Numerical modeling of CO2 storage in geological formations - recent developments and challenges

Holger Class, Anozie Ebigbo, Andreas Kopp
Lehrstuhl für Hydromechanik und Hydrosystemmodellierung
Institut für Wasserbau
Universität Stuttgart

1 Introduction

The development of numerical modeling capabilities for simulating CO_2-injection and storage in geological formations has been enormously intensified in the last decade. Meanwhile, there are many working groups world-wide that address with their models different aspects of the injection and storage processes, trapping mechanisms, etc. In general, the models currently available focus on one of the different aspects like geohydraulic, geomechanical or geochemical processes.

It can be observed that the dominant physical processes change both in space and time. For example, viscous forces and buoyancy govern the behavior of the CO_2 plume during the injection in the near-field of the injection well. Considering the need for storage over centuries, viscous and buoyant forces will lose their influence and other processes become relevant such as dissolution, diffusion, geochemical reactions etc.

We believe that numerical modeling is an indispensable tool for the large-scale implementation of CO_2 storage in the underground. Therefore, it is essential to identify the appropriate numerical model concept for a given problem or question. For example, modeling the pressure built-up in the near-field of an injection well depends predominantly on viscous forces due to the high velocities caused by the injection. This can be modeled with a multiphase model neglecting compositional effects or geochemical reactions. On the other hand, if one is interested in the long-term fate of the CO_2 in the reservoir, it requires a more sophisticated model that allows simulating compositional effects and geochemical reactions.

We suggest for the near future to evaluate the existing modeling capabilities and to develop strategies for an efficient and robust coupling of existing models. This can only

be done by thoroughly understanding the interaction and scale-dependence (both in space and time) of the ongoing physical and chemical processes. It is necessary to improve the analytical description of the processes and to quantify their influence, for example, by dimensional analyses and sensitivity studies.

2 Physical/Chemical Processes and Time Scales

The understanding of the interactions of the physical and chemical processes on different scales is necessary for choosing an appropriate model concept according to the desired information. The major physical and chemical processes that become relevant for injection of CO_2 into a reservoir are explained in the following.

Advection due to viscous forces caused by the injection itself and buoyancy. Furthermore, capillary-driven flow of the fluid phase is advection. For the modeling of advective flow of CO_2 and water (brine) in a reservoir, a multiphase model concept in porous media is required including the effects of relative permeabilities and capillary pressures which both are - currently still more or less unknown - functions of the phase saturations. Advective processes typically lose gradually their influence after the injection since the CO_2 plume spreads and tends to find a state of rest in residual saturation or due to structural or stratigraphic barriers.

Dissolution and evaporation.
Mass transfer processes play a role on the early to medium-term time scale. Once CO_2 and brine are in contact, a mutual transfer of mass components between the fluid phases begins and increases in relevance. After the plume of the CO_2 phase is at rest, this will be the limiting process regarding the further spreading of the CO_2. Another important effect is the evaporation of water into the supercritical or gaseous CO_2 phase. This can cause a drying-out of the porous medium and a precipitation of salt which may potentially reduce the permeability and porosity in the vicinity of the injection well and would thus limit the feasible injection rates. Models that are able to simulate mass transfer need to take compositional effects into account.

Diffusion and dispersion.
The dissolution of CO_2 into ambient brine in the reservoir causes a concentration gradient. Thus, a diffusive/dispersive spreading occurs that is superimposed on the advective phase

movement and eventually will be the dominant spreading process after the CO_2 phase is trapped.

Density-driven current.
The density of brine increases with the amount of dissolved CO_2. Thus, CO_2-rich brine tends to sink down into deeper regions of the reservoir. Since the density-increase is relatively small, this process is rather slow. Furthermore, this effect requires more investigation in order to quantify the time scale on which it is relevant and how it interacts with an increased dissolution rate [2].

Geochemical reactions.
It is expected that mineral trapping of CO_2 will contribute to a safe long-term storage of the CO_2 in the reservoir. However, in order to assess the capacities for mineral trapping quantitatively it is very important to improve the understanding of the geochemical reactions. This concerns the knowledge of the reactions themselves, the optimum ambient conditions, the kinetics etc. Another point is to investigate whether or not geochemical reactions can affect the permeability and porosity of the reservoir during injection. Such scenarios are in particular interesting for the industry that has to provide the required infrastructure. And finally, geochemical investigations will be essential to evaluate the influence of CO_2 injection on the fauna and flora outside of the target reservoir which might be affected, for example, by propagating acidification.

Non-isothermal effects. Some authors already showed that non-isothermal effects can have a significant influence on the spreading of the CO_2 phase in the subsurface [13, 5]. An expansion of the CO_2 due to a pressure reduction causes a cooling of the phase and the ambient rock. Varying temperatures and pressures also have a strong influence on the fluid properties. Thus, at least in the near-field of the injection well, it is urgently recommendable not to forget non-isothermal effects.

Figure 1 shows a schematic of the trapping mechanisms and the dominant processes and how their influence or contribution changes over the time scales. Obviously, this schematic simplifies the reality strongly and the changes occur rather gradually. For example, as mentioned above, this illustration should not lead to the wrong assumption that geochemical reactions cannot play a role in the short-term during injection, since under certain circumstances they can. Nevertheless, for the coupling of models it is necessary to be able to separate the time scales on which the processes interact. It is in the nature of a model that it is designed to represent certain processes while neglecting others. Therefore, the coupling of models has to take the spatial and time scales of the

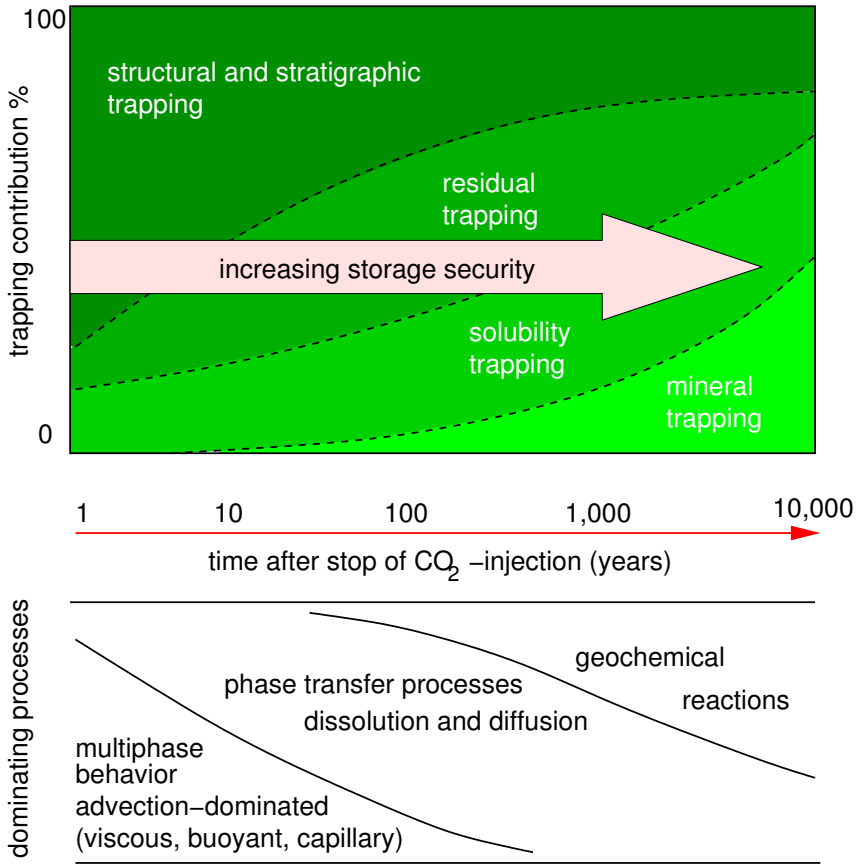

Figure 1: Variation of the trapping mechanisms and the dominating processes on different time scales (modified after [7]).

processes into account.

3 Overview of Model Concepts

Presently, there are already a number of simulators that are able to model the geohydraulic processes during and after the injection of CO_2 into a geological formation, c.f. [15, 6, 14]. These models can describe the multiphase behavior of the phases CO_2 and brine. However, they use different approaches to approximate the fluid properties and - if implemented - the multicomponent behavior, i.e. the mutual dissolution or evaporation of the components and their dependence on the content of salt or other minerals in the brine.

Only very few models exist that can handle geochemical reactions quantitatively

for large-scale applications, cf. Shemat [4], TOUGHREACT [20]. Commonly, they are able to model the transport of the reaction partners, the reactions themselves, and the change of the rock properties by simple phenomenological approaches. However, they mostly cannot account for the multiphase behavior and they are in great need of data for validating their results. A coupling of chemical reactions with multiphase flow is done in [19].

Within the context of enhanced oil recovery (EOR), CO_2 injection into oil reservoirs has been studied intensively, c.f. [10]. In the research field of Enhanced coalbed methane recovery, i.e. CO_2 is injected into deep unminable coal seams causing a desorption of methane (which is produced), the sorption processes play an important role as well as the alteration of the porous medium (coal swelling). Various investigations have been carried out by, for example, [9], [3], and [16]. Some investigations on mechanical effects caused by carbon dioxide injection have been conducted by [18], [17].

Beside numerical methods, analytical solutions for CO_2 migration in the subsurface have also been developed, c.f. [12].

A comprehensive overview of existing models can be found in [2].

4 Challenges

In the following, we point out some of the challenges that we believe are important to work on in the near future. We are aware that this overview is incomplete and gives only a narrow view from the perspective of multiphase modeling.

4.1 Field Scale Modeling

The need for implementing large-scale CO_2 storage projects is obvious since the time to mitigate the greenhouse effect is short. Thus, modelers have to provide concepts to calculate the scenarios on a reservoir scale. Assuming that the models are capable of simulating the physical/chemical processes correctly, this further requires stable and robust numerical algorithms, fast and efficient solution methods, but also a concept for the handling of the geometric data. Interfaces between the simulators, powerful CAD-systems and mesh generators are indispensable.

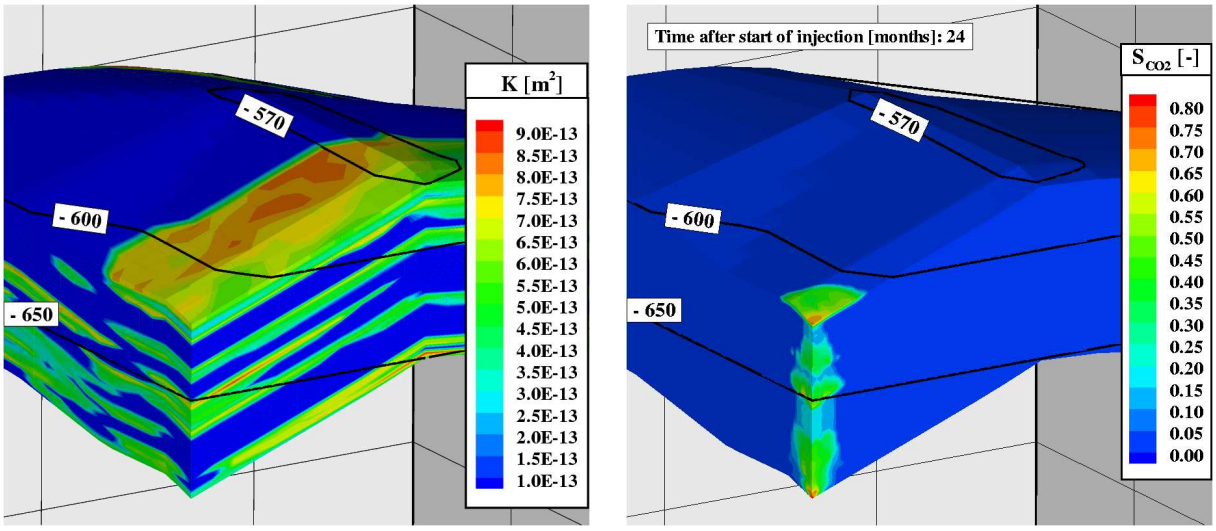

Figure 2: Realization of the permeability distribution (left) and CO_2 saturation after an injection into the Ketzin reservoir [8].

Figure 2 shows, for example, an application of the multiphase simulator MUFTE-UG [1] on the reservoir scale, in this case the Ketzin reservoir which will be used for the storage of 60 000 tons of CO_2 in the frame of the EU-project CO2SINK. The model size extends to 25 km$^2 times$80 m. The left picture represents the distribution of absolute permeability generated by a geostatistical model, the right one gives the saturation of free-phase CO_2 after 24 months of injection. For details, see [8].

However, we should emphasize here that even the results of the best model are useless if the available input data are not sufficient. Thus, site exploration and data monitoring is the precondition for any meaningful field-scale simulation.

4.2 Model Coupling

As emphasized earlier, the coupling of models of different complexity according to the spatially and temporally changing relevance of physical and chemical processes appears to be attractive. Therefore, it is necessary to thoroughly analyze the criteria that the coupled models have to fulfill. For example, a sequential coupling of models requires that the processes, for which the individual models are tailored can be considered to be decoupled in time (see Fig. 1). It may also be necessary to consider different complexities of the models with respect to their spatial distribution. For example, non-isothermal

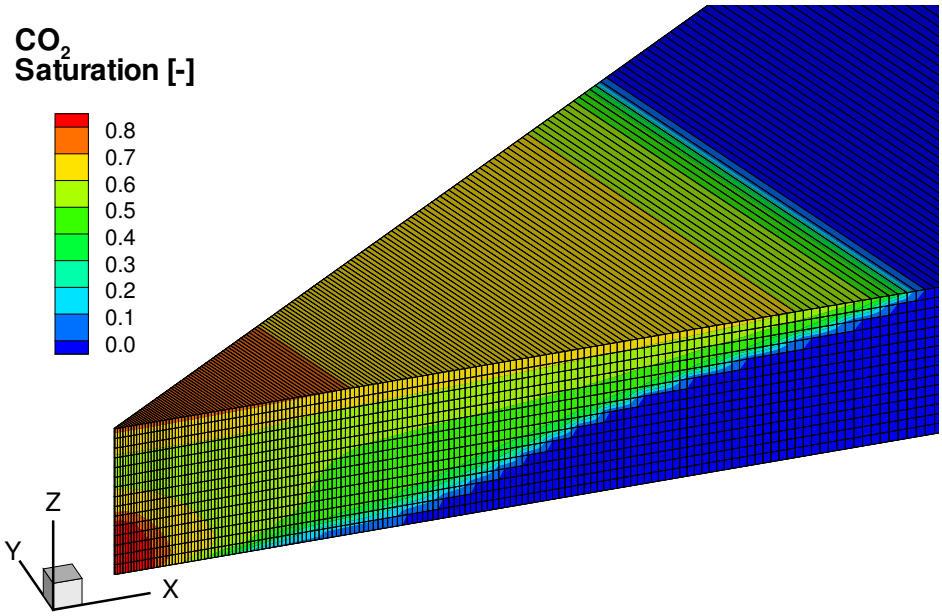

Figure 3: Code intercomparison MUFTE-UG versus ECLIPSE100: Model domain (incomplete), mesh and CO_2 saturation after the injection.

effects are presumably important in the near-field of an injection while they are probably much less significant far away from the injection well. In this case, it is appropriate to use multi-scale models, cf. [11].

4.3 The Influence of Phase Composition: Salt Content, Non-Pure CO_2

The ambient waters in target formations for CO_2 storage have characteristically high salt contents. This challenges modelers since it increases the complexity of constitutive functions for the description of the brine properties and the dissolution of CO_2 in brine. On the other hand, salt can precipitate in case of a dry-out of the formations. This may occur in the vicinity of the injection well, where the CO_2 displaces the ambient brine down to its residual saturation. This effect can be observed, for example, in the scenario that was used for a code intercomparison between the black oil reservoir simulator ECLIPSE100 and the simulator MUFTE-UG.

Figure 3 gives the model domain, the mesh and a snapshot of the propagating CO_2 plume. A CO_2 injection occurs over 2 years into a radially symmetric, homogeneous

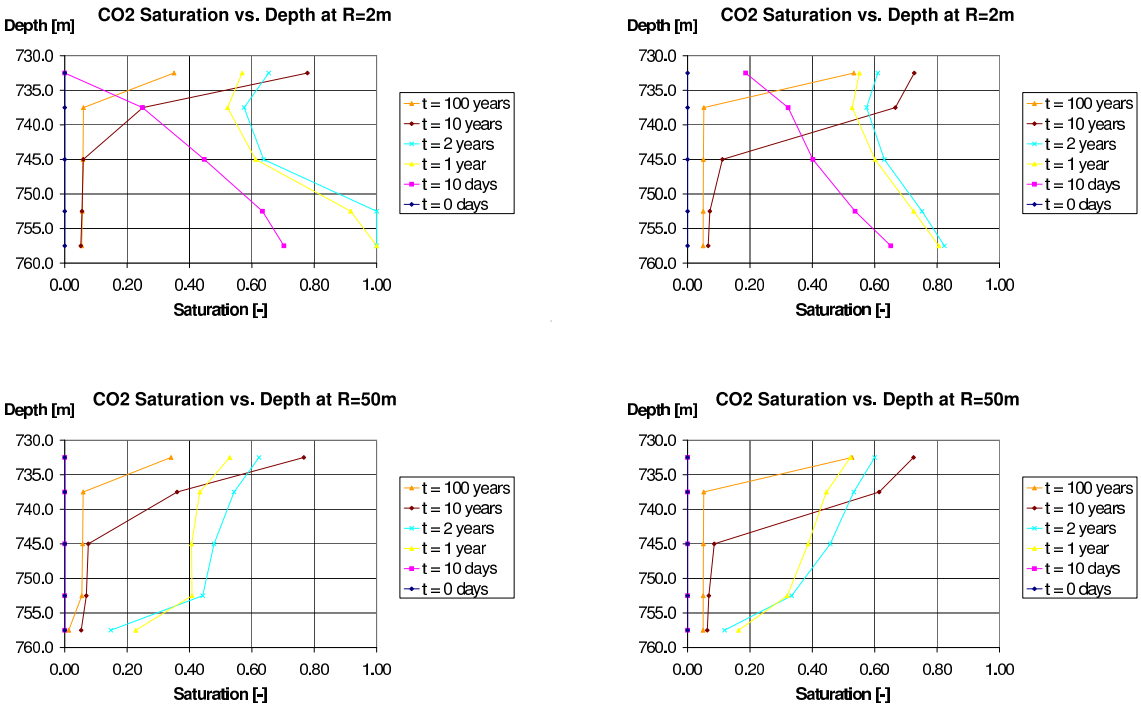

Figure 4: Comparison of the CO_2 saturation from simulations with MUFTE-UG (left) and ECLIPSE100 (right).

reservoir. In a distance of 2 m, 50 m, and 1 000 m from the injection wells, the profiles of the CO_2 saturation, the CO_2 concentrations in the brine, and the brine pressures were compared after 10 d, 1 a, 2 a, 10 a, and 100 a.

The profiles for the CO_2 saturations 2 m away from the injection well are shown for both the MUFTE-UG and the ECLIPSE100 results in Fig. 4. We do not discuss here the differences between both simulators in detail. We are also aware that ECLIPSE100 is not designed for simulating the detailed compositional effects that we are interested in here. For this purpose, ECLIPSE300 is expected to give better results. Anyway, comparing MUFTE-UG and ECLIPSE100 revealed some discrepancies in the description of the fluid properties and the mutual dissolution behavior of the phases and components. Nevertheless, the results as shown in Fig. 4 are in good agreement except for the profile after 2 years. While the MUFTE-UG results predict a complete drying-out of the rock, brine remains in residual saturation in the ECLIPSE100 simulations. The reason is simply that this version of ECLIPSE100 neglects the dissolution or evaporation of water into the CO_2 phase so that the brine saturation cannot become less than residual. Still, both

models do not account for the precipitation of the salt. They both neglect possible alterations of the permeability and porosity, and thus of the injectivity.

Another feature that is not implemented in the majority of the simulators is the effect of non-pure CO_2. Additional components in the injected gas would significantly change the fluid properties. If such scenarios should be modeled, there is still a great demand for fundamental research to find thermodynamic models that can represent the fluid properties.

4.4 Benchmarking

In order to build confidence in the existing models, a first code intercomparison study focussing on CO_2 injection was conducted 6 years ago [14] at an early stage of model development for CO_2-water and CO_2-CH_4 systems. Meanwhile, due to intensive further developments, the need for new intercomparisons grew. The project *Benchmarks* within the German *Geotechnologien* program aims at providing new problem-oriented benchmark examples. This is done in cooperation with international partners in order to include the problems that are currently in the focus of international research in this field. The benchmark examples will be published, for example, cf. [6], and they will be discussed at a workshop in Stuttgart, April 2.-4., 2008 (*www.iws.uni-stuttgart.de/co2-workshop*).

Fig. 5 shows an example of a benchmark scenario for modeling the escape of CO_2 through a leaky well [6].

5 Summary

The presently available modeling capabilities for CO_2 storage in geological formations comprise already very sophisticated models, particularly for simulating the hydraulic multiphase behavior. However, all the existing models are based on certain simplifying assumptions and neglect some of the processes described in Sec. 2. A key issue for modelers in the near future is developing strategies to cover the different time scales and spatial scales with appropriate models. Coupling of specifically designed models promises to be a way to bridge this gap. Yet, it requires a thorough understanding of the physical and geochemical processes, but also a powerful technical concept for robust and efficient interfaces.

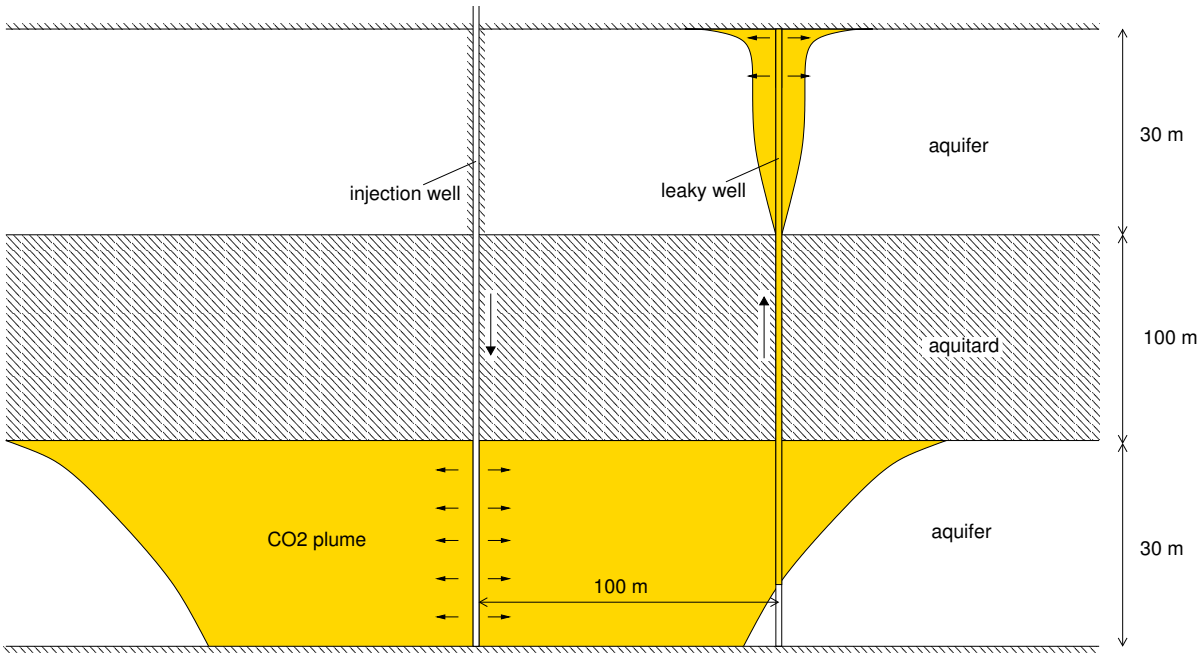

Figure 5: Benchmark example: leaky well scenario.

A further issue is the improvement of the confidence into the results of numerical models. Benchmarking and model intercomparison appears to be the most reasonable way of addressing this, since measurements and field data are typically rare.

References

[1] A. Assteerawatt, P. Bastian, A. Bielinski, T. Breiting, H. Class, A. Ebigbo, H. Eichel, S. Freiboth, R. Helmig, A. Kopp, J. Niessner, S. O. Ochs, A. Papafotiou, M. Paul, H. Sheta, D. Werner, and U. Ölmann. MUFTE-UG: Structure, Applications and Numerical Methods. *Newsletter, International Groundwater Modeling Centre, Colorado School of Mines*, 23(2), 10/2005.

[2] A. Bielinski. *Numerical Simulation of CO_2 Sequestration in Geological Formations*. PhD thesis, Institut für Wasserbau, Universität Stuttgart, 2006.

[3] A. Busch, Y. Gensterblum, and B.M. Krooss. Methane and CO2 sorption and desorption on dry Argonne Premium Coals: Pure components and mixtures. *International Journal of Coal Geology*, 55:205–224, 2003.

[4] C. Clauser. *Numerical Simulation of Reactive Flow in Hot Aquifers, SHEMAT and Processing SHEMAT*. Springer, 2003.

[5] A. Ebigbo. Thermal Effects of Carbon Dioxide Sequestration in the Subsurface. Master's thesis, Institut für Wasserbau, Universität Stuttgart, 2005.

[6] A. Ebigbo, H. Class, and R. Helmig. CO2 Leakage through an Abandoned Well: Problem-Oriented Benchmarks. *Computional Geosciences*, 2006. DOI:10.1007/s10596-006-9033-7.

[7] IPCC. Special Report on Carbon Dioxide Capture and Storage. Technical report, Intergovernmental Panel on Climate Change (IPCC), prepared by Working Group III (Metz, B., O. Davidson, H.C. de Conink, M. Loos, and L.A. Meyer (eds), Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2005.

[8] A. Kopp, A. Bielinski, A. Ebigbo, H. Class, and R. Helmig. Numerical Investigation of Temperature Effects during the Injection of Carbon Dioxide into Brine Aquifers. 8th International Conference on Greenhouse Gas Control Technologies, Trondheim, Norway, 2006.

[9] B.M. Krooss, F. van Bergen, Y. Gensterblum, N. Siemons, H.J.M. Pagnier, and P. David. High-pressure methane and carbon dioxide adsorption on dry and moisture-equilibrated Pennsylvanian coals. *International Journal of Coal Geology*, 51:69–92, 2002.

[10] L.W. Lake. *Enhanced Oil Recovery*. Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1989.

[11] J. Niessner. *Multi-Scale Modeling of Multi-Phase - Multi-Component Processes in Heterogeneous Porous Media.* PhD thesis, Mitteilungsheft 151, Institut für Wasserbau, Universität Stuttgart, 2006.

[12] J.M. Nordbotten, M.A. Celia, and S. Bachu. Injection and Storage of CO_2 in Deep Saline Aquifers: Analytical Solution for CO_2 Plume Evolution During Injection. *Transport in Porous Media*, 58(3):339–360, 2005.

[13] K. Pruess. Thermal Effects During CO2 Leakage from a Geologic Storage Reservoir. *Lawrence Berkeley National Laboratory Report LBNL-55913*, 2004.

[14] K. Pruess, A. Bielinski, J. Ennis-King, R. Fabriol, Y. Le Gallo, J. Garcia, K. Jessen, T. Kovscek, D.H.-S. Law, P. Lichtner, C. Oldenburg, R. Pawar, J. Rutqvist, C. Steefel, B. Travis, C.-F. Tsang, S. White, and T. Xu. Code Intercomparison Builds Confidence in Numerical Models for Geologic Disposal of CO2. In *Gale, J. and Kaya, Y. (Editors): GHGT-6 Conference Proceedings: Greenhouse Gas Control Technologies*, pages 463–470, 2003.

[15] K. Pruess and J.E. Garcia. Multiphase Flow Dynamics during CO2 Injection into Saline Aquifers. *Environmental Geology*, 42:282–295, 2002.

[16] S. Reeves and L. Pekot. Advanced Reservoir Modeling in Desorption-Controlled Reservoirs. *Society of Petroleum Engineers*, SPE 71090, 2001.

[17] M.N. Watson, C.J. Boreham, and P.R. Tingate. Carbon Dioxide and Carbonate Cements in the Otway Basin: Implications for Geological Storage of Carbon Dioxide. *The APPEA Journal*, pages 703–720, 2004.

[18] M.N. Watson, N. Zwingmann, N.M. Lemon, and P.R. Tingate. Onshore Otway Basin Carbon Dioxide Accumulations: CO_2-induced Diagenesis in Natural Analogous for Underground Storage of Greenhouse Gas. *The APPEA Journal*, pages 637–653, 2003.

[19] T. Xu, J.A. Apps, and K. Pruess. Reactive Geochemical Transport Simulation to Study Mineral Trapping for CO_2 Disposal in Deep Saline Arenaceous Aquifers. *Lawrence Berkeley National Laboratory Report LBNL–50089*, 2002.

[20] T. Xu, E. Sonnenthal, N. Spycher, and K. Pruess. TOUGHREACT - A simulation program for non-isothermal multiphase reactive geochemical transport in variably saturated geologic media: Applications to geothermal injectivity and CO2 geological sequestration. *Computers & Geosciences*, 32:145–165, 2006.