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Non-isothermal effects on two-phase flow in porous medium: CO₂ disposal into a saline aquifer

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Abstract

This paper presents non-isothermal effects on disposal of carbon dioxide into a saline aquifer. Carbon dioxide storage in the subsurface could be an important part of the present climate control initiative to reduce the carbon dioxide concentration of the atmosphere. Layer of water-bearing permeable rock is assumed as a saturated porous medium, and the contained water can be replaced by compressed carbon dioxide. In such environment, water vapor flow can be developed from the thermal gradient caused by geothermal energy. High injection pressure is required to remove the fluid already present in the pores of solid skeleton hence accurate density calculation is important. So we use an extended ideal gas law to calculate the compressed carbon dioxide gas density. Temperature dependent entry pressure is accounting the surface tension and wetting angle role on the sorption equilibrium. Governing equations for numerical simulations are: mass balance equations for each component, i.e., water, vapor and carbon dioxide; energy balance equation. We have used a combined monolithic and staggered coupling scheme to solve these equations numerically using an automatic time stepping scheme. The numerical model is implemented into an open source in-house scientific finite element code allowing for simulations of applications in various geotechnical areas.

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Keywords: Non-isothermal two phase flow; OpenGeoSys project; partially saturated porous media; super compressibility factor

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1. Introduction

Depleted oil and gas reservoirs have limited capacity to store carbon dioxide within the context of the Carbon Capture and Storage (CCS) strategy, and are often not located near the carbon dioxide emitters (Koide et al. [1]). That makes disposal of carbon dioxide into deep saline aquifers as the most promising storage technology. For such disposal, it will need to remove carbon dioxide gas from the flue gases produced by power station and compress it to a pressure of about 60 bars, at ambient temperature about 283.15 K. Under these conditions the carbon dioxide will be a relatively pure liquid. Supercritical carbon dioxide is considered as a necessary attribute in any significant carbon dioxide disposal system due to its high density. Supercritical state is defined at any pressure above 73.8 bars, when handling pure carbon dioxide. Supercritical carbon dioxide acts much like a gas, with much greater changes in density as pressure and temperature are varied.

The critical temperature at which carbon dioxide will be in a supercritical stage is 304.2 K. Above this temperature carbon dioxide cannot exist as a liquid, and supercritical carbon dioxide is non-polar. Experiences in the operation of fluid injection yields possible limitation on the injection pressure to avoid well damage during carbon dioxide storage into aquifers (van der Meer [2]). A general approach to evaluate sedimentary basins for carbon dioxide disposal is presented by Bachu et al. [3]. The underground disposal of industrial quantities of carbon dioxide is entirely feasible (Holloway [4]). Numerical simulations are presented by Pruess and Garcia [5] for injection of carbon dioxide into a brine aquifer.

This paper presents heat and mass transport in a saline aquifer during injection of compressed carbon dioxide. Moreover, interests of non-isothermal effects are in utilization of geothermal energy through two-phase flow modelling. Normally liquid phase flow is very slow intact with low permeable host medium. Therefore, consideration of heat transport in two-phase flow is important. Vapor pressure offers a comprehensive image of the complexity. It is characteristic of such compositional model to consider the flow of more than one fluid phase. Inter-phase mass transport is accounted through vaporization under local thermal equilibrium, where mechanical work done by change in phase densities is neglected.

Non-isothermal two-phase flow model needs the mass balance equations for each species and energy balance equation to describe the system of carbon dioxide disposal into saline aquifers. This system is constituted by an undeformable solid matrix and compressible fluids. This numerical modelling requires consideration of multiphase, multicomponent approach to derive the mass balance equations, as done by Forsyth [6] for steam injection methods for clean the non-aqueous phase liquid (NAPL) contamination of groundwater. Considered gas phase is a multicomponent system composed of vapor and carbon dioxide. It is more convenient to separate vapor and carbon dioxide masses, and to formulate a mass balance equation for each phase. Heat transfer occurs due to conduction and multiphase convection which includes latent heat effects (Falta et al. [7]). Since the solid phase is assumed to be undeformable, therefore advective heat-flux is contributed only by liquid and gas phases. The heat source term $m\Delta h_{vap}$ of the energy balance equation expresses the amount of heat, which has lost due to latent heat of vaporization. The source term m of the gas balance equation is the quantity of water lost through vaporization. Primary variables of this formulation are capillary pressure, gas pressure and temperature. We have used a modified version of the Peng-Robinson equations of state (Peng and Robinson, [8]) for gas density. The account of the compressibility factor reveals the real behavior of the gas phase. A large group of constitutive relations are provided, such as: saturated vapor pressure from the Kelvin equation; heat of evaporation from the Watson formula, water saturation from the Brooks-Corey relation. In Brooks-Corey relation entry pressure is changing with temperature which provides derivative of the water saturation with respect to temperature. Along with this, temperature dependent material parameters are used, which is responsible for coupling of the heat and flow processes.

In general, such partial differential equations are not solvable because of the complex geometry of the porous media. But, it is possible by using the volume-averaging technique which can be achieved by averaging these governing partial differential equations on a representative elementary volume (REV) of the porous medium. The macroscopic balance equations are discretized in space and time within the context of the finite element method (FEM). In particular, a Galerkin's procedure is used for the discretization in space. We have used a staggered scheme for the coupling of mass and energy balance equations with automatic control of time stepping. The finite element module is embedded in the object-oriented framework of the scientific open source code OpenGeoSys (Kolditz et al. [9]; Wang et al. [10]).

2. Governing Equations

Modelling non-isothermal multiphase multicomponent flow and transport processes in the porous media requires the consideration of the transfer of mass and heat between the phases by such as advection and diffusion. More details on this formulation can be found in Class et al. [11] and Kolditz [12];

- *Mass balance equations*

The mass balance equations for liquid and gas phase are

$$\frac{\partial [n(1-S^l)\rho_{vap}^g]}{\partial t} - \nabla \cdot \left[\rho_{vap}^g \frac{\mathbf{k}k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] - \nabla \cdot \left[\rho^g \frac{M_{co_2} M_w}{M^2} \mathbf{D}_{eff} \nabla \left(\frac{p_{vap}^g}{p^g} \right) \right] = m$$

$$\frac{\partial[n(1-S^l)\rho_{CO_2}^g]}{\partial t} - \nabla \cdot \left[\rho^g \frac{\mathbf{k}k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] + \nabla \cdot \left[\rho^s \frac{M_{CO_2} M_w}{M^2} \mathbf{D}_{eff} \nabla \left(\frac{p_{vap}^g}{p^s} \right) \right] = 0$$

Here, n is porosity; S^l is saturation; ρ is density; p is pressure; μ is viscosity; \mathbf{k} is intrinsic permeability; k_{rel} is relative permeability; \mathbf{D}_{eff} is effective diffusion coefficient and M is molecular weight. Superscripts l, g, s stand for liquid, gas and solid phase, respectively. Subscripts CO_2, vap, w stand for carbon dioxide, vapor and water, respectively. Mass source m , can be find from mass balance equation for water component.

- *Energy balance equation*

Under local thermodynamical equilibrium heat flow through porous medium in terms of temperature T , is described by following equation

$$(\rho c_p)_{eff} \frac{\partial T}{\partial t} - \left[\rho_w^l c_p^l \frac{\mathbf{k}k_{rel}^l}{\mu^l} (\nabla p^l - \rho_w^l \mathbf{g}) + \rho^s c_p^s \frac{\mathbf{k}k_{rel}^s}{\mu^s} (\nabla p^s - \rho^s \mathbf{g}) \right] \cdot \nabla T - \nabla \cdot [\kappa_{eff} \nabla T] = \dot{m} \Delta h_{vap}$$

Where, $(\rho c_p)_{eff}$ and κ_{eff} are the volumetric heat capacity and thermal conductivity of the porous media, respectively. The above mentioned equation includes heat transport by advection (only for liquid and gas phase), conduction and latent heat of vaporization. The right hand side term is heat source, expresses latent heat of the vaporization with mass source term, being the quantity of liquid water lost through vaporization.

3. Numerical Example

In this study numerical simulation has been performed about injection of compressed carbon dioxide to the pressure 60 bars at temperature of 283.15 K. We assume that column is a partially saturated porous medium; initially the pores of the solid skeleton are filled with water and vapor. We solve the problem in one-dimensional domain with 260 linear finite elements up to the time duration 4000 s. The non-linear iteration is restricted with maximum of 25 iterations. Material parameters of the porous medium are presented in Table 1.

Meaning	Symbol	Value	Unit
Length	L	2.6	m
Density	ρ^s	2046	kg m ⁻³
Heat capacity	c_p^s	1200	J kg ⁻¹ K ⁻¹
Thermal conductivity	κ^s	2.5	W m ⁻¹ K ⁻¹
Intrinsic permeability	\mathbf{k}	1.0x10 ⁻¹⁰	m ²
Porosity	n	0.3	-

Table 1 Material parameters of the solid phase used in the simulations.

$$p^c = 5.0 \times 10^3 \text{ Pa}, \quad p^g = 4.0 \times 10^6 \text{ Pa}, \quad T = 353.15^\circ\text{K}$$



Fig. 1 Layer of water-bearing permeable rock and physical conditions.

Water saturation is defined as extensive quantity per unit volume of the pore space. In this study, water saturation is depending on capillary pressure and temperature. Brooks and Corey [13] presented the relationship between water saturation and capillary pressure. From the temperature dependent entry pressure it is possible to estimate how the water saturation varies with temperature. Entry pressure is the measure of capillary pressure regarding to the start of the displacement of wetting pore fluid. Surface tension on the phase interface and wetting angle induces a movement of fluids until a local equilibrium is reached. This equilibrium depends on several physical quantities and temperature is one of them. Hence, it is possible to define a temperature dependent relation for entry pressure. Since capillary pressure can be scaled with surface tension along with wetting angle so the entry pressure can be expressed as (Olivella and Gens [14])

$$p_d(T) = p_d(T_0) \frac{\sigma(T) \cos \theta_w(T_0)}{\sigma(T_0) \cos \theta_w(T)}$$

$$\sigma(T) = 0.3258(1-a)^{1.256} - 0.148(1-a)^{2.256}; \theta_w(T) = \theta_w(T_0) [0.97 + 0.65a - 1.3a^2]$$

Where $a = \frac{T}{647.3K}$, p_d is assumed 5×10^3 Pa and wetting angle $\theta_w(T) = 69.8^\circ$ at $T_0 = 353.15$ K for water solid system.

In left side of Fig. 2 we present the water saturation S^d profile from isothermal and non-isothermal injection of carbon dioxide at time steps: 100; 1000; 4000 s. From Fig. 2a it is clear that, in the non-isothermal case the injected carbon dioxide could displace the water sufficiently more than in case of isothermal injection. This is due to the increment in the entry pressure as surface tension and wetting angle decrease with temperature. We found that decrease in the water saturation is partially assisted by vaporization but primarily due to surface tension and wetting angle effects. Increased water saturation can also increase the movement of the phases (liquid, gas) as Brooks-Corey relative permeability of both phases gets enhanced. Enthalpy of vaporization for water is according to Watson formula as given in Benes and Mayer [15]. The Kelvin’s equation relates the capillary and vapor pressures, whereas saturated vapor pressure is obtained from the Clausius-Clapeyron relation. Here, density of liquid water is decreasing with temperature linearly.

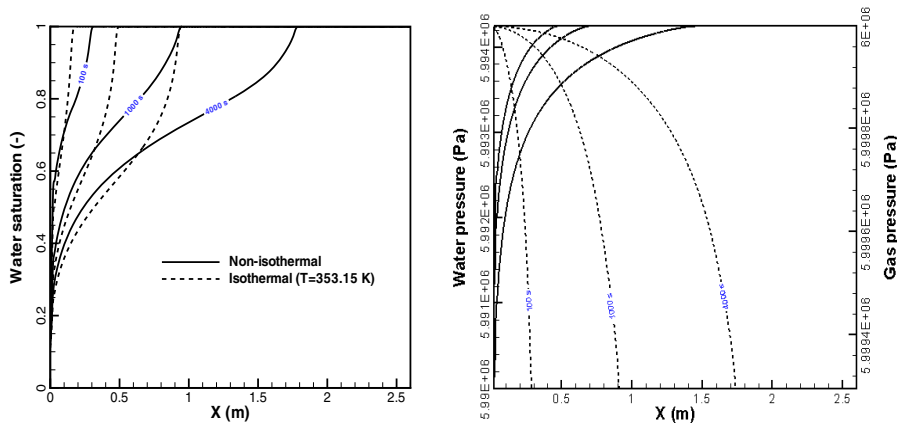


Fig. 2 Water saturation; gas and water pressure in the one-dimensional column for selected time steps.

Fig. 2 (right) shows horizontal profiles of the obtained gas pressure p^g and water pressure p^l at different time steps. The pressure gradient illustrates that mass-flux of water is in the opposite direction of the injected gas mass-flux, i.e. carbon dioxide. From this pressure profiles it is observed that up to a certain distance from the injection point carbon dioxide is displacing water smoothly (see Figs 4a-c), beyond that point gas pressure falls sharply. This reveals the suppression of water in the closed column. Hence, to balance the mass-fluxes, water pressure starts rising from its minimum value to the initial water pressure.

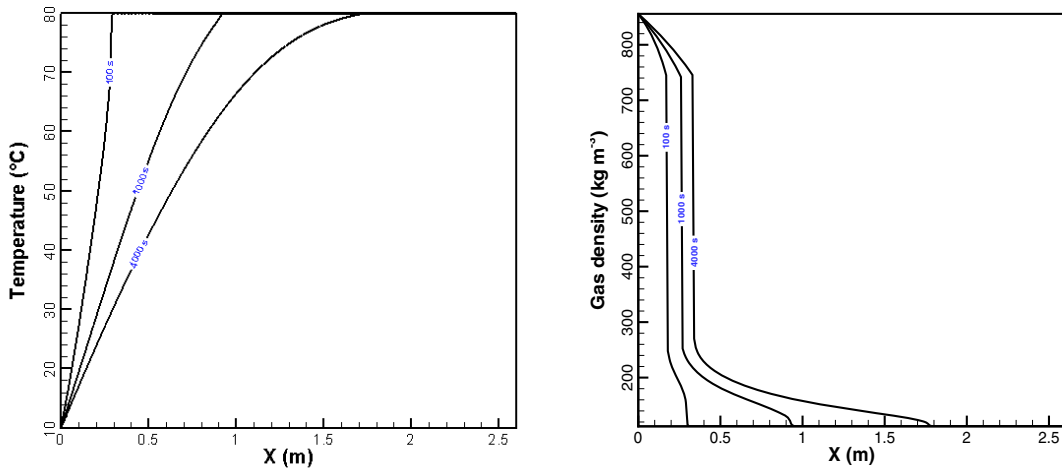


Fig. 3 Temperature and gas density distribution in one-dimensional column for selected time steps.

Temperature T and gas phase density ρ^g are presented in Fig. 3. Water density varies linearly with temperature and gas phase density is composed of vapor density and carbon dioxide density. Density of vapor can be directly calculated by using the Clausius-Clapeyron relation through Watson formula. Carbon dioxide density is very sensitive to the pressure near the critical temperature; hence using the ideal gas law will be not good. So we calculate this with an extended ideal gas law accurately close to reality. Within this context, the cubic equation of the compressibility factor corresponds to Peng-Robinson equations of state. This is solved analytically at any temperature and pressure for given critical constant and the acentric factor. Out of three roots, maximum one is used for gas phase in the extended ideal gas equation. Fig. 3 (right) shows that the sudden decrease in density corresponds to the region where temperature is close to the critical temperature of carbon dioxide, i.e. 304.2 K.

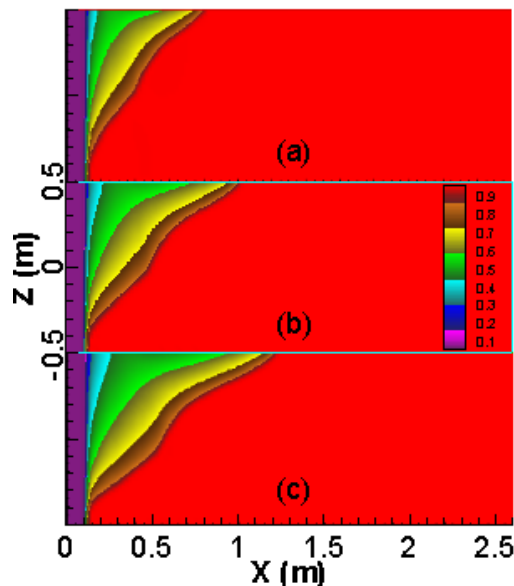


Fig. 4 Water saturation distribution in a two-dimensional porous cross-section of 1m thickness.

In Figs. 4a-c we present the water saturation S^l for selected time steps 100, 1000, 4000 s. This figure shows that up to a distance about $x=0.2$ m, injected carbon dioxide displaced water like in a piston. But beyond this distance gravity generates a sufficient vertical pressure gradient, and the lighter carbon dioxide moves upwards reaching the top of the column. Therefore for permanent disposal of carbon dioxide, the structure of the saline aquifer must contain a barrier of impermeable or low-permeable strata to prevent the escape of carbon dioxide.

4. Conclusions

In this work we have developed a numerical model for carbon dioxide disposal into saline aquifers. Following progress is achieved in this work.

- A ppT - formulation of the governing equations for non-isothermal two-phase flow through a partially saturated porous medium has been developed i.e., the chosen primary variables are capillary pressure, gas pressure and temperature. We have experienced that, in comparison to commonly used pST formulations the ppT concept has advantages in particular for the accuracy of the finite element method with no upwind technique.
- Temperature effects have been included by means of the general Clausius-Clapeyron equation for phase change. Density of compressed carbon dioxide has been calculated accurately by extended ideal gas.
- The variability of the complete material properties of porous medium and fluids such as capillarity, relative permeability, mobility, density, viscosity, heat capacity and thermal conductivity has been investigated in detail.
- We used a combined monolithic / staggered coupling scheme with automatic control of time stepping i.e., monolithic for the two-phase flow and staggered for the heat transport. We have considered the latent heat of vaporization for heat transfer in addition to advection and conduction.
- In a previous work Olivella and Gens [14] estimated the entry pressure required to initiate the desaturation process in an unsaturated porous medium. We further developed this scaling technique to investigate temperature dependent entry pressure as well as wetting angle for fluid displacement. The entry pressure and wetting angle can be used to estimate temperature effects on sorption equilibrium due to curvature of concave meniscus separating water and vapor. We used this sorption equilibrium to study how the water saturation changes with temperature through variability of entry pressure.
- The numerical scheme has been implemented in the framework of object-oriented FEM and, therefore, allows an easy extension of the numerical non-isothermal two-phase model for multi-dimensional problems.

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