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The coupled multiphase flow and reactive transport simulator OGS-Eclipse for CO_2 storage simulations

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Abstract The long-term prognosis of the behaviour of CO_2 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; CO_2 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 CO_2 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 CO_2 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 CO_2 phase and of the formation brine. Main parameters influencing the movement of CO_2 are buoyancy, due to the lower density of CO_2 compared to that of the resident brine, and the pressure gradient caused by the injection. Furthermore, dissolution of CO_2 in brine has to be considered, as it changes the CO_2 density and may initiate convective mixing. Dissolved CO_2 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 CO_2 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 CO_2 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 CO_2 geological storage.

METHODS

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

$$\frac{\partial(n\rho_\alpha S_\alpha)}{\partial t} - \nabla\left(\rho_\alpha \frac{k_{r\alpha}k}{\mu_\alpha}\left(\nabla p_\alpha - \rho_\alpha g\right)\right) - \rho_\alpha q_\alpha = 0 \tag{1}$$

where n is the porosity, S_α the phase saturation, ρ_α the phase density, q_α the phase source/sink term

and v_α the phase velocity, where index α 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_{ra} the relative permeability, μ_α 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:

$$\frac{\partial\left(nS_\alpha\rho_\alpha X_\alpha^\kappa\right)}{\partial t} + \nabla\left(v_\alpha\rho_\alpha X_\alpha^\kappa - nS_\alpha D_\alpha^\kappa\nabla\left(\rho_\alpha X_\alpha^\kappa\right)\right) - q_\alpha^\kappa = 0 \tag{2}$$

with X the component mass fraction and D the coefficient of hydrodynamic dispersion. Upper index κ 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.
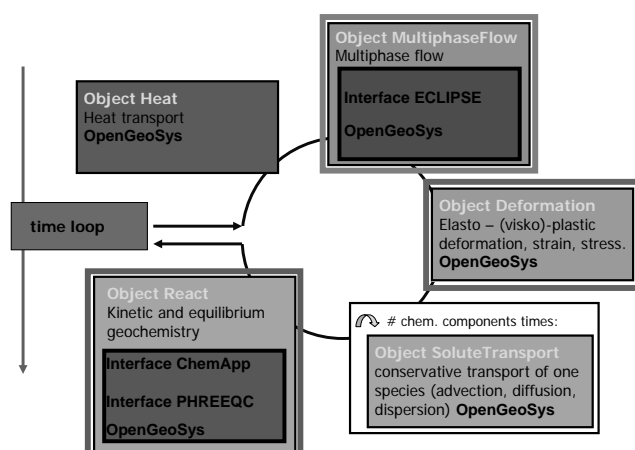
Fig. 1 OpenGeoSys Code structure with the interface Eclipse in the MultiphaseFlow object.

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 CO_2 concentration occur within the multiphase flow and within the chemical reaction processes. Whereas the equilibrium between dissolved CO_2 in water and the CO_2 phase is calculated within the multiphase flow process, chemical reactions might consume or produce CO_2. This change in CO_2 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 CO_2 in water between the multiphase flow and the geochemical reaction objects. Finally Benchmark 9 represents the

Table 1 Classification of the considered benchmarks for testing the developed interface Eclipse-OpenGeoSys.

Nr	Name	Analytical solution or Source for comparison	Phases	Dimension	Flow orientation	Transport
1	1D uniform	Kolditz & Shao (2010)	1	1	Parallel	Conservative
2	2D uniform	Hewson (1976)	1	2	Parallel	Conservative
3	2D radial	Moench & Ogata (1981)	1	2	Radial	Conservative
4	Buckley-Leverett (2D)	Buckley & Leverett (1942)	2	1	Parallel	–
5	CO_2 injection (2D)		2	3	Radial	–
6	CO_2 injection (2D)		2	3	Parallel	Conservative
7	Appearing CO_2 phase (2D)		2	2	Parallel	–
8	Disappearing CO_2 phase (2D)		2	2	Parallel	–
9	Leaky well (3D)	Class *et al.* (2009)	2	3	Radial	–

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, Mufte (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.
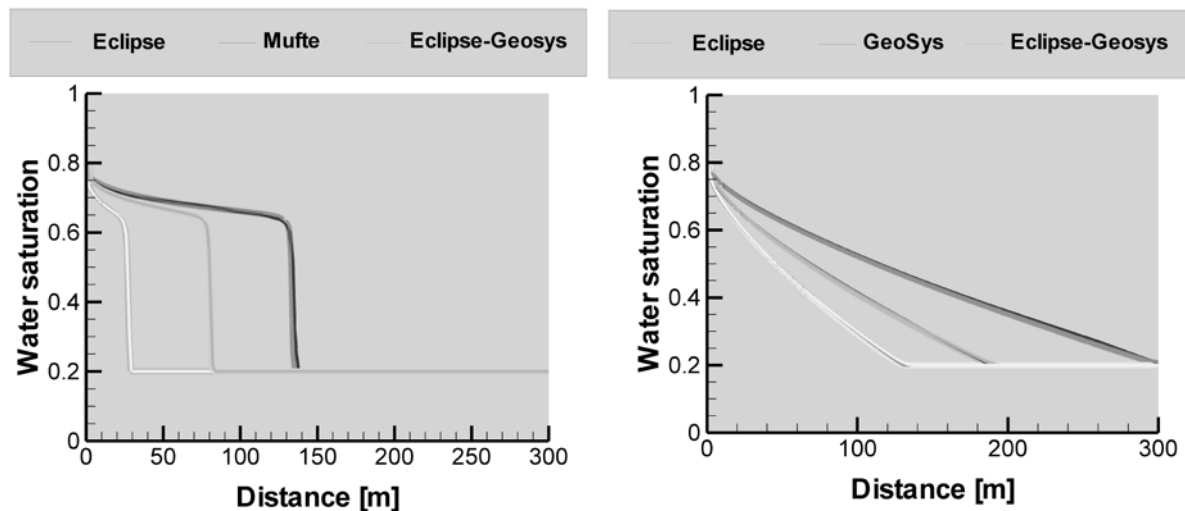

Fig. 2 Comparison of simulation results from the simulators Eclipse, Mufte, OpenGeoSys and OpenGeoSys-Eclipse. Left: Saturation profiles for 100, 300 and 500 days using Brooks-Corey p_c–S and k_r–S relation without capillary pressure. Right Saturation profiles for 50, 100 and 231 days using a linear p_c–S, k_r–S relation with capillary pressure.

Results of Benchmark 5 are shown in Fig. 3. A CO_2 injection at the left side of a 20-m high and 100 m long radial model is simulated. The breakthrough of the CO_2 phase is observed at the upper-most point (20 m above ground) and at 16 m above ground. A CO_2 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 CO_2-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 CO_2 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 satura-tion 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).
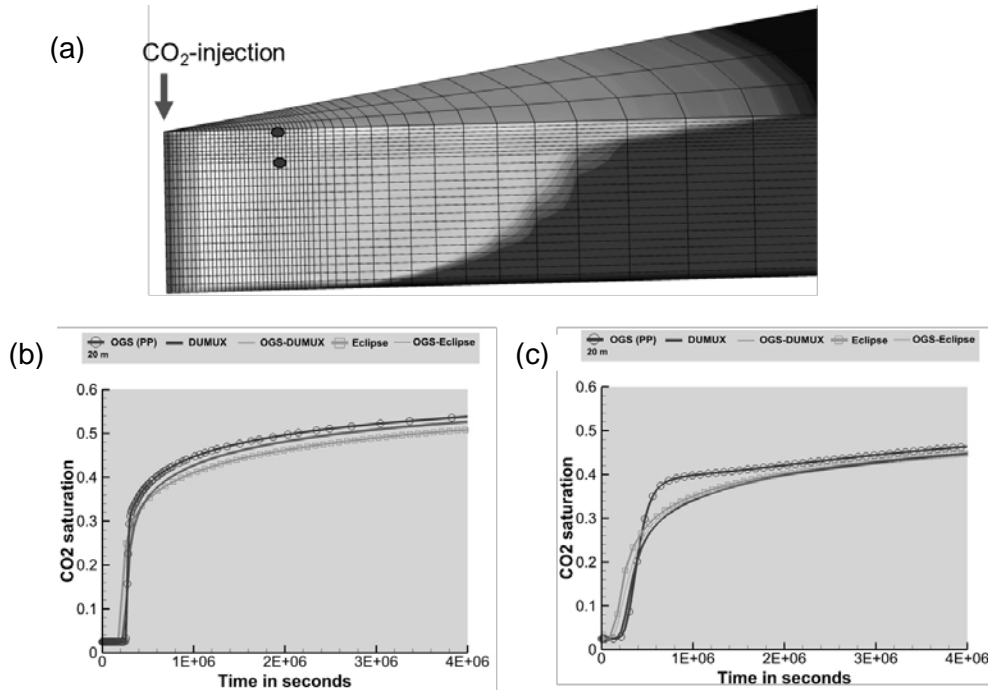
Fig. 3 (a) Model set-up for Benchmark 5. The dark grey spots show the location of the two observation points at 20 m and 16 m above the bottom of the formation, the dark filling shows the CO_2 phase distribution. Comparison of the CO_2 phase saturation over time at (b) upper and (c) lower observation point for the simulators OGS, DuMux, OGS-DuMux, Eclipse and OGS-Eclipse.
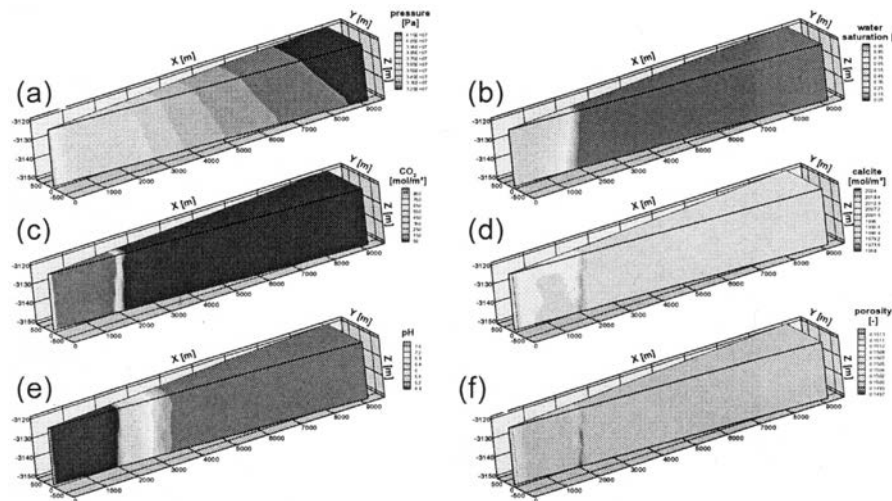
Fig. 4 Model results for a radial injection into a sandstone formation showing (a) pressure, (b) CO_2 saturation, (c) dissolved CO2 in water, (d) calcite concentrations in the solid phase, (e) pH and (f) porosity change due to mineral dissolution.

APPLICATION

To test the applicability of the developed code for real site conditions, as a first step a radial injection model was used. CO_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, CO_2 spreads and shows only little gravity separation (Fig. 4(b)), as a rather low hydraulic permeability is applied. The dissolved CO_2 (Fig. 4(c)) closely follows the CO_2 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 CO_2 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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