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MODELING OF MULTI-PHASE TRANSPORT AND DEFORMATION PROCESSES IN SALINE AQUIFERS DURING CO_2 SEQUESTRATION

Uwe-Jens Görke*, Chan-Hee Park*, Joshua Taron*, Wenqing Wang*, Olaf Kolditz*,†

* Department of Environmental Informatics
Helmholtz Centre for Environmental Research - UFZ
Permoserstr. 15, D-04318 Leipzig, Germany
e-mail: uwe-jens.goerke@ufz.de, web page: http://www.ufz.de/

† University of Technology Dresden, Germany

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Summary. In this paper, the conceptual modeling and the numerical simulation of two-phase flow during CO_2 injection into deep saline aquifers is presented. The work focuses on isothermal short-term transport and deformation processes in the vicinity of the injection well, including hydromechanical failure analyses. Governing differential equations are based on balance laws for mass and momentum, and completed by constitutive relations for the fluid and solid phases as well as their mutual interactions. Constraint conditions for the partial saturations and the pressure fractions of CO_2 and brine are defined. To characterize the stress state in the solid matrix the effective stress principle is applied. The coupled problem is solved using the in-house scientific code OpenGeoSys (an open source finite element code) and verified with benchmarks.

1 INTRODUCTION

Carbon dioxide sequestration is at the concluding and most persistent stage of Carbon Capture and Storage (CCS) procedures and a promising transition technology for the mitigation of anthropogenic greenhouse gas emissions. Currently, the modeling of various transport and reactive processes as well as deformation aspects during CO_2 injection and storage in deep geological formations is subject of worldwide research activities. The simulation of the injection and the propagation of carbon dioxide in the subsurface is essential for the proper understanding of the physical and chemical processes at different length and time scales, to ascertain migration and trapping of CO_2 in the porous formations, and in assessing the capacity as well as the safety (possible leakage, fracturing) of

the reservoir and the caprock layers. Usually, the multiple coupled problems are analyzed numerically based on physically founded complex mathematical models.

The modeling of CO_2 migration in geological formations is a fairly new subject of investigations in different research areas (e.g., hydrology, geotechnology, computational mechanics, and mathematics). About ten years ago only a few publications have been dedicated to this topic[1,2], and recently an increasing number of numerical[3,4,5,6], semi-analytical[7,8], and analytical studies[9,10] have been published.

Within the context of numerical simulations, more complex problems can be solved (e.g., coupling of different processes, consideration of heterogeneities and various geological conditions). As most of the numerical codes are focused on a subset of the thermo-hydro-mechanical-chemical (THMC) processes, at present, capabilities for a comprehensive treatment of the coupled system are still restricted. To compare several numerical simulators with respect to their capabilities, studies for the code comparison of efficiency and accuracy have been conducted[11,12].

Modeling CO_2 storage is very demanding with respect to the computational cost due to the complex geometries that need to be described and due to the diversity of interacting hydraulic, thermal, mechanical, and geochemical processes. According to the evolving processes at various time and length scales we propose a successive model development with the final goal of a comprehensive coupled simulation of the relevant physico-chemical effects, but starting with the most significant effects at CO_2 injection near the injection well. Since the model complexity is adapted to these dominating processes, other phenomena having less contribution to the event under consideration are neglected for computational efficiency (e.g., dissolution and mineral trapping). For the mechanical failure, fairly few studies induced by CO_2 injection have been conducted numerically[13]. Therefore, in this paper, the study is focussed to hydromechanical (H^2M) effects of the CO_2 injection into deep saline aquifers at isothermal conditions. Special attention is paid to the interfaces between the caprock and the aquifer as well as the CO_2 and saline water fluid phases (assumed to be immiscible) in the analysis.

2 CONCEPTUAL MODELING

2.1 Balance equations

Within the context of two-phase flow in deformable porous media, neglecting mass exchange between the phases (no dissolution and sorption processes), and assuming material incompressibility of the solid phase, the mass balance relations for the fluid constituents can be defined with respect to the solid phase motion.

$$nS^\gamma \frac{d_s \rho^{\gamma R}}{dt} + n\rho^{\gamma R} \frac{d_s S^\gamma}{dt} + \operatorname{div}(\rho^{\gamma R} \boldsymbol{w}^{\gamma s}) + S^\gamma \rho^{\gamma R} \operatorname{div} \dot{\boldsymbol{u}}^s = 0 \tag{1}$$

Here, the superscript $\gamma = CO_2, l$ refer to the pore fluid constituents (phases), n is the porosity, S^γ is the saturation, $\rho^{\gamma R}$ is the material mass density, $\dot{\boldsymbol{u}}^s$ is the solid phase veloc-

ity, and $\boldsymbol{w}^{\gamma s}$ is usually known as filter velocity of the motion of the pore fluid constituents. The derivative $d_s()/dt$ denotes the material time derivative with respect to the motion of a material point of the solid phase.

In geotechnical problems, the internal fluid friction forces can be neglected in comparison to the interaction terms between fluid and skeleton motions. Thus, the total Cauchy stress tensor $\boldsymbol{\sigma}$ referring to the local loading state of the overall aggregate is given by the sum of all partial stresses of the constituents. Consequently, the stress tensor is defined according to the well-known effective stress concept:

$$\boldsymbol{\sigma} \;=\; \boldsymbol{\sigma}^{'} \;-\; \left(\sum_{\gamma} S^{\gamma} p^{\gamma}\right) \boldsymbol{I} \tag{2}$$

with the solid effective stress tensor $\boldsymbol{\sigma}^{'}$, the fluid pressure fractions p^{γ} and the identity tensor $\boldsymbol{I}$.

Completing the set of necessary balance relations, the stress field in the saline aquifers is governed by the overall local momentum balance relation

$$\operatorname{div}\left(\boldsymbol{\sigma}^{'} - \left(\sum_{\gamma} S^{\gamma} p^{\gamma}\right) \boldsymbol{I}\right) \;+\; \rho \boldsymbol{g} \;=\; \boldsymbol{0} \tag{3}$$

where $\rho \boldsymbol{g}$ is the volume force with the mass density of the porous medium (homogenized overall aggregate) and the gravity vector $\boldsymbol{g}$.

2.2 Constitutive relations

Constitutive equations are required for selected production terms of the specific balance relations of the individual constituents, for pore fluid properties like pressure and saturation, and for the partial effective stress tensor of the solid skeleton.

It can be shown that, based on appropriate constitutive relations for the momentum production terms, the fluid momentum balances are represented by modified Darcy's law

$$\boldsymbol{w}^{\gamma s} = -\frac{k^{\gamma}_{\mathrm{rel}}}{\mu^{\gamma}} \boldsymbol{k} \cdot \left(\operatorname{grad} p^{\gamma} - \rho^{\gamma R} \boldsymbol{g}\right) \tag{4}$$

for multiphase flow as a constitutive flux expression, with $k^{\gamma}_{\mathrm{rel}}$ denoting the relative permeability, μ^{γ} the dynamic viscosity, and $\boldsymbol{k}$ the intrinsic permeability of the solid skeleton.

We define the capillary pressure in the usual way as the difference between the non-wetting and wetting fluid pressures fractions ($p^c = p^{CO_2} - p^l$).

The capillary pressure-saturation functions as well as the relations between relative permeability and saturation are substantial constitutive equations required for multiphase flow. Within this context, usually algebraic expressions are fit to the corresponding experimentally observed curves. Among the widely-used of these algebraic expressions are the Brooks-Corey and van Genuchten relations. Both are realized within the scientific software code OpenGeoSys. Additionally to the constitutive relations characterizing media

properties, appropriate equations of state for pressure dependent fluid properties (density, viscosity) are considered.

The host rock of the reservoirs under consideration is assumed to be linear elastic, and the solid effective stress is governed by the well-known generalized Hookean law.

2.3 Failure modes

For the coupled H^{2}M problems in deformable porous media we consider two potential failure modes. The first assumes, conservatively, that hydraulic fracturing (e.g., tensile failure) may occur when the pore fluid pressure p exceeds the current minimum principal stress, σ_3. This defines a factor of safety for hydraulic fracturing,

$$f_S^H = \frac{p}{\sigma_3} \tag{5}$$

The second mode allows for shear slip/failure along an optimally oriented fracture plane. In two dimensions, the Mohr-Coulomb failure criterion says that the failure is favorable when the current maximum shear stress, $\tau_m = 1/2(\sigma_1 - \sigma_3)$, becomes $|\tau_m| \geq C_k \cos\theta + (\sigma_m - p)\sin\theta$, where σ_1 is the maximum principal stress, $\sigma_m = 1/2(\sigma_1 + \sigma_3)$ is the mean normal stress, C_k is the cohesion, and θ is the internal friction angle. This relationship defines a factor of safety for shear slip/failure,

$$f_S^S = \frac{|\tau_m|}{C_k \cos\theta + (\sigma_m - p)\sin\theta} \tag{6}$$

The safety factors $f_S^H \geq 1$ and $f_S^S \geq 1$ imply incipient failure.

3 NUMERICAL SCHEME

The numerical treatment of the coupled problem of single- or multiphase flow in deformable porous media is based on the governing field equations together with discretization methods in the space and time domains. The method of weighted residuals is applied to derive the weak formulations of all the governing equations given above. Within the framework of a standard Galerkin procedure, the local balance equations are multiplied by appropriate test functions, and integrated over the current domain bounded by the solid skeleton.

For two-phase flow problems, the choice of primary variables is of crucial importance for the stability of the employed numerical scheme[14]. A pressure-pressure (pp) scheme (e.g., capillary pressure and CO_2 pressure) as well as a pressure-saturation (pS) scheme (using the pressure of the wetting phase and the saturation of the nonwetting phase) have been realized. Naturally, the solid phase displacements serve as the primary variable modeling the deformation processes.

As usual, in the finite element space the continuous functions of the selected primary variables are interpolated based on their nodal values and appropriately defined shape functions. After discretizing the weak forms of the balance relations a system of nonlinear

algebraic equations can be obtained. For the required time discretization we use the generalized first order difference scheme.

The nonlinear coupled boundary value problem is solved iteratively using the Picard linearization within the context of the finite element method[15]. Within this context, usually all unknowns can be solved at the same time with a so called monolithic scheme. We adopt a mixture of monolithic and staggered schemes to avoid possible memory or solver problems without losing the accuracy of the solutions. Within this context, at first the two-phase flow problem is solved monolithically, and subsequently, the deformation problem is solved separately considering the results from the flow problem. This iteration cycle repeated until the converged solution of all primary variables is achieved.

For the sake of benchmark simplicity, two-phase flow to elastic deformation coupling is conducted in one way only: pore pressure and phase saturation changes influence mechanical deformation, without the inverse feedback. This indicates that the last term in the mass balance equation (1) containing the term $\operatorname{div} \dot{\boldsymbol{u}}^s$ is ignored, as are other coefficient changes such as porosity and permeability due to mechanical deformation.

4 RESULTS

For the simulation of two-phase flow in deformable porous media, a problem is formulated to study mechanical failure at the interface of a caprock and aquifer for a time-scale allowing the return of mechanical stability. Geometrical characteristics are adapted to data from a real site (Hou, M., 2009, unpublished report), and the corresponding problem domain is chosen to be a vertical cross-section 100 m in length and 10 m in depth, with the caprock/aquifer interface located at 6 m above the bottom impermeable boundary.

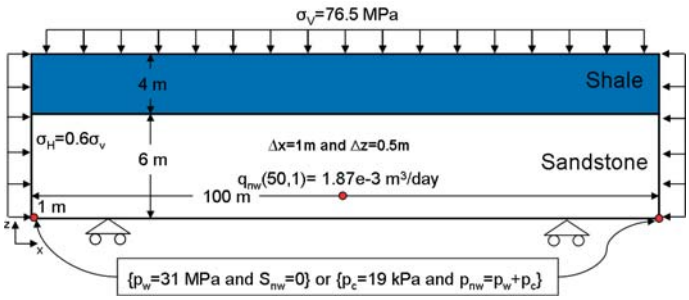

Figure 1: Model domain and boundary conditions for two-phase flow and elastic mechanical deformation for CO_2 benchmark

The lower boundary is located at 3010 m from the surface (cf. Fig. 1). The reservoir is assumed to be filled with a liquid pore fluid, and the supercritical carbon dioxide is injected at a point source centrally located in the vertical cross section; in this case, located 1 m from the lower boundary. A volumetric injection rate of $1.87 \cdot 10^{-3}$ m^3/day over a 20 year life is calculated from an assumed equivalent total injection rate of 500 tons/year.

For simplicity of the example, isothermal conditions are assumed. The density of brine and supercritical CO_2 under a geothermal gradient of 25°C/km from a surface temperature of 10°C are calculated as 1173 kg/m^3 and 734.27 kg/m^3, their viscosity is $1.252{\cdot}10^{-3}$ Pa·s and $6.24{\cdot}10^{-5}$ Pa·s, respectively. The residual saturation of both the fluid phases is assumed to be 0.1, and the maximum saturation is consistently 0.9. The properties for the media are summarized in Tab. 1. Initial conditions are set as hydrostatic for fluids and lithostatic for rocks at 3 km depth. This hydrostatic condition for two-phase flow is also used for the boundary conditions at the two lower corner points of the problem domain. The state of stress on aquifer boundaries is approximated by applying 0.6 of the vertical, lithostatic stress to the horizontal. All of these boundary conditions and sources for the different numerical schemes are depicted in Fig. 1.

Property	Unit	Caprock (shale)	Reservoir (sandstone)
Young's modulus	GPa	0.2	21
Poisson's ratio	–	0.2	0.25
Porosity	–	0.01	0.15
Intrinsic permeability	m^2	$1.0 \cdot 10^{-20}$	$1.0 \cdot 10^{-17}$
Brooks-Corey's index	–	2.0	2.0
Entry pressure	kPa	3100	19.6

Table 1: Media properties for the CO_2 example

The different choices of primary variables influence CO_2 distribution in the reservoir-caprock system: While the *pS*-scheme tends to penetrate into the caprock from the aquifer vertically, the *pp*-scheme tends to propagate horizontally over 100 years of simulation time. The maximum saturation of CO_2 obtained from the *pS*-scheme is higher than that obtained from the *pp*-scheme (Fig.2).

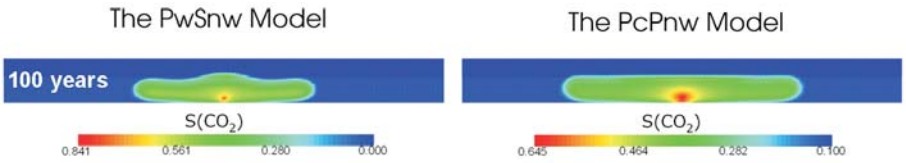

Figure 2: CO_2 saturation with 20 years of the injection at 100 years: Comparison of results for the *pS*-scheme and the *pp*-scheme

From calculated pore pressure and density, safety factors defined in Eqs. (5) and (6) are analyzed over time for the two numerical schemes. For a uniform injection rate, mechanical stability is generally observed to increase with time (safety factors decrease) and therefore with greater spatial extent of the CO_2 plume.

The spatial distribution of mechanical instability due to potential hydraulic fracture and shear failure follow a similar trend, concentrating at the edges of the CO_2 plume.

In contrast to hydraulic failure, however, the magnitude of shear failure safety factor is clearly in excess of the threshold (unity) in early times, with shear slip likely to occur both at the bottom of the caprock and in the aquifer coinciding with the outer edge of the CO_2 plume (see Fig. 3).

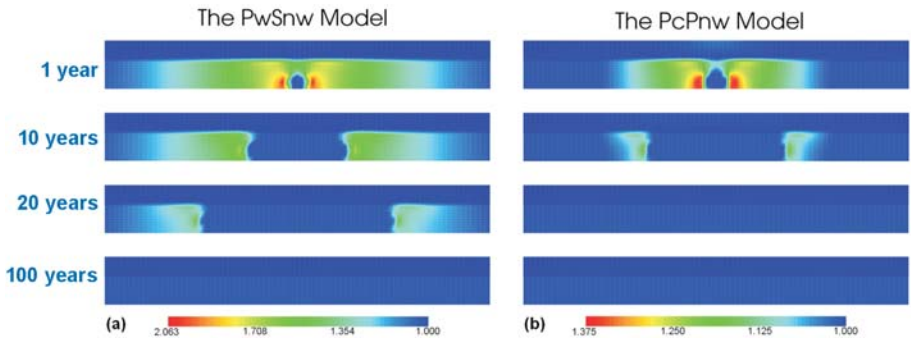

Figure 3: Safety factors for shear slip with 20 years of the injection at 1, 10, 20, and 100 years (from top to bottom): (a) the pS-scheme and (b) the pp-scheme

The pS- and pp-schemes lead to significant differences in characteristics of CO_2 spreading. Thus, the selection of a primary variable scheme has observable and potentially significant consequences for the prediction of mechanical stability during CO_2 injection. In general, and for the geometry explored here, results indicate a higher likelihood of mechanical failure when a pS-scheme is enacted.

5 CONCLUSIONS

We have investigated two-phase flow and deformation processes caused by CO_2 injection for CCS in deep saline aquifers, with special attention to damage scenarios. The analysis is conducted with two different numerical schemes of multiphase flow models consisted of two different sets of primary variables: the capillary pressure and non-wetting pressure model and the wetting phase pressure and non-wetting phase saturation model. The coupling scheme between multiphase flow and elastic deformation is realized within the context of a mixed monolithic/staggered scheme. The choice of the primary variables in multiphase flow has consequences for CO_2 distribution and, subsequently, impacts the evolution of mechanical stress and the deformation response. For reasonable parameter values and the aquifer geometry, significant mechanical failure (and potential breach of integrity) is expected in the shale caprock for all but low injection rates. This indicates that the analysis of the hydromechanical response is crucial for proper selection of injection sites, injection rates, and total storage capacity.

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