back on the CO2
spreading by multiphase flow itself. These complex and interacting processes require adequate
software for their numerical simulation for prognosis of phase spreading or risk assessment. For
this purpose, this paper presents the implementation and verification of a coupled software for
simulation of multiphase flow and reactive transport processes for CO2 geological storage.

METHODS
Multiphase flow in porous media is described for each phase by the corresponding balance
equation (e.g. Bear & Bachmat, 1990):

\[
\frac{\partial (n \rho_a S_a)}{\partial t} - \nabla \left( \rho_a \frac{k_a}{\mu_a} \nabla p_a - \rho_a g \right) - \rho_a q_a = 0
\]  

(1)

where \( n \) is the porosity, \( S_a \) the phase saturation, \( \rho_a \) the phase density, \( q_a \) the phase source/sink term
and $v_\alpha$ the phase velocity, where index $\alpha$ indicates the fluid phases brine and CO$_2$. The phase velocity is calculated according to the extended Darcy’s law, where $k$ is intrinsic permeability, $k_{rel}$ the relative permeability, $\mu_\alpha$ the phase viscosity and $p$ phase pressure.

Transport of the individual components is described by a balance equation for each component in each phase (e.g. Bear & Bachmat, 1990) as:

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

with $X$ the component mass fraction and $D$ the coefficient of hydrodynamic dispersion. Upper index $\kappa$ designates the component. The source and sink term includes the geochemical reactions, which couple the individual components with each other.

The open-source scientific software OpenGeoSys is used in this investigation. OpenGeoSys is a finite element code for simulation of thermal, hydrological and mechanical problems in porous media (Kolditz & Bauer, 2004; Wang & Kolditz, 2007; Kolditz et al., 2010). OpenGeoSys uses an object-oriented and process oriented approach that allows the solution of partial differential equations for different physical problems using a generic object structure (Kolditz & Bauer, 2004). This includes also multiphase flow, which can be solved either in the pressure-pressure or in a pressure-saturation formulation. Chemical reactions are simulated using interfaces to PhreeqC (Parkhurst & Appelo, 1999) or ChemApp (Erikson & Konigsberger, 2008).

The simulation of multiphase flow has become standard in both scientific as well as power company work and a variety of computer codes like e.g. Eclipse (Schlumberger Information Systems) are available. Fewer codes are able to solve multiphase flow with multi-component transport and reactions, e.g. ToughReact (Xu et al., 2006). Often, power companies build site models of potential CO$_2$ storage sites using the standard simulator Eclipse. In order to use these existing site models and extend the modelled processes also to reactive transport in multiphase flow, an interface coupling Eclipse to OpenGeoSys is developed. The CO$_2$ injection and multiphase flow can be simulated using Eclipse. The interface adds the possibility of including multi-component transport in both phases as well as geochemical reactions based on an equilibrium as well as a kinetic approach. This allows representing the hydraulic and geochemical alteration during CO$_2$ sequestration under reservoir conditions without creating a new site specific reservoir model.

The processes simulated by OpenGeoSys are processed within a time loop for each time step (Fig. 1). The interface to Eclipse needs to be part of this object-oriented process structure and therefore was implemented as an alternative flow simulator within the “MultiphaseFlow” process (see Fig. 1). A MultiPhaseFlow process is generated within OpenGeoSys, which does not solve the balance equations itself but rather obtains the results of the Eclipse simulation. Using this approach, all required variables, data structures and methods are available. Results of the multiphase flow simulation are passed for each time step from Eclipse to OpenGeoSys, where the transport and geochemical reactions of dissolved and mineral species are calculated.

Whereas Eclipse uses a finite difference method, OpenGeoSys uses a finite element method for the discretization of the balance equations. This makes a transformation of the flow results necessary at each time step. For this purpose, an identical grid using regular hexahedron elements for both simulators is used. The mesh can be created within Eclipse or Petrel or within any compatible software. A mesh converter was developed to transform the Eclipse grid into the grid format of OpenGeoSys.

Currently the data exchange is based on the input and output files of Eclipse. When Eclipse is called for the first time, the interface reads the grid file and creates the data structure for storing the multiphase flow results. Besides the grid structure, this encloses all element faces with their orientation and the distance to the corresponding nodes. After the data structures are set up, the interface reads for all time steps the flow results depending on the number of phases used in the simulation. Phase pressures and phase saturations are interpolated to the nodes of the Finite-Element mesh and the phase velocities are transferred to the Gauss points. Thus the multi-phase flow velocities obtained by Eclipse are directly used, which allows for a high precision. Subsequently, transport of all species considered for the geochemical reactions is simulated in OpenGeoSys.
For simulation of geochemical reactions, existing interfaces to equilibrium speciation simulators like PhreeqC or ChemApp have been implemented in OpenGeoSys. Chemical reactions as well as the mass transport are calculated at the nodes. Changes in the dissolved CO2 concentration occur within the multiphase flow and within the chemical reaction processes. Whereas the equilibrium between dissolved CO2 in water and the CO2 phase is calculated within the multiphase flow process, chemical reactions might consume or produce CO2. This change in CO2 is transferred to the multiphase flow process and accounted for in the next multiphase flow time step.

**BENCHMARK TESTS**

The interface OpenGeoSys-Eclipse, as described above, was applied to several benchmarks to test the data exchange, the implemented transport processes and the program interfaces in 2 and 3 dimensions. Table 1 provides an overview on the number of phases, the dimension used, the simulation type and the flow orientation of the benchmarks investigated.

Benchmarks 1 and 2 were used to test the correctness of single-phase transport. With benchmarks 3 and 4 the multiphase flow process and the variable transfer was tested. Benchmark 6 was used to test the conservative transport in two phases together with multiphase flow. Benchmarks 7 and 8 are used to verify the transfer of dissolved CO2 in water between the multiphase flow and the geochemical reaction objects. Finally Benchmark 9 represents the

<table>
<thead>
<tr>
<th>Nr</th>
<th>Name</th>
<th>Analytical solution or Source for comparison</th>
<th>Phases</th>
<th>Dimension</th>
<th>Flow orientation</th>
<th>Transport</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1D uniform</td>
<td>Kolditz &amp; Shao (2010)</td>
<td>1</td>
<td>1</td>
<td>Parallel</td>
<td>Conservative</td>
</tr>
<tr>
<td>2</td>
<td>2D uniform</td>
<td>Hewson (1976)</td>
<td>1</td>
<td>2</td>
<td>Parallel</td>
<td>Conservative</td>
</tr>
<tr>
<td>3</td>
<td>2D radial</td>
<td>Moench &amp; Ogata (1981)</td>
<td>1</td>
<td>2</td>
<td>Radial</td>
<td>Conservative</td>
</tr>
<tr>
<td>4</td>
<td>Buckley-Leverett (2D)</td>
<td>Buckley &amp; Leverett (1942)</td>
<td>2</td>
<td>1</td>
<td>Parallel</td>
<td>–</td>
</tr>
<tr>
<td>5</td>
<td>CO2 injection (2D)</td>
<td></td>
<td>2</td>
<td>3</td>
<td>Radial</td>
<td>–</td>
</tr>
<tr>
<td>6</td>
<td>CO2 injection (2D)</td>
<td></td>
<td>2</td>
<td>3</td>
<td>Parallel</td>
<td>Conservative</td>
</tr>
<tr>
<td>7</td>
<td>Appearing CO2 phase (2D)</td>
<td></td>
<td>2</td>
<td>2</td>
<td>Parallel</td>
<td>–</td>
</tr>
<tr>
<td>8</td>
<td>Disappearing CO2 phase (2D)</td>
<td></td>
<td>2</td>
<td>2</td>
<td>Parallel</td>
<td>–</td>
</tr>
<tr>
<td>9</td>
<td>Leaky well (3D)</td>
<td>Class et al. (2009)</td>
<td>2</td>
<td>3</td>
<td>Radial</td>
<td>–</td>
</tr>
</tbody>
</table>
application of the multiphase flow simulation on a virtual large scale application focusing on possible leakage scenarios.

The coupled simulator was found to yield good results for all benchmarks considered. Exemplarily, results are shown for the Benchmarks 4 and 5.

For Benchmark 4 (Buckley & Leverett, 1942), the displacement of an incompressible fluid by another incompressible fluid of equal density is simulated for a one-dimensional set-up. Figure 2 compares the results from the simulators Eclipse, Muft (Assteerawatt et al., 2005) and OpenGeoSys-Eclipse for different times and different capillary pressures. Results from the simulators used are in good agreement with each other, which verifies the implemented interface for OpenGeoSys-Eclipse.

Results of Benchmark 5 are shown in Fig. 3. A CO₂ injection at the left side of a 20-m high and 100 m long radial model is simulated. The breakthrough of the CO₂ phase is observed at the uppermost point (20 m above ground) and at 16 m above ground. A CO₂ saturation of zero and hydrostatic pressure conditions are defined at the right model boundary. Figure 3(a) depicts the model set-up and a typical phase distribution, which shows the density separation further away from the injection well. Figure 3(b) shows a comparison of CO₂-phase saturations at the top of the formation.

Generally, a good agreement between the different simulators used is achieved. The differences that can still be seen are due to the different numerical and mathematical methods used. Because the grid nodes for a Finite-Element mesh (OpenGeoSys) are directly at the model boundary, while the grid nodes for a Finite Difference method (Eclipse) are located in the centre of the uppermost model cell, the locations for measuring the CO₂ saturations are slightly different.

The higher saturation shown by OpenGeoSys is thus consistent with the numerical methods used. Figure 3(b) therefore shows a comparison at 16 m above the formation bottom, where this effect should be smaller. Correspondingly, the saturations converge for larger times. At shorter times, again differences between the results of the different simulators used can be seen. The saturation rise is sharpest for OpenGeoSys and smoother for Eclipse or DuMux. The reason this time is that OpenGeoSys employs a pressure–pressure scheme, which is nearly free of numerical dispersion, while Eclipse and DuMux use implicit upwinding schemes, which show numerical dispersion and thus a smearing of the front. The differences between the simulators become smaller, when finer grids and shorter time steps are used, as was tested in a grid convergence study (results not shown).
The coupled simulator OpenGeoSys-Eclipse

Fig. 3 (a) Model set-up for Benchmark 5. The dark grey spots show the location of the two observation points at 20 m and 16 m above the bottom of the formation, the dark filling shows the CO\textsubscript{2} phase distribution. Comparison of the CO\textsubscript{2} phase saturation over time at (b) upper and (c) lower observation point for the simulators OGS, DuMux, OGS-DuMux, Eclipse and OGS-Eclipse.

Fig. 4 Model results for a radial injection into a sandstone formation showing (a) pressure, (b) CO\textsubscript{2} saturation, (c) dissolved CO\textsubscript{2} in water, (d) calcite concentrations in the solid phase, (e) pH and (f) porosity change due to mineral dissolution.

APPLICATION

To test the applicability of the developed code for real site conditions, as a first step a radial injection model was used. CO\textsubscript{2} is injected at the left boundary for 20 years with a 50 years post-injection period.

Hydrostatic conditions are applied at the right hand side boundary. The model length is 9000 m. A typical geochemical composition of a sandstone rock in the North German Basin was used for the geochemical system. This includes the minerals Calcite and Dolomite and the
corresponding aqueous species. A total of 12 geochemical components is included in the model and geochemical kinetic as well as equilibrium reactions are simulated. Results (exemplarily) are shown in Fig. 4. Due to the injection, CO2 spreads and shows only little gravity separation (Fig. 4(b)), as a rather low hydraulic permeability is applied. The dissolved CO2 (Fig. 4(c)) closely follows the CO2 phase, and thus determines the area of geochemical reactions. A pH-change is clearly visible in this area, dropping from about 7 to 5 (Fig. 4(e)), as well as small changes to the porosity (Fig. 4(f)).

CONCLUSIONS

The coupled simulator OpenGeoSys-Eclipse has been developed, implemented and successfully verified for a number of test cases of increasing complexity. Results show that the implementation is correct and the coupled simulator is thus able to simulate the hydraulic behaviour of a CO2 injection into a saline formation. Within OpenGeoSys, multiphase flow and reactive multi-component transport were successfully coupled. The simulator is applicable to geochemical systems, as found in saline aquifer formations, and a first geochemical investigation using a simplified radial model was performed. Future work will extend these simulations to full scale site models and test the simulator using a variety of geochemical systems.

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