MUSTANG

A MUltiple Space and Time scale Approach for the quaNtification of deep saline formations for CO2 storaGe

Project Number:227286

Work-Package: WP7

WP Title
Numerical model development and modeling

Deliverable D7.4
Updates CODEBRIGHT-RETRASO and TOUGH2

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Executive summary

The finite element numerical code CODE_BRIGHT has been extended to simulate CO_2 injection in deep saline aquifers. CO_2 density is calculated using the Redlich and Kwong (1949) equation of state with the parameters proposed for CO_2 by Spycher *et al*. (2003). CO_2 viscosity is computed using an empirical expression, assumed to be the most precise expression for CO_2 viscosity. Several applications have been performed, including the validation of analytical solutions and a semianalytical solution for predicting the CO_2 plume position; the injection of CO_2 in sloping aquifers; and the assessment of the caprock mechanical stability solving coupled hydro-mechanical simulations.

Additionally, the thermal properties of CO_2 have been implemented using the Redlich and Kwong (1949) equation of state. Non-isothermal CO_2 injection simulations were carried out to analyze the effects on the caprock mechanical stability of injecting cold CO_2 in a deep saline aquifer. Surprisingly, injecting cold CO_2 improves the caprock mechanical stability because even though the thermal contraction of the rock induces a reduction of the effective stresses in the saline aquifer, which could induce microseismic events, the horizontal total stresses increase in the caprock tightening it.

Finally, chemical reactions have been incorporated to CODE_BRIGHT to allow solving geochemical reactions that can be calculated as a function of the state variables of CODE_BRIGHT (e.g. liquid pressure, gas pressure, temperature). Though this method presents some limitations, it permits to solve some chemical reactions, like calcite dissolution, in an easy way.

TOUGH2 family of codes have been extensively used in the MUSTANG project, including the versions for both the supercritical and gaseous CO2, the inverse version iTOUGH for extensive parameter estimation problems when designing the MUSTANG CO2 injection tests, the massively parallel version TOUGH2MP for large scale CO2 storage capacity estimates, the version including the well-module T2WELL for estimating the coupled effects of wellbore and reservoir during CO2 injection. Since the code was already at the onset of MUSTANG project suitable for CO2 injection containing the features considered necessary for extensive analysis of the CO2 injection and storage problem, no actual extensive model development has been carried out during MUSTANG, but what could be considered more minor modifications to the code, to enable the multitude of applications that have been carried out, such as updating of the characteristic functions to accommodate the experimental findings, analysis of stochastically heterogeneous systems etc. We here report a number of model applications to

(i) various site studies, and (ii) to studies addressing heterogeneous systems. In the latter studies, TOUGH has been used both as the main method and as a validation or support for new alternative approaches (Gaussian Process Emulators and Invasion Percolation models). We also report in this context (iii) the development of a new two-phase CO2-brine flow and transport code where kinetic tracer transport from one phase to another can take place. Being able to model such behaviour was necessary for analysing the tracers developed within the MUSTANG project and due to the internal architecture of the TOUGH codes, where an equilibrium assumption for species transfer from one phase to another is characteristic, writing a new code was deemed more suitable than attempting modifying TOUGH2.

Keywords	Multiphase flow, CO2 density, Analytical solution, Interface, Gravity forces, Reactive transport, Tracers, CO2 injection experiments

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1 Introduction

Modelling of multiphase and coupled flow and reactive transport processes related to CO_2 storage is a challenging task. The problem of geological storage of CO_2 involves a complex combination of coupled thermo-hydro-mechanical processes in a system with multiple scales. The major issues to be resolved in terms of modeling CO_2 storage have been identified to be (e.g. Pruess, 2006, Tsang et al. 2005) (i) the great range of *space and time scales* to be encountered in CO_2 storage and (ii) the importance of the various couplings between flow, chemical and geomechanical processes. The third major issue is related to development of reliable probabilistic methods (ICPP 2007) for predicting the leakage rates from storage sites. Such approaches are greatly needed due to the heterogeneity effects.

This report summarized the developments, updates and many applications with the two main CO2 reservoir simulators used in the MUSTANG project, namely the CODEBRIGHT-RETRASO code that was updated during the course of the project to handle several of CO2 related coupled processes and TOUGH2 family of codes that were already mature codes for CO2 storage at the onset of the project but have here been here applied to a number of studies, uncludind site analyses, probabilistic problems etc.

2 Updates to CODEBRIGHT-RETRASO

The finite element numerical code CODE_BRIGHT (Olivella et al., 1994; 1996) has been extended by CSIC to simulate CO_2 injection in deep saline aquifers. CO_2 density is calculated using the Redlich and Kwong (1949) equation of state with the parameters proposed for CO_2 by Spycher *et al*. (2003). CO_2 viscosity is computed using the empirical expression proposed by Altunin and Sakhabetdinov (1972), which according to Sovova and Prochazka (1993) is the most precise expression for CO_2 viscosity. Several applications have been performed, including the validation of analytical solutions (Vilarrasa et al., 2010a) and a semianalytical solution (Vilarrasa et al., 2013a) for predicting the CO_2 plume position; the injection of CO_2 in sloping aquifers (Vilarrasa et al., 2011a); and the assessment of the caprock mechanical stability solving coupled hydro-mechanical simulations (Vilarrasa et al., 2010b, 2011b, 2013c).

Additionally, the thermal properties of CO_2 have been implemented using the Redlich and Kwong (1949) equation of state. Non-isothermal CO_2 injection simulations were carried out to analyze the effects on the caprock mechanical stability of injecting cold CO_2 in a deep saline aquifer (Vilarrasa et al., 2013b). Surprisingly, injecting cold CO_2 improves the caprock mechanical stability because even though the thermal contraction of the rock induces a reduction of the effective stresses in the saline aquifer, which could induce microseismic events, the horizontal total stresses increase in the caprock tightening it.

Finally, chemical reactions have been incorporated to CODE_BRIGHT by following the method proposed by Saaltink et al. (2012) that allows solving geochemical reactions that can be calculated as a function of the state variables of CODE_BRIGHT (e.g. liquid pressure, gas pressure, temperature). Though this method presents some limitations, it permits to solve some chemical reactions, like calcite dissolution, in an easy way.

2.1 Effects of CO_2 Compressibility on CO_2 Storage in Deep Saline Aquifers

The injection of supercritical CO_2 in deep saline aquifers leads to the formation of a CO_2 plume that tends to float above the formation brine. As pressure builds up, CO_2 properties, i.e. density and viscosity, can vary significantly. Current analytical solutions do not account for CO_2 compressibility. In this article, we investigated numerically and analytically the effect of this variability on the position of the interface between the CO_2-rich phase and the formation brine. We introduced a correction to account for CO_2 compressibility (density variations) and viscosity variations in current analytical solutions. We found that the error in the interface position caused by neglecting CO_2 compressibility is relatively small when viscous forces dominate. However, it can become significant when gravity forces dominate, which is likely to occur at late times of injection. (Vilarrasa et al., 2010a)

2.2 Coupled hydromechanical modeling of CO_2 sequestration in deep saline aquifers

Sequestration of carbon dioxide (CO_2) in deep saline aquifers has emerged as an option for reducing greenhouse gas emissions to the atmosphere. The large amounts of supercritical CO_2 that need to be injected into deep saline aquifers may cause large fluid pressure increases. The resulting overpressure may promote reactivation of sealed fractures or the creation of new ones in the caprock seal. This could lead to escape routes for CO_2.

In order to assess the probability of such an event, Vilarrasa et al. (2010b) have modelled an axisymmetric horizontal aquifer–caprock system, including hydromechanical coupling. We studied the failure mechanisms, using a viscoplastic approach.

Simulations illustrate that, depending on boundary conditions, the least favorable moment takes place at the beginning of injection. Initially, fluid pressure rises sharply because of a reduction in permeability due to desaturation. Once CO_2 fills the pores in the vicinity of the injection well and a capillary fringe is fully developed, the less viscous CO_2 displaces the brine and the capillary fringe laterally. The overpressure caused by the permeability reduction within the capillary fringe due to desaturation decreases with distance from the injection well. This results in a drop in fluid pressure buildup with time, which leads to a safer situation. Nevertheless, in the presence of low-permeability boundaries, fluid pressure continues to rise in the whole aquifer. This occurs when the radius of influence of the injection reaches the outer boundary. Thus, caprock integrity might be compromised in the long term. (Vilarrasa, 2010b)

2.3 CO_2 injection in deep saline sloping aquifers through a vertical well

Vilarrasa et al. (2011a) describe how CODE_BRIGHT was adapted to simulate CO2 injection. To do so, an equation of state for CO_2 has been implemented. CO_2 density follows a Redlich-Kwong equation of state type with the parameters proposed by Spycher et al. (2003). CO_2 viscosity has been taken from Altunin & Sakhabetdinov (1972). These expressions for CO2 density and viscosity are valid regardless of the temperature and pressure conditions.

To model CO_2 injection of 100 t of CO2 during 1 week in a sloping homogeneous aquifer, we used a 3D model. We modeled half of the domain, 200x70x10 m^3, by making use of the symmetry in the direction of maximum slope. The upslope and downslope boundaries were treated as constant head boundaries. The aquifer permeability was 10^{-13} m^2 and its porosity 0.1. The slope of the aquifer ranged from 0º to 20º. Results showed that the implemented density and viscosity functions are general and cover the whole range of depths and geothermal gradients of potential aquifers.

2.4 Geomechanical stability of the caprock during CO_2 sequestration in deep saline aquifers

Sequestration of carbon dioxide (CO_2) in deep saline aquifers has emerged as a mitigation strategy for reducing greenhouse gas emissions to the atmosphere. The large amounts of supercritical CO_2 that need to be injected into deep saline aquifers may cause large fluid pressure buildup. The resulting overpressure will produce changes in the effective stress field. This will deform the rock and may promote reactivation of sealed fractures or the creation of new ones in the caprock seal, which could lead to escape paths for CO_2.

To understand these coupled hydromechanical phenomena, Vilarrasa et al. (2011b) modelled an axisymmetric horizontal aquifer-caprock system. We studied plastic strain propagation patterns using a viscoplastic approach. Simulations illustrate that plastic strain may propagate through the whole thickness of the caprock if horizontal stress is lower than vertical stress. In contrast, plastic strain concentrates in the contact between the aquifer and the caprock if horizontal stress is larger than vertical stress. Aquifers that present a low-permeability boundary experience an additional fluid pressure increase once the pressure buildup cone reaches the outer boundary. However, fluid pressure does not evolve uniformly in the aquifer. While it increases in the low-permeability boundary, it drops in the vicinity of the injection well because of the lower viscosity of CO_2. Thus, caprock stability does not get worse in semi-closed aquifers compared to open aquifers. Overall, the caprock acts as a plate that bends because of pressure buildup, producing a horizontal extension of the upper part of the caprock. This implies a vertical compression of this zone, which may produce settlements instead of uplift in low-permeability ($k \leq 10^{-18}$ m^2) caprocks at early times of injection. (Vilarrasa et al., 2011b)

2.5 Hydromechanical characterization of CO_2 injection sites

Clear understanding of coupled hydromechanical effects, such as ground deformation, induced microseismicity and fault reactivation, will be crucial to convince the public that geologic carbon storage is secure. These effects depend on hydromechanical properties, which are usually determined at metric scale. However, their value at the field scale may differ in orders of magnitude.

To address this shortcoming, Vilarrasa et al. (2013c) we propose a hydromechanical characterization test to estimate the hydromechanical properties of the aquifer and caprock at the field scale. We propose injecting water at high pressure and, possibly, low temperature while monitoring fluid pressure and rock deformation. Here, we analyzed the problem and performed numerical simulations and a dimensional analysis of the hydromechanical equations to obtain curves for overpressure and vertical displacement as a function of the volumetric strain term. We found that these curves do not depend much on the Poisson ratio, except for the dimensionless vertical displacement at the top of the caprock, which does. We then estimated the values of the

Young's modulus and the Poisson ratio of the aquifer and the caprock by introducing field measurements in these plots.

Hydraulic parameters can be determined from the interpretation of fluid pressure evolution in the aquifer. Reverse-water level fluctuations are observed, i.e. fluid pressure drops in the caprock as a result of the induced deformation that undergoes the aquifer-caprock system when injecting in the aquifer. We find that induced microseismicity is more likely to occur in the aquifer than in the caprock and depends little on their stiffness. Monitoring microseismicity is a useful tool to track the opening of fractures. The propagation pattern depends on the stress regime, i.e. normal, strike slip or reverse faulting. The onset of microseismicity in the caprock can be used to define the maximum sustainable injection pressure to ensure a permanent CO_2 storage. (Vilarrasa et al., 2013c)

2.6 Semi-analytical solution for CO_2 plume shape and pressure evolution during CO_2 injection in deep saline formations

The injection of supercritical carbon dioxide (CO_2) in deep saline aquifers leads to the formation of a CO_2 rich phase plume that tends to float over the resident brine. As pressure builds up, CO_2 density will increase because of its high compressibility. Current analytical solutions do not account for CO_2 compressibility and consider a volumetric injection rate that is uniformly distributed along the whole thickness of the aquifer, which is unrealistic. Furthermore, the slope of the CO_2 pressure with respect to the logarithm of distance obtained from these solutions differs from that of numerical solutions. We develop a semianalytical solution for the CO_2 plume geometry and fluid pressure evolution, accounting for CO_2 compressibility and buoyancy effects in the injection well, so CO_2 is not uniformly injected along the aquifer thickness. We formulate the problem in terms of a CO_2 potential that facilitates solution in horizontal layers, with which we discretize the aquifer. Capillary pressure is considered at the interface between the CO_2 rich phase and the aqueous phase.

When a prescribed CO_2 mass flow rate is injected, CO_2 advances initially through the top portion of the aquifer. As CO_2 is being injected, the CO_2 plume advances not only laterally, but also vertically downwards. However, the CO_2 plume does not necessarily occupy the whole thickness of the aquifer. We found that even in the cases in which the CO_2 plume reaches the bottom of the aquifer, most of the injected CO_2 enters the aquifer through the layers at the top. Both CO_2 plume position and fluid pressure compare well with numerical simulations. This solution permits quick evaluations of the CO_2 plume position and fluid pressure distribution when injecting supercritical CO_2 in a deep saline aquifer. (Vilarrasa et al., 2013a)

2.7 Liquid CO_2 injection for geological storage in deep saline aquifers

CO2 will remain in supercritical (SC) state (i.e. p > 7.382 MPa and T > 31.04 °C) under the pressure (p) and temperature (T) conditions appropriate for geological storage. Thus, it is usually assumed that CO2 will reach the aquifer in SC conditions. However, inflowing CO_2 does not need to be in thermal equilibrium with the aquifer. In fact, surface operations are simpler for liquid than for SC CO2, because CO2 is transported in liquid state. Yet, problems might arise because of

thermal stresses induced by cold CO_2 injection and because of phase changes in the injection tubing or in the formation.

Here, we propose liquid CO_2 injection and analyze its evolution and the thermo-hydro-mechanical response of the formation and the caprock. We find that injecting CO_2 in liquid state is energetically more efficient than in SC state because liquid CO_2 is denser than SC CO_2, leading to a lower overpressure not only at the wellhead, but also in the reservoir because a smaller fluid volume is displaced. Cold CO_2 injection cools down the formation around the injection well. Further away, CO_2 equilibrates thermally with the medium in an abrupt front.
The liquid CO_2 region close to the injection well advances far behind the SC CO_2 interface. While the SC CO_2 region is dominated by gravity override, the liquid CO_2 region displays a steeper front because viscous forces dominate (liquid CO_2 is not only denser, but also more viscous than SC CO_2).

The temperature decrease close to the injection well induces a stress reduction due to thermal contraction of the media. This can lead to shear slip of pre-existing fractures in the aquifer for large temperature contrasts in stiff rocks, which could enhance injectivity. In contrast, the mechanical stability of the caprock is improved in stress regimes where the maximum principal stress is the vertical. (Vilarrasa et al., 2013b)

2.8 A Method for Incorporating Equilibrium Chemical Reactions into Multiphase Flow Models for CO_2 Storage

CO_2 injection in deep saline aquifers involves many coupled processes, including multiphase flow, heat and mass transport, rock deformation and mineral precipitation and dissolution. Their modeling requires complex computer codes. We present a simple methodology to incorporate chemical reactions into multiphase flow codes for chemical systems that can be calculated as a function of the state variables of the multiphase flow model (i.e., liquid pressure, gas pressure, temperature). Basically, we redefine the conservative components of the multiphase flow code (traditionally, water and CO_2), so that they can yield the full chemical composition of the system. We applied this method to incorporate the chemical reactions of the $H_2O–CO_2–Na–Cl–CaCO_3$ system into CodeBright, a code to handle multiphase flow, heat transfer, mass transport and deformation. We used this code to model CO_2 injection into a carbonate aquifer containing salt water, which was feared to produce large dissolution features. The model could simulate well the interaction between the development of the CO_2 plume, dissolution of CO_2 into the brine, calcite dissolution and density dependent flow. We find that porosity development near the injection well is small because of the low solubility of calcite. Moreover, dissolution concentrates at the front of the advancing CO_2 plume because the resident brine tends to equilibrate with calcite quite rapidly. (Saaltink et al., 2013)

3 Updates to TOUGH2

TOUGH2 family of codes have been extensively used in the MUSTANG project, including the versions for both the supercriticial and gaseous CO2, the inverse version iTOUGH for extensive parameter estimation problems when designing the MUSTANG CO2 injection tests, the massively parallel version TOUGH2MP for large scale CO2 storage capacity estimates, the version including the well-module T2WELL for estimating the coupled effects of wellbore and reservoir during CO2 injection. Since the code was already at the onset of MUSTANG project suitable for CO2 injection containing the features considered necessary for extensive analysis of the CO2 injection and storage problem, no actual extensive model development has been carried out during MUSTANG, but what could be considered more minor modifications to the code, to enable the multitude of applications that have been carried out, such as updating of the characteristic functions to accommodate the experimental findings, analysis of stochastically heterogeneous systems etc. We here report a number of model applications to (i) various site studies, and (ii) to studies addressing heterogeneous systems. In the latter studies, TOUGH has been used both as the main method and as a validation or support for new alternative approaches (Gaussian Process Emulators and Invasion Percolation models). We also report in this context (iii) the development of a new two-phase CO2-brine flow and transport code where kinetic tracer transport from one phase to another can take place. Being able to model such behaviour was necessary for analysing the tracers developed within the MUSTANG project and due to the internal architecture of the TOUGH codes, where an equilibrium assumption for species transfer from one phase to another is characteristic, writing a new code was deemed more suitable than attempting modifying TOUGH2.

3.1 Site-specific models

3.1.1 Modeling of the push-pull test for characterizing residual carbon dioxide saturation, Heletz site

Different alternative sequences and ways to carry out the single-well push-pull (injection-withdrawal) test designs for the Heletz (Niemi et al, 2012) have been extensively modelled with the TOUGH2 (Pruess et al, 1999) simulators. The test scenarios simulated combine thermal, hydraulic and tracer tests in line with the work by Zhang et al (2011), where the test sequences have three main stages divided into (i) reference tests, (ii) creation of a zone of residual gas saturation and (iii) testing during residual gas saturation conditions. One of the main interests have been to compare different ways of creating the residual zone, the two principal approaches being to push the mobile CO2 away by injecting CO2 saturated water, thus leaving the residual zone behind or by pumping the mobile CO2 back. Inverse modeling with the iTOUGH2 simulator and the EOS7c module have been used to analyze the ability of the competing test designs to accurately determine parameters of main interest during CO2 sequestration, in particular the

residual gas saturation. The modelling has been presented in a number of project reports, seminar presentations and summarized e.g. in Rasmusson et al., (2014a).

3.1.2 Interwell test to quantify residual and dissolution trapping, Heletz site

A two-well test sequence aimed at quantifying field values of both residual and dissolution trapping of CO2 has also been developed and applied to the Heletz site using numerical modelling (Fagerlund et al., 2013a, b). Minor modifications to the existing codes TOUGH2/ECO2N (Pruess at al, 1999, 2007) and iTOUGH2/EOS7C (Finsterle et al, 2007, Oldenburg et al, 2004) were implemented to model the simultaneous CO2 dissolution and tracer transport. The proposed and modelled tracer technique uses a tracer with negligible aqueous solubility, which is injected with the scCO2 and enriched in the scCO2 phase as CO2 dissolves. As illustrated in Fagerlund et al, 2013, we show that this tracer can provide direct information about the dissolution of mobile scCO2. We also show that the rate of abstracted dissolved CO2 can be used to predict the total rate of CO2 dissolution, provided that the amount of dissolved CO2 in the formation stabilizes, and that this can be achieved with the proposed abstraction scheme. We conclude that the combination of these measurements is a promising tool for detailed field-scale characterization of residual and dissolution trapping processes. (Fagerlund et al 2013a,b)

3.1.3 Distribution of injected CO_2 in a stratified saline reservoir accounting for coupled wellbore-reservoir flow

Alternating high and low permeability strata are common in prospective CO2 storage basins. The distribution of injected CO2 among such layers affects e.g. CO2 storage efficiency, capacity and plume footprint. A numerical study on the distribution of injected CO2 into a multi-layered reservoir, accounting for coupled wellbore-reservoir flow, was carried out using T2Well/ECO2N simulator (Pan et al, 2011). A site-specific case, reflecting the properties of Heletz site, as well as a more general case were considered.

Properties and processes governing the distribution of sequestrated CO2 were identified and the potential to operationally modify the distribution was investigated. The distribution of CO2 was seen to differ from that of injected water, i.e. it was not proportional to the transmissivity of the layers. The results indicate that caution should be taken when performing numerical simulations of CO2 injection into layered formations. Ignoring coupled wellbore-reservoir flow and instead adopting a simple boundary condition at the injection well, such as an inflow rate proportional to the transmissivity of each layer, may result in significant underestimation of the proportion of CO2 ending up in the shallower layers, as not all relevant processes are accounted for. This discrepancy has been thoroughly investigated and quantified for several CO2 sequestration scenarios. (Rasmusson et al, 2014b)

3.1.4 Modeling of shallow injection experiments, Maguelone site

Maguelone experiment (SIMEx) is a part of Mustang project consists of a series of Nitrogen and CO_2 injection experiments in shallow aquifer and Application of different monitoring techniques

(Lofi et al, 2012). We used TOUGH2 code (Pruess et al., 1999) with module EOS7CA (Oldenburg et al., 2003) to simulate the injection-monitoring experiment carried out during 2012 and 2013. Our main objectives are to improve our understanding of gas transport in the shallow subsurface as well as to develop and validate the model to monitor it (Basirat et al, 2013).

The Module EOS7CA is including the equation of states to treat a two phase flow (gas and liquid), five components (water, brine, CO_2 or N_2, a gas tracer, and air) system in near ambient pressure/ temperature conditions. According to the site information, a series of axisymmetric 2D and 3D numerical simulations, with three different geological layers, were done. The host layer in the bottom and top layer have high hydraulic conductivity and the middle layer is impermeable to fluid flow. Leaky path near injection well connects to permeable layers and injected gas can also flow into the top layer. The modelling has been successful and has so far been presented in [4] with work going on to further analyse the most recent experiments. Numerical simulations with TOUGH2 show a good agreement with the pressure data from WestBay systems. The CO_2 gas plumes from modelling qualitatively supports the monitoring techniques. Work is presently going on to incorporate the experimental data into the numerical simulation further.

3.1.5 Large-scale modeling for evaluating CO2 storage capacity, South Scania site

For the MUSTANG project, five sites with different geological and geographical settings were selected for detailed site analysis. These sites are South Scania, Heletz, Horstberg, Hontomin and Valcele. Comprehensive data analysis and construction of conceptual/geological models were carried out and various model simulations were carried out, mainly to consider their suitability for large scale CO2 storage. For modelling the South Scania site, both standard TOUGH and massively parallel version of TOUGH (TOUGH-MP) were used, along with more simplified analytical and semi-analytical models, to allow model comparison.

South Scania site, Sweden, is a saline aquifer with a sequence of alternating reservoir and sealing layers. A potential CO2 injection from an existing well was modeled and capacity estimates for this scenario presented. A three-step modeling approach was used where first a semi-analytical approach is used to determine a viable injection rate based on pressure response, followed first by simulations with a multi-layer vertical equilibrium model to explore the spatial and temporal scale of the injected CO_2 and a finally, by full simulation with the massive parallel version of the TOUGH2 code, TOUGH2MP/ECO2N to calculate the CO_2 inventory in greater detail (Tian et al, 2014 and Mustang Deliverable D07.3).

TOUGH2MP (Zhang et al., 2008) is designed for the more computational demanding 3D simulations. By coupling with the equation of state module ECO2N, TOUGH2MP/ECO2N is capable in resolving large scale CO2 storage simulations. A full scale 3D model was constructed in Groundwater Modeling System (GMS, Aquaveo LLC) with 19 model layers representing 5 hydro geological units. The site model of South Scania consists of a total number of 71174 grid elements. The TOUGH2MP simulation was performed on cluster Glenn from SNIC (Swedish National Infrastructure for Computing). The total CPU time was about 90 hours using 16 CPUs for 1000 years simulation.

In another, more simplified study only the pressure response to CO2 injection in the same domain was analyzed by means of different analytical, semi-analytical and numerical TOUGH2 models. (Yang et al, 2014)

3.2 Studies for Stochastic Heterogeneity

3.2.1 Model for Heterogeneous Systems and Uncertainty Analysis using TOUGH2 simulations and Gaussian Process Emulator

Simulations of CO2 sequestration in geological formations are subject to uncertainties from a number of sources. For simulation to make a useful contribution to the understanding of CO2 migration and its associated storage, these uncertainties must be identified, characterized and their consequences quantified. In MUSTANG the uncertainties quantification on modelling the evolution of the CO2 plume due to the lack of detailed knowledge of the spatial variation of the permeability field has been addressed both by means of TOUGH2 modeling and by means of a novel Gaussian Process Emulator (GPE) approach.

The system under consideration is a reservoir layer idealized as a two-dimensional slice with an injection well at one vertical edge. The dimensions are selected to correspond to a relatively thin reservoir layer of confined by low-permeability layers from above and below. The other boundary conditions are constant pressure at injection borehole and open boundary away from injection well, up to which point the spreading of CO2 is studied and break-out time as well as sweep efficiency analyzed for a large number of heterogeneous realizations. The first set of modeling was performed by using standard version of TOUGH2 (Pruess *et al.*, 1999) and the equation of state module ECO2N (Pruess and Spycher, 2007). The focus of the first study is to look at the role of geological heterogeneity on sweep efficiency and CO2 break-through (Tian et al, 2014).

In the second study the focus is on replacing traditional TOUGH2 based Monte Carlo simulations with a Gaussian process emulators (GPE) approach, to considerably mitigate the computational cost of the Monte Carlo scheme. The analysis a truncated Karhunen-Loève (KL) expansion of the logarithm of the permeability field is used so that the input to the calculation can be characterized by a finite number of parameters, which are the coefficients in the KL expansion. In this way, a Monte-Carlo simulation is effectively achieved by running the emulator many times with the input parameters (the KL coefficients) drawn from the appropriate multivariate normal distribution. In a traditional Monte-Carlo method the full simulation has to be run for a large number of realizations, whereas in the GPE approach a relatively small number of realizations of the full problem are run first with the TOUGH2 simulator to train the emulator. The basic idea is that the GPE produces a good approximation to the output of the full simulation from where the statistical properties of the output can be computed from the emulator runs. We also used the TOUGH2 simulation results to evaluate the emulator performance. (Wilkinson et al, 2014)

3.2.2 Numerical upscaling for complex heterogeneity

Due to computational resource constraints, reservoir scale models have limitations in accounting for the details of the multi-scale heterogeneities. Appropriately averaged medium parameters are needed for the full scale modeling. In this study, we apply the macroscopic theory and present large-scale capillary pressure-relative permeability-saturation relationships that may be used as grid-block properties in the full-scale modeling.

A macroscopic Invasion Percolation (MIP) model is developed, based on the assumption of capillary force dominance. Comparison of the MIP model with the numerical simulator TOUGH2/ECO2N for simulations of large-scale drainage capillary pressure curves shows a reasonably good match between results from the two models. We consider a two-dimensional heterogeneous section which is composed of a rectangular array of cells. The array is assigned a local permeability value to each cell, assuming that the permeability follows a multimodal distribution. Based on the well log data from deep borehole FFC-1 at the South Scania Site (Sweden), we generate realizations of the heterogeneous medium using geostatistical methods.

Large-scale constitutive relationships are obtained through simulation procedures of CO_2 displacing brine in multimodal heterogeneous media for ten cases with different geostatistical parameters. The large-scale constitutive relationships are mainly controlled by the proportion and the permeability variability of the background (framework) material, while the existence of the non-framework materials and their permeability variabilities may contribute, in a complex way, to the uncertainty in the large-scale constitutive relationships. In addition, the Leverett equation may well describe the relationship between the large-scale capillary pressure and absolute permeability when the sandstone (background material) proportion is high (>0.7). For cases with smaller sandstone proportions it may not be appropriate to link capillary pressure and absolute permeability through the Leverett equation. (Yang et al, 2013a).

3.3 A numerical model of tracer transport in a non-isothermal two-phase flow system for CO_2 geological storage characterization

For the purpose of characterizing geologically stored CO2 including its phase partitioning and migration in deep saline formations, different types of tracers are being developed. Such tracers can be injected with CO2 or water, and their partitioning and/or reactive transfer from one phase to another can give information on the interactions between the two fluid phases and the development of their interfacial area.

New models or further developments of existing models are needed to provide the capability for interpreting the signals of novel tracers, including tracers with kinetic/time-dependent interface transfer. Such new numerical model of tracer transport in a non-isothermal two-phase flow system was developed in MUSTANG (Tong et al., 2013). The model consists of five different governing equations describing liquid phase (aqueous) flow, gas (CO2) flow, heat transport and the movement of the tracers within the two phases, as well as allowing kinetic transport of the tracers between the two phases. A finite element method is adopted for the spatial discretization and a finite difference approach is used for temporal discretization. Some special technologies and solution strategies are adopted for increasing the convergence, ensuring the numerical stability and eliminating non-physical oscillations. The new numerical model is validated against the code TOUGH2/ECO2N as well as some analytical/semi-analytical solutions. Good agreement between the simulated and analytical results indicates that the model has capability to simulate two-phase flow and tracer transport in a non-isothermal two-phase flow system with high confidence. Finally, the capability to model transport and kinetic mass transfer of tracers between the two fluid phases is demonstrated through examples. (Tong et al, 2013)

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