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The coupled simulator ECLIPSE – OpenGeoSys for the simulation of CO_2 storage in saline formations

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Abstract

The storage of CO_2 in deep saline aquifers is due to the large available capacities and the common occurrence of these formations one of the major options for carbon dioxide sequestration. Besides the multiphase flow aspects geochemical, thermal and mechanical processes may alter the conditions within the reservoir as well as in the cap rock. Whereas single aspects of these processes can be investigated with experiments a multi-process simulator allows evaluating their combined consequences for the storage system over short and long time scales. In this paper the newly coupled software ECLIPSE-OpenGeoSys is presented that allows a combined simulation of multiphase flow, transport and geochemical reactions. ECLIPSE provides a fast and efficient solution for the multiphase flow whereas the open-source scientific software OpenGeoSys is used for calculating transport and geochemical reactions. This paper presents the code structure of the interface. Furthermore the coupled software is successfully applied to benchmarks

Keywords: CO2, ECLIPSE; OpenGeoSys; CCS; saline aquifers

1. Introduction

Saline aquifers are one of the main targets for carbon dioxide sequestration [1]. During CO2 injection many processes are involved that might influence storage efficiency and storage safety within the reservoir (e.g. [1]). Multiphase flow is the dominating process that describes the movement of the CO2 phase as well as its dissolution within the brine. Main parameters influencing the movement of CO2 are buoyancy due to the lower density compared to brine and the pressure gradient due to injection. Furthermore the dissolution of CO2 in brine changes the density. Therefore convective mixing is expected to enhance CO2 dissolution. Dissolved CO2 in brine changes strongly the chemical conditions. Whereas the brine was in equilibrium with the minerals before injection dissolved CO2 reduces the pH significantly. The rising weathering potential of the fluid causes the dissolution of minerals like calcite or feldspar. Very close to the injection well the high saturation of the CO2 phase causes the vaporizing of the

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residual brine phase at specific pressure and temperature conditions. Due to the large amount of solvents within the brine this will lead to salt precipitation. The dissolution as well as the precipitation of minerals changes the porosity and permeability and thus the multiphase flow itself.

The multiphase flow in general for each phase can be described depending on the porosity n, the densityρ, the saturation S, the pressure p and a sink/source term q (e.g. [2]):

$$\frac{\partial(n\rho_\alpha S_\alpha)}{\partial t} + \mathrm{div}\left(\rho_\alpha \overrightarrow{v_\alpha}\right) - \rho_\alpha q_\alpha = 0 \qquad (1)$$

The open-source scientific software OpenGeoSys was used in this investigation. It is a finite element code for simulation of thermal, hydro and mechanical problems in porous media ([3]; [4]). OpenGeoSys uses an object-oriented process based approach that allows the solution of partial differential equations for different physical problems in the same way ([5]). This includes also multiphase flow, which can be solved either in the pressure-pressure or in a pressure-saturation formulation. Chemical reactions might be considered as well via interfaces to PhreeqC ([6]) or ChemApp ([7]).

Whereas the simulation of multiphase flow is possible in a wide variety of computer codes like e.g. Eclipse (Schlumberger Information Systems) , fewer codes are able to solve multiphase flow with multi-component transport and reactions like e.g. ToughReact ([8]). Commonly local models of potential CO2 storage sites are build by power companies that frequently use the simulator Eclipse. To extend the capabilities for simulating CO2 storage with these existing models as a multiphase flow and reactive transport process a newly developed interface is presented that couples Eclipse to OpenGeoSys. This allows representing the hydraulic and geochemical alteration during CO2 sequestration under reservoir conditions without creating a new site specific reservoir model.

2. Method

For the use of Eclipse as multiphase flow simulator during an OpenGeoSys run the interface needs to be part of the process structure of OpenGeoSys. Thus it is implemented as alternative flow simulator within the "MultiphaseFlow" process, see Figure 1. Eclipse and OpenGeoSys are coupled using an operator splitting approach where OpenGeoSys defines the length of each flow time step. Results of the multiphase flow simulation are passed for each time step from Eclipse to OpenGeoSys where transport of dissolved species is calculated. Whereas Eclipse uses finite differences, OpenGeoSys is a finite element simulator, which makes a transformation of the flow results necessary at each time step.

To simplify the data exchange an identical grid structure for both simulators is used. OpenGeoSys provides a range of 1D (lines), 2D (triangles, quadrilaterals) and 3D (tetrahedron, hexahedron) elements. The different element shapes allow a close fit to complex model boundaries and geological structures. But the finite element approach requires that all elements are connected to each other. Compared to this Eclipse achieves the flexibility of its hexahedron mesh with using regular or non regular elements together with non neighbor connections. Bringing the possibilities as well as the needs of both simulators together requires a mesh of regular hexahedrons without non-neighbor connections. The mesh can be created within Eclipse or within any software that is able to provide the corresponding "grd" file. A mesh converter was developed to translate it into the format of OpenGeoSys.

Within the coupling the multiphase flow model with all necessary initial and boundary conditions is built in Eclipse. Despite the fact that OpenGeoSys does only use flow results from Eclipse it still requires the corresponding data structures. Therefore it is necessary to provide a multiphase flow process with the model dimension, the converted mesh and material properties that are necessary for component transport as well. Flow related initial and boundary conditions can be omitted.

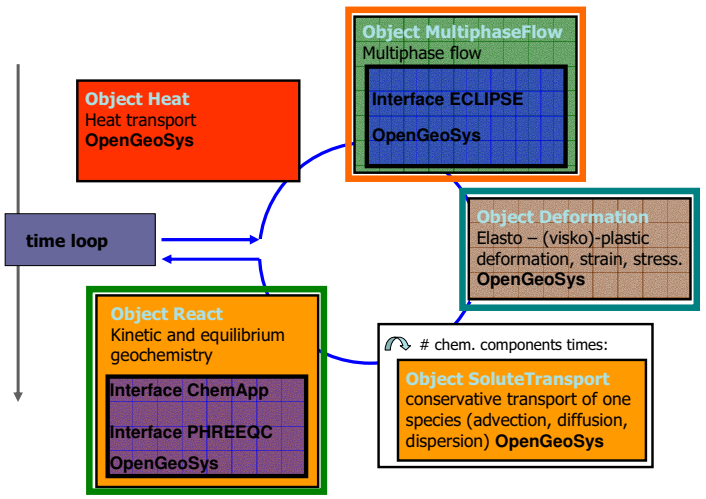

Figure 1 OpenGeoSys Code structure with the interface Eclipse for multiphase flow.

The course of a model run follows the process order within OpenGeoSys that calls each considered process in the order shown in Figure 1 with the process related time step. If the flow process is called, the interface itself calls Eclipse and provides the length of the current time step. After the ECLIPSE simulation the results are transformed to the FE mesh. Currently the data exchange is based on the output files of Eclipse. If Eclipse is called the first time the interfaces 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 structure is provided the interface reads for any time step the flow results depending on the number of phases used in the simulation. Phase pressure and phase saturation are stored at the elements and the phase velocities are stored at the element faces. Flow over the element faces is than transferred to the nodes and in a second step from the nodes to the Gauss points in OpenGeoSys. Thus the multi-phase flow velocities obtained by Eclipse are directly used instead of recalculating them from the pressure distribution. This allows keeping a high data precision with the general possibility of using non-neighbor connections. Due to this procedure, the phase pressures and saturations at nodes are not required for the transport simulation but are used for output purposes. An inverse volume weighted interpolation scheme is used for this data transfer. Additionally the pressure can be provided at the elements for considering mechanical deformation, which needs no further transformation. Subsequently, transport of all species considered for the geochemical reactions is simulated in OpenGeoSys. For geochemical reactions existing interfaces to equilibrium speciation simulators like PhreeqC or ChemApp are available. Possible changes in the permeability and porosity, which are induced by the geochemical reactions due to mineral dissolution or precipitation, will in future be considered for the multiphase simulations.

3. Benchmark tests

The interface Eclipse-OpenGeoSys, 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, the simulation type and the flow orientation of the benchmarks used.

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

Nr.	Name	Analytical solution or Source for comparison	Phases	Dimen-sion	Flow orientation	Transport
1	1D uniform	[4]	1	1	Parallel	Conservative
2	2D uniform	[9]	1	2	Parallel	Conservative
3	2D radial	[10]	1	2	Radial	Conservative
4	Buckley-Leverett	[11]	2	1	Parallel	-
5	CO_2 injection		2	3	Radial	-
6	Leacky well benchmark Stuttgart	[12]	2	3	Radial	-

The coupled simulator was found to yield good results for all of them. Exemplarily results are shown for the benchmarks 3, 4 and 5.

Benchmark 3 tests radial flow and transport in two dimensions that usually will occur during CO2 injection. It is based on the analytical solution from [10] and compared to simulation results obtained using OpenGeoSys, Eclipse and the interface Eclipse-OpenGeoSys. Thereby an injection rate of 100 m³/d was assumed. The results are depicted in Figure 2, and show the resulting radial distribution of the conservative compound as well as the good agreement of the results from the coupled Eclipse-OpenGeoSys simulator with the analytical solution, which verifies the implementation of the interface.

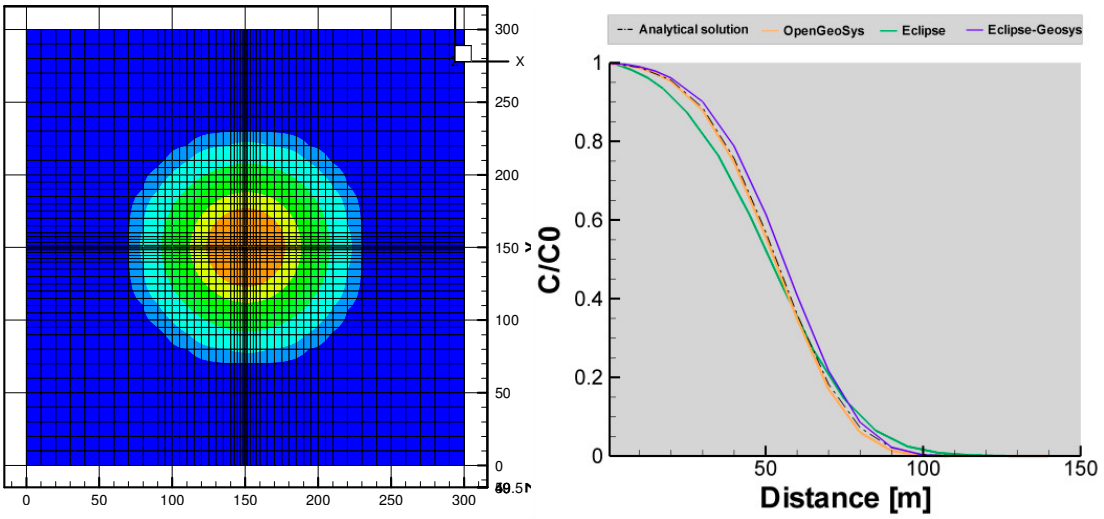

Figure 2 2D radial Benchmark, spread of a conservative tracer from the injection well top view (left) and comparison of radial profiles using the simulators OpenGeoSys, Eclipse and Eclipse-OpenGeosys (right)

The up scaling from one to two-phase flow is tested using Benchmark 4 [11]. The displacement of one incompressible fluid by another incompressible fluid of equal density is simulated for a one-dimensional set-up.

Figure 3 compares the results from different simulators (Eclipse, Mufte ([13]) and Eclipse-GeoSys) for different times and different capillary pressures. The figures show a good correspondence of the individual results, which again verifies the implemented interface.

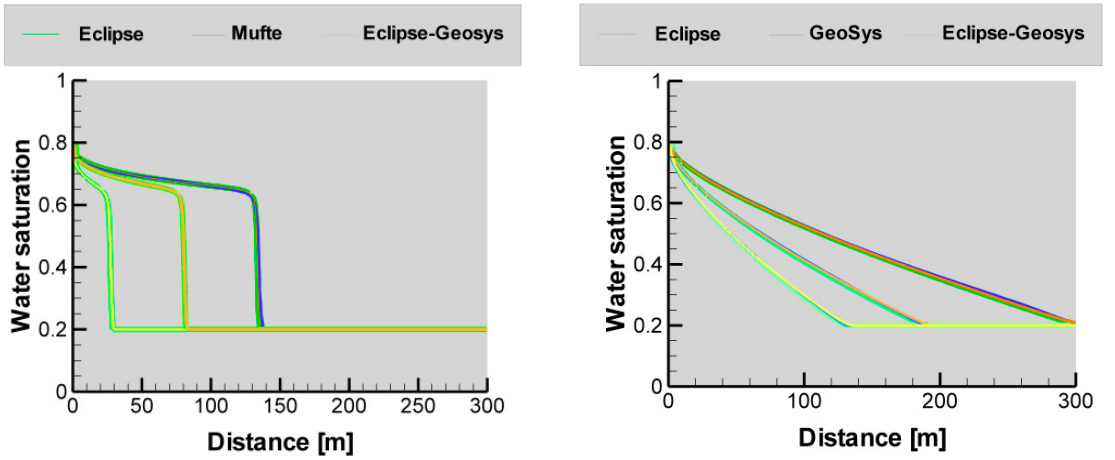

Figure 3 Comparison of results between Eclipse, Mufte, OpenGeoSys and Eclipse-OpenGeoSys: left after: 100, 300 and 500 days, Brooks-Corey pc-S, kr-S relation without capillary pressure; right after: 50, 100 and 231 days, linear pc-S, kr-S relation with capillary pressure.

The last example covers the injection of CO2 into a deep saline aquifer, see Figure 4. The aquifer is at a depth of around 3000 m thus the injected CO2 stays supercritical. The spread of the CO2 phase between Eclipse and the Eclipse-OpenGeoSys interface is compared after 1000 days of injection with a rate of 1600 m³/d. For the simulation several simplifying assumptions were used. The density of CO2 ρCO2 = 479 kg/m³ and of brine ρbrine = 1045 kg/m³ as well as the viscosities ηCO2 = 3.95.10-5 Pa.s and ηbrine = 2.535.10-4 Pa.s were assumed constant, as in the benchmark study of [12].

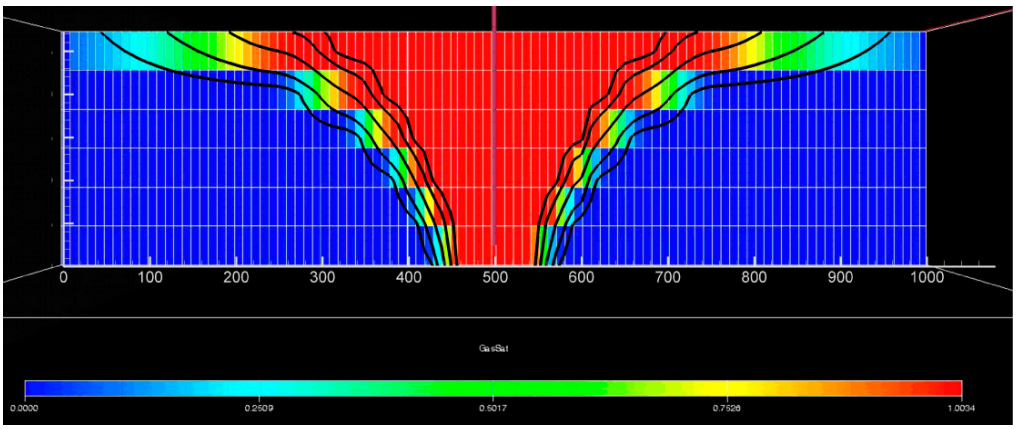

Figure 4 Spread of the CO2 phase in a saline aquifer after 300 days with an injection rate of 1600 m³/d. Full block contours: Eclipse, black contour lines: Eclipse-OpenGeoSys, showing contour lines at sCO2 = 0.1, 0.25, 0.5, 0.75 und 0.9.

Overall the comparison of simulation results between the interface Eclipe-OpenGeoSys and analytical solutions in the benchmarks 1, 2, 3 and 4 showed that the accuracy of describing the transport phenomena was improved compared to Eclipse. The reason for this is the possibility of solving the transport equation in OpenGeoSys using a semi-implicit time stepping, whereas this option is not included in the Eclipse software. Furthermore the solution of the coupled software shows less numerical dispersion compared to Eclipse. This might be of importance for the prediction of the impact range of CO2 injection with slow moving fronts of CO2 containing brine.

The advantage of a high efficiency for solving multiphase flow is underlined with the last benchmark. Results show that the computation time of the interface Eclipse-OpenGeoSys is up to 10 times faster compared to multiphase flow calculations within OpenGeoSys. The higher computation speed is achieved despite the fact that the results of the multiphase flow are obtained from files and interpolated to the OpenGeoSys mesh. The efficiency could be increased even more if the ECLIPSE developer interface is used for data exchange. This interface allows to pause the ECLIPSE simulation after a certain time step. The data exchange could be performed based on data stored within the memory. Thus the data exchange itself speeds up and the calculations are faster because the initialization procedure is carried out only once.

Acknowledgements

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