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Protection of caprock integrity for large-scale CO₂ storage on the Norwegian continental shelf

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Abstract

Large-scale CO₂ storage requires advanced understanding of the geomechanical response of the caprock subject to pressure build-up in the reservoir. CO₂ injection into basin systems will need to approach rates of 100 Mt/y in order to achieve significant reduction in worldwide emissions and realize the large capacity of saline aquifers. High pressure build-up is expected, which may activate existing fractures and faults in the seal and create leakage pathways for the CO₂ plume. New fractures may also evolve at higher pressures. To avoid creating leakage pathways for the CO₂ plume, the pressure must be kept under an upper bound that is determined by the caprock weakest point or initial stress. To date, there has been great uncertainty in critical knowledge needed for planning and execution of safe large-scale CO₂ storage projects. Within the PROTECT project, we advance methods and reduce uncertainty regarding the mechanical response. The research study focuses on three subareas: data collection, experimental studies and computational tasks. The studies are performed at small scale (scale of individual cracks, cm to m) and at large scale (reservoir or basin scale, 10 m to km). Data are synthesized, and a benchmark study of large-scale geomechanical simulation is performed. The Utsira Formation on the Norwegian continental shelf has been used as a common case study for integration and benchmarking activities. Finally, recommendations are made for future research based on knowledge gained in this study.

Keywords: caprock integrity; large-scale CO₂ storage; fractured shale; geomechanical characterization; geophysical monitoring; fracture flow modeling; hydromechanical simulation; geochemical fracture alteration; Utsira Formation

1. Introduction

The capacity of saline aquifers on the Norwegian continental shelf (NCS) for storing large quantities of injected CO₂ has been well established [1-2]. However, the ability to unlock this theoretical capacity in a safe and economically

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feasible manner is hampered by significant uncertainties. The largest risk factors in carbon capture and storage (CCS) include low injectivity, excess overpressures, and leakage risk [3]. Assessing and managing these risks requires reliable prediction of geomechanical integrity of the caprock when subjected to overpressure in the reservoir. Caprock integrity has been identified as a critical research area in which data, process understanding, and modeling capabilities are still lacking. These deficiencies limit our ability to reliably assure mechanical integrity, especially for gigatonne-scale CO₂ storage. Optimal use of basin-scale storage resources and cost-effective storage operations rely on reducing uncertainty and improving model confidence beyond the current state-of-the-art.

The mechanical integrity of the caprock is connected to a range of processes including thermal, chemical and physical, all which can impact the mechanical behavior of the storage reservoir and surrounding over- and underburden. Understanding coupled complex processes requires a multi-disciplinary effort that combines complementary laboratory and computational investigations stemming from geomechanics, geophysics, geochemistry and mathematical modeling.

An interdisciplinary study to advance understanding of caprock integrity was performed within the PROTECT project [4] financed through the CLIMIT program of the Research Council of Norway, TOTAL and the SUCCESS center for environment-friendly energy research. is to advance our understanding of the complex nature of caprock integrity. In this study, we combine these approaches to advance new knowledge in three key areas: (1) characterizing fractured rocks, including the impact of chemical and physical processes on fracture activation, propagation and/or healing; (2) identifying computational methods best suited to study fractures at the small-scale and monitor for leakage; and (3) integrating understanding from detailed data and models into large-scale hydromechanical simulations of CO₂ injection.

2. Laboratory experiments and analysis of fractured caprock

In this section, we summarize the data and analysis performed on relevant caprock samples. In this study, fresh samples of the Draupne shale (Ling Depression, North Sea) and from the Rurikfjellet shale (Longyearbyen CO₂ Lab, Svalbard) were tested. The laboratory tests examine several different parameters relevant to classical loading, shearing, and drying mechanisms that are influenced by the presence of CO₂. Simulations are performed to interpret the data when necessary. Bench-scale experiments are also performed to provide insight into chemical parameters of fractured rock.

2.1. Hydromechanical characterization

Direct shear box testing that allows for large displacement was performed on pre-fractured Rurikfjellet shale. The data were used to quantify the shear strength parameters (friction coefficient and cohesion) of the sample under varying conditions [5]. Running shear box tests to large displacements is an advantage since rock behavior may vary with increasing displacement. These data give insight in to the impact of flow along the fracture on fracture shear strength, and also quantify the relationship of shear strength with normal stress [6]. The results of the direct shear tests are shown in Fig. 1. The tests were run at different normal stresses in the range of 6.4 to 12 MPa. Frictional strength increases with increasing normal stress. The effect of flowing water on the shear strength of rock is dramatic, the peak strength is reduced to about 50% of the dry sample and the residual strength is close to zero (see LYB21 and LYB21-flow in Fig. 1 upper). These data were used to derive friction angle and cohesion of Rurikfjellet shale samples (Fig. 1, lower).

Stress-dependent fracture permeability in artificially fractured caprocks has also been investigated as a function of the flowing fluid. During experiments different fluids (CO₂ (gas), water and oil) were injected at different confining pressures (effective stress). Fracture permeability to CO₂ (Fig. 2a) shows that organic rich shales are highly stress sensitive and show considerable hysteresis during loading and unloading cycles. This hysteretic behavior can also be shown in cases where there are two subsequent loading and unloading cycles (Fig. 2a). These results imply that fracture aperture may be significantly reduced at deep burial depths. Similar results were seen in another study [7] showing that permeability to liquid/supercritical CO₂ is different to that of water or oil (Fig. 2b-c). These results indicate that fracture surfaces undergo alteration, i.e. swelling/shrinking or other surface effects, which impacts the hydraulic properties of fractured caprock material. Studies on shale powder pellets have not seen evidence of direct

impacts of swelling/shrinkage on permeability [8], but additional research is needed to quantify this effect on natural shale samples.

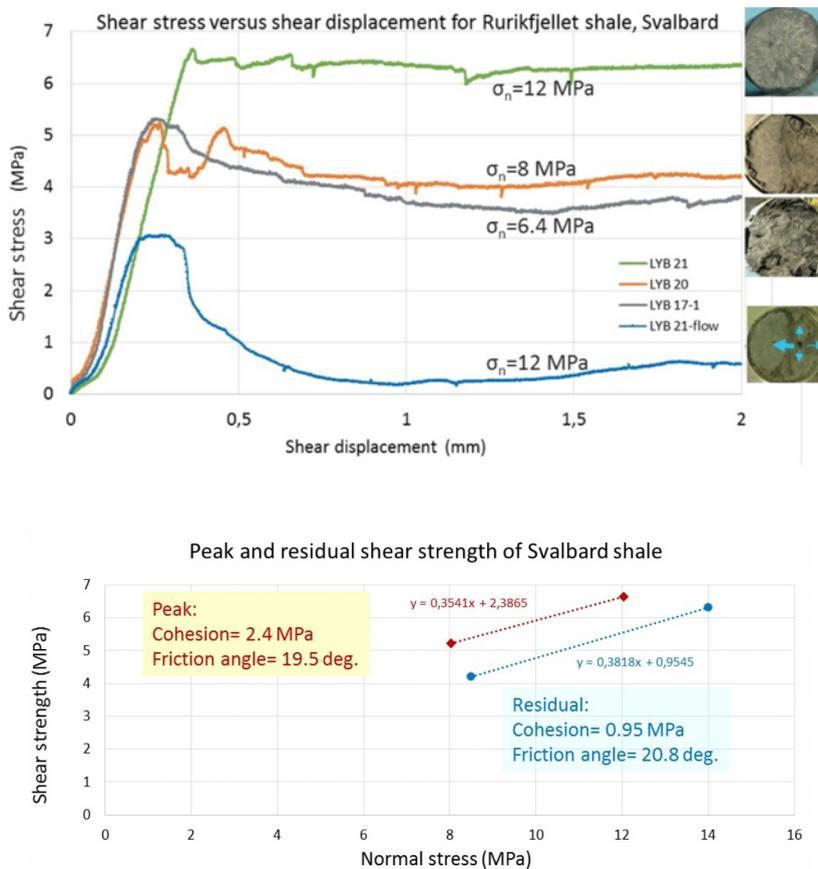


Fig. 1. Results from direct shear box testing of Rurikjellet shale, Svalbard [6]. Top panel shows the failure curves under different levels of normal stress. Photos of sheared samples are shown inset. Bottom panel show the correlation of shear strength parameters: cohesion and friction angle for both peak and residual portions of the test.

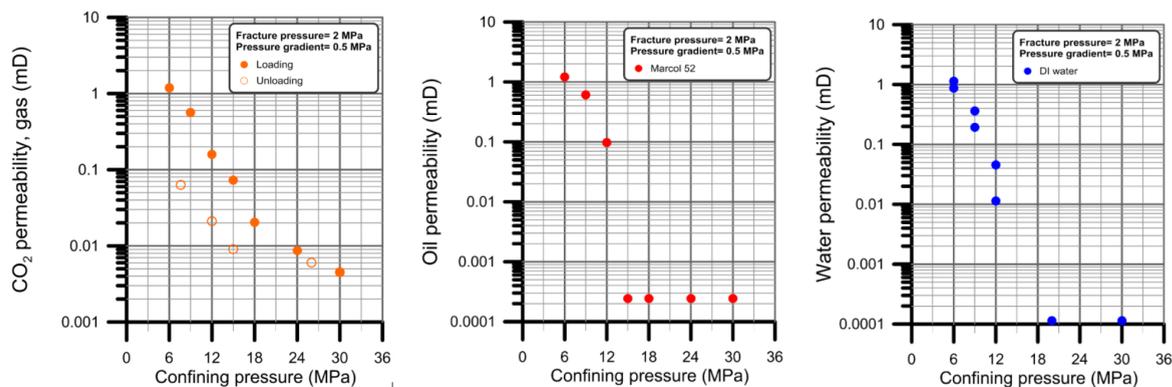


Fig. 2. Fracture permeability (mD) as a function of confining pressure for different fluids, CO₂ gas (left), oil (middle), and water (right).

2.2. Salt precipitation and fracture clogging

A series of microfluidic experiments have been performed to investigate how salt crystals, precipitated in the fractures, can affect the flow inside the fractures [9]. During these experiments laser-scribed samples of organic-rich Draupne shale samples are used as the substrate to represent the real fractured rock. CO₂ in three phases (gas, supercritical and liquid) is injected into the sample at different field-relevant injection rates so that the dynamics of salt precipitation is visually observed. The development of micrometer-sized salt crystals toward the inlet of the fracture (Fig. 3), the affinity of salt bodies to become connected, and extent of accumulations suggest that the salt precipitation during injection of CO₂ into the geological formations can be considered as a fracture healing mechanism.

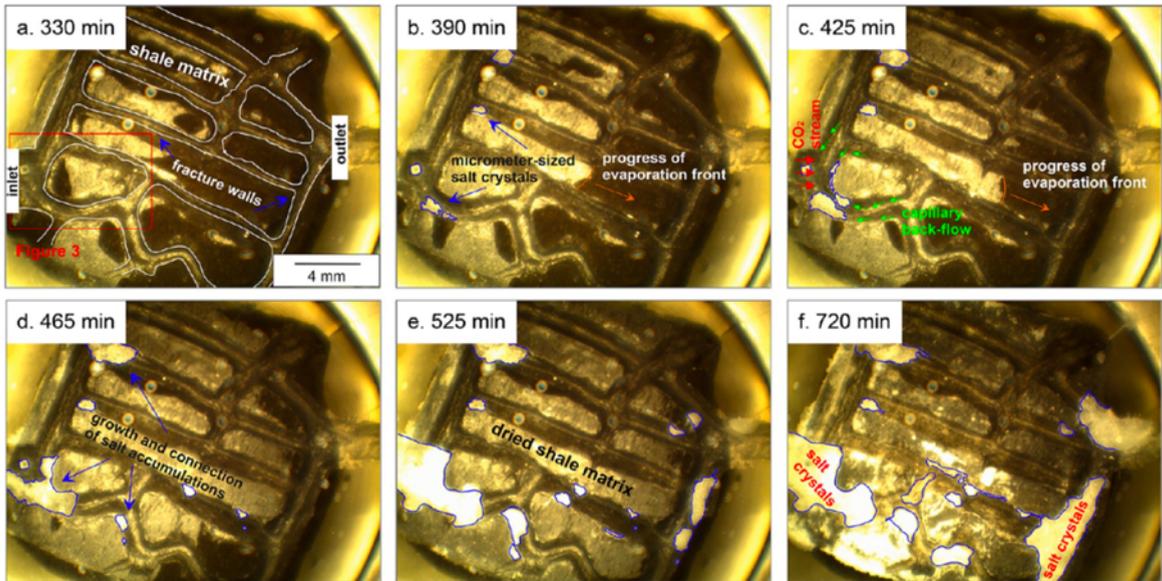


Fig. 3. Dynamics of salt precipitation for micrometer-sized crystals of halite that form on the interface of rock and CO₂ stream. The subfigures are time-lapse images of an experiment at pressure = 1 MPa, temperature = 22 °C, and flow rate = 20 cm³ CO₂/min. The white-outlined surfaces describe the fracture walls, and the blue-outlined areas inside the fractures are precipitated salt crystals. Image taken from [9].

2.3. Chemical alteration

Shale powders (Draupne shale) were exposed to supercritical CO₂ under dry conditions [10]. No chemical alteration was detected by thermal analysis (TGA). This result does not rule out other possible changes. For example, preliminary results indicate microcracking of unconfined shale cubes exposed to dry supercritical CO₂ occurs. It is believed that shale shrinking/swelling is the cause of the cracking, however, the precise mechanisms for these observations are yet to be determined [8].

3. Geophysical data interpretation and leakage detection

Geophysical data is important for monitoring pressure and saturation within the reservoir over time. In addition, data may be an important tool for leakage detection, either through detection of discrepancies in the injected plume or of an anomalous plume outside of the storage reservoir. In both cases, joint utilization of different datatypes improves detection capabilities. This approach improves the data interpretation and gives more reliable estimates of where the CO₂ plume and pressure pulse are located, which is important for assessing and monitoring the risk of leakage due to overpressure.

3.1. Improving seismic inversion through joint utilization

Seismic PP surveys are the standard geophysical monitoring technique but can be challenged in differentiating between changes in pressure or changes in saturation. Joint utilization of PP seismic with PS seismic, electromagnetic (EM) or gravimetric signals has the potential to differentiate saturation from pressure, and thus may greatly improve the value of PP seismic surveys [11]. A methodology where results from EM or gravimetric inversion are utilized in the prior model for seismic inversion has been developed and tested on the Skade formation synthetic data study (Fig. 4) with advantageous results [12].

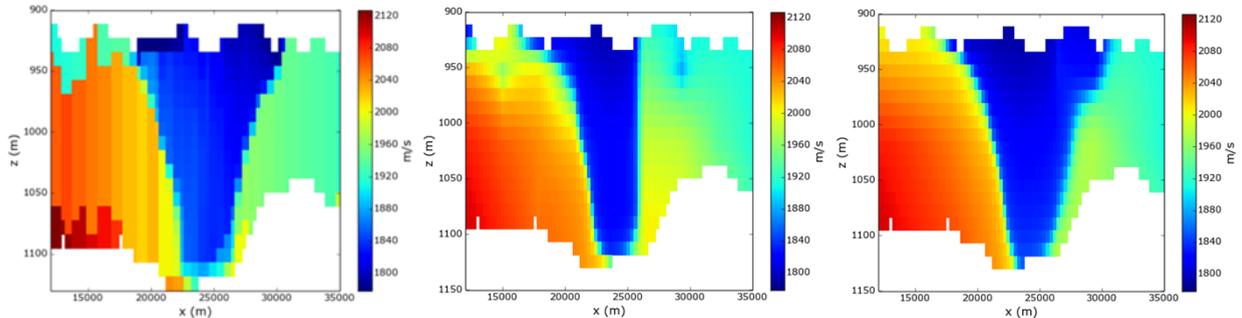


Fig. 4. Vertically exaggerated cross section of seismic inversion of synthetic data from the Skade formation [12]. Panels show seismic P-velocity. Left: true V_p . Middle: mean estimate using seismic data only. Right: mean estimate using novel methodology with seismic and gravimetric data.

3.2. Leak detection using gravity data

Gravimetric data may be used alone or in combination with seismic and/or electromagnetic (EM) to detect CO_2 leaked from an injection plume. Investigations using data from the Utsira Sleipner CO_2 injection site were used to determine the effectiveness of gravity data for leak detection. Results show that gravity data alone is insufficient for leak detection. Densely sampled ($\ll 1\text{km}$) gravity data (with noise of ca $3 \mu\text{Gal}$) can be used to measure density of leaked plumes only if plume position is given by seismic data [13].

4. Fracture flow models

The details of processes occurring within fractures and fracture systems require specialized modeling tools. We investigate hydraulic stimulation, chemical interaction, drying and thermal processes, leading to insights into mechanical behavior that affect fracture generation and growth. In some cases, entirely new mathematical frameworks are developed, while building upon existing modeling tools and expertise elsewhere.

4.1. Hydraulic stimulation and fracture growth

A 2D volume conservative numerical model of hydraulic fracturing has been developed for propagation of fractures away from an injection well [14]. The model utilizes a regular finite element grid at the reservoir scale without any special gridding of the fracture. A constitutive model for the critical fluid pressure necessary for fracture propagation is based on fracture surface energy. Numerical experiments indicate that most of the fluid injected during hydraulic fracturing resides in the fracture. It is difficult to maintain a fracture pressure when leak-off is dominating the volume of fluid in the fracture. The code has been used successfully to reproduce wellhead pressure during water injection and fracture stimulation in the Adventalen formation on Svalbard [15].

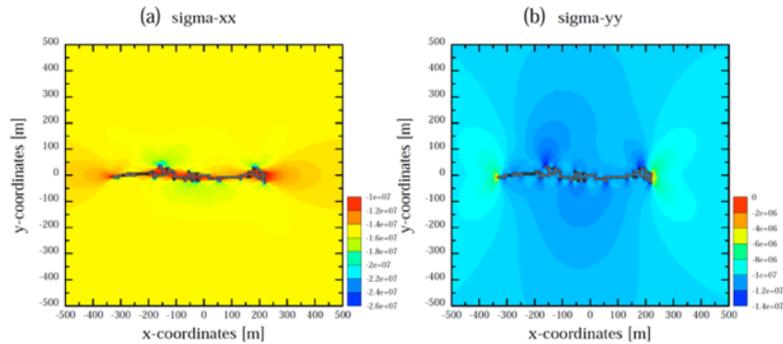


Fig. 5. The plots show the stress around a hydraulic fracture that has developed in a heterogeneous rock [14] (a) The stress σ_{xx} and (b) the stress σ_{yy} . Negative values give compressive stress. We notice that there is a stress enhancement at the fracture tips. Figure (b) shows that opening of the fracture compresses the rock along its sides.

4.2. Multi-dimension discretization for fracture-matrix models

A new, stable and convergent fracture-matrix discretization scheme has been developed that allows for accurate simulation of flow in finely discretized fractures [16,17]. The analysis of the fracture flow model has led to a new theory of coupled partial differential equations defined in 3D and 2D, as well as lower dimensions [18]. The method can be solved on non-matching grids and gives more flexibility for modeling fracture-matrix interactions (e.g. discontinuous pressure) as well as including intersecting fractures and dead-end fractures in coupled systems (see Fig. 2.2.1). The method and its analysis are moreover applicable to problems in 3D (see Fig. 2.2.2) The scheme has participated in a benchmark study concerning single-phase flow in fractured porous media where it is shown to perform well in comparison to the other participating methods [19]. The same principles are being extended to elasticity problems with thin inclusions, and further development towards poroelasticity is planned. Sharp interface models are closely related to this mathematical framework, especially if the location of the interface is governed by a lower-dimensional, partial differential equation [20]. This concept has been applied to form a water table evolution discretization based on domain transformation. The domain transformation scheme has been applied to investigate ground flow patterns in the vicinity of meandering streams, both in synthetic model problems as well as a real-world test case [21].

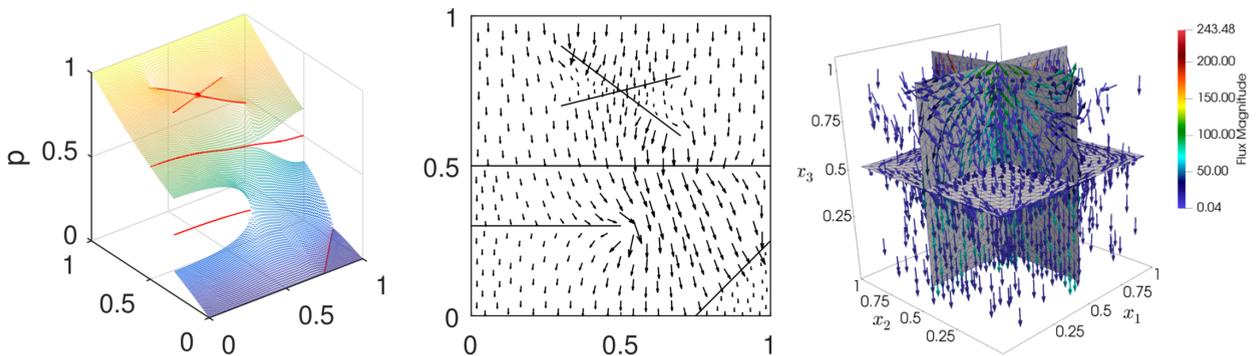


Fig. 6. Example of new fracture-matrix discretization [16,17] (Left) The pressure distribution for the two-dimensional test case. The effects of abrupt fracture endings as opposed to gradual closure of fractures is apparent around the tips of the blocking features. Continuity of the solution is visible where the aperture equals zero. (Center) The flow in 2D uses conducting fractures as preferential flow paths whereas it is forced around the features with low permeability. (Right) The flux field in the regular three-dimensional case. The solution is qualitatively consistent with expectations for a problem with conducting fractures.

4.3. Lattice-Boltzmann methods for reactive transport in fractures

Existing lattice Boltzmann (LB) software for pore-scale simulation of reactive-transport processes has been further developed for dissolution and precipitation reactions relevant for CO₂ storage. The extended numerical model has been coupled to the geochemical solver PHREEQC and can be used for 2D and 3D simulations. The model has been used to investigate the alteration of a single fracture surrounded by a heterogeneous rock surface composed of reactive and nonreactive minerals. The mineral composition of the fracture surface was varied to test the impact of heterogeneity on fracture permeability. The presence of non-reactive minerals inhibits uniform dissolution of the fracture surface, thus hindering the impact of dissolution on fracture permeability (Fig. 7) [22]. Also, the LB solver has been used to simulate the fracture geometry evolution in a fractured carbonate-rich caprock sample. The input geometry for the simulation was taken from CT scan data. 3D simulations also showed that presence of non-reactive minerals can negatively impact the permeability enhancement and that the power law formulations, used for porosity-permeability relations in large scale reactive transport simulators, need to account for presence of non-reactive (or less reactive) minerals in the system [23].

The LB solver is currently being used to simulate the nucleation and precipitation in fracture networks and investigate effect of mineral substrate on the precipitation pattern.

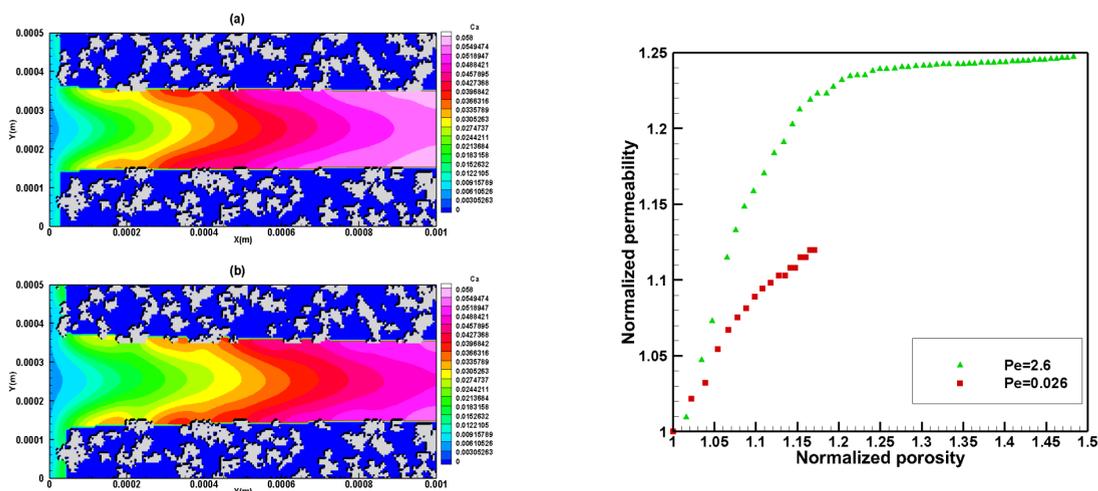


Fig. 7. Ca concentrations (mol/L) at (a) $t = 1.5$ hr, (b) $t = 4.9$ hr. In all three cases $Pe = 2.6$. Kaolinite mineral is depicted in light gray and zero concentrations (blue) are showing the calcite [22]. Right panel shows normalized permeability vs normalized porosity at two different Pe numbers for initially mixed mineral assemblage [22].

4.4. Saturation-dependent fracturing

Saturation-dependent processes in deformable porous media requires an understanding of the interrelation between flow and mechanics. A finite-volume numerical model has been developed for two-phase flow and deformation [24]. Richards' assumption (inviscid flow of the non-wetting phase) has been applied for the flow problem, while linear elasticity behavior is assumed for mechanics. Unlike saturated flow in deformable porous media (Biot's equations), unsaturated flow results in a highly non-linear coupled system due to use of water retention curves which are necessary to compute the saturation and relative permeability as a function of pressure. The model has been implemented in Matlab and used to study desiccation processes in clayey soils. Mudcracks form as water evaporates from the soil, shrinking the soil, and inducing stresses above the critical value. We simulate the evaporative process of a clayey soil contained in a Petri dish. Numerical results show an increase in tensile stress as the soil evaporates, with highest stress at the walls of the dish. We can infer that cracks will initiate at the walls and propagate inwards, which is in agreement with experimental results.

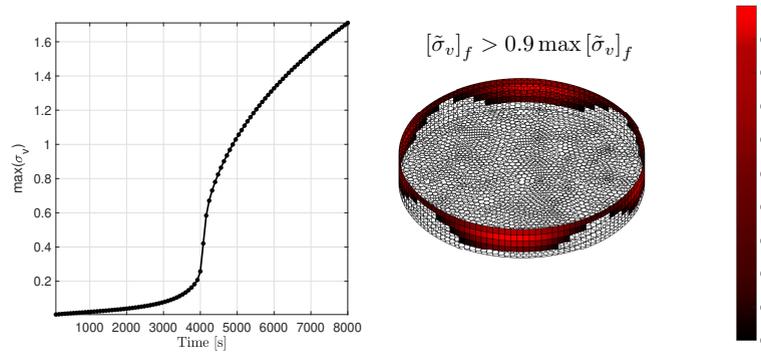


Fig. 8. 3D simulation of water evaporation from a clayey soil in a Petri dish [24]. (Left) Plot shows the evolution of maximum tensile stress that lead to tensile cracks. (Right) The highest values of tensile strength are located on the walls of the Petri Dish where mudcracks would be initiated.

5. Large-scale hydromechanical simulation

To consider large-scale injection systems of up to tens to hundreds of megatons per year, new large-scale computational models have been developed specifically to address the response of the caprock under massive injection into deep storage reservoirs. These large-scale systems are well beyond the scale of individual fractures, and therefore simpler techniques must be used in order to be computationally efficient. The project has compared different approaches and demonstrated that analytical estimates of seabed uplift are reasonably accurate and save time. Again, a benchmark study has been carried out to determine the effectiveness of different (yet necessary) simplifications on model predictions. This study shows that more accurate representation of CO₂ in the storage reservoir is as, or more, important than accurate geomechanical representation of the over- and under-burden. This allows for simplification of the mechanical system, which is advantageous when many simulations are needed to evaluate uncertainty and sensitivity to input data.

5.1. Simplified mechanical deformation model

A simple analytical 1D poroelastic model has been proposed to estimate reservoir expansion and seabed uplift caused by perturbations of the reservoir pressure [25]. The validity of the simplified 1D model was examined by plane-strain analysis using the method of Fourier decomposition. The 1D estimate is found to be accurate for pressure wavelengths larger than 2π times the maximum of the reservoir thickness and the overburden thickness. This implies that the 1D estimate will perform better for systems of large areal extent, and with improved accuracy at greater distance from the injection well (see Fig. 9). These results, in terms of wavelength, are useful because they identify the amplitudes in a Fourier decomposition of an overpressure distribution that produce reservoir expansion and surface uplift.

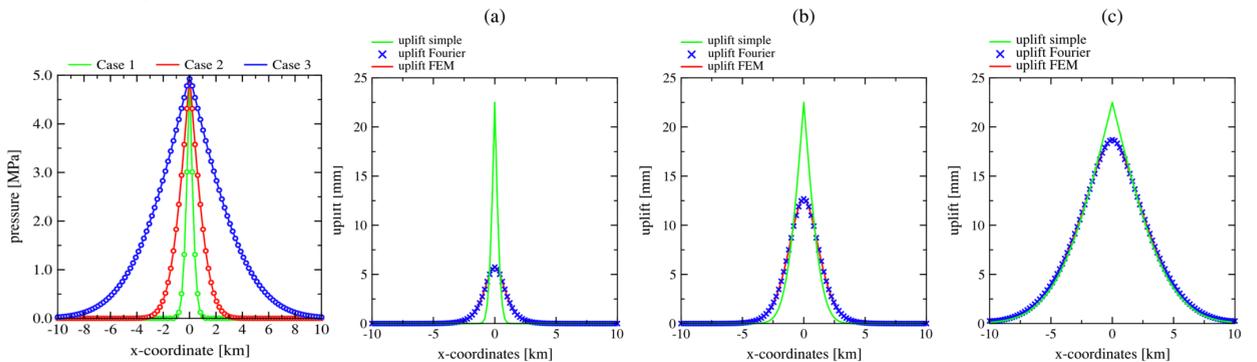


Fig. 9. Analysis of simple uplift model [25]. (Left) The thick line shows the three pressure distributions of the cases 1, 2 and 3, which corresponds to 0.1, 1 and 10 years of injection, respectively. The circular markers show the Fourier representation of the pressure distributions. (Right) The uplift calculated by three different models created by the three pressure distributions at (a) 0.1 y, (b) 1 y, (c) 10 y.

5.4. Mixed-dimensional coupled flow and mechanics

A third model developed at NGI [29,30] uses a simplified description of the flow and mechanical processes in the storage reservoir through the method of dimensional reduction. The governing equations for both two-phase immiscible flow and poroelasticity are integrated across the thickness of the reservoir, transforming the relevant variables and equations into integrated and averaged quantities and equations. The equations are solve using FEM in COMSOL Multiphysics software. The dimensionally reduced reservoir is embedded in a three-dimensional environment, accounting for the full stress tensor in the overburden and underburden. The method does not only reduce the number of degrees of freedom that needs to be solved by reducing the dimensionality of the reservoir, it also leads to a less stiff nonlinear system of equations, allowing the numerical solver to progress with longer time steps and consequently further reduce computational time. It has also been demonstrated that the model retains reasonable accuracy when applied to realistic field data as it was tested and validated against a full-dimensional model inspired by the conditions at now decommissioned CO₂-storage plant in In Salah, Algeria [31]. The range of applicability of the dimensionally reduced model is to a leading order the thickness of the reduced domain, the reservoir. A convergence test for a range of aquifer thickness values indicates that accurate solutions in the order of 0.1% and less difference in solution compared to the full-dimensional formulation for reservoirs up to 100-m thick are achieved.

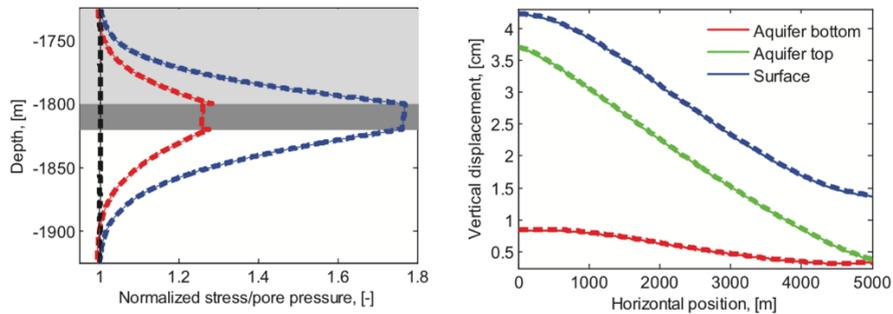


Fig. 11. Coupled flow and mechanical simulations of reservoir based on In Salah CCS injection using a simplified approach [31]. Left: Vertical profiles of various normalized stress components (normalized to initial values) measured 100 meters away from the symmetry line. Black: vertical stress. Red: horizontal stress. Blue: Pore pressure. Dark gray area indicates the reservoir. Right: Vertical displacement along the bottom of the aquifer (red line), top of aquifer (green line) and surface (surface heave, blue line), cf. Figure 1 (left). In both figure the thin lines are from the simplified model and thick dashed lines are for the fully resolved model.

5.5. Utsira benchmark and model comparison

The three different mechanical and flow simulators presented in sections 5.2-5.4 have been applied to a common benchmark problem based on the Utsira aquifer [32]. The objective of this study was to build confidence in different complexity simulators to predict pressure and deformation for large-scale CO₂ injection. Three simulators were compared for a single-well injection into the southern Utsira at different rates for 25 years. Compressibility of the Utsira sand was varied between stiff and soft values to reflect a realistic range for unconsolidated sand.

The main differences between the simulators can be summarized: the IFE model (described in 5.3) is a fully coupled hydromechanical simulator that solves only single-phase water injection, the VESA model (described in 5.2) solves for two-phase flow in the reservoir using dimension reduction coupled to an analytical model for deformation (see section 5.1); and the COMSOL model (described in 5.4) solves the full hydromechanical problem with reduced physics in the reservoir and static CO₂ properties. The results show that the models compare very well for the simplest problem of water injection (Fig. 12). However, when comparing for CO₂ injection, the single-phase model overestimates the pressure build-up and subsequent deformation (Fig. 13). The discrepancy in model predictions becomes progressively worse with higher injection rates and stiffer media.

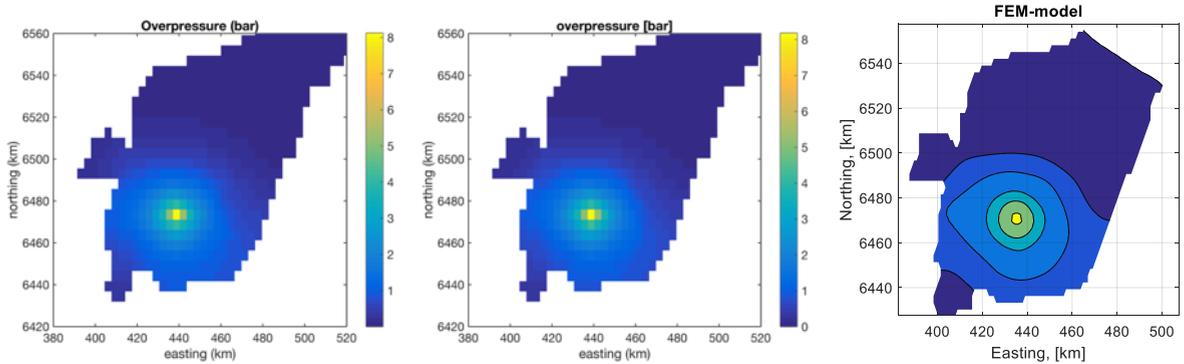


Fig. 12. Comparison of pore pressure from two-phase flow simulations using three different simulators: (left) IFE, (middle) VESA, (right) COMSOL-FEM. used in the benchmark test, two-phase flow, constant properties, soft reservoir, injection rate is 10 Mton/year.

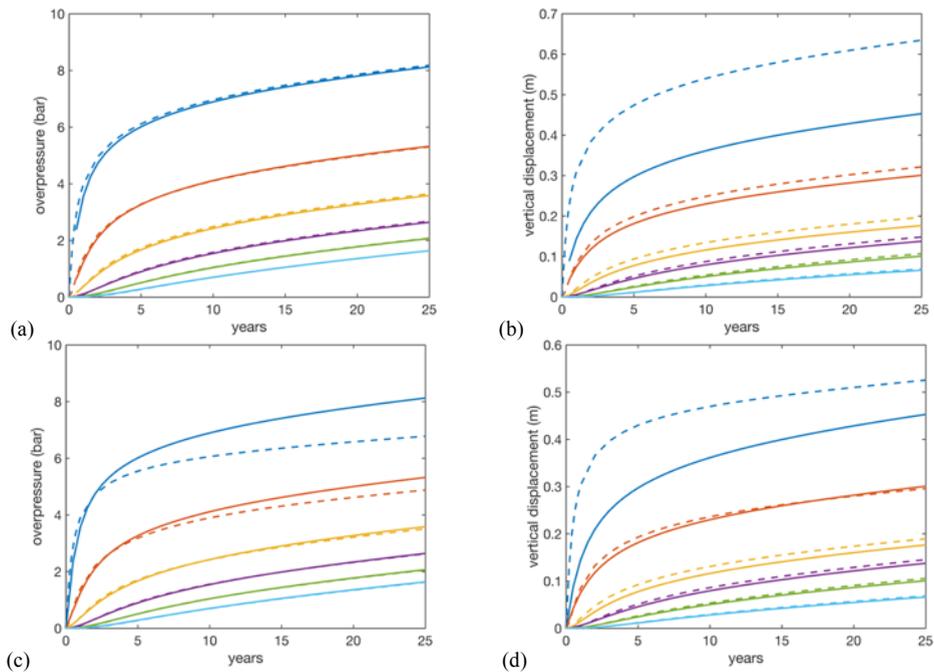


Fig. 13. Comparison of pore pressure (a,c) and surface uplift (b,d) in time for two different simulators (IFE in solid and VESA in dashed) at increasing distance from the injection cell (blue curves is located the injection cell and subsequent curves increase in distance by increments of 3.2 km). Panels show two comparisons: (top panels: a-b) water injection for both IFE and VESA; (bottom panels: c-d) water injection for IFE model and CO₂ injection for VESA model.

6. Integration and basin-scale case study

New technological developments in this study were then integrated into regional-scale studies to help understand practical capacity of NCS aquifers. The Utsira formation was used as a relevant case study was designed to demonstrate this workflow [33]. According to the Norwegian Storage Atlas, the theoretical capacity of the Utsira for CO₂ is exceptionally high [1]. However, effective use of the theoretical capacity requires that CO₂ be injected at rates that are tens or hundreds of times larger than the Sleipner CCS project. As CO₂ injection volumes increase, the Utsira will become pressurized, leading to overpressures that exceed the allowable pressure the caprock can withstand.

Understanding the impact of these pressure limits of the Utsira requires very sophisticated simulation tools and a good estimation of rock properties. Using all available data for the Utsira assembled within this study, we investigated the maximum allowable injection rate that can be sustained over a 50-year storage project (total 5 Gt CO₂ injected at 100 Mt/y for 50 years) without water production and closed boundaries. Sensitivity to rock properties and boundary conditions at the very large scale was performed based on input from other aspects of the study. Different simulation methods lead to the same conclusion that the Utsira can potentially withstand injection rates 100 times the current Sleipner injection rate, with lower capacity estimates for a lower compressibility in the Utsira sand before reaching the estimated fracture pressure limit of the caprock.

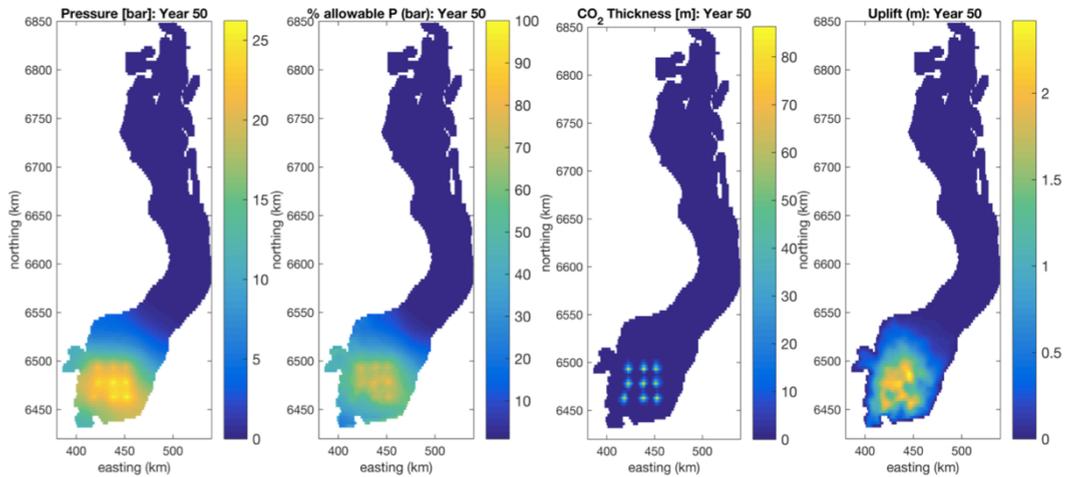


Fig. 14. VESA simulation results at 50 years of 100 Mt/y CO₂ injection into the Utsira formation [33] Panels from left to right show overpressure (bar), overpressure as a fraction of fracture pressure (%), CO₂ plume thickness (m), and seabed uplift (m).

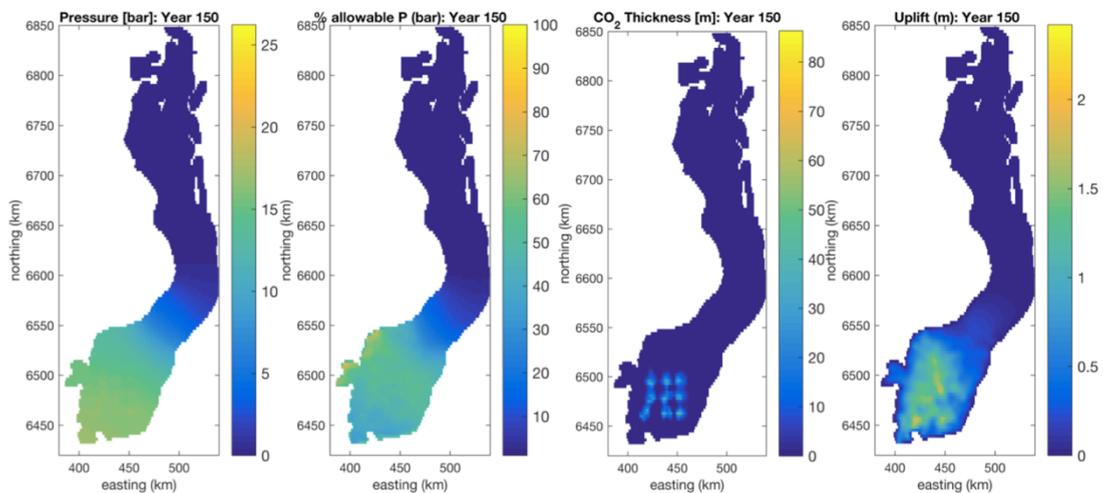


Fig. 14. VESA simulation results at 100 years post-injection after a 5-Gt injection into the Utsira formation [33] Panels from left to right show overpressure (bar), overpressure as a fraction of fracture pressure (%), CO₂ plume thickness (m), and seabed uplift (m).

7. Summary and Recommendations

In this paper, we have described new developments in laboratory studies and numerical modeling that have contributed to our understanding of caprock integrity and its response to large-scale CO₂ injection. The main focus has been on understanding the controls on initiation and/or activation of fractures in caprocks, specifically mudstones

and shales. The series of investigations have focused on different facets of this problem, covering mechanical, chemical, hydrological and multiphase flow impacts. New data have been collected and novel numerical methods have been derived. These studies have ranged from core-scale to basin-scale investigations.

The results from this study, although extensive, are not exhaustive. Many of the results were quite fundamental, yet with important implications for our ability to predict the impact of CO₂ injection on caprock integrity. The value of such a wide-ranging study is that it allows us to propose recommendations for future research and innovation that target needed data and models.

- **Mechanical properties of fractured media:** Data obtained in this study, as in many others, are restricted to clean fractures (either natural or artificially created) within a single “uniform” material. The mechanical properties of composite fractures are largely unexplored. Particularly with regard to faults, there is a need for composite fractures that represent the rock types found within a fault core, i.e. sands, clays, shales, basement, etc. The standard suite of testing also does not explore the impact of field conditions on fractures, i.e. exposure to continue stress and also CO₂ exposure. Fractures that slip in the field will continue to be exposed to stress after failure, and data are needed to quantify not just the initial failure point, but also repeated failure curves in a sequence. For example, more studies are needed to quantify how compaction and/or dilation after a shear event enhances or reduces mechanical integrity. For CO₂ exposure, studies are needed to understand whether clay smear in the fault core become more brittle or ductile when CO₂ enters the system.
- **Geochemical aspects of fracture leakage:** Intriguing evidence from small laboratory and theoretical studies point to fast-evolving geochemical reaction along fracture surfaces as having impact on flow behavior if a fracture becomes activated. Little is known about the extent to which sub-microscale (surface processes) affect meter-scale processes. Chemical impacts need to be expanded from small-scale experiments of isolated processes (calcite, salt precipitation, swelling) to large-scale hydro-chemical-thermal-mechanical simulation studies of a flowing fracture under realistic input and boundary conditions. Studies are needed at scale to determine if fractures will clog/disintegrate, or swell/shrink when exposed to reactive CO₂-laden fluids. For example, larger-scale simulation studies can be designed to model the calcite deposits observed in shale outcrops, such as the Kimmeridge clay. Benchmarked simulations can be used to understand the conditions when geochemical reactions in faulted shales are important and if they impact fault flow properties.
- **CO₂ impact on mechanical stability:** As the mudcrack numerical experiments have showed, change in fluid saturation can have a significant impact on the stress environment, leading to significant fracturing in dried out clays. These experiments were for air-water systems at the ground surface, but it raises important questions about whether the impact of CO₂ fluid saturation at depth may be important for the mechanical stability of caprocks. More research is needed to explore the possible saturation-dependent impacts of CO₂ on shales, particularly in shallow, unconsolidated zones. The possible impact of chemistry on mechanical stability is also a largely unexplored area of research. More investigations are needed to understand how CO₂ exposure affect mechanical properties of a fracture, i.e. how cohesion/friction parameters change with exposure to a reactive fluid. Here, the impacts may be due not just to CO₂ but also to other reservoir treatments that the reservoir may have experience in a previous EOR setting (e.g. low-salinity, seawater injection).
- **Moving across scales from a single fracture to multi-fracture systems and quantification of effective parameters:** There is a very large gap between our understanding of single-fracture deformation and flow to large-scale behavior of fracture systems connected to pressure dynamics within a CO₂ storage reservoir. We currently have all of the components: high-resolution datasets of single fracture deformation and flow, state-of-the-art numerical methods for a meter-scale multi-fracture network subject to changes in stress and pressure, and robust reservoir simulators for the larger scale system. However, there are critical gaps at the interface between these various components. First, more sophisticated analysis is needed of existing data to build constitutive models for fracture permeability. These need to be incorporated into multi-fracture flow models at the 10-meter scale to simulate the dynamics of a fracture network subject to realistic boundary conditions, ideally provided by the reservoir simulator. But in the end, complex fracture systems (most likely associated with faults) must be reduced to only the essential information and processes when fully coupled into a reservoir system. More research is needed to bridge the gap between fine-scale detailed fracture characterization and effective fracture/fault models for use in large-scale simulation studies, thus improving existing workflow for fault and fracture seal analysis.

- **Large-scale reservoir simulation and fracture/fault leakage:** Simulation technology at the reservoir scale is quite mature, and very large-scale methods such as VE have advanced quite significantly in recent years. The main research should be directed towards handling of fracture/fault fluid migration within very coarse grids and streamlining software with other methodologies such as needed for uncertainty quantification and optimization. For fault fluid migration, improvements beyond the standard approach in commercial simulation, which tunes transmissibility factors to get the desired cross-fault flow but are not able to handle the more complex dynamics of vertical/along-fault fluid flow. Semi-analytical solutions are available that have taken the same approach for handling sub-scale leakage along abandoned wells, and these should be explored to see if they can be practically and efficiently implemented into reservoir simulations. Analytical solutions can be adapted to account for time-dependent permeability changes with fault deformation (with relations developed from the upscaling workflow and not through modeling of fault deformation itself).
- **Geophysical monitoring:** The importance of integration of various geophysical data (seismic, EM, gravity) has been long emphasized for reliable and efficient monitoring strategy of CO₂ injection. This concept has been well demonstrated for a synthetic data study. In the near future, we believe, a field-scale demonstration of applicability of all learnings from the synthetic data study should be realized so that we can better evaluate the true feasibility for practical cases, not just for desktop study cases.
- **Uncertainty characterization and quantification:** It is well understood that uncertainty is a main concern in all aspects of CO₂ storage. For caprock integrity, the uncertainty problem has significant implications for predicting caprock failure, quantifying subsequent leakage and understanding its large-scale impacts. First, the characterization of uncertainty should be addressed in the laboratory, with several repeat experiments required to build statistical distributions. Secondly, it is often assumed that propagation of uncertainty requires an ensemble approach where many realizations are needed to explore the extensive parameter space. In order to reduce the computational burden of uncertainty quantification, more efficient methods need to be developed, most likely by tailoring existing stochastic or multi-step ensemble methods to the fracture initiation/activation and leakage problem.

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