Numerical simulation of two-phase flow in deformable porous media: application to carbon dioxide storage in the subsurface

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Abstract In this paper, numerical simulation of two-phase flow in deep, deformable geological formations induced by CO_2 injection is presented. The underlying conceptual approach is based on balance equations for mass, momentum and energy completed by appropriate constitutive relations for the fluid phases as well as the solid matrix. Within the context of the primary effects under consideration, the fluid motion will be expressed by modified Darcy's law for two phase flow. To characterize the stress state in the solid matrix, the effective stress principle is applied. Furthermore, interaction of fluid and solid phases is specified by constitutive models for capillary pressure, porosity and permeability as functions of saturation. Based on the conceptual model, a coupled system of nonlinear differential equations is formulated for non-isothermal two-phase flow in a deformable porous matrix (TH^2M model). The finite element method is used to solve the multi-field problem numerically. The capabilities of the model and the numerical tools to treat complex processes during CO_2 sequestration is checked by benchmarking within a wider scope of a benchmarking scheme, which is also presented and illustrated using two examples: (1) a new benchmark test for H^2M processes, and (2) a 3-D demonstration example to test the stability and computational costs of the H^2 model for real applications.

Key words porous media; two-phase flow; deformation; benchmarking; carbon capture storage (CCS)

LIST OF SYMBOLS

	Symbol	Meaning	Units
General	c	Specific heat capacity	J/(kg K)
	C	Elasticity matrix	
	D_w^g	Vapour diffusion coefficient	m^2/s
	H	Hydraulic coefficient matrix	
	HM	Hydro-mechanical coefficient matrix	
	HT	Hydro-thermal coefficient matrix	
	g	Gravity acceleration	m/s^2
	k	Saturated permeability tensor	m^2
	k_{rel}	Relative permeability of a phase	-
	M	Molar mass of a species	kg
	n	Porosity	m^3/m^3
	p	Pressure	Pa
	p_w^g	Vapour pressure	Pa
	q	Flux, process related	
	Q	Source / sink terms, process related	
	S	Saturation	m^3/m^3
	t	Time	s
	T	Temperature	K
	u	Displacement vector	m
	v	Velocity vector	m/s
Greek	α	Biot coefficient	
	β_T	Thermal expansion coefficient	1/K
	γ	Phase indicator (l,g,s)	
	ε	Volume fraction	m^3/m^3
	μ	Dynamic viscosity	Pa s
	ρ	Density	kg/m^3
	ρ_w^g	Water vapour density	kg/m^3
	$\boldsymbol{\sigma}$	Stress tensor	Pa

Superscripts	1,2	Phase number	
	g	Gas phase	
	l	Liquid phase	
	s	Solid phase	
	T	Transpose	
Subscripts	a	Air species in different phases	
	c	Capillary	
	H,M,T	Process related source terms	
	t	Time discretization	
	w	Water species in different phases	
	x	Space discretization	
Other	∇	Nabla operator, space derivative	1/m
	$\dot{A}$	Dot over symbol is time derivative	1/s

INTRODUCTION

In 2005, the Intergovernmental Panel on Climate Change (IPCC) published a report (Metz *et al.*, 2005) addressing the state-of-the-art, the perspectives and various knowledge gaps related to the long-term storage (sequestration) of CO_2 in the subsurface. Three types of geological formations are considered particularly for the safe storage of CO_2: (nearly) depleted hydrocarbon reservoirs, deep saline aquifers and non-minable coal seams. In cases of hydrocarbon reservoirs and deep aquifers, carbon dioxide is injected in a dense form into porous rock formations, filling out the pore space and partially displacing *in situ* residing fluids. According to various studies, deep saline aquifers provide the largest geological carbon dioxide storage capacity (Arts *et al.*, 2004; Förster *et al.*, 2008).

To ascertain migration and trapping of CO_2 in the formations and assess the capacity and the safety (possible leakage) of the reservoir, numerical simulation of injection and spreading of carbon dioxide in the underground is essential for understanding the physical and chemical processes at different length and time scales. Currently, numerical studies of carbon dioxide storage are mostly based on simulators developed for use in oil, gas and geothermal energy production. They represent starting points for specialized model and code adaptations targeted at modelling the geological storage of CO_2 (Tsang, 1991; Pruess & Garcia, 2002). Little attention has so far been focused on geomechanical effects. The injection of supercritical CO_2 into deep saline aquifers results in high pressure in the vicinity of the injection well, which may significantly change the stress distribution in this reservoir region. High pressure induced medium deformation therefore must be considered when assessing the safety of the injection process. In the present study, we utilize numerical methods to analyse the stress changes caused by the interaction with the pore fluids during the injection. We focus on a conceptual model, which represents the non-isothermal two-phase fluid flow process of CO_2 and water, and also the deformation process in the near field in deep saline aquifers. Furthermore, we propose a system for benchmarking CO_2 models and present two selected examples.

GOVERNING EQUATIONS

From the mechanical point of view we consider non-isothermal flow of two fluid phases (compressible and incompressible fluids) in a deformable thermo-poro-elastic porous medium based on Biot's consolidation concept – a thermo-hydro-mechanical (THM) coupled field problem. Similar multi-field problems need to be solved for geotechnical applications such as subsurface waste deposition (Lewis & Schrefler, 1998; Rutqvist *et al.*, 2008; Wang *et al.*, 2009).

Based on the fundamental balance equations of mass, momentum and energy in combination with the constitutive equations for the specific geological material as well as the fluids (CO_2 and groundwater) we derive the governing equations for the TH^2M problem in terms of primary variables (see Tables 1–4). Symbols are listed above. A p-p and a p-S formulation for the two-phase flow problem are provided (see Table 1) (Wang & Kolditz, 2007; Görke *et al.*, 2010).

Table 1 Primary variables of the TH²M problem.

Process	H	H	T	M
pp formulation	$p^1 == p_c$	$p^2 == p^g$	T	$\mathbf{u}^s$
pS formulation	$p^1 = p^l$	$S^2 = S^g$	T	$\mathbf{u}^s$

Table 2 Non-isothermal two-phase flow in a deformable porous medium.

The general flow equation of the TH²M problem is:	with the following equation coefficients:
$$H_t^1 \dot{p}^1 + H_{xx}^1 \nabla^T \cdot \nabla p^1 + H_{xx}^2 \nabla^T \cdot \nabla p^2 + HT_t \dot{T} + HM_{tx} \nabla \dot{\mathbf{u}} + = Q_H + Q_{HT} \quad (1)$$	$$H_t^1 = n\left((\rho^l - \rho_w^g)\frac{\partial S^l}{\partial p_c} + (1-S^l)\frac{\partial \rho_w^g}{\partial p_c}\right)$$ $$H_{xx}^1 = \rho^l \frac{\mathbf{k}k^l{}_{rel}}{\mu^l}$$ $$H_{xx}^2 = \rho_w^g \frac{\mathbf{k}k^g{}_{rel}}{\mu^g} - \rho^l \frac{\mathbf{k}k^l{}_{rel}}{\mu^l}$$ $$HT_t = n\left((\rho^l - \rho_w^g)\frac{\partial S^l}{\partial T} + (1-S^l)\frac{\partial \rho_w^g}{\partial T}\right) - \beta_T$$ $$HM_{tx} = S^l \rho^l + (1-S^l)\rho_w^l$$ $$Q_H = -\left(\rho^l \frac{\mathbf{k}k^l{}_{rel}}{\mu^l}\rho^l + \rho_w^g \frac{\mathbf{k}k^g{}_{rel}}{\mu^g}\rho^g\right)\mathbf{g}$$ $$Q_{HT} = \nabla\left(\rho^g \frac{M_a M_w}{M_g^2} D_w^g \nabla(\frac{p_w^g}{p^g})\right) \quad (2)$$

Table 3 Two-phase flow heat transport in a deformable porous medium.

The general heat transport equation of the TH²M problem is:	with the following equation coefficients:
$$T_t \dot{T} + T_x \nabla T + T_{xx} \nabla^T \cdot \nabla T = Q_T + Q_{TM} \quad (3)$$	$$T_t = \sum_i \varepsilon^i c^i \rho^i$$ $$T_x = n \sum_\gamma S^\gamma c^\gamma \rho^\gamma \mathbf{v}^{\gamma s}$$ $$T_{xx} = \sum_i \varepsilon^i \lambda^i$$ $$Q_T = \rho q_T$$ $$Q_{TM} = \mathbf{v} \cdot \nabla \boldsymbol{\sigma} \quad (4)$$

Table 4 Non-isothermal two-phase flow consolidation.

The general equation for stress equilibrium of the TH²M problem is:	with the following equation coefficients:
$$MH_x^1 \nabla p^1 + MH_x^2 \nabla p^2 + MT_x \nabla T + M_{xx} \nabla^T \cdot \nabla \mathbf{u} + Q_M \quad (5)$$	$$MH_x^1 = \alpha S^1$$ $$MH_x^2 = \alpha S^2$$ $$MT_x = \beta_T = \sum_i \varepsilon^i \beta_T^i$$ $$M_{xx} = \mathbf{C}$$ $$Q_M = \rho \mathbf{g} = \left(\sum_i \varepsilon^i \rho^i\right)\mathbf{g} \quad (6)$$

BENCHMARKING CONCEPT

Benchmarking of process simulation is one of the cross-cutting activities within the CO_2 modeller community. This initiative includes a systematic development of appropriate test cases for CO_2 injection and storage as well as the verification procedure itself. Verification methods rely on both classic test cases and inter-code comparison (Kolditz *et al*., 2010). The proposed benchmarking strategy comprises three aspects:

– Process-based: Numerical analysis of individual and coupled processes related to CO_2 injection and storage with increasing complexity, i.e. compressible flow (H), two-phase flow (H^2), consolidation (H^2M), thermo-mechanics (TM) up to non-isothermal two-phase flow consolidation (TH^2M processes) (see Table 5).
– Thermodynamics-based: Increasing complexity of material behaviour, i.e. from constant to highly nonlinear material functions.
– Scenario-based: Development of site-specific test cases (application benchmarks, see Table 6).

The system of benchmarking by processes is given in Table 5. We start from the flow processes, then include mechanical effects (consolidation) and finally consider non-isothermal phenomena (heat transport and phase changes). Chemical reactions are not yet incorporated into this benchmark systematic. The last column (DBB) shows the related chapter of the *OpenGeoSys Developer Benchmark Book* (Kolditz & Shao, 2010, available through the web site www.opengeosys.net; Kolditz *et al*., 2008), where the reader can find a detailed description of the benchmark tests as well as the results obtained.

Table 5 Benchmarking by processes.

Problem type	Process type	Dimension	DBB
Compressible flow	H	1-D	7
Two-phase flow (Buckley-Leverett)	H^2	1-D	20.3
Two-phase flow (McWorther-Sunada)	H^2	1-D	20.4
Two-phase flow (Keuper)	H^2	2-D	20.5
Unsaturated consolidation	HM	2-D	14.3
Two-phase flow consolidation	H^2M	2-D	14.4
Thermo-mechanics	TM	2-D / 3-D	15
Non-isothermal compressible flow	TH	1-D	7
Non-isothermal two-phase flow	TH^2	1-D	17
Non-isothermal unsaturated consolidation	THM	2-D	16
Non-isothermal two-phase flow consolidation	TH^2M	2-D	17

The third classification is denoted as “scenario-or-site-based” (Table 6). Within this study, buoyancy effects in two-phase flows are studied, i.e. density differences between CO_2 and brine. “EGR” is a scenario benchmark for enhanced gas recovery using specific geological stratigraphy of a depleted gas reservoir. This case study is dedicated to the scenario when CO_2 is injected in a gaseous state into a depleted gas reservoir. Therefore we deal with non-isothermal compressible flow. “Stuttgart” and “Svalbard” can be called community benchmarks (Dahle *et al*., 2009; Class *et al*., 2010). These examples have been developed and intensely discussed during two workshops in Stuttgart and Svalbard, respectively (Table 6).

Table 6 Benchmarking by scenarios.

Problem type	Process type	Dimension
Buoyancy	H^2M	2-D(r)
EGR	THC^n	2-D(r)
Svalbard	H^2	2-D
Stuttgart	H^2	3-D
Shear slip	H^2M	2-D

EXAMPLES

Numerical simulation of coupled TH^2M processes, including possible phase changes, is a complex task. In order to verify the computational schemes a systematic collection of benchmarks needs to be developed. Here we present two examples proposed to the benchmark collection: (1) a 2-D vertical cross-section to study multiphase consolidation (Buoyancy benchmark), and (2) a 3-D case to test the stability and computational costs of the two-phase flow models for real applications (Stuttgart benchmark).

Two-phase flow consolidation

The first example simulates the effects of CO_2 injection into a saline aquifer, located at a depth of 770 m from the ground surface and 6 m thick (Fig. 1). The saline aquifer is fully saturated with water before injection.

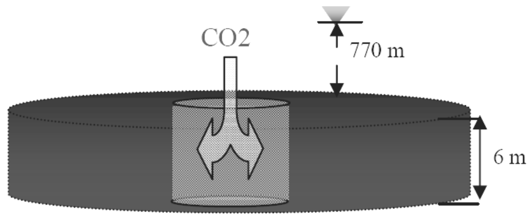

Fig. 1 Buoyancy benchmark set-up.

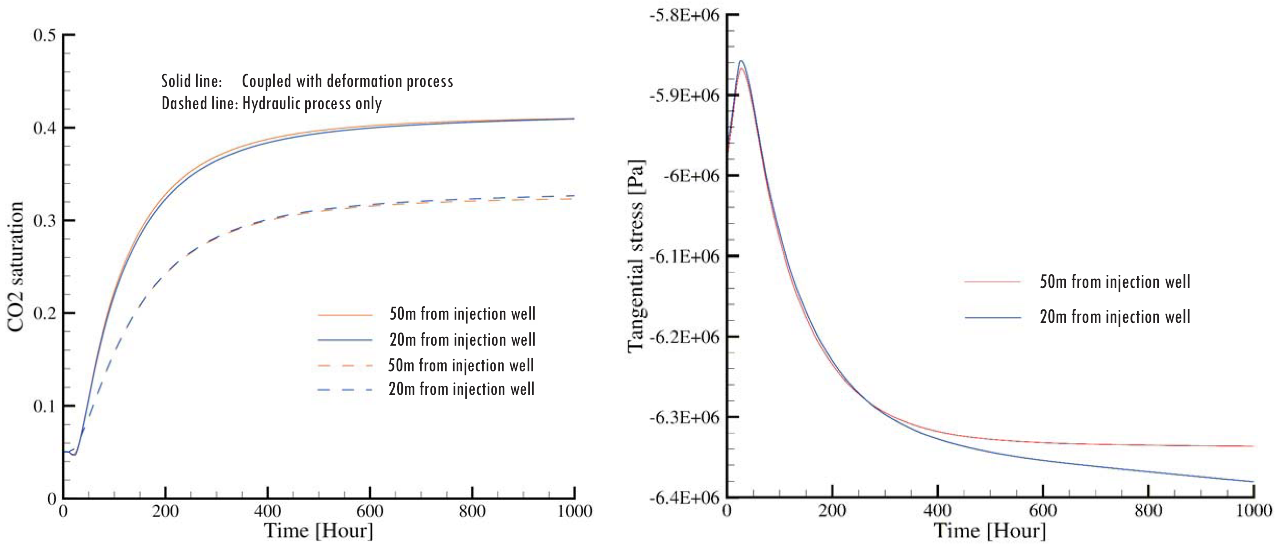

Fig. 2 Density benchmark: calculated CO_2 saturations (left) and tangential stresses (right).

In the present study, the near field is the domain of interest. To this purpose, we assume the problem is axisymmetrical in both geometry and physics. By taking the injection well's radius as 0.2 m and cutting the domain at the radius of 200 m, we generalise a finite mesh. In the simulation, the density of the liquid phases and the solid phase are assumed to be constant. The Brooks-Corey model is employed to characterise the hydraulic properties of liquid CO_2 and water. Initially, the stresses in the deep saline aquifer are assumed to be produced by the gravity force only, which is calculated by solving the stress equilibrium equation with the volume force term. Later on, the stress results obtained by the initial distribution analysis are used as the initial stress status for CO_2 injection modelling. Although the saturations are not much affected by including deformation, we can clearly see stress changes at 20 and 50 m from the injection location, which are induced by the elevated injection pressure (Fig. 2). The tangent stress decreases at the beginning of the injection due to the extension at the well surface, and then increases due to propagation of the injection pressure. Since we assume the initial stress is only induced by the gravity force, the stress distribution in the analysed domain is vertically oriented.

Two-phase flow – approaching reality

The test case is a 3-D model of two aquifers connected by a leaky borehole. CO_2 is injected into the lower aquifer. The purpose of the modelling study is to analyse the CO_2 leakage to the upper aquifer through a borehole 400 m from the injection well. Figure 3 shows the results of the 3-D two-phase (H^2) simulations. Liquid pressure and saturation of CO_2 is plotted for a selected time. The plots show the radial propagation of the carbon dioxide. We see the buoyancy effect of up-coning CO_2 due to it is smaller density in comparison to the saline water. The carbon dioxide reaches the leaky well after about 100 days.

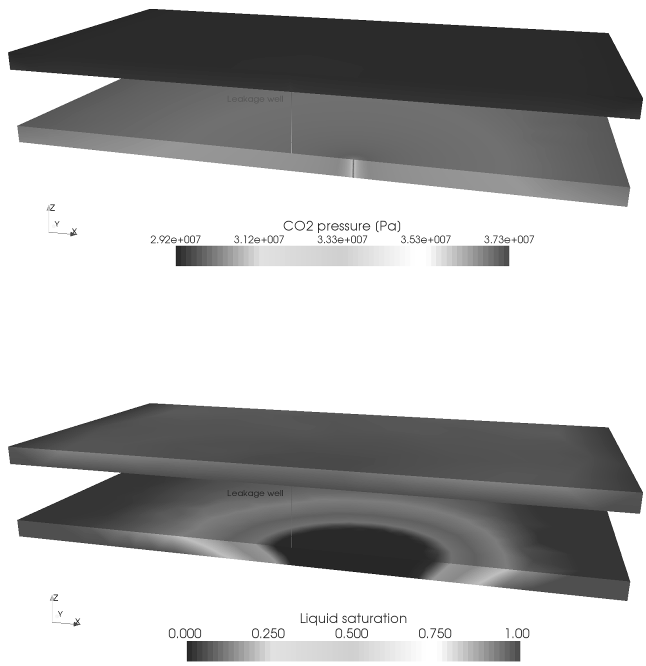

Fig. 3 Results of two-phase flow simulation: phase pressure of CO_2 (top), CO_2 saturation (bottom).

CONCLUSIONS AND FUTURE WORK

This paper describes ongoing work on developing the theoretical and numerical framework as well as object-oriented software for the solution of thermo-hydro-mechanical-chemical (THMC) coupled problems related to CO_2 storage in the geological subsurface. In this paper we present a conceptual approach for non-isothermal multi-phase flow consolidation in porous media. The corresponding TH^2M model is numerically solved using the finite element method. Two test examples are presented in order to discuss details of H^2M processes, such as variable fluid properties exhibiting phase changes, interaction of capillarity and buoyancy forces, and two-phase flow in 3-D aquifer structures. The current status of TH^2M is not solving the problem but rather pointing to important details of the coupled system. In the numerical analysis of CO_2 storage, most of the done work focuses on the hydraulic and mechanical changes during injection or storage.

With a simple axisymmetrical example of two-phase flow and deformation coupled processes in the saline aquifers, we demonstrated that the stress change in the vicinity of the CO_2 injection well is distinct from the initial stress state, and such coupling must be considered as an issue for the assessment of safety of injection and storage. The present TH^2M concept can be extended to geothermal reservoir analysis and safety assessment of nuclear waste repositories. To this purpose the properties of the corresponding geofluids and geological environment, i.e. equations of state and constitutive equations, need to be taking into account.

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