



STATE OF THE ART REPORT

Dealing with uncertainty
associated with long-term
CO₂ geological storage

ULTimate
CO₂



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PARTNERS



BUREAU DE RECHERCHES GEOLOGIQUES ET MINIERES (BRGM), France



BUNDESANSTALT FÜR GEOWISSENSCHAFTEN UND ROHSTOFFE (BGR), Germany



BRITISH GEOLOGICAL SURVEY (NERC), UK



CO2Sense CIC, UK



EUROPAISCHES INSTITUT FÜR ENERGIEFORSCHUNG EDF-KIT EWIV (EIFER), Germany



GEOGREEN, France



THE GEOLOGICAL SURVEY OF DENMARK AND GREENLAND (GEUS), Denmark



IFP ENERGIES NOUVELLES (IFPEN), France



CONSIGLIO NAZIONALE DELLE RICERCHE (IGG-CNR), Italy



PHI-MECA ENGINEERING (PHIMECA), France



NETHERLANDS ORGANIZATION FOR APPLIED SCIENTIFIC RESEARCH (TNO), Netherlands



UNIVERSITEIT UTRECHT (UU), Netherlands

ABOUT ULTimateCO₂

The ULTimateCO₂ project is financed by the 7th Framework Program (FP7) of European Union Research policy under the program topic "ENERGY.2011.5.2-1: Understanding the long-term fate of geologically stored CO₂". Contract Number: 281196".

The aim of ULTimateCO₂ is to significantly advance our knowledge of specific processes that could influence the long-term fate of geologically stored CO₂ and to develop validated tools for predicting the performance of long-term storage sites. This 4-year collaborative programme includes detailed laboratory, field and modelling studies of the main physical and chemical processes involved and their long-term impact on: a) trapping mechanisms in the reservoir (structural, dissolution, residual, mineral), b) fluid-rock interactions and effects on mechanical integrity of fractured caprock and faulted systems and c) leakage due to mechanical and chemical damage in the well vicinity.

Integration of the results will enable an assessment to be made of the overall long-term behaviour of storage sites at a regional scale in terms of efficiency and security. This will also include other important aspects such as far-field brine displacement and fluid mixing.

The long-term prediction of CO₂ evolution during geological storage will thus become more robust, not only by addressing the uncertainty associated with numerical modelling, but also by applying realistic contexts and scale. This will be ensured through close collaboration with, at least, two demonstration sites in deep saline sandstone formations: the onshore NER300 Ouest Lorraine candidate in France (ArcelorMittal GeoLorraine) and the offshore EPR Hatfield site in UK (National Grid).

ULTimateCO₂ will develop recommendations for operators and regulators that will enable a robust demonstration to be made of the assessment of the long-term storage site performance. Scientific knowledge on the long-term efficiency and safety of CO₂ storage will be disseminated widely to a broad audience, so that this work will not only benefit the operators of the demonstration sites but also other stakeholder groups, including policy makers and regulators, storage developers, investors, the scientific community, and representatives of the general public (NGOs and CCS initiatives), thereby helping to improve public understanding of CO₂ storage.



INTRODUCTION

CCS could contribute as much as 20% of the total reduction in emissions needed

Carbon dioxide Capture and Storage (CCS) offers the possibility of reducing atmospheric greenhouse gas emissions by confining carbon dioxide (CO₂) permanently in geological formations deep underground. The International Energy Agency (IEA) has recently estimated that CCS could contribute as much as 20% of the total reduction in emissions needed to keep global warming below 2°C. The recent European Strategic Energy Technology (SET) Plan aims to support research programmes and industrial pilots in order to accelerate the deployment of such low carbon technologies.

However, although the SET Plan recognises that the technical feasibility of CCS has been proven with the development of small-scale pilot sites that draw on oil and gas industry experience, the EC Directive on the Geological Storage of CO₂ requires operators to demonstrate that the long-term fate of the CO₂ in the reservoir will constitute permanent containment. Other stakeholders, notably the general public and their representatives, seek answers to questions on the behaviour and impact of the injected CO₂: "What will happen to the CO₂?", "Will it leak from the chosen reservoir?", "Will it stay underground?", "For how long?".

Such questions, at whatever level, can only be answered convincingly through a better understanding of a chain of complex physical and chemical processes. This requires a significant increase in scientific knowledge beyond the current state of the art since, unlike other domains, we require evidence from experiments and simulations to support the limited experience obtained to date. The European Commission's Directive on geological storage Annex 1 specifies the need to perform "long-term simulation (to establish CO₂ fate and behaviour over decades and millennia, including the rate of dissolution of CO₂ in water)". Although some long-term issues have been indirectly investigated previously (FP6 NASCENT, FP7 CO₂CARE projects), the present work specifically considers the "post-abandonment" phase of a CCS project, after site closure and 'de-licencing' and during which the stored CO₂ continues to migrate, dissolve and react with the host rock. Demonstrating the safety of the storage site and building the confidence of stakeholders in this new technology will rely on a sound scientific knowledge of all the physicochemical processes affecting the geological storage formation, the surrounding area and overlying aquifers.

The specific targeted research proposed in ULTimateCO₂ is intended to fill this knowledge gap. The four-year ULTimateCO₂ programme (2011-2015) comprises seven work packages (WPs). WP1 concentrates on project management and coordination. WP2 is aimed at integrating and compiling the results of the detailed study of three main aspects developed in WPs 3, 4 and 5, in order to assess long-term impacts of geological storage at the basin scale. It will also address other important aspects, such as hydro-regional flow, water quality and native fluid displacement. This modelling will incorporate field data from CO₂ storage demonstration sites to provide test cases. WPs 3, 4 and 5 are focused on understanding the three main aspects determining long-term confinement efficiency looking at (i) the reservoir, (ii) the caprock, and (iii) the well. Each WP in ULTimateCO₂ will integrate numerical modelling, laboratory experiments and geological evidence. WP6 is dedicated to uncertainty assessment and supports all the other work packages by providing them with a framework for addressing the confidence that can be placed on the long-term extrapolation of identified processes, and numerical simulation results. WP7 will develop clear guidelines for storage projects enabling site-specific evaluation of the long-term fate of geologically stored CO₂.

The ULTimateCO₂ consortium is composed of experts in a variety of geoscience disciplines covering geology, geochemistry, geomechanics, reservoir engineering, and numerical modelling. In addition, collaboration with CSLF members from USA and Canada will contribute to the scientific and technological content and will provide a more international context to the project in terms of data exchange and dissemination of results.

ULTimateCO₂ will
integrate numerical
modelling,
laboratory
experiments
and geological
evidence

Near the beginning of the project, each WP leader provided their latest information on the uncertainty associated with long-term CO₂ geological storage. To support the pilot sites being set up under EEPR (Don Valley in UK) and NER300 (ULCOS in France) this information was used to produce this state of the art report, which contains the partners' pooled knowledge in answer to pertinent questions from project owners, site operators and national authorities about their post-abandonment exposure to uncertainty. The report has been compiled for CO₂ storage developers (particularly those involved in EEPR and NER300 projects), the GCCSI, CSLF, IEAGHG, CO₂GeoNet and CCSA, EU wide regulators and NGOs such as the Bellona Foundation, Green Alliance, Zero, E3G and WWF informing civic society.

This document provides a view of the current state of the art for the issues addressed by this project:

- The long-term reservoir trapping efficiency (WP3)
- The long-term sealing integrity of faulted and fractured caprock (WP4)
- The near-well leakage characterisation and chemical processes (WP5)
- The long-term behavior of stored CO₂ looking at the basin scale (WP2)
- Uncertainty assessment (WP6)

Each chapter is divided into two sections: (i) a summary which explains in "simple words" the main issues and objectives of the WP, and (ii) a current state of the art section which provides a more sound review on the specific studied processes.

This report will be available on the project website and virtual network, linked to the external project newsletter.

Long-term reservoir trapping efficiency

SUMMARY

Being less dense than formation water, supercritical CO₂, when it is injected into a reservoir, will tend to rise upwards from the point of injection under buoyancy and therefore create a plume. Rocks with a low permeability, such as mudstones and evaporites, prevent the vast majority of the CO₂ from migrating away from the reservoir although a small amount will still occur through diffusion. As the volume of CO₂ increases, through continuous injection, the plume will continue to spread along the base of these impermeable layers as a result of buoyant flow.

To constrain this flow many storage sites require a physical structure to contain the CO₂ and this structural trapping is the principal form of containment for the injected CO₂. Most CO₂ storage sites are likely to have some form of structural or stratigraphic trap that enables the CO₂ plume to be physically retained as the primary containment feature.

At the trailing edge of the CO₂ plume, the CO₂ saturation decreases gradually as the plume migrates. As the CO₂ concentration decreases, the non-wetting CO₂ becomes disconnected and separated because of capillary pressures. CO₂ becomes trapped in large pores from which it can no longer move due to the capillary pressures occurring in the thinner pore throat. This relatively fast trapping mechanism is known as residual trapping, hysteresis trapping or capillary trapping.

As the amount of residually-trapped gas increases with time, it has been proposed as the principle form of containment in large open aquifers, where an injected CO₂ plume may move slowly updip. Most of the CO₂ is trapped as a residual phase as well as a dissolved phase – so called migration assisted storage. It has been proposed that injection schemes should be optimised to maximise the potential for residual gas trapping. Some reservoirs contain mudstone strata of variable lateral extent which may serve to spread the plume laterally.

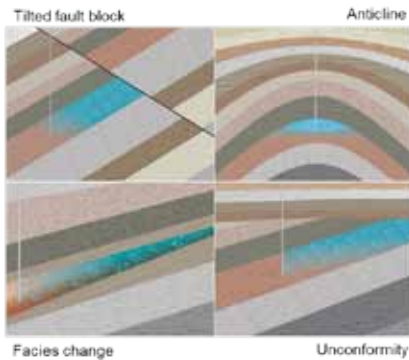
The permeability of the cap rocks, the effect the CO₂ has on them and the mechanisms with which CO₂ is trapped in these reservoirs forms the subject of this work package.

CURRENT STATE OF THE ART

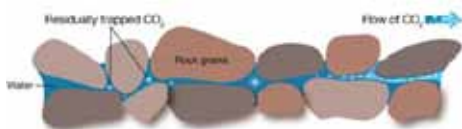
Residual trapping is considered to be the most rapid mode of trapping^{1,2,3} and has three consequences: the gas immobilisation itself, changes in the capillary pressure and a variation in relative permeability curves. These effects have been integrated, progressively, in the modelling efforts undertaken to describe plume migration⁴. Analytically, several works considered a residual gas saturation in sharp-interface models^{3,5} and in Buckley-Leverett models but the hysteretic effects were ignored.

It has been estimated¹ that the proportion of CO₂ residually trapped in Japanese reservoir rocks may be between 24.8% and 28.2% whilst studies in other reservoirs indicate between 11% and 25% of the CO₂ can be residually trapped^{6,7}. Residual trapping may be enhanced during injection by the co-injection of water⁸. As the CO₂ moves through the formation, some of it will dissolve in the formation water, leading to further solubility trapping. Initially a small amount of dissolution will also take place in the residual brine contained in the CO₂ plume, like in a depleted gas field. Dissolution is relatively slow at the reservoir scale because it is limited by the rate of CO₂ diffusion into the water and the contact area of the CO₂ plume itself.

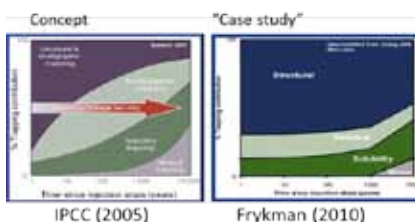
In addition, CO₂ injected into depleted hydrocarbon fields, for either CO₂ storage or enhanced oil recovery⁹, may also dissolve in any remaining oil as well as any brine present. Hence, reservoirs in which intraformational mudstone strata allow the plume to migrate laterally and radially from the injection point(s) may enhance solubility trapping



CO₂ (in blue) is lighter than the brines and tends to migrate upward during and after injection, being trapped by geological structural trapping



Residual trapping of CO₂ flowing through porous media: The tail of the plume of free-phase CO₂ migration is trapped by capillary pressure from the water in the pore spaces between the rock and stops flowing.



Concept of Trapping evolution with time hypothetical (on left, from the International Panel on Climate Change document in 2005) and based form case study from Frykman 2010.

relative to reservoirs in which plumes contact less unsaturated formation waters ^{10,11,12}.

Local capillary trapping and rates of dissolution trapping increase with increases in small-scale variations in permeability and porosity ¹³. The amount of residual trapping can be overestimated if this micro-heterogeneity is not taken into account, though the overall amount of CO₂ contained by local capillary trapping can compensate for this ^{14,15}.

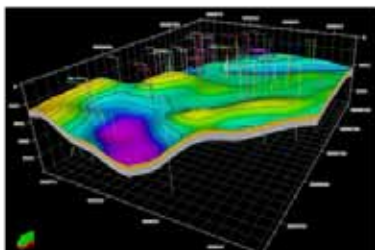
One effect that dissolved CO₂ can have is to shift the pre-existing equilibrium between the formation water and minerals present in the reservoir. This may lead to increased dissolution and precipitation reactions ¹⁶. However, these reactions are generally very slow, although reactions involving the dissolution and precipitation of carbonate minerals tend to be quicker than those involving silicate minerals, such as feldspars and clay minerals. Consequently, in mature reservoir sandstones of the North Sea, in which the proportion of 'reactive' minerals is generally low, the amount of CO₂ dissolution and subsequent reaction could be very limited ^{17,18}.

However, mineral reactions will also be influenced by impurities present in the CO₂ stream, and it is important to determine whether these effects will be beneficial or deleterious. For example in the presence of SO₂ hydrolysis will form H₂SO₃ (a weak acid) and oxidation will form H₂SO₄ (a strong acid); from which H₂SO₄ and H₂S ¹⁹ may form. Modelling studies suggest that SO₂ will enhance acidification ²⁰ since it is more soluble than CO₂. However, it has also been suggested ²¹ that this may be moderated by limitations of mass transfer of SO₂ through the mixed gas phase. Studies of co-injection of H₂S indicate that the preferential dissolution of H₂S over CO₂ inhibits H₂S breakthrough ²². Other studies ²³ suggest the impacts of co-injected species may be relatively limited.

Where the reservoir rock is poor in sources of calcium or magnesium, such as the mature sandstones in the North Sea, reactions that liberate iron from iron oxides can be particularly important since FeCO₃ (siderite) might provide a stable mineral trap for injected CO₂ ²⁴. The key to this process are redox reactions that can reduce iron oxides in grain coatings to reduced Fe in solution. These reactions can be facilitated by the presence of impurities such as H₂S ²⁵ or residual CH₄/hydrocarbons in depleted gas fields. Natural analogues of bleached sandstones in exhumed hydrocarbon reservoirs reflect the reaction of iron oxides with methane or oil.

Over time, the contributions of the different trapping mechanisms change and different reservoirs will have different amounts of CO₂ trapped by the different mechanisms previously described. Reservoir characteristics such as structural geometry, porosity and permeability, wettability and injection rates will all influence the relative contributions of each trapping mechanism. For example, calculations for CO₂ storage in the Mt Simon Sandstone in the US Midwest suggest CO₂ may almost completely dissolve in 10,000 years when regional groundwater flow is taken into account. This dissolution also leads to extensive dissolution of feldspars and precipitation of secondary minerals ²⁶. However, structurally trapped CO₂ may persist for many thousands of years in reservoirs where capillary and solubility trapping is limited ²⁷.

To date, SRDM (structural, residual, dissolution and mineral) trapping effects have only been extrapolated to long timescales through numerical modelling ^{28,29}. Simulations predict a high contribution of dissolution trapping of the CO₂ remaining as free phase in the structural geological traps or in pore structure by capillary forces. However, long-term mineral trapping efficiency is expected to be low ^{30,31,27}. All these modelling studies suffer from an over-simplification of the reservoir geology (heterogeneity, groundwater flow, diagenesis, etc.) and there are still questions over the real impact and the uncertainty level of each SDRM trapping mechanism, especially for long time scales. The study of natural analogues might serve to calibrate these geochemical models with regard to mineral trapping.



Map (on top) and 3D model (bottom) of The Bunter closure 3/44, an analogue of the EEPR UK demonstration site in North Sea, Yorkshire.

There is still a great need to evaluate data quality, validity ranges, and inconsistencies

Currently available thermodynamic databases typically used by geochemical simulators are based on data sets that are valid only for limited pressure, temperature and salinity ranges as they were mostly derived from less saline, lower pressure and temperature applications (e.g. shallower groundwater studies). Despite increasing efforts to improve geochemical data bases by studies such as the "Yucca Mountain Project" or the "Thermoddem" project, there is still a great need to evaluate data quality, validity ranges, and inconsistencies.

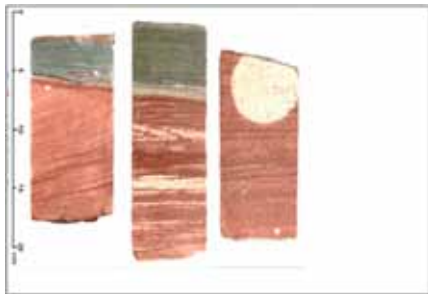
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Long-term sealing integrity of faulted and fractured caprock systems



Bundsandstein samples from natural CO₂ analogue site in Baden-Württemberg, Germany. These sandstone samples are also of special interest to analysis in workpackage 3 on reservoir trapping evolution



Figure 2: Opalinus clay from Mont Terri site. Cylindrical and gouged samples from these blocks will be used in laboratory investigations in workpackage 4



Figure 3: 4 by 8 cm cylindrical Opalinus clay sample of Mont Terri site

SUMMARY

Deep saline aquifers, together with depleted oil and gas reservoirs, have long been regarded as promising sites for the geological storage of CO₂. A crucial component for the success of long-term storage is the sealing integrity of the caprock on top of the reservoir.

Caprocks are typically dense, clay-rich or highly cemented rocks, or evaporites (crystalline sedimentary rocks) with a low permeability. However, due to the large-scale tectonic processes that helped form them they may contain fault zones or networks of fractures which could be further affected by the injection of CO₂. In particular, the resulting increase in reservoir pressure is predicted to partially counteract the force pressing opposing fault blocks or fracture walls together. This will decrease the friction between the blocks and could lead to movement along pre-existing faults or fractures. In addition, at higher pore pressures so-called tensile fractures may form. This interaction between fluid pressure and mechanical rock behaviour is called hydro-mechanical coupling.

Besides these hydro-mechanical processes, the potential chemical fluid-rock interaction is also important for the long-term sealing integrity of the caprock. The dissolution of minerals along fractures may cause, or accelerate, leakage and weaken the caprock. However, to counter this effect, the precipitation of minerals can also inhibit leakage. The actual chemical reactions are dependent on the reservoir itself, the caprock and brine composition, as well as the temperature, pressure and the presence of impurities in the injected gas.

ULTimateCO₂ is investigating the long-term sealing integrity of faulted and fractured caprock systems using a combination of data from petroleum field analogues, natural analogue studies, laboratory experiments, and numerical modelling. Although the petroleum industry has collected a large amount of data on the mechanical and flow properties of caprocks, this data typically only refers to caprocks unaffected by CO₂. ULTimateCO₂ will use laboratory experiments to contribute quantitative data on the evolution of the hydro-mechanical behaviour of fracture and faulted caprock as a consequence of chemical fluid-rock interaction. In addition, it is hoped that studies of the natural analogue can validate these reactions and the resulting short- and long-term changes in mineralogy. Finally, the chemical effects on the hydro-mechanical caprock integrity will be integrated in micro- and macro-scale numerical models. This will allow the upscaling of results to larger spatial and temporal scales and therefore an assessment of the caprock sealing integrity and quantification of possible leakage rates.

CURRENT STATE OF THE ART

The subsurface storage of CO₂ is only technically feasible if the long-term sealing integrity of the caprock, preventing leakage of CO₂ to the surface, can be guaranteed³². Analysis of caprock integrity is therefore an important part in the evaluation of storage sites^{33, 34, 35}.

Previous work conducted for the petroleum industry has provided a lot of information regarding fault stability and the role it plays in the migration and trapping of hydrocarbons³⁶. It is known that caprocks may contain pre-existing fractures and faults, as a result of mechanical loading during tectonic processes, and that the reactivation of a fault or fracture is dependent on the pore fluid pressure, stress orientation, stress magnitude, fault and fracture orientation and strength³⁷. Therefore, fractures may be induced or faults may be partially reactivated during gas extraction or the injection of CO₂ into depleted gas fields or deep saline aquifers.



Figure 4: Experimental setup for mechanical characterisation of fractured and chemically altered caprock samples

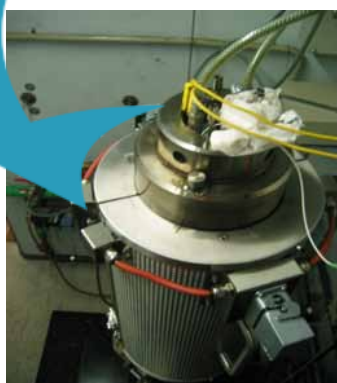
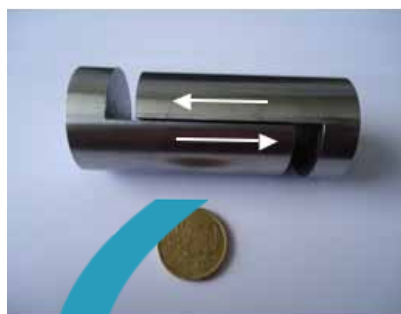


Figure 5: Experimental setup for direct shear experiments on simulated gouge-filled faults. During the experiment the direct shear assembly resides in the triaxial cell to simulate in situ pressure and temperature

As well as these hydro-mechanically coupled processes, the chemical fluid-rock interactions are important for the long-term caprock sealing integrity^{38, 39, 40}. The injection of CO₂, and its subsequent dissolution into the reservoir brine, may induce mineral dissolution and chemical reactions, thereby altering the mineralogy and the microstructure of the caprock. Although such fluid-rock chemical effects are generally slow⁴¹, a positive feedback between the reactive flow of CO₂-rich fluids and fracture propagation or fault reactivation may significantly alter caprock integrity in the long term. This is especially possible in the case of depleted gas reservoirs compartmentalised by sealed faults like K12B in the North Sea^{42, 43}.

Most studies focus on the mechanical integrity of, initially, intact caprock over timescales of a similar order as the injection phase^{1, 4, 44, 45, 46}. Accordingly, in order to assess the long-term sealing integrity of a caprock, it is necessary to quantify the interrelated effects of (1) the presence of discontinuities (i.e. faults and fractures) in the caprock and (2) interaction between CO₂-rich fluids and the caprock.

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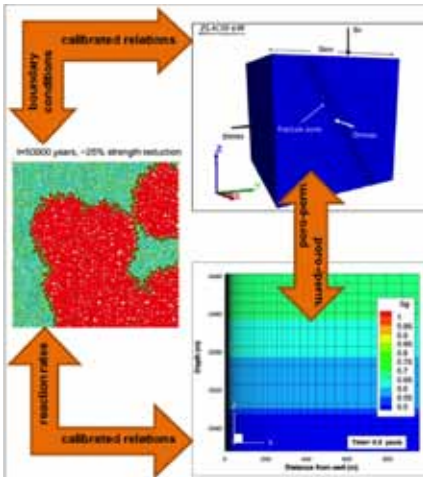


Figure 6: Coupled chemo-hydro-mechanical modelling at micro- and macro-scale using geomechanical (PFC, FLAC) and geochemical software (TOUGHREACT, PHREEQC)

reservoir at the K12-B field, North Sea, in M.

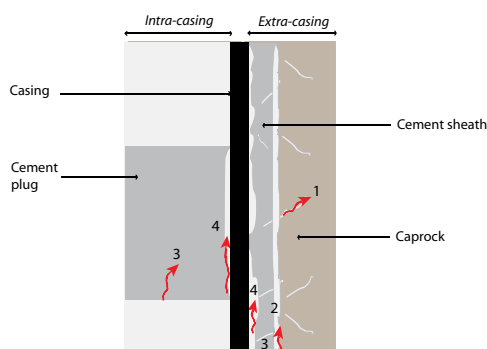
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Near-well leakage characterisation and chemical processes



Representation of possible leakage pathways through an abandoned well

The integrity of a well over time is essential for the fluids' confinement



Cement/Formation interface samples from a CO₂ production well (from Crow et al., 2010)

SUMMARY

Wells (decommissioned or active) drilled through a low-permeable caprock into a geological CO₂ storage site could act as potential connections between the CO₂ storage reservoir and overlying sensitive targets like aquifers. The integrity of a well over time is essential for the fluids' confinement (brine with or without dissolved CO₂ or buoyant gaseous CO₂).

Well integrity is defined as the capacity of the well to maintain the isolation of fluids in the subsurface reservoirs. To ensure this isolation, the well casing and the caprock are bonded by a cement sheath and, after abandonment, a cement plug is used to avoid upward migration within the casing. The behavior of this complete wellbore system and its long-term sealing integrity under influence of CO₂ is the issue addressed in this work package

CURRENT STATE OF THE ART

Well integrity has been the topic of a number of detailed reviews^{47,48} and, according to these, wellbore integrity might be compromised in several ways:

1. Operational defects – operational defects can be created by in situ operations. During the drilling, the caprock adjacent to the borehole can be damaged leading to potential fractures or other disturbances⁴⁹. The cementing process is also important and poor cement/caprock or cement/casing bonding might occur as a result of poor cement mixing or placement, or gas migration during cementing²⁷. During the life of the well, the pressure and temperature conditions might evolve, changing stress conditions, which might displace the casing, damage the cement sheet and lead to a loss in integrity of the cement sheet and of the bonding with the casing or the host rock²⁷. Well abandonment could also lead to the potential loss of internal isolation depending on the method and material used for the well plugging⁵⁰.
2. Chemical degradation – the wellbore could be potentially degraded through chemical interactions. In the context of geological CO₂ storage, several chemical environments are likely to exist around an existing well such as: dry supercritical CO₂ near the injection well, wet CO₂ (supercritical or gaseous CO₂ in equilibrium with the formation water) and CO₂-rich brine and native brine. Wet CO₂ and CO₂-rich brine have been shown to be the most aggressive environments²⁷. In these environments, the evolution of the well integrity according to the reactivity needs to be understood. Cement reactivity is of first concern and a significant amount of studies have already been carried out to characterise these interactions^{51,52,53,54,55}. However, some uncertainties still prevail regarding the impacts on cement degradation^{26,35}. Casing corrosion by CO₂ has also been studied as a potential reaction impacting the wellbore integrity⁵⁶.

The operational defects and the potential degradation induced by geochemical interactions may constitute leakage pathways. The location, in the wellbore environment, of these potential pathways is shown in Figure 1 and can be summarised as such:

- Migration through damaged zone in the caprock (1);
- Migration through the caprock/cement interface (2);
- Migration through degraded or fractured cement (sheath or plug) (3);
- Migration through the cement (sheath or plug)/casing interface (4).

The evolution of the well integrity is therefore a combination of several physical processes (including hydrological, mechanical, chemical...) on several materials and elements (formation, cement, casing, interfaces, annuli)²⁶. In addition to the previous and

The evolution of the well integrity according to the reactivity needs to be understood



Percolation bench used to assess well sealing integrity at the core scale in the ULTimateCO₂ project



Experimental setup installation at Mont Terri Underground Rock Laboratory to assess well sealing integrity at the well system scale in the ULTimateCO₂ project

ongoing work dedicated, mainly, to individual elements, some supplementary work has been focused on the interactions and/or evolution of flow occurring at the interfaces or defects between elements such as the casing/cement interface^{35,57} and the caprock/cement interface^{34, 58}.

Some field studies have assessed the consequences of the contact between wellbores and CO₂ in an EOR field⁵⁹ and at a natural CO₂ reservoir⁶⁰. A new methodology has been proposed to evaluate the effective permeability of the wellbore close environment considered as a damaged zone⁴⁹. This test has been performed on a number of existing wells^{39, 61, 41} and these studies show that the effective permeability in this region is higher than the permeability of cement or formation matrices. This suggests that some preferential flow takes place as these interfaces or through the damaged caprock and cement^{39, 62}. Although the results of these tests do not provide exact flowing paths, they give an indication of the hydraulic properties to be used in large-scale models.

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The long-term behaviour of stored CO₂, looking at the basin scale

SUMMARY

Saline aquifers are the main targets envisaged for large-scale CO₂ injection projects. These geological formations are represented by a deep (below 1000 m depth) underground layer of non drinkable water-bearing permeable and porous rock, which can cover large areas (up to 100 x 100 km²) to constitute a geological structure so-called "basin". For industrial-scale carbon capture and storage projects the amount of CO₂ injected into an aquifer could be as much as several million tons every year. The continuous injection of CO₂ over several decades could lead to the build-up of groundwater pressure over a much larger area (100 km) than that directly affected by the CO₂ injection itself (~km). And as the CO₂ is injected, the brine initially present will be displaced with a risk to migrate through faults or wellbore to reach overlying formations containing drinkable groundwaters. This effect will be directly influenced by the geological characteristics of the aquifer as well as the groundwater composition and its natural flow. Therefore there is a need to better characterise and understand these processes affecting the natural hydrological equilibrium of a geological basin.

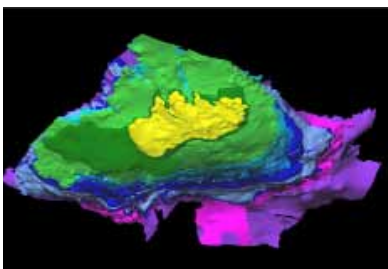


Geological map of the Paris basin (BRGM)

METHODS

In order to predict the potential effects of the build up in aquifer pressure, accurate modelling at a basin scale of the groundwater flow, together with any changes that might occur due to the injection of CO₂, is required. However, integrating complex physical processes that could occur simultaneously at different scales is not straightforward. For example, the flow of water through/along an aquifer can be considered large scale (100 km) whilst the movement of free CO₂, its dissolution into the water and capillary and mineral trapping occurs on a much smaller scale (from km to micrometer, respectively).

The numerical modeling of such basins consists in reproducing the different geological layers that evolved for several millions of years. To build such a static geological model, 3D grids are used and populated with properties like permeability and porosity to calculate dynamic processes like CO₂ or brine migration and pressure build up.



3D Numerical Geomodel of the 12 main horizons (from basement to surface) of the Paris basin

Using a small grid size to capture all these interactions would require a huge amount of computing time whilst using a larger resolution risks trivialising important factors and missing the impact that relatively small objects, such as fractures and wells, could make to the overall picture. To incorporate these issues and take into account all the physical and chemical processes within a reasonable computing time, it has been proposed to model brine displacement, due to CO₂ injection, with a multi-scale approach. The idea of the multi-scale approach is to use results from a fine-scale model (~10 km large) and transpose it into a large basin-scale model. This transposition can be made using upscaling methods or by locally refining the large-scale model in order to focus on a particular physical behaviour and/or to follow the movement of injected CO₂, the plume.

STATE OF THE ART

Whilst it is understood that continuous long-term injection of CO₂ for more than several decades will build up groundwater pressures in extensive regions, it has recently been suggested this may also have a hydrological impact on shallow groundwater resources^{63, 64}. In particular, investigations on regional groundwater at the Texas Gulf Coast Basin¹ suggest that CO₂ injection could cause groundwater pressure perturbation at up-dip aquifers. Other studies² suggest that seal permeability has a significant impact on pressure build up, and that pressure perturbation of shallow units may occur only when the permeability of sealing layers is higher than a microdarcy.

Integrating complex physical processes that could occur simultaneously at different scales is not straightforward

However, overall, brine migration has only been studied to a limited extent with the latest results indicating the importance of the geological properties of the storage site, including site heterogeneities, boundary connections (permeability) and overlying formations.

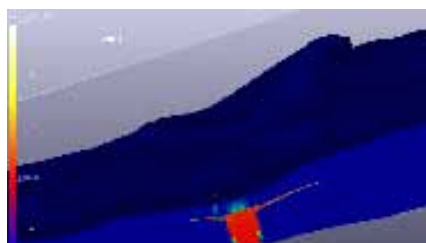
The simulation of CO₂-rich fluid migration inside a storage complex requires the use of a multi-scale approach to account for the complex physical processes that occur at different scales. It is known that the accuracy of the finite difference solution of flow equations is significantly affected by the grid size. A finer grid system⁶⁵ will lead to a smaller truncation error, more accurate modelling of the displacement front and, consequently, a more accurate solution but requires a long computation time. One solution to this issue could be the local grid refinement technique^{66,67} which could save computation time without compromising the accuracy.

Some of the potential issues that have to be addressed by this multi-scale modeling include:

- a) The pressure pulse caused by the injection of CO₂ could modify the hydro-mechanical properties of the borehole cement and existing faults allowing fluid leakage from the storage area^{68,69}.
- b) Possible changes in the hydrodynamic flow regime, the migration of brine through abandoned wells or permeable faults from deep reservoirs, driven by pressure increases resulting from CO₂ injection⁷⁰. This upward fluid migration could cause the chemical degradation, pollution, of groundwater reserves with brine, free CO₂ and/or water enriched with dissolved CO₂.
- c) Acidification due to CO₂ injection could induce mineral dissolution, thus triggering trace elements mobilisation, which could have a severe impact on the chemical water quality^{71,72}.

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Numerical modelling of CO₂ (in red) plume injected into a deep saline aquifer (in blue)

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SUMMARY

The main objective of ULTimateCO₂ is to gain a better understanding of specific physical and chemical processes involved in the long-term fate of geologically stored CO₂ and their impact on the long-term performance assessment of potential geological CO₂ storage sites. In this context, the role of uncertainty is of primary interest in addressing the following issues ⁷³ :

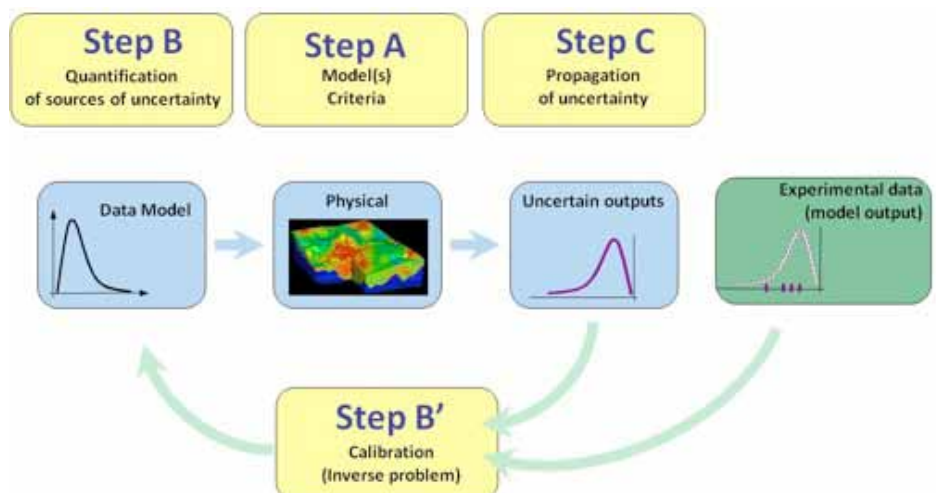
- What is the accuracy/best estimate value of the model's prediction?
- What level of confidence can be associated with the result?
- What sources of uncertainty are the most important to account for?
- What effort should be spent to characterise such a parameter?

These issues constitute the generic objectives of any uncertainty analysis ^{74 75} . However, the scientific and technical issues tackled by ULTimateCO₂ introduce major challenges for quantifying, comprehensively and with the least possible bias, the uncertainties in a storage site's performance prediction. Standard and commonly applied tools are inadequate to quantify, based on all major sources of uncertainty, performance prediction uncertainty. Moreover, how improved physics modelling reduces the bias and prediction uncertainty from models that use the currently available physics, is unknown. New methods will have to be developed to research this.

Apart from the classical performance prediction uncertainty due to the model's parametric uncertainty (poorly known permeability, etc.), using known and validated physics, difficulties in quantifying prediction uncertainty, i.e. comprehensively and with the least possible bias, arise from:

- Poorly known physical FCMT phenomena (Flow-Mechanical-Chemical-Temperature), which in principle should be coupled: multiphase flow, mechanical, geochemistry, temperature effects, etc.
- The sensitivity of the site's performance prediction uncertainty to these coupled phenomena, especially on the long-term scales applicable to CCS (several years to a few centuries);
- How the model's spatial resolution should be selected as a function of the (highly) non-linear (and long-term) processes is unknown.
- Particular challenges with up-scaling the problem where different types of data and information need to be combined and fed to the reservoir simulation model: lab tests, in-site tests, static models, dynamic simulation results, literature data, experts' information, etc.

Therefore, ULTimateCO₂ is seeking to address a compounded problem: a poorly defined reservoir and poorly defined (long term) physics. The challenge is to better understand how to distinguish parametric uncertainty from modeling uncertainty.

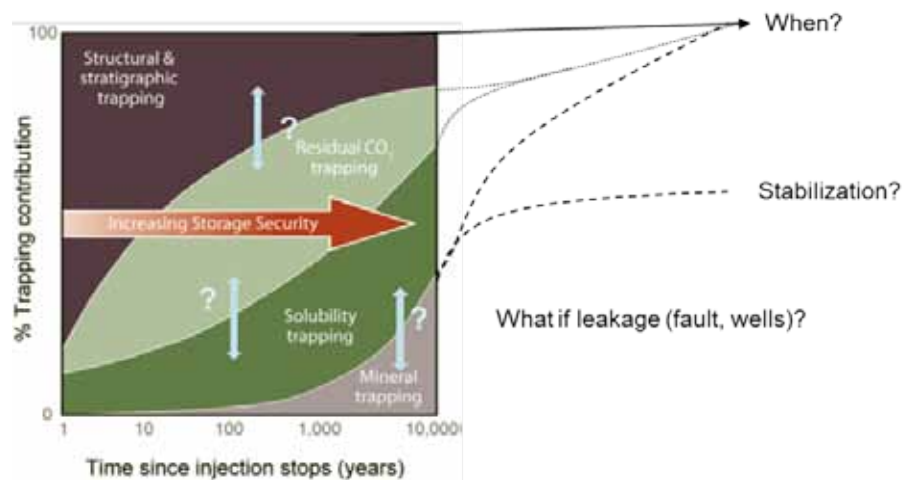


In this context, this work package is composed of two main parts:

1. The first part is focused on methodological developments to enhance and adapt existing methods to this new context;
2. The second part concentrates on transfer the uncertainty methodology and implementing it in the other work packages.

The objective is to generate generic learning, rather than case-specific lessons, although the uncertainty in the performance forecast will be a function of both the parametric uncertainty (i.e. case-specific) and the uncertainty in the physical relationships between these parameters (i.e. the generic part of the forecast uncertainty problem). Having a better understanding of how reduced/simplified/incomplete physics results in a forecast uncertainty bias, and how this bias can be reduced, is a major goal of ULTimateCO₂. In this context, this work package will develop "uncertainty quantification protocols" that will help the other work packages by:

1. Assisting in the design of modeling experiments that are likely to result in generic lessons;
2. Identifying the main sources of uncertainty in the modeling of the physical processes;
3. Assessing, in the context of scarce data and new data acquisition during a storage site's operations, how new information reduces performance forecast uncertainty;
4. Providing support and tools to assist in carrying out uncertainty assessment studies.



Uncertainty related to long-term fate of geologically stored CO₂

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EXPECTED OUTCOMES

Improving scientific knowledge on the long-term fate of geologically stored CO₂

Each technical work package will advance the knowledge of a specific long-term process

It is intended that the ULTimateCO₂ project will "provide the necessary insights to support the characterisation and assessment of potential storage sites and their surrounding areas as required in the Directive on geological storage, thus facilitating the large-scale deployment of CCS". Such a major, and broad, impact can only be achieved through a series of smaller, interrelated, steps.

IMPROVING SCIENTIFIC KNOWLEDGE ON THE LONG-TERM FATE OF GEOLOGICALLY STORED CO₂

The results of each technical work package will advance the knowledge of a specific long-term process: i) trapping mechanisms of CO₂ in underground geological reservoirs, ii) the sealing integrity of fractured caprock and faulted systems, and iii) the sealing integrity of wells. The results, based on laboratory and field experiments, plus real demonstration site data, will be combined and integrated to true-scale context. This will help define what to look for during the characterisation of a site for long-term CO₂ storage and also what to avoid, i.e. identification of any processes that might prevent permanent containment (potential leakage pathways, fluid mixing, etc.). The dissemination of this criteria to operators and regulators will help demonstrate under what conditions long-term site performance is likely to lead to permanent containment. Dissemination of this knowledge to the scientific community, through publications, participation in conferences and links with international and European networks (IEAGHG, CO₂GeoNet, etc.), will enable other parties working in CO₂ storage to benefit from these advances and, in turn, help to facilitate the large-scale demonstration of this technology.

INCREASING CONFIDENCE IN THE USE OF CCS

Confidence in the use of CCS will be increased through the dissemination of the project's results and the envisaged improved scientific knowledge to a wide audience of specific target stakeholder groups. This project will enable questions on the safety and efficiency of long-term CO₂ geological storage to be answered with increased confidence and backed up by scientific facts. This will play a significant role in increasing the social acceptance of CCS. The fact that the results will be based on real site data and contexts provided by at least two large-scale CCS demonstration sites associated with the project will bring additional credibility to the results.

The experience and confidence gained through ULTimateCO₂ will also benefit subsequent demonstration sites. Links have already been established with the appropriate French and UK governmental authorities as well as policy makers within the European Commission in order to facilitate the flow of information. Another way that ULTimateCO₂ will increase confidence is by tackling the uncertainty associated with long-term CO₂ storage, with assessments made throughout all the technical work.

RECOMMENDATIONS FOR CONSIDERING THE LONG-TERM PROCESS OF GEOLOGICALLY STORED CO₂

ULTimateCO₂ will develop a series of recommendations that should be considered when determining future sites for the long-term geological storage of CO₂. The improved understanding of long-term processes gained through ULTimateCO₂ will form the basis for these recommendations, drawn up in collaboration with a range of key stakeholders, to provide improved technical criteria for establishing the long-term permanent containment of CO₂. This will greatly improve the robustness and clarity of CO₂ storage regulations, a critical step in both the licensing process and also provide wider confidence that storage

operations will be safely decommissioned after site closure. This step is currently not specifically addressed as a separate issue in the European Directive 2009/31/EC on the geological storage of CO₂, and ULTimateCO₂ will help fill this knowledge gap and reduce the uncertainty associated with whether or not the stored CO₂ will be completely and permanently contained. The in-depth studies based on known geology (case studies), well location, fractures and faults, will help improve site selection, not only on the basis of reservoir capacity, but also in terms of global safety and integrity at basin scale.

