NUMERICAL MODELING OF CO_2 SEQUESTRATION WITH MUFTE-UG

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ABSTRACT

In this presentation, we outline the recently developed modeling capabilities of our numerical simulator MUFTE-UG in the field of simulating the non-isothermal multi-phase multi-component processes occuring during the sequestration of CO_2 in deep geological formations. The relation of this work to other currently ongoing research projects in which the authors are involved will be discussed. A benchmark example related to our current research activities in this field is then discussed in more detail.

We use MUFTE-UG as a development platform for our new conceptual models and their mathematical-numerical implementation. Based on existing moduls, MUFTE-UG has been extended by a non-isothermal two-phase two-component model concept for the simulation of CO_2 sequestration in geological formations. It takes into account the two phases CO_2 and brine and the components CO_2 and water which can dissolve in the different phases. Presently, we assume chemical equilibrium and neglect all kinds of mineralization processes in the code.

The presented benchmark example is oriented at certain key questions that have to be answered in the run-up to any large-scale implementation of the CO_2 sequestration technology. In this case, we focus particularly on leaky well scenarios.

1. INTRODUCTION

CO_2 sequestration in geological formations is considered for reducing carbon dioxide emissions into the atmosphere and thereby mitigating the greenhouse effect. This method is to be investigated with all available scientific means to assess feasibility, problems, and limitations. One possibility to study this technology is the formulation of mathematical models that take into account the relevant processes in the subsurface. These are, for example, the flow and transport behavior of multiple phases, geochemical reactions and geomechanical effects. The various processes involved lead to very complex mathematical problems which cannot be solved analytically, at least not in their full complexity. Available (semi-)analytical approaches [Nordbotten et al., 2005] use significant simplifications. Therefore, numerical methods have to be applied. Nevertheless, (semi-)analytical solutions are very valuable for an improved understanding of the coupled processes. Furthermore, they can be used to verify the developed numerical models.

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In this paper, we first describe the conceptual model for a non-isothermal compositional CO_2-water (brine) model based on the simulator MUFTE-UG as the development platform. A focus will be on the partitioning of the components in the phases and the temperature and pressure dependence of the fluid properties. We introduce the major model assumptions, the physical processes taken into account, and the arising system of strongly coupled non-linear partial differential equations. The numerical treatment of non-linearities and the discretization in space and time is shortly discussed. The second pillar of this paper is then the application of the model for a benchmark example which is particularly related to the problem of CO_2 leakage through a fracture or an abandoned well.

2. MODEL

For the description of the flow and transport processes of carbon dioxide and brine in a rock formation, a two-phase two-component model concept is used. This means that two separate fluid phases, a CO_2 phase and a brine phase are moving in the subsurface while the rock matrix is assumed to be rigid and incompressible. However, the hydraulics of the fluid flow is strongly influenced by the properties of the porous medium like permeability and porosity. Furthermore, the interaction between fluid phases and rock matrix is expressed by highly non-linear constitutive relationships for capillary pressure and relative permeabilities as functions of saturation. The considered components are CO_2 and water. The carbon dioxide component can dissolve in the aqueous phase while the water content of the CO_2 is considered to be negligible. Furthermore, high salinities of the formation water are taken into account by considering their effect on the fluid properties of the brine phase and the amount of dissolved carbon dioxide (salting-out). The model concept also takes into account non-isothermal processes that occur while the carbon dioxide is migrating in the subsurface. Details of the presented model can be found in [Bielinski, 2006] and [Bielinski et al., 2006].

2.1. **Fluid properties.** The essential fluid properties needed for the description of the non-isothermal multi-phase flow and transport problem are density, enthalpy, and viscosity of each phase. An overview of these properties is given in table 1. The CO_2 fluid properties vary significantly depending on temperature and pressure conditions in the subsurface. This is because the carbon dioxide can occur in gaseous, liquid, or supercritical state of aggregation. Figure 1 illustrates this behavior showing the density as a function of pressure at various temperatures. A significant density difference between, e.g., gaseous and liquid CO_2 can be observed.

2.2. **Component partitioning.** The component partitioning in this work only addresses the dissolution of CO_2 in the brine phase. An approach after [Duan and Sun, 2003] is used for taking into account the effect of temperature, pressure, and salinity on the dissolution behavior.

2.3. **Mathematical model.** This involves balance equations for mass and energy, constitutive relationships and supplementary constraints for saturations, mass fractions and pressures. Important physical processes such as transient storage, advective transport of the components with the phase flow, diffusion in the brine phase need to be taken into

TABLE 1. Fluid properties of brine and CO_2.

Fluid property	function of	literature
CO_2 density ϱ_{CO2}	$f(T, p)$	[Span and Wagner, 1996]
CO_2 enthalpy h_{CO2}	$f(T, p)$	[Span and Wagner, 1996]
CO_2 viscosity μ_{CO2}	$f(T, p)$	[Fenghour et al., 1998]
Brine density ϱ_b	$f(T, p, S, X_w^{CO2})$	[Batzle and Wang, 1992], [Garcia, 2001, IAPWS, 1997]
Brine enthalpy h_b	$f(T, p, S, X_w^{CO2})$	[Daubert and Danner, 1989], [Duan and Sun, 2003, IAPWS, 1997], [Michaelides, 1981]
Brine viscosity μ_b	$f(T, S)$	[Batzle and Wang, 1992]

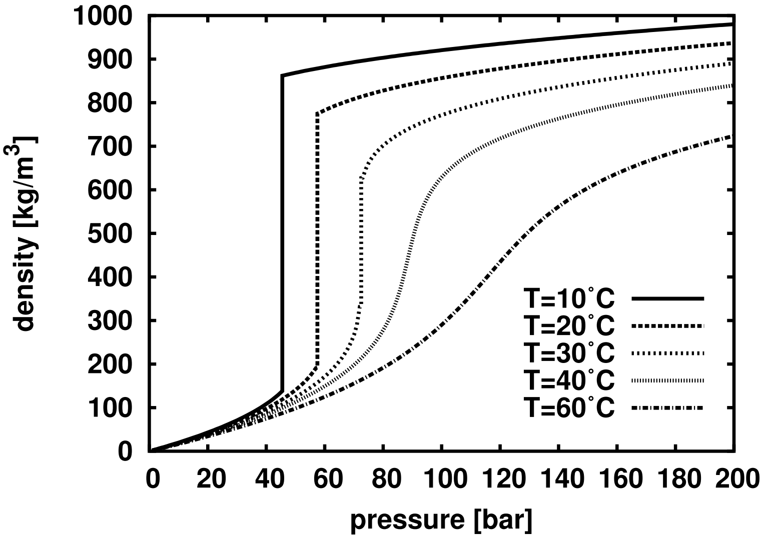

FIGURE 1. Density of CO_2 as a function of pressure at various temperatures using the correlations of [Span and Wagner, 1996].

account. The velocity of the advective phase flow is calculated using the multi-phase version of the Darcy equation. The diffusion in the brine phase is calculated using a Fickian approach. The mass balance equations for each component is given in equation (1). The constitutive relationships necessary for the closure of the balance equations is given by [Bielinski et al., 2006]. In equations (1) and (2), ϱ_α is the density of the phase α, S is saturation, X_α^κ is the mass fraction of the component κ in the phase α, k_r and $\mathbf{K}$ are the relative and intrinsic permeabilities respectively, μ denotes dynamic viscosity, D_{pm} is a diffusion coefficient, u is internal energy, c_s is the specific heat capacity of the solid matrix, T is temperature, p is pressure, λ_{pm} is heat conductivity and h is specific heat capacity.

$$
\begin{array}{lr}
\phi \frac{\partial(\Sigma_\alpha \varrho_\alpha X_\alpha^\kappa S_\alpha)}{\partial t} & \text{storage} \\[2ex]
-\Sigma_\alpha \nabla \cdot \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \varrho_\alpha X_\alpha^\kappa \mathbf{K} \cdot (\nabla p_\alpha - \varrho_\alpha \mathbf{g}) \right\} & \text{advective transport} \\[2ex]
-\nabla \cdot \left\{ D_{pm}^\kappa \varrho_w \nabla X_w^\kappa \right\} & \text{diffusive transport} \\[2ex]
-q^\kappa & \text{source/sink} \\[2ex]
= 0, & \kappa \in \{w, CO_2\}, \quad \alpha \in \{w, CO_2\}.
\end{array}
\tag{1}
$$

Non-isothermal processes can be quite important in the context of CO_2 sequestration in geological formations. An energy balance equation under the assumption of local thermal equilibrium is used to describe such processes. This is given in equation (2).

$$
\begin{array}{lr}
\phi \frac{\partial(\Sigma_\alpha \varrho_\alpha u_\alpha S_\alpha)}{\partial t} + (1-\phi) \frac{\partial \varrho_s c_s T}{\partial t} & \text{storage} \\[2ex]
-\nabla \cdot (\lambda_{pm} \nabla T) & \text{conduction} \\[2ex]
-\Sigma_\alpha \nabla \cdot \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \varrho_\alpha h_\alpha \mathbf{K} \cdot (\nabla p_\alpha - \varrho_\alpha \mathbf{g}) \right\} & \text{convection} \\[2ex]
-\Sigma_\kappa \nabla \cdot \left\{ D_{pm}^\kappa \varrho_w h_w^\kappa \nabla X_w^\kappa \right\} & \text{heat transport due to diffusion} \\[2ex]
-q^h & \text{source/sink} \\[2ex]
= 0, & \kappa \in \{w, CO_2\}, \quad \alpha \in \{w, CO_2\}.
\end{array}
\tag{2}
$$

The storage term accounts for the storage of energy in the fluid phases and in the formation matrix. Heat conduction and convection as well as a source/sink term are also included in the equation.

2.4. **Numerical model.** Above, we outlined the arising system of partial differential equations that has to be solved with appropriate numerical methods. A key issue of the numerical solution process is the application of robust, fast and efficient algorithms on the one hand and the generation of accurate and stable solutions on the other hand. The numerical simulator MUFTE-UG ([Helmig et al., 1998]) that we use as the development platform for our work provides a variety of numerical algorithms and solution methods. MUFTE-UG was jointly developed by work groups at the University of Stuttgart and the University of Heidelberg. It is conceptually designed as a research code with a strictly modular and hierarchical architecture that allows to combine different physical-mathematical model concepts with a number of discretization and numerical solution methods.

For the above-mentioned PDEs we use a Newton-Raphson linearization for the treatment of the non-linearities. The derivations of the equations with respect to the primary variables is achieved by numerical differentiation (first order central differences method). Out of this linearization arises a linear system of equations which we solve with a BiCGStab solver. Optionally, we can use this in combination with a multigrid preconditioner. However, the efficiency and applicability of the multigrid method depends on the method of grid generation and degree of heterogeneity on the coarsest grid.

Time is discretized fully implicit (Euler). Higher-order time discretization methods revealed non-physically oscillating solutions. The discretization in space is done with a subdomain-collocation method. The so-called BOX method is based on the weighted residuals approach and can be formally distinguished from a finite-element method by the choice of the weighting functions. The BOX method uses a dual mesh with piecewise constant weighting functions in the boxes (secondary mesh). The interpolation of the parameters is done with shape functions that are based on the primary mesh. For details, we refer here to [Helmig, 1997] and [Bastian, 1999].

Another important issue of the solution process is the choice of the primary variables. Since we can have situations where phases appear or disappear, the set of primary variables is not necessarily the same throughout the domain and can locally change during a simulation. The algorithm that switches the primary variables dependent on the physical processes (displacement, dissolution, condensation, etc.) therefore requires switching criteria that indicate a change of the phase state. For the disappearance of phases this is simply achieved by negative values of saturations. The appearance of phases, however, needs to be done by considering the responsible physical process. This is explained in detail in [Class et al., 2002] and [Bielinski et al., 2006].

3. APPLICATIONS

Current research projects which involve the modeling of CO_2 sequestration in geological formations with MUFTE-UG include:

- *CO_2SINK.* This project aims at testing subsurface storage of CO_2 in an area near Berlin and by this means improve the general understanding of the processes and the techniques involved in geological CO_2 sequestration. Our work package involves large-scale numerical simulations of the CO_2 injection process to help predict the evolution of the CO_2 plume. CO_2SINK is funded by the EU.
- *CO2-TRAP.* The objectives of this project include the development of physical and mathematical model approaches for the CO_2 adsorption in coal seams and simultaneous desorption of methane (CH_4), the implementation of these approaches in a numerical multi-phase simulator and the validation of the models by comparison with laboratory experiments.
- *Numerical Investigation of CO_2 Sequestration in Geological Formations - Problem-OrientedBenchmarks.* This project and the CO2-TRAP project are funded by the German Research Foundation (DFG) and the Federal Ministry of Education and Research in Germany (BMBF) in the context of the geoscientific research and development program [GEOTECHNOLOGIEN, 2005].

  The project aims at developing benchmark problems related to CO_2 sequestration for the comparison of different numerical codes. The problems are meant to be oriented around topics that are often dealt with in the context of CO_2 sequestration e.g. storage-capacity estimation, enhanced coalbed methane recovery. In the following, one benchmark problem will be addressed as an example of the modeling of CO_2 sequestration with MUFTE-UG.

Benchmark problem: CO_2 leakage from a geological reservoir. This benchmark deals with the problem of CO_2 leakage from a geological reservoir through an abandoned well. The importance of the investigation of such scenarios is obvious. The goal of CO_2 capture and storage in geological formations over long periods of time is undermined if the CO_2 can leak back to the atmosphere. Moreover, CO_2 leaking into the atmosphere in large quantities poses a serious threat to human lives, since high concentrations of CO_2 cause suffocation. Leakage can occur through abandoned wells or through fractures in the formation. In North America, for example, many potential formations for CO_2 sequestration are perforated by between thousands and millions of oil and gas wells. Since CO_2 is less dense than water (even as a supercritical fluid), it would upon reaching such a well rise towards the surface. The thermal effects involved while the CO_2 is rising are just as important especially if phase changes are involved.

The numerical simulation of scenarios involving such leakage is a major part of this benchmark.

Numerical simulation. A model has been set up to simulate such a leakage scenario (see figure 2). The model domain is located 640 m to 800 m below the surface and has the following dimensions: 1000 m x 1000 m x 160 m. The distance between the injection and the leaky well is 100 m and the injection rate is 8.87 kg/s. The leaky well is treated as a porous medium with a higher permeability ($1{\cdot}10^{-12}$ m^2) than the formation ($2{\cdot}10^{-14}$ m^2). The porosities of the well and the formation are both 0.15.

Figure 3 is a slice taken from the three-dimensional domain and shows the distribution of the CO_2 saturation after 200 days of injection. Part of the CO_2 dissolves in the brine. In this case, after 200 days about 9% ($1.36{\cdot}10^7$ kg) of the injected CO_2 had dissolved. The leakage rate as a function of time is shown in figure 4. The leakage rate is calculated as the CO_2 flux at the middle of the leaky well (z = 80 m, see figures 2 and 3). Leakage starts with the upward brine flux when the mass fraction of CO_2 in the brine becomes significant. This is however a small amount compared to the CO_2 flux as a separate phase which sets in later, increases to a maximum value and slowly drops. This drop in the leakage rate can be attributed to the lateral boundary conditions which influence the pressure in the domain. For an infinitely large domain, the CO_2 flux would be expected to continue increasing ([Nordbotten et al., 2005]).

Figure 4 also shows the temperature at the top of the leaky well (z = 130 m, see figures 2 and 3). The temperature initially rises a bit as warm brine from lower regions in the formation flows upwards. As soon as the CO_2 phase arrives, there is sudden temperature decrease which is as a result of the phase change of the CO_2 (liquid to gas) in that region and the accompanying volume/density and temperature changes.

Within the project, it is planned to adapt this example for a comparison with a semi-analytical solution based on the work of [Nordbotten et al., 2005].

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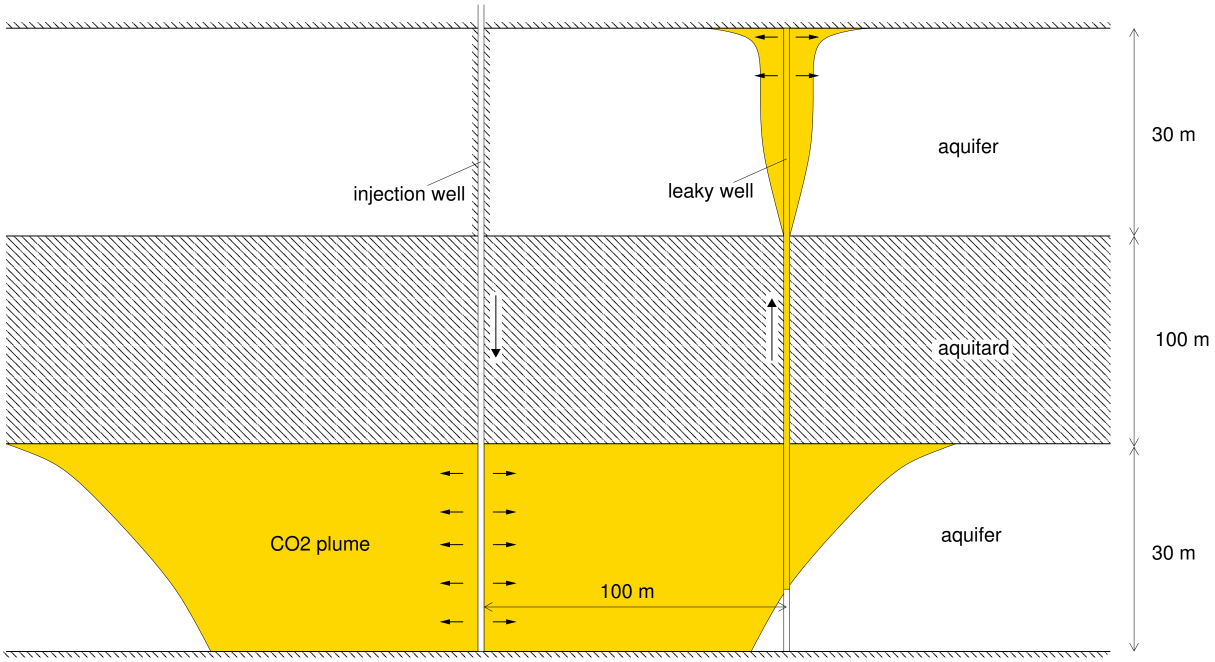

Figure 2. Simulated leakage scenario

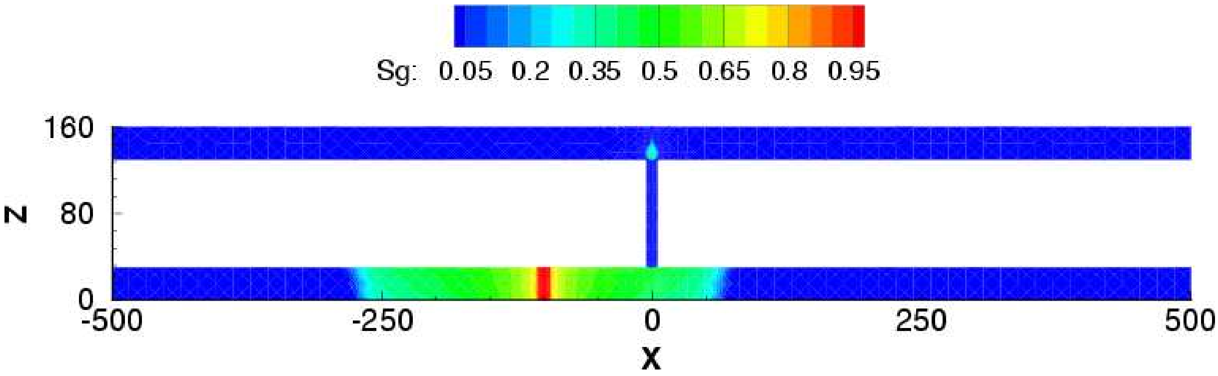

Figure 3. Numerical results: CO_2 saturation at t = 200 days

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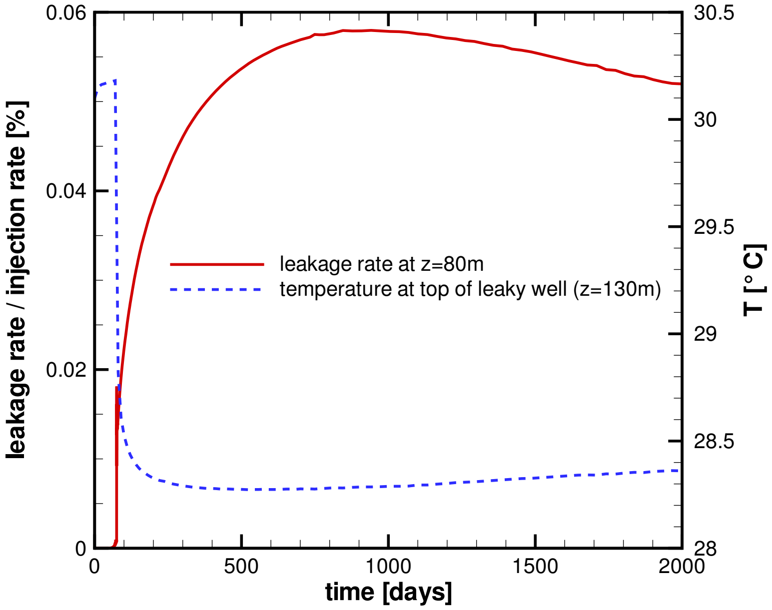

FIGURE 4. The continuous line shows the CO_2 leakage rate through the leaky well, calculated as the CO_2 flux at the middle of the well (z = 80 m, see figures 2 and 3). The dashed line shows the temperature at the top of the leaky well (z = 130 m, see figures 2 and 3).

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