CATO-2 Deliverable WP3.03-D07

Preliminary data on gas/CO_2 transport through intact caprocks, plus parameter computation and interpretation based on numerical simulations (1st Year Progress Report, 2010)

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1 Executive Summary (restricted)

Subsurface storage of CO2 is beneficial only if long-term containment in storage sites can be ensured. Therefore, scenarios for the development of potential leakage pathways for CO2 through the caprock need to be analysed.

This report (deliverable WP3.3-D07) describes the preliminary data and simulations for CO2 transport through caprocks. In this task, experimental data on reactions between CO2-rich fluids and caprock is combined with numerical modelling of mineral reactions, reactive flow and coupled chemical-mechanical deformation of the caprock.

In the first year of the CATO-2 program, the following activities have been performed relevant to CO2 transport through caprocks have been performed: (1) Experimental facilities for reactions between caprock and CO2-rich fluids have been set up (c.f. WP3.3-D04, D08, D09), (2) data for the P18 reservoir caprock was collected and a model (TOUGHREACT) for reactive flow through the caprock was set up, (3) a discrete element model (PFC2D) of an anhydrite caprock sample was developed and initial simulations of the effect of chemical reactions with CO2 on the caprock mechanical properties were performed.

Initial data and models show that fluid penetration in the caprock and reaction rates between caprock and CO2-rich fluids are generally very slow. However, some long-term weakening of caprock by reactions with CO2 occurs. More data and simulations are needed to evaluate the effect of such weakening on top seal integrity and determine the feasibility of CO2 leakage through the caprock.

Distribution List

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Document Change Record

(this section shows the historical versions, with a short description of the updates)

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2010-08-30	9	Initial report by TNO	1-9

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2 Applicable/Reference documents and Abbreviations

2.1 Applicable Documents

(Applicable Documents, including their version, are documents that are the "legal" basis to the work performed)

	Title	Doc nr	Version date
AD-01	Beschikking (Subsidieverlening CATO-2 programma verplichtingnummer 1-6843	ET/ED/90780 40	2009.07.09
AD-02	Consortium Agreement	CATO-2-CA	2009.09.07
AD-03	Program Plan	CATO2-WPD-3.03-D.03	2009.09.29

2.2 Reference Documents

(Reference Documents are referred to in the document)

	Title	Doc nr	Version/issue	Date

2.3 Abbreviations

(this refers to abbreviations used in this document)

3 General Text

3.1 Introduction

Long-term containment of CO2 in subsurface storage sites requires that leakage of CO2 through (intact) caprock is insignificant. Several processes can give rise to enhanced transport of CO2 through caprocks: (1) Changes of properties of reservoir fluid (e.g., viscosity) due to introduction of CO2 in reservoir, (2) changes in transport properties of caprock (e.g., capillary entry pressure, permeability) due to reactive flow of CO2-rich fluids, (3) changes in mechanical properties of caprock due to reactive flow of CO2-rich fluids potentially leading to caprock fracturing. This work package focuses on the last two processes, i.e. chemo-hydro-mechanical modelling of the transport properties of caprock.

This report represents the first year progress report on "*Preliminary data on gas/CO2 transport through intact caprocks, plus parameter computation and interpretation based on numerical simulations"* (deliverable D07), which is a part of the WP3.3 *"Caprock and Fault Integrity"* of the CATO-2 project. The reporting period is from project start 2009.04.15 until 2010.08.31 and addresses task T3.3.1 related to "*Geomechanical evolution of the reservoir-seal system and induced deformation*". The objective is to investigate transport of CO2 through caprock using a combination of reaction experiments and numerical modelling. Reactive flow through the caprock is modelled using TOUGHREACT software. Coupled chemical-mechanical modelling is performed using PFC2D with reaction rates from experiments or direct coupling with TOUGHREACT. The experiments are described elsewhere (WP3.3-D04, D08, D09).

In the first year, activities were focussed on (1) setting up experimental facilities for reactions between caprock and CO2-rich fluids (c.f. WP3.3-D04), (2) collecting data and setting up a TOUGHREACT model for the P18 reservoir caprock (section 3.2), (3) developing a discrete element model (PFC2D) of an anhydrite caprock sample and performing initial simulations of the effect of chemical reactions with CO2 on the caprock mechanical properties (section 3.3).

The deliverables achieved in the 1st year of the project are in agreement with the project plan, although activities were focussed on collecting data for a site-specific model of the P18 reservoir caprock and investigating the effect of chemical reactions on the mechanical properties of anhydrite caprock samples rather than on collecting preliminary experimental data.

3.2 Setup of TOUGHREACT model of P18 reservoir caprock

Introduction

The P18 reservoir is part of the Main Buntersandstein Subgroup, overlain by a clay layers seal from Triassic age (the Upper Germanic Trias Group) and possibly, above that, shales from the Posidonia formation. No core samples were analyzed for the P18 field. As outlined by Spain and Conrad (1997) the knowledge of the true top seals in the P18 area and associated P- and Q-blocks in the Dutch offshore is limited. The same study describes an assessment of the sealing characteristics of these caprocks in the P-blocks, based on a core from the P15 well. The caprock analyses of P15 is therefore taken as representative for the P18 reservoir.

Analyses

The results of the X-Ray Diffraction measurements of 37 seal core samples, over the range of 3117 to 3152.5 m, are described by Spain (1991). Averages of these measurements were taken and the final result shows a significant amount of quartz (60.7%), as well as illite, feldspars, dolomite, and anhydrite. Table 1 shows the computed mineralogical composition.

Table 1: Mineralogical composition of the P18 caprock, based on analyzed core samples of the P15 seal.

Mineral	Amount (wt%)
Quartz	60.73
Anorthite	2.89
K-Feldspar	3.65
Calcite	0.00
Dolomite	11.84
Pyrite	0.54
Anhydrite	6.97
Siderite	2.38
Albite	0.00
Kaolinite	0.00
Clinochlore-14a	0.73
Illite	10.14
Smectite-Na	0.14

The porosity values range from 0.7% to 5.4% and the permeability values range from 0.00155 mD to 0.240 mD. Based on all the data given in the report of Spain (1991), the average porosity is estimated to be 2.5 and the average permeability to 0.01 mD. The caprock is assumed to be fully water saturated.

Future work

The mineralogical composition and the caprock properties given above will be compared with freshly analyzed samples from analogues in German outcrops, as characterized by Utrecht University. The final resuls will be used for future reactive transport modeling studies with *TOUGHREACT*, together with the parameters of the reservoir below the caprock (see WP3.2).

3.3 Long term chemical effects on the integrity of fault- and top seals at CO_2 storage sites

The long term integrity of fault and top seals at CO_2 storage sites can be affected by chemical reactions of CO_2-rich fluids with fault- or caprock as altered rock mechanical properties in combination with changed stress conditions may result in fault reactivation and fracture initiation or propagation. The mechanical properties of fault- or caprock can be significantly altered if reaction products with different volume and geomechanical properties are produced. Considering the low permeability of seals, a positive feedback between reactive flow of CO_2-rich fluids and fracture propagation is critical for this to occur. Such coupled chemical-hydromechanical processes are difficult to investigate using field examples or laboratory experiments as reaction kinetics are generally slow.

This investigation aims to explore modelling techniques for coupled chemical-mechanical modelling suitable for assessing the feasibility of leakage by fault reactivation or fracturing of fault- and caprock as a result of long-term reactive transport of CO_2-rich fluids. As a first step, we have investigated the long term mechanical effects of chemical reactions between CO_2 and anhydrite caprock.

We used a discrete element model (PFC2D, [1]) for simulation of reactions and deformation of a typical anhydrite caprock sample in contact with CO_2-rich fluids (Figure 1). Discrete element models are particular suitable for simulating grain-scale processes, such as chemical reactions and fracture propagation (e.g., [2]). We chose to closely simulate a sample of representative anhydrite caprock from the Permian Zechstein formation in the Netherlands as used in an experimental study by Hangx et al. [3] to be able to use experimentally-derived reaction rates and compare experimental and model results. The model consists of mm-sized clusters of circular elements representing acicular rosettes (60 vol%) embedded in a matrix of 50-83 μm-sized clusters of 3 overlapping circular elements representing euhedral to subhedral anhydrite (40 vol%) (c.f. [3]). The model is kept relatively small (2.5x2.5 mm) to be able to simulate reactions between anhydrite and CO_2 at the grain scale and maintain reasonable computation times. The initial sample strength is calibrated using experiments on wet anhydrite from [3] by changing inter- and intracluster bond strengths. We simulated the following reaction of anhydrite with CO_2 and water at high CO_2 pressure occurring at a rate of ~10^{-8} mol/m^{2}s, resulting in a 20% volume decrease in the solid phases [3];

$$CaSO_4 + CO_2 + H_2O \rightarrow CaCO_3 + H_2SO_4 \qquad (1)$$

Changes in mechanical behaviour of the sample due to the volume decrease associated with this reaction were simulated at stress and temperature conditions representative for a caprock buried at ~ 2.5 km depth (σ_v = 50 MPa, σ_h = 40 MPa, T = 80 ºC) for 50000 years. Simulations were performed for time intervals of 100 years, with for each time interval (1) a volume change of matrix grains and edges of rosettes according to the reaction rate of equation 1, (2) re-equilibration of applied stresses and associated volume decrease, failure of intergranular bonds and grain rearrangement at the end of each time interval, (3) determination of sample strength at different horizontal stresses using (virtual) biaxial tests on the sample. It is assumed that the entire sample is in contact with CO_2-rich fluids. In reality fluid penetration in the caprock is likely to be very slow due to the low permeability of the caprock, although this process may be aided by fracture propagation. The model is therefore representative of caprock at the reservoir-caprock boundary or near open fractures rather than for intact caprock.

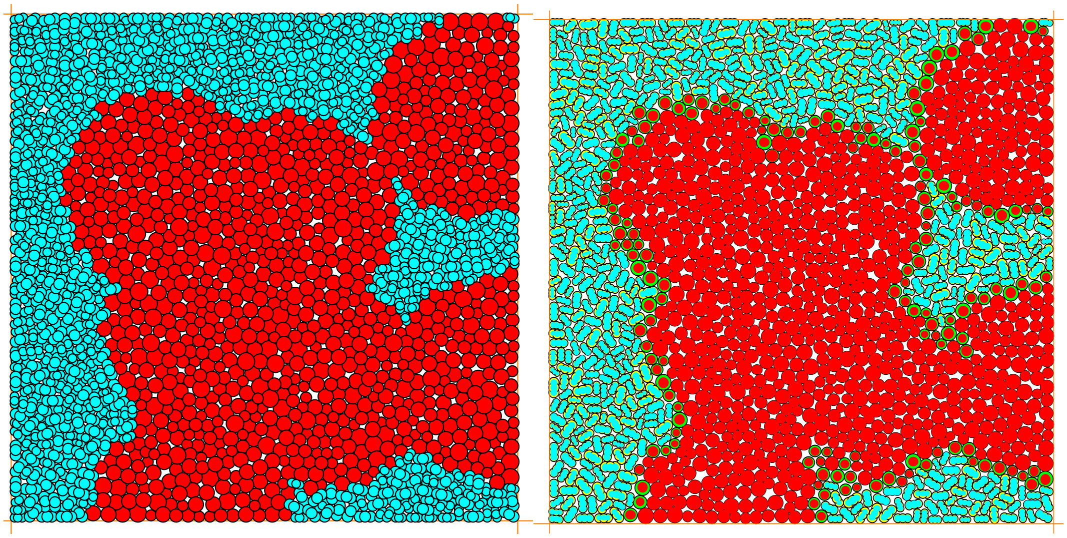

Figure 1. *Discrete element model of anhydrite caprock before reaction with CO_2 (left) and after 50000 years exposure to CO_2-rich fluids. Matrix anhydrite grains (blue), anhydrite rosettes (red), reaction rims of calcite in matrix grains (yellow) and rosettes (green) are indicated.*

Figure 1 shows the anhydrite-calcite alteration in the grain (edges) as a result of the reaction with CO_2-rich fluids in the model. The biaxial tests show that anhydrite failure strength is only significantly reduced for very long reaction times (~25% reduction after 50000 years). For reaction times of ~1000 years, changes in failure strength are insignificant. This observation is in agreement with conclusions of Hangx et al. [3]. It means that reaction of CO_2-rich fluids with caprock is unlikely to significantly change caprock permeability, unless aided by other processes not considered in our simple model.

This study shows that coupled chemical-mechanical modeling of the effect of reactive flow on caprock deformation using discrete element models is feasible. In future work, this modeling technique can be used to more rigorously test leakage scenarios related to coupling between reactive flow and deformation.

3.4 References

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