

## TOWARDS THE GENERIC CONCEPTUAL AND NUMERICAL FRAMEWORK FOR THE SIMULATION OF CO<sub>2</sub> SEQUESTRATION IN DIFFERENT TYPES OF GEORESERVOIRS

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**Abstract.** In this paper, conceptual and numerical modeling of coupled thermo-hydro-mechanical (THM) processes during CO<sub>2</sub> injection and storage is presented. The commonly used averaging procedure combining the Theory of Mixtures and the Concept of Volume Fractions serves as background for the complex porous media approach presented here. Numerical models are based on a generalized formulation of the individual and overall balance equations for mass and momentum, as well as, in non-isothermal case, the energy balance equation. Within the framework of a standard Galerkin approach, the method of weighted residuals is applied to derive the weak forms of governing equations. After discretizing spatially these weak forms, a system of nonlinear algebraic equations can be obtained. For the required time discretization a generalized first order difference scheme is applied, linearization is performed using Picard or Newton-Raphson methods. The corresponding models are implemented within the scientific open source finite element code OpenGeoSys (OGS) developed by the authors, which is based on object oriented programming concepts. This assists the efficient treatment of different physical processes, whose mathematical models are of similar structure. Thus, the paper is mainly focused on a generic theoretical framework for the coupled processes under consideration. Within this context, CO<sub>2</sub> sequestration in georeservoirs of different type can be simulated (e.g., saline aquifers, (nearly) depleted hydrocarbon reservoirs).

## 1 INTRODUCTION

Carbon Capture and Storage (CCS) is counted among the most promising transition technologies for the mitigation of anthropogenic greenhouse gas emissions. Recently, CO<sub>2</sub> sequestration as an essential part of CCS procedures has become a subject of worldwide investigation.

Three types of geological formations are particularly considered for the safe storage of CO<sub>2</sub>: (nearly) depleted hydrocarbon reservoirs, deep saline aquifers and unminable coal seams. The migration of the carbon dioxide in the subsurface, and its interaction with the formation fluids as well as with the porous reservoir media is characterized by various complex transport, reaction and deformation phenomena. Several trapping mechanisms (e.g., stratigraphic, structural, solubility, mineral effects), which prevent the migration of the buoyant CO<sub>2</sub> back to the surface, are based on these phenomena. Within the context of mechanical loading, the injection of carbon dioxide into the subsurface results in high pressure in the vicinity of the injection well. Due to the injection pressure, the stress distribution in this reservoir region can be changed significantly. To consider high pressure induced medium deformation is very important for the integrity of potential geological storage sites. Fluid and matrix properties of the porous subsurface media are also affected by prevailing thermal conditions. In particular, high temperature differences between injected fluid and reservoir environment have the potential of possible reservoir failure (e.g., thermal matrix damage).

The coupling of multiple physical-chemical processes requires numerical analysis based on physically grounded complex mathematical models. Within this context, the modeling and simulation of the injection and the spreading of carbon dioxide in the underground 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<sub>2</sub> in the porous formations, and in assessing the capacity as well as the safety of the reservoir. Sophisticated mathematical models, numerical algorithms and software tools have to be developed taking into account all relevant physico-chemical phenomena during migration and storage of CO<sub>2</sub> in the subsurface, such as flow and transport of multiple phases including dissolution and mixing effects, hydrodynamic instabilities (e.g. viscous fingering), rock deformation as well as fracturing, heat transport and phase changes. In most cases it is not necessary to be able to describe all these processes for the whole simulation time period or for the entire model domain. The formulation of specific model concepts has to consider the spatial and temporal scale of the problem and the dominating processes in each case.

While transport and deformation processes in porous media have been studied for several decades considering various applications (e.g. groundwater flow and consolidation problem), the modeling of carbon dioxide migration in geological formations is a fairly new subject of investigations in different research areas (e.g. hydrology, geotechnology, computational mechanics and mathematics). As about ten years ago only a few publications have been dedicated to this topic (cf. [1, 2]), recently an increasing number of

numerical (see e.g., [3–7]), semi-analytical (cf. [8, 9]) and analytical (cf. [10–12]) studies have been published. Within the context of numerical simulations, more complex problems can be treated (e.g. coupling of different processes, consideration of heterogeneities and various geological conditions), although the development of efficient and stable algorithms is challenging. Among hydromechanical site specific simulations of CO<sub>2</sub> injection, hypothetical cases are reported (e.g., [13], saline aquifer) as well as real field studies (e.g., [14], depleted hydrocarbon reservoir). For the state of the art in model and software development for geological CO<sub>2</sub> storage see also [2, 15] and literature cited there. To compare several numerical simulators with respect to their capabilities, efficiency and accuracy code comparison studies have been conducted [16, 17]. Within this context, benchmark problems and real site studies have been defined addressing various aspects of CO<sub>2</sub> storage at different reservoir conditions.

Modeling of CO<sub>2</sub> storage on a reservoir scale for feasibility studies and risk analyses is very demanding with respect to the computational costs due to the complex geometry that needs 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 all relevant physico-chemical effects, but starting with the most relevant effects at CO<sub>2</sub> injection near the injection well. Since the model complexity is adapted to these dominating processes, other processes having less contribution to the event under consideration are neglected for computational efficiency (e.g., mineral trapping for short-term processes). Within this context, in this paper, the investigation is restricted to thermo-hydro-mechanical (THM) effects of the CO<sub>2</sub> injection into different types of reservoirs.

In this study, we present the generalized conceptual model, the governing equations and numerical aspects of a finite element approach to analyze THM coupled processes at geological CO<sub>2</sub> storage. To this purpose, we focus on basic ideas and relations, not discussing here specific formulations of governing equations, which are related to typical processes in different storage sites (e.g., multiphase flow in deformable porous media in the case of saline aquifers, non-isothermal compositional gas flow for enhanced gas recovery in gas reservoirs). With the present assumption, the changes in thermal, flow and deformation fields of the model are simulated by using the standard Galerkin finite element method, which is realized in an object oriented scientific tool, OpenGeoSys (an open source finite element code) developed by the authors. Specific model formulations, simulation results and discussion are presented in two complementary conference papers.

In the following, vectors and higher order tensors will be denoted by boldface characters. Their scalar product is characterized by a single dot while double dots indicate the summation product (double inner product)  $\mathbf{a} \cdot \cdot \mathbf{b} = a_{ij} b_{ji}$ . A superposed dot indicates the material rate of a vector or a tensor. The individual constituents  $\alpha$  of a porous material represent the phases of the overall aggregate or components within a phase. Below, superscript  $\alpha = s$  marks the solid phase, and  $\alpha = \gamma$  denote several pore fluid phases.

## 2 CONCEPTUAL MODELING

### 2.1 Preliminary Remarks

Based on Biot's studies on the macroscopic theory of saturated wet soils (cf. [18]), the Theory of Mixtures has been widely accepted to model the complex behavior of porous media (concerning basic assumptions see e.g., [19, 20]). For the realistic modeling of the mutual interactions of the porous media constituents, the Theory of Mixtures has been combined with the Concept of Volume Fractions by, e.g., [21, 22]. Within the context of this enhanced Theory of Mixtures (also known as Theory of Porous Media), all kinematical and physical quantities can be considered at the macroscale as local statistical averages of their values at the underlying microscale. Comprehensive studies about the theoretical foundation and numerical algorithms for the simulation of coupled problems of multiphase continua are given in, e.g., [23–25] and the quotations therein. Recent developments of enhanced numerical approaches for the porous media modeling in geotechnical applications are reported in, e.g., [26–28].

In the following, the subsurface formation designated as carbon dioxide reservoir is considered as a mixture of a solid skeleton and a pore fluid content, which can either be

- a single liquid or gas (single-phase flow in porous media),
- an immiscible fluid mixture of gas and liquids (multiphase flow in porous media) or
- a miscible fluid mixture of different reacting constituents allowing phase transitions due to evaporation, condensation, precipitation (multiphase multicomponent flow in porous media).

Within the framework of the Concept of Volume Fractions, various scalar variables are defined to describe the microstructure of a porous medium in a macroscopic manner neglecting the real topology and distribution of the pores. These variables serve as measures of local fractions of the individual constituents. In this context, the volume fractions  $n^\alpha$  represent the ratio of the partial volume of the corresponding constituent of a multiphase body with respect to the overall volume of a representative elementary volume (REV) of the control domain under consideration. One of the most characteristic media properties of a porous material is the porosity  $n$ , the local amount of fluid volume fractions.

$$n = \sum_{\gamma} n^{\gamma} = 1 - n^s \quad (1)$$

Since, in general, the overall medium is completely filled with matter, from the definition of the volume fractions follows the saturation condition regarding the overall aggregate.

$$\sum_{\alpha} n^{\alpha} = 1 \quad (2)$$

If multiphase flow occurs, it is more convenient for various applications to use the (partial) fluid saturations  $S^\gamma$  instead of the volume fractions. These local functions are given by

$$S^\gamma = \frac{n^\gamma}{n} \quad \text{with the pore content saturation condition} \quad \sum_{\gamma} S^\gamma = 1 \quad (3)$$

In the following, two different formulations of mass density related to the constituents of a porous medium are introduced. The so-called material (effective, realistic) density  $\rho^{\alpha R}$  is defined as the ratio of the mass fraction  $dm^\alpha$  of the individual constituent under consideration with respect to its partial volume fraction  $dv^\alpha$ .

$$\rho^{\alpha R} = \frac{dm^\alpha}{dv^\alpha} \quad (4)$$

The so-called partial (global, bulk) density is given by the ratio of the mass fraction of the given constituent with respect to the volume fraction of the overall aggregate  $dv$ .

$$\rho^\alpha = \frac{dm^\alpha}{dv} \quad \text{with the correlation} \quad \rho^\alpha = n^\alpha \rho^{\alpha R} \quad (5)$$

Obviously, the mass density of the porous medium (homogenized overall aggregate) is defined as the sum of the partial densities of its constituents.

$$\rho = \sum_{\alpha} \rho^\alpha \quad (6)$$

The conceptual idea behind the formulations and relations presented above consists in the assumption that the mass fractions of all constituents of the multiphase medium are simultaneously present and statistically uniformly distributed over the entire control domain. Within this context, the material body under consideration is theoretically substituted by an aggregate completely and continuously filled by superimposed (overlapping) homogenized partial continua with reduced mass densities. Consequently, the motion and physics of the individual constituents as well as the overall aggregate can be specified by well-accepted phenomenological methods of continuum mechanics.

Describing the transport and deformation of the constituents of porous media within the framework of continuum mechanics it is assumed that the geometry of the control domain under consideration is characterized at each time by the solid skeleton, whereas the fluid pore content is able to flow across the boundary of the surface. Thus, it proves to be reasonable not to model the absolute motion state of the pore content, but its motion relative to the motion of the solid phase, considering the porous medium as a local thermodynamic open system with the solid skeleton as volume under observation.

## 2.2 Governing Equations

The governing field equations for the modeling of transport and deformation processes of non-isothermal multiphase flow in deformable porous media are formulated based on the local individual balance relations of the constituents, particularly mass, momentum and

energy balances. Within this context, the application of the fundamental balance relations on the analysis of multiphase materials is based on Truesdell's *metaphysical principles* [29]. The crucial idea behind these principles is the assumption that the balance relations of the constituents as well as the balance relations of the overall aggregate of a porous medium can be formulated in accordance to the corresponding classical relations of single-phase continuum mechanics. Additionally, to account for the interaction mechanisms between the constituents, so-called production terms are introduced for the individual balance relations of the constituents (cf. [24]). Following, superposition is used to define the balance relations of the overall aggregate based on the individual balance relations of the constituents.

Neglecting mass exchange between the phases (no dissolution and sorption processes), the local mass balance for any individual constituent of the porous medium is given by

$$\frac{d_\alpha \rho^\alpha}{dt} + \rho^\alpha \nabla \cdot \mathbf{v}^\alpha = \frac{\partial \rho^\alpha}{\partial t} + \nabla \cdot (\rho^\alpha \mathbf{v}^\alpha) = 0 \quad (7)$$

with the velocity  $\mathbf{v}^\alpha$  of the constituent under consideration, and the usual divergence operator  $\nabla \cdot (\cdot)$ . From the velocity-displacement relation for the solid skeleton follows  $\mathbf{v}^s = \dot{\mathbf{u}}^s$  with the solid displacement vector  $\mathbf{u}^s$ . The derivative

$$\frac{d_\alpha a}{dt} = \frac{\partial a}{\partial t} + \mathbf{v}^\alpha \cdot \nabla a \quad (8)$$

with the usual gradient operator  $\nabla(\cdot)$  denotes the material time derivative of an arbitrary variable  $a$  with respect to the motion of a material point of the constituent. For the further discussion, the relations between the material time derivatives (here, of an arbitrary variable  $a$ ) with respect to the solid skeleton, and with respect to an individual fluid constituent is of crucial interest in terms of a unified numerical characterization of the different processes.

$$\frac{d_\gamma a}{dt} = \frac{d_s a}{dt} + \mathbf{v}^{\gamma s} \cdot \nabla a \quad (9)$$

Here,  $\mathbf{v}^{\gamma s} = \mathbf{v}^\gamma - \dot{\mathbf{u}}^s$  is the so-called seepage velocity describing the fluid motion with respect to the deforming skeleton material.

According to the generalized formulation Eq. (7), considering Eqs. (1) and (5), the local solid phase mass balance is given by

$$\frac{d_s [(1-n)\rho^{sR}]}{dt} + (1-n)\rho^{sR} \nabla \cdot \dot{\mathbf{u}}^s = 0 \quad (10)$$

serving as basis for the calculation of porosity changes. Following the same procedure, additionally considering Eqs. (3) and (9), the mass balance relations for fluid constituents can be defined with respect to the solid phase motion.

$$\frac{d_s (nS^\gamma \rho^{\gamma R})}{dt} + \nabla \cdot (nS^\gamma \rho^{\gamma R} \mathbf{v}^{\gamma s}) + nS^\gamma \rho^{\gamma R} \nabla \cdot \dot{\mathbf{u}}^s = 0 \quad (11)$$

Assuming material incompressibility of the solid phase, i.e.  $d_s \rho^{sR}/dt=0$ , and applying the solid phase mass balance Eq. (10), Eq. (11) can be represented in a more detailed description.

$$nS^\gamma \frac{d_s \rho^{\gamma R}}{dt} + n\rho^{\gamma R} \frac{d_s S^\gamma}{dt} + \nabla \cdot (\rho^{\gamma R} \mathbf{w}^{\gamma s}) + S^\gamma \rho^{\gamma R} \nabla \cdot \dot{\mathbf{u}}^s = 0 \quad (12)$$

Here  $\mathbf{w}^{\gamma s} = nS^\gamma \mathbf{v}^{\gamma s}$  is usually known as filter velocity of the motion of the pore fluid constituent  $\varphi^\gamma$ . For non-isothermal problems, the saturations  $S^\gamma$  and the mass densities  $\rho^{\gamma R}$  represent functions of temperature  $T$  and the fluid pressure fractions  $p^\gamma$

Deformation processes in porous media are described by the momentum balance equation in terms of the total Cauchy stress tensor  $\boldsymbol{\sigma}$  referring to the local loading state of the overall aggregate. In geotechnical problems, the internal fluid friction forces can be neglected in comparison to the interaction terms between fluid and skeleton motions. Thus,  $\boldsymbol{\sigma}$  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 [30]:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_E^s - p\mathbf{I} \quad (13)$$

with the solid effective stress tensor  $\boldsymbol{\sigma}_E^s$  and the identity tensor  $\mathbf{I}$ . Therein, the pore pressure  $p$  is given in analogy to Dalton's law.

$$p = \sum_{\gamma} S^\gamma p^\gamma \quad (14)$$

Finally, in non-isothermal case, the specific local overall linear momentum balance equation for fluid saturated porous media is defined as follows:

$$\nabla \cdot \left[ \boldsymbol{\sigma}_E^s - \left( \sum_{\gamma} S^\gamma p^\gamma \right) \mathbf{I} - \alpha \Delta T \left( \underset{\mathbf{D}}{\mathbf{D}} \cdot \cdot \mathbf{I} \right) \right] + \rho \mathbf{g} = \mathbf{0} \quad (15)$$

where  $\alpha$  is the thermal expansion coefficient,  $\underset{\mathbf{D}}{\mathbf{D}}$  is the fourth-order elastic material tensor, and  $\rho \mathbf{g}$  is the volume force with the gravity vector  $\mathbf{g}$ .

The heat transport equations for individual constituents of a porous medium are based on their local partial energy balance equations.

$$\rho^\alpha C_{p\alpha} \frac{d_\alpha T^\alpha}{dt} - \nabla \cdot (\lambda_\alpha \nabla T^\alpha) + Q_\alpha = 0 \quad (16)$$

Here,  $C_{p\alpha}$  denotes the heat capacity and  $\lambda_\alpha$  the thermal conductivity of the given constituent, respectively,  $T^\alpha$  is the individual temperature of the constituent, and  $Q_\alpha$  characterize source/sink terms. Assuming that the constituents are locally in a thermodynamical equilibrium state, i.e., locally all phases are at the same temperature  $T$  at each material point of the homogenized continuum, and using Eq. (9), the set of necessary balance

equations according to the generalized problem under consideration is completed by the heat transport equation for the overall aggregate.

$$(\rho C_p)_{\text{eff}} \frac{d_s T}{dt} + \sum_{\gamma} (C_{p\gamma} n S^{\gamma} \rho^{\gamma R} \mathbf{v}^{\gamma s}) \cdot \nabla T - \nabla \cdot (\lambda_{\text{eff}} \nabla T) + Q_T = 0 \quad (17)$$

Considering the above mentioned Truesdell's metaphysical principles, the effective heat capacity and the thermal conductivity of the overall porous medium are calculated according to the following equations, which allows for the coupling of thermal and hydraulic properties.

$$(\rho C_p)_{\text{eff}} = (1 - n) \rho^{sR} C_{ps} + n \sum_{\gamma} C_{p\gamma} S^{\gamma} \rho^{\gamma R} \quad (18)$$

$$\lambda_{\text{eff}} = \sum_{\alpha} \lambda_{\alpha} \quad (19)$$

Based on specific material functions for the state variables and appropriate formulations of different production terms to characterize the interaction between the constituents of the overall aggregate (e.g., phase transition, mixing), specific formulations for the above mentioned balance equations have to be defined considering the site specific situation.

### 2.3 Constitutive Relations

If the balance relations characterize fundamental physical and thermodynamical properties of the matter independently of specific material properties, in real applications the response of a physical body on similar interactions with the external environment differs for various materials. Thus, so-called constitutive relations have to be defined to characterize the specific material behavior. In terms of the mathematical modeling of physico-chemical processes this observation is equivalent to the formulation of closed systems of equations, which should consist of balance as well as constitutive relations.

Within the context of the multiphase problem under consideration, constitutive equations are required for selected production terms of the specific balance relations of the individual constituents, as mentioned above, for pore fluid properties like pressure and saturation, for the partial effective stress tensor of the solid skeleton, and for several thermal properties. Among others, specific formulations of Darcy's, Fick's and Fourier's law, equations of state, capillary pressure-saturation functions as well as the relations between relative permeability and saturation, and deformation laws relating the effective stress to the strain and/or strain rate of the solid matrix are substantial constitutive equations required for porous media mechanics.

## 3 NUMERICAL SCHEME

The numerical treatment of the coupled problem of THM processes in deformable porous media is based on the governing field equations together with discretization meth-



ods in the space and time domains. Some general representations of corresponding numerical approaches to solve the problem under consideration can be found in [25, 31–33].

Usually, 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 corresponding local individual or overall balance equations are multiplied by arbitrary test functions, which are defined in appropriate spaces and meet the corresponding homogeneous Dirichlet boundary conditions, and are integrated subsequently over the domain of interest bounded by the solid skeleton.

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 spatially the weak forms of the balance relations a system of nonlinear algebraic equations can be obtained. For the required time discretization we use a generalized first order difference scheme, but in most applications, a fully implicit Euler scheme is used, which is unconditionally stable and can be applied to complex coupled problems. However, numerical diffusion is introduced into the system by time discretization. This problem is reduced by an adaptive time-stepping scheme.

The nonlinear coupled boundary value problem is solved iteratively using the Picard or Newton-Raphson linearization. Within this context, usually all unknowns can be solved at the same time in the context of a so called monolithic scheme. However, solving the whole system of equations monolithically may lead to memory problems when employing a fine mesh due to a large number of freedoms per element node of the coupled problem under consideration. We adopt a mixture of monolithic and staggered schemes to avoid this bottleneck without losing the accuracy of the solutions.

The discussed numerical scheme is realized in an object oriented scientific software tool, OpenGeoSys, developed by the authors, and has been verified by several classic benchmarks. The presented generalized model has been adopted to several site specific applications (e.g., two-phase flow in deformable porous media in the case of saline aquifers, compositional gas flow for enhanced gas recovery in gas reservoirs - for details see [34, 35])

## 4 CONCLUSIONS

We have presented the conceptual model and the governing equations for the simulation of coupled thermo-hydro-mechanical processes, which are observed for geological storage of carbon dioxide in porous subsurface materials. The presented generalized numerical model is based on balance laws for the overall porous medium as well as for its different fluid and solid phases. Using well-established discretization procedures (in space and time), a coupled multiphysics finite element model is developed from the weak formulations of the governing equations. Monolithic or staggered monolithic/staggered coupling schemes are available to solve the discretized system of equations. The presented generalized approach represents the basis for specific formulations of numerical models for the simulation of different application oriented situations within the context of geological CO<sub>2</sub> storage (e.g., saline aquifers, nearly depleted hydrocarbon reservoirs). For this purpose, the appropriate

choice of relevant primary variables and constitutive relations has a high priority, and is subject of intense scientific studies. This indicates that the analysis of the thermo-hydro-mechanical response is crucial for proper selection of injection sites, injection rates, and total storage capacity of potential CO<sub>2</sub> reservoirs.

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