

Modelling of CO₂ storage in geological formations with DuMu^x, a free-open-source numerical framework. A possible tool to assess geological storage of carbon dioxide in Romania

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Abstract. Geological storage of carbon dioxide represents a viable solution to reduce the greenhouse gases in the atmosphere. Romania has initiatives to build a large-scale integrated CO₂ capture and storage demonstration project and find suitable on-shore and off-shore CO₂ storage locations. Numerical simulators are essential tools helping the design process. These simulators are required to be capable to represent the complex thermo-hydro-mechanical-chemical and biological phenomena accompanying the geological CO₂ storage such as, multi-phase flow, compositional effects due to dissolution of CO₂ into the brine, non-isothermal effects due to cold CO₂ injection, geomechanical effects, mineralization at the reservoir-scale. These processes can be simulated accurately and efficiently with DuMu^x (www.dumux.org), a free- and open-source simulator. This article presents and reviews briefly these mathematical and numerical models.

1 Introduction

Reduction of greenhouse gas emissions has been proposed by United Nations beginning with the 1997 Kyoto Protocol and the most recent Paris Agreement negotiated in 2015 Climate Change Conference. Among the technologies able to reduce the greenhouse gas emissions, *carbon capture and storage* (CCS) in geological formations represents most viable option for storage [1]–[4]. Generally, the geological CO₂ storage can be done in depleted oil/gas fields, coal seams, salt caverns, or in deep saline formations below 800 meters, which also have the highest estimated storage capacity of more than 1000 Gt [2]. The main criteria for selecting a long-term CO₂ storage site are the size (reservoir extent), porosity and permeability, i.e. large porosities ensure the volume for storage while a large permeability a good injectivity, depth below 800 m to guarantee the CO₂ is in supercritical form, and an overlying impervious cap rock (e.g., Tatomir et al. 2016). Current state of the art of CCS is at a stage where the transition from pilot to large-(industrial-) scale projects is required.

Another technology to reduce the greenhouse gas emissions is the Carbon Capture Utilization and Storage (CCUS). CCUS aims to increase the economic viability of the CO₂ storage by making use of the CO₂ and subsequently reducing the emissions to the atmosphere; for instance, increasing the oil/gas recovery by injecting CO₂. Unlike CO₂ storage, the enhanced oil recovery (EOR) and enhanced gas recovery (EGR) using CO₂, i.e., CO₂-EOR, are already operating on a commercial scale [6]. CCUS technologies list CO₂-EOR, CO₂-EGR, CO₂-

enhanced coal bed methane production, CO₂-enhanced shale gas production, CO₂-enhanced geothermal systems, etc.

Global CCS pilot plants and initiatives are reviewed in [4], [7], [8].

The main objective of this article is to introduce mainly to the Romanian scientific community the open source numerical simulator DuMu^x [9] and review its applicability to geological storage of CO₂. We do not present any modelling results of potential storage sites but refer the reader to the literature sources where such studies have already been conducted at field and regional scales.

1.1 CCS in Romania

Assessing the GCS in Romania has been conducted in a number of studies. [10] investigates the potential of Romanian Black Sea shelf for CO₂ storage, in particular the deep saline formations of the Histria Depression. The authors identify three potential locations in the Lower and Upper Cretaceous and Middle Eocene formations, composed mainly of sands and sandstones. The depths range from 1820 – 2850 m, with a permeability up to 200 mD and a porosity of up to 30%. Available well data provide a good representation of the layers in the three identified reservoirs.

[11] aims to identify suitable locations for a CCS Demo Project in the Oltenia Region in an area 50 km around Turceni Power Plant. The formation unit is called Getic Depression, a sedimentary basin at the contact between South Carpathians and the Moesian Platform. The large scale GETICA CCS Demo project aims to

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demonstrate the application of large-scale integrated CCS to an existing coal-fired power plant in Romania [12].

Possibilities to deploy CO₂-EOR in Romania are discussed by [13]. The authors select 10 out of 130 oil fields and couple them with a major emission source (i.e., power plants, cement factories, refinery, chemical plant). Furthermore, they report designing CO₂-EOR injection experiments for eight oil fields (i.e., Bradu Albota – Meoșian, Siliștea – Sarmatian, Satchinez – Pannonian, Calacea – Miocene, Bradesti – Triassic, Turnu - Pannonian, Moreni – Meotian and Cerdac – Oligocene). The study concludes that Romania has large potential for using the CO₂ captured from industrial sources for enhanced oil and gas production, estimating an increase of the estimated oil reserves by 20 to 80 million tons.

The reviewed literature does not present any forward modelling results for the selected CCS or CCUS sites in Romania.

1.2 Available numerical simulators for GCS

For CCS deployment at industrial scale it is crucial to have available efficient numerical tools. These modelling tools are necessary during the project planning phase, during the injection operations and post-injection. Numerical simulations are essential to estimate the capacity of the reservoir, for the risk assessment and feasibility studies, for developing efficient injection strategies, and implementing efficient monitoring strategies.

Available numerical simulators capable of dealing with non-isothermal multiphase multicomponent transport processes can be found in the code inter-comparison studies e.g., [14]–[17]. There are more than 20 simulators available, e.g., COORES, CODEBRIGHT, COMSOL Multiphysics, DuMu^x, ECLIPSE, ELSA, EWOMS, FEHM, GEM, GPRS, IPARS-CO₂, MoReS, MRST, MUFTE, OpenGeoSys, PFLOTRAN, ROCKFLOW, RTAFF2, ELSA, TOUGH2, TOUGH2/ECO2N, VESA. Commonly, the oil and gas industry use ECLIPSE, which has two software packages, the E100 for black oil model and E300 for simulating the compositional effects.

2 Modelling CO₂ storage in geological formations using DuMu^x

The physical chemical processes involved in GCS and described by the models (section 1.2) are highly coupled and non-linear. The fluid properties are functions of pressure, temperature, salinity, and composition.

DuMu^x [17] (www.dumux.org) stands for DUNE for Multi-{Phase, Component, Scale, Physics, ...} and is mainly developed at the University of Stuttgart, Germany since 2007. It is a free and open-source simulator for multiphase flow, multicomponent transport in porous media. DuMu^x has been applied to a number of geological CO₂ storage scenarios [13]–[15], [18], [19]. DuMu^x is based on the Distributed and Unified Numerics Environment DUNE (www.dune-project.org).

The spatial discretization methods available for different models are the vertex-centered finite volume method (or, the box method) [20], cell-centered finite volume method, and the standard Galerkin finite element method. The time discretization is a fully implicit Euler method. The models can be solved fully coupled or sequentially. By choosing a model with sequential coupling larger speed-up factors are usually obtained [21].

The practical modelling of flow and transport processes in porous media at reservoir-scale applications requires the definition of the properties, quantities and processes on a representative elementary volume (REV) [20]. Generally, all models implemented in DuMu^x are constructed on the assumption that a REV exists at the Darcy scale. Exceptions use for instance pore-network models to couple mass, momentum and energy at the interface between free flow and porous media flow [22].

For CO₂ storage in porous media the relevant processes can be described by the multiphase flow in porous media equations, the multiphase multicomponent balance equations, the non-isothermal multiphase flow and non-isothermal multi-phase multi-component equations, and by hydrogeomechanical equations when accounting for the deformations of the porous media. These processes can be simulated with the DuMu^x models given in Table 1. During the CO₂ injection period the most important processes can be modelled with the **2pni** or **2p2cni** models. After several hundreds of years when the temperature effects become negligible, the **2p2c** model is computationally more efficient.

The mass balance equations for multi-phase flow in porous media can be formulated as:

$$\frac{\partial(\phi S_{\alpha} \rho_{\alpha})}{\partial t} - \nabla \cdot \left\{ \rho_{\alpha} \frac{k_{r,\alpha} K}{\mu_{\alpha}} (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}) \right\} - q_{\alpha} = 0 \quad (1)$$

The system of partial differential equations (1) is closed with the following equations:

$$S_w + S_n = 1, \quad (2)$$

$$p_n - p_w = p_c, \quad (3)$$

where α denotes the phase (with w , as the wetting phase and n as the non-wetting phase), S_{α} is the phase saturation, ρ_{α} is the phase density, ϕ is the porosity of the matrix q_{α} is the phase source or sink term, K is the intrinsic permeability, $k_{r\alpha}$ is the relative permeability, μ_{α} is the phase dynamic viscosity, g is the gravity term, p_{α} is the phase pressure, and p_c denotes the capillary pressure. If the solid matrix is allowed to deform the effective porosity ϕ and intrinsic permeability K are determined as functions of the solid displacement.

The CO₂ rich phase may consist of two components, i.e., CO₂, H₂O as water vapors, while the brine phase can consist of CO₂, H₂O and dissolved NaCl. A compositional model accounts for the mass balance of each component present in each phase following Eq.(4). The salinity is assumed constant and accounted through the mutual solubility functions.

$$\begin{aligned}
 & \sum_{\alpha} \frac{\partial(\phi S_{\alpha} \rho_{\alpha} x_{\alpha}^{\kappa})}{\partial t} - \\
 & -\nabla \cdot \sum_{\alpha} \left\{ \rho_{\alpha} x_{\alpha}^{\kappa} \frac{k_{r,\alpha} \mathbf{K}}{\mu_{\alpha}} (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}) \right\} - \\
 & -\nabla \cdot \sum_{\alpha} \left\{ \rho_{\alpha} D_{pm,\alpha}^{\kappa} \nabla x_{\alpha}^{\kappa} \right\} - q_{\alpha}^{\kappa} - r_{\alpha \rightarrow \beta}^{\kappa} = 0
 \end{aligned} \quad (4)$$

The injected CO₂ has a different temperature, usually lower, than the formation fluids. In this sense, the non-isothermal processes occurring during the CO₂ injection can be represented with the energy balance equation, assuming local thermal equilibrium [20], [21]:

$$\begin{aligned}
 & \phi \frac{\partial(\sum_{\alpha} \rho_{\alpha} u_{\alpha} S_{\alpha})}{\partial t} + (1 - \phi) \frac{\partial(\rho_s c_v T)}{\partial t} \\
 & -\nabla \cdot \sum_{\alpha} \left\{ \rho_{\alpha} h_{\alpha} \frac{k_{r,\alpha} \mathbf{K}}{\mu_{\alpha}} (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}) \right\} \\
 & -\nabla \cdot (\lambda_{pm} \nabla T) - q_h = 0
 \end{aligned} \quad (5)$$

The energy balance equation (5) is solved by the **2pni** and the **2p2cni**.

The momentum balance equation of the solid-fluid system can be written to describe the linear elastic deformations during CO₂ injection as [18]:

$$\nabla \cdot (\Delta \sigma' + \Delta p_{eff} \mathbf{l}) + \phi S_n (\rho_n - \rho_w) \mathbf{g} = 0 \quad (6)$$

where $\Delta \sigma'$ is the effective stress change. Equation (6) is implemented in the **el2p** model.

CO₂ migration in fractured reservoirs can be simulated with the **2pdfm** model using a lower-dimensional representations of the discrete fractures [19].

Table 1: DuMu^x models for GCS and the primary variables (modified after [18]).

Individual models		Balance equations		Primary variables
2p	Two-phase model	mass	Eq. (1)	p_w, S_n
2p2c	Two-phase two-component model	mass	Eq. (4)	p_w, S_n $/ X_w^{CO_2}$ $/ X_n^{H_2O}$
2pni	Non-isothermal two-phase model	mass, energy	Eq. (1) and (5)	p_w, S_n, T
2p2cni	Non-isothermal two-phase two-component model	mass, energy	Eq. (4) and (5)	p_w, S_n $/ X_w^{CO_2}$ $/ X_n^{H_2O}, T$
el2p	Linear elastic two-phase model	mass, momentum	Eq. (1) and (6)	$p_w, S_n,$ u_x, u_y, u_z
2pdfm	Two-phase discrete fracture model	mass	Eq. (1) and variations	p_w, S_n

In DuMu^x the mutual solubility model for the calculation of the phase composition for the CO₂-H₂O-NaCl fluid system is implemented according to the Spycher and Pruess approach [20]. Implemented

constitutive relations and fluid properties for the DuMu^x CO₂ models are summarized in Table 2.

Table 2 Fluid property and solubility functions implemented in DuMu^x (after [18]).

Secondary variable	Symbol	Function of	Function used
Brine phase density	ρ_b	$f(p, T, x_b^{sal}, x_w^{CO_2})$	[21]
CO ₂ -rich phase density	ρ_{CO_2}	$f(T, p)$	[22]
Brine phase viscosity	μ_b	$f(p, T, x_b^{sal}, x_w^{CO_2})$	[23][21]
CO ₂ -rich phase viscosity	μ_{CO_2}	$f(T, p)$	[24]
Mass fraction water in CO ₂ phase	$x_g^{H_2O}$	$f(T, p, x_b^{sal})$	[20]
Mass fraction of CO ₂ in brine	$x_b^{CO_2}$	$f(T, p, x_b^{sal})$	[20]
Relative permeability brine	$k_{rel,b}$	$f(S_b)$	[25], [26]
Relative permeability CO ₂	$k_{rel,g}$	$f(S_{CO_2})$	[25], [26]
Capillary pressure	p_c	$f(S_b)$	[25], [26]
Salinity	X_b^{sal}	$f(X_b^{NaCl})$	-
Diffusion coefficient of H ₂ O in gas	$D_{pm,g}^{H_2O}$	$f(p, T)$	[27]
Diffusion coefficient of CO ₂ in brine phase	$D_{pm,w}^{CO_2}$	$f(p, T)$	

3 Relevant studies applying DuMu^x for modelling GCS

The total number of scientific peer-reviewed journal articles using DuMu^x is more than 100 (Oct. 2018). We provide a summary of the key peer-reviewed articles using DuMu^x for simulating geological storage of CO₂. The models used in these publications can simulate the most important thermo-hydro-mechanical-chemical and biological processes occurring during the lifetime of the CO₂ storage reservoir. First DuMu^x overview paper summarizing the capabilities of the simulator has been peer reviewed and published in the journal *Advances in Water Resources* [9]. Until now, the publication was cited more than 224 times. Since 2008, DuMu^x was used and developed in 22 PhD theses.

CO₂ storage sites

A number of numerical studies using DuMu^x were conducted to assess the storage efficiency in North German Basin and are described in [28], [29]. DuMu^x was applied to model the CO₂ storage at the Ketzin pilot site located in Brandenburg, Germany, which is the longest-operating on-shore CO₂ storage site in Europe [30], [31]. Intercomparison modelling studies on the Stuttgart formation at Ketzin pilot site were conducted in [32] using DuMu^x, OpenGeosys, TOUGH2 and Eclipse 100. One

focus was to test the simulator capabilities on a complex heterogeneous reservoir. Their study concludes that DuMu^x is a reliable simulator showing excellent agreement of simulated and observed pressures.

Walter et al. [33] provides estimates of the risk of brine discharge into freshwater aquifers due to CO₂ injection into geological formations. Key parameters influencing the CO₂ migration process from the gas reservoir in the Snøvit area, Barents Sea were determined by means of numerical modelling with DuMu^x [34]. The authors identify potential migration pathways and their extent, i.e., faults, gas chimneys in an off-shore mostly sandy reservoir located in the Tubåen Formation (at 2560-2670 m below sea surface).

Geomechanics

The geomechanical effects are not only important for CO₂ injection in the geologic formations, but also for technologies such as geothermal stimulation, hydraulic fracturing, or wastewater injections. Here the understanding of the rock stresses and deformation is essential. Surpassing the strength of the rock can lead to failure and fractures in the caprock which may induce leakage. A volume-based model of fault reactivation in porous media and its implementation within DuMu^x framework is discussed in [35]. The modelling approach is compared to the well-established models of Rutqvist et al. [36].

For understanding of the mechanical damage in weak sandstone reservoirs due to high CO₂ injection pressure a 2p2c-DuMu^x – discrete element method coupled model is proposed in [37]. The capabilities of the approach are tested on the CO₂ pilot site located at Heletz, Israel [38], [39].

Fractured Porous Media

Modelling of single- and multi-phase flow in discrete fractured porous media was done in DuMu^x by considering a box-method implementation [19], [40]. [41] present the method and implementation in DuMu^x of a discrete fracture model on the basis of a cell-centred finite volume scheme with multi-point flux approximation. Furthermore, an efficient workflow for modelling discrete fracture networks in DuMu^x using the vertex-centered finite volume scheme for spatial discretization is presented in [42]. An upscaling technique of CO₂ migration in an interconnected fractured porous medium, i.e., extended multiple interacting continua (MINC) method is described in [19]. The comparison with the discrete fracture model shows very good agreement while obtaining computational speed-up factors over 100 times.

The development of a mathematical and numerical model for fracture flow in porous media using the eXtended finite element method (XFEM) is described in [43]. The XFEM is based on the hybrid-dimensional problem formulation and non-conforming meshing. A comparison of the box-DFM and XFEM methods is shown in [17]. The XFEM model in DuMu^x however, has not been tested yet on CO₂ storage problems.

Reactive transport

Reactive transport models are also available under DuMu^x. A numerical model for microbially induced calcite precipitation is developed by [44] and compared to laboratory column experiments. The microbial induced

calcite precipitation is related to the reduction of porosity and permeability and can potentially be used to cut off highly permeable pathways such as fractures and faults. This can be used to increase storage security near wellbores of CO₂ storage sites. The change of pore space (porosity, permeability) as a result of the reactive transport processes, e.g., mineral dissolution and precipitation, biomass growth is further discussed in [45].

A numerical model capable to reproduce reactive transport of a new category of tracers, termed kinetic interface sensitive (KIS) tracers in CO₂-brine systems is described in [46], [47]. KIS tracers are intended to be a monitoring technique providing information about the dynamic evolution of fluid-fluid interfacial area. This can be used to optimize the CO₂ injection such that the interfacial area is maximized. An increased CO₂-brine interfacial area leads to higher dissolution of CO₂ into the water phase and increase the efficiency of trapping. Following [48], CO₂ storage efficiency is defined as the ratio of the volume of CO₂ injected into an aquifer rock volume to the pore space in that volume.

Benchmarking DuMu^x

Benchmarks (code intercomparison) are important instruments for building confidence in the numerical simulator and better understanding the thermo-hydro-mechanical-chemical-biological processes occurring during injection and storing of the CO₂ in the subsurface. Benchmarking studies are a necessary to verify the algorithms and the software. [14], [15]

First code intercomparison studies related to GCS were done by [49] and [14]. Several workshops aimed at harmonizing and discussing the modelling results obtained with the various codes were held in Stuttgart (2008) and Svalbard (Norway, 2009). DuMu^x has participated in these workshops showing a good performance (see [14]). Most commonly the sources of errors come from gridding, wrong assignment of model input parameters by human error, different interpretations of problem descriptions. A systematic approach for developing benchmarking concepts for CO₂ injection problems is proposed in [50]. Even though DuMu^x has not directly participated in their benchmarking study, the authors address a problem (i.e., DSA#1) initially defined in [14].

Another benchmarking study on GCS, investigated the variability in model predictions obtained by different participants in response to the benchmark problem definition [15]. The conclusions of the study are very interesting, stressing the importance of modelling choices on the outcome of predictions even for simple, idealized problems. These choices the modeler has to take are similar to “real life” situations, where no problem statement is defined perfectly. Therefore, the choices are made as a function of the time availability, human and computational resources, independent interpretation of the problem. The sources of error in this case include the specific interpretation of the physical processes to be modelled, the choice of numerical scheme, upscaling procedure, if at all, and, the interpretation of problem definition and results.

A recent code intercomparison study involving DuMu^x is described in [16]. The study was initiated within

the European Framework 7 funded project TRUST. Three benchmark test problems with increasing degree of complexity are defined to investigate and compare the effects arising during the CO₂ injection, i.e., CO₂ plume shape, fluid pressure and temperature evolution, deformation, etc. Simulators participating in the benchmarking are DuMu^x, PFLOTRAN, CODE_BRIGHT, eWoms, and TOUGH2. The results are in good agreement with each other.

4 Summary and conclusions

CCS represents a viable mitigation technology which is ready to be implemented commercially at industrial scales. Numerical simulators are necessary tools to assist the dimensioning, planning and monitoring of operations during all stages of the project.

The paper gave an overview of DuMu^x simulator capabilities to address the complex phenomena accompanying the CO₂ storage in geological formations. The models can deal with the non-isothermal multiphase flow, in fractured heterogeneous porous media systems, reactive transport, dissolution and mixing, modelling of rock deformation and stresses, (bio) mineralization, etc.

Our literature review on the possible geological storage locations in Romania showed that there are initiatives both on-shore and off-shore, either as storage in deep saline aquifers or as CCUS. The reviewed geological sites fulfil the conditions required for CO₂ storage, i.e., a depth below 800m, high permeabilities and high porosities.

Due to increasing physical complexity of the modelling tools benchmarking is receiving increasing attention from the scientific community. DuMu^x participated in more than three benchmarking studies aimed modelling CO₂ storage in geological formations, where the results were compared with the ones of 23 academic and commercial simulators. Another benchmarking study was aimed at modelling single-phase flow in lower-dimensional fractured porous media. Further benchmarking studies are currently being planned and conducted, such as the call for participation "Verification benchmarks for single-phase flow in three-dimensional fractured porous media" [51]. Intercomparison studies have shown broad agreements in most areas but also highlighted sensitive points, mostly related to human/modeller choices in handling the benchmark problem.

The free open-source, numerical simulator DuMu^x, the manual, a list of current research projects, modelling examples and an up-to-date list of publications using the simulator can be obtained at the website <http://www.dumux.org>.

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