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ULTimateCO2: A FP7 European Project dedicated to the understanding of the long term fate of geologically stored CO2

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Abstract

ULTimateCO2 will assess the long-term CO2 storage behaviour in terms of efficiency and security. The project is dedicated to studying the main physical processes needed to develop a better, quantitative understanding of the long-term geological storage of CO2, namely: (i) reservoir trapping, (ii) sealing integrity of caprock, and (iii) well leakage. Close collaboration with the NER300 candidates and EEPR demonstration sites will underpin all investigation with relevant supply of data industrial context. ULTimateCO2 will define a set of recommendations that will enable both regulators and operators to demonstrate that site specific long-term site performance will lead to permanent and safe CO2 containment.

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Keywords: Long-term, storage, demonstration, guidelines

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1. Introduction

Although 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 EU Directive on the Geological Storage of CO2 requires operators to demonstrate that the long-term fate of the CO2 in the reservoir will ensure 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 state-of-the-art since, unlike other domains we currently have limited experience to draw on for this new technology.

2. Objectives of ULTimateCO2 FP7 Project

The aim of the ULTimateCO2 project is to significantly advance our knowledge of specific processes that may affect the long-term fate of geologically stored CO2 and yield improved and validated tools for predicting long-term storage site performance through a dedicated four-year collaborative programme covering:

i) Detailed laboratory, field and modelling studies of the most relevant physical and chemical processes and their impacts in the long-term, namely:
- o trapping mechanisms in the reservoir (structural, dissolution, residual and mineral [SDRM]);
- o fluid-rock interactions and effects on mechanical integrity of the caprock and the sealed faults;
- o leakage associated with mechanical and chemical damage in the well vicinity;

ii) Integration of the results into assessing the overall long-term behaviour of storage sites at reservoir and basin scale in terms of efficiency and security, and including other important aspects, such as far-field brine displacement and fluid mixing, integrity of sealed faults compartmentalising depleted gas reservoirs, and chemistry change in overlying groundwater resources due to leakage through abandoned wells.

The long-term prediction of CO2 evolution during geological storage will be made more robust by addressing the uncertainty associated with numerical modelling at all stages.

Several major funding programmes have been recently launched to promote the deployment of the CCS technology in Europe. In July 2009, the European Council and the European Parliament adopted the Commission's proposal for a European Energy Programme for Recovery (EEPR). The European Commission granted financial assistance to six projects judged best suited to making substantial progress in terms of demonstrating the CCS chain and facilitating future deployment. More recently, the NER300 funding programme was launched to grant 300 million EU emission unit allowances (EUAs) to fund about four CCS projects.

ULTimateCO2 will benefit from this rapidly evolving European CCS context by integrating data from such large-scale demonstration projects into its work programme, which was not easily possible until now. Demonstration sites will serve as a basis for investigating both long-term efficiency and safety of

CO2 storage at reservoir and regional scale, thus giving greater credibility to the results. Collaboration is already underway with two demonstration sites (Fig1):

• NER300 candidate ULCOS-BF in France operated by ArcelorMittal GeoLorraine (onshore sandstone deep saline formation in the North East of France);

• EEPR Don Valley demonstration site in the UK operated by National Grid (offshore North Sea sandstone deep saline formation and/or depleted hydrocarbon formations);

a) b)

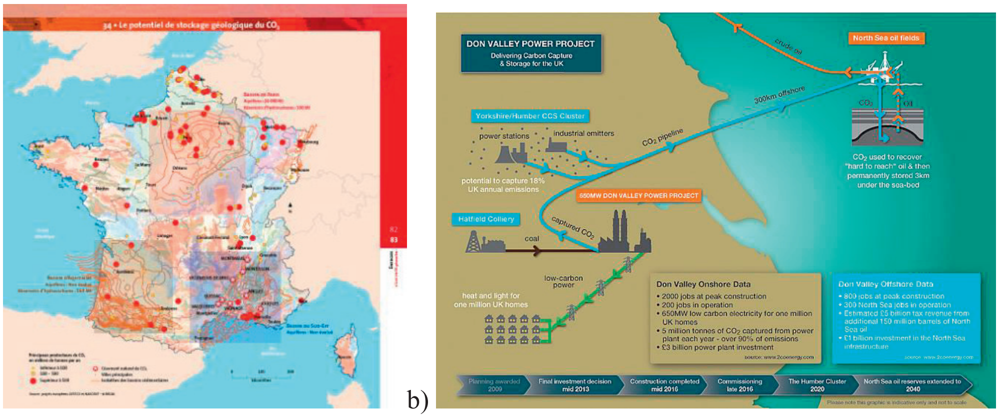

Fig 1: the onshore NER300 Ouest Lorraine candidate in France (ArcelorMittal GeoLorraine), the offshore EEPR Don Valley (ex-Hatfield) site in UK (National Grid) (picture taken from http://www.medstor.fr and http://www.energyroyd.org.uk).

In addition, the use of the Underground Rock Laboratory of Mont Terri (Switzerland) will also offer access through galleries to representative samples of caprock clay in order to perform unique experiments on well-leakage assessment (Fig 2).

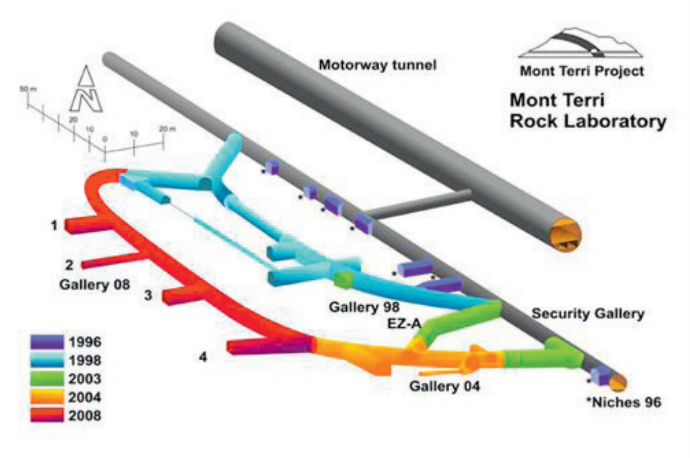

Fig 2: The Mont Terri Rock Laboratory

ULTimateCO2 will develop recommendations for operators and regulators to enable a robust demonstration of the assessment of long-term storage site performance, including an assessment of

appropriate timescales to establish safe 'permanent' storage. These will be developed by drawing on the lessons learned within the project, as well as relevant research internationally and through dialogue with targeted stakeholders.

3. Methodology for studying the long term fate of CO2 geological storage

The ULTimateCO2 project will foster progress and understanding in several domains of long-term processes of geologically stored CO2, as outlined below:

1.1. Far-field brine displacement and fluid mixing

Continuous long-term injections for more than several decades will build up groundwater pressure over extensive areas inducing fluid displacement and possible fluid mixing. Although brine migration due to CO2 injection has only been studied to a limited extent up to now, the results reveal the importance of having a good geological characterization of a potential storage site, taking into account heterogeneities, boundary conditions and overlying formations. Recently, it has been suggested that large-scale CO2 injections could have a hydrological impact on groundwater pressure perturbation at up-dip aquifers and even shallow groundwater resources (IEAGHG [1]; Nicot [2]; Person et al. [3]). The concern with upward fluid migration is that if there is intrusion into aquifers containing fresh water resources, the incoming fluid (brine, free CO2 and/or water enriched in dissolved CO2) may chemically degrade the groundwater. Acidification due to CO2 injection will induce mineral dissolution, thus triggering trace elements mobilisation, which can have a severe impact on the chemical water quality (Zheng et al. [4]).

ULTimateCO2 will address these issues by proposing a multi-scale approach to modeling brine displacement, associated with far-field pressure changes and pressure relaxation, after injection has ceased (see WP2 description of the project). The geological contexts of the demonstration sites and available field data will enforce the pertinence of the scenario framework. Modelling will be carried out at the basin scale and will include water quality assessment of both the storage formation but also the overlying groundwaters. The proposed modelling scenarios will help site operators in their investigations on appropriate technical elements required by the EU Directive for improving the long-term monitoring of the storage site.

1.2. Long-term reservoir trapping efficiency

To date, SDRM (structural, dissolution, residual and mineral) trapping effects have only been extrapolated to long timescales through numerical modelling (Le Gallo, [5]; Yamamoto et al. [6]). 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 (Audigane et al. [7]; Mito et al. [8]; Zhang et al. [9]). All these modelling studies suffer from the over-simplification of the reservoir geology (heterogeneity, groundwater flow, diagenesis, etc.) and questions are still raised concerning the real impact and the uncertainty level of each SDRM trapping mechanism, especially for long time scales. ULTimateCO2 will develop an extensive modelling strategy to assess and predict the long-term evolution of the SDRM trapping mechanisms as identified above (WP3). The interactions between the trapping processes will also be investigated through the coupling of mechanisms at reservoir scale. Eventually, new trapping vs. time plots will be delivered supported by a solid uncertainty assessment methodology (WP6).

Residual trapping is considered as the most rapid mode of trapping (Qi et al. [10]; Juanes et al. [11]). Residual trapping has two consequences: the gas immobilization itself and changes in capillary pressure and relative permeability curves. It has been integrated progressively in the modelling efforts undertaken to describe plume migration (e.g. Doughty [12]). Analytically, several works considered a residual gas saturation in sharp-interface models (Juanes et al. [11]; MacMinn et al. [13]) and in Buckley-Leverett models (Noh et al. [14]) but the hysteretic effects were ignored. UltimateCO2 proposes to develop a numerical modelling study taking into account history dependant phenomena and estimating the evolution of immobile gaseous CO2 across time according to different aquifer conditions, such as groundwater flow, aquifer tilt and the specific injection strategy, which could lead to wetting of the plume. Reactions with minerals may be influenced by impurities present in the CO2 stream, and it is important to determine whether they will be beneficial or deleterious. Take SO2 for example, hydrolysis will form H2SO3 (a weak acid); oxidation, will form H2SO4 (a strong acid); and disproportionateness will form H2SO4 and H2S (Palandri and Kharaka [15]). Modelling studies suggest that SO2 will enhance acidification (Knauss et al. [16]) since it is more soluble than CO2. However, Ellis et al. [17] suggested that this may be moderated by limitations of mass transfer of SO2 though the mixed gas phase. ULTimateCO2 will investigate through laboratory experimental approach and numerical modelling the potential for enhanced mineral trapping when trace gases present in the CO2 stream are co-injected, to test the results of previous modelling studies and identify most-likely reactions for given stream compositions and reservoirs. In cases where the reservoir rock is poor in Ca or Mg, such as the mature sandstones in the North Sea, reactions that liberate Fe from iron oxides can be particularly important since

FeCO3 (siderite) might provide a stable mineral trap for injected CO2. The key to this process is redox reactions that can reduce Fe oxides in grain coatings to reduced Fe in solution, and these can be facilitated by the presence of impurities such as SO2 or residual CH4/hydrocarbons in depleted gas fields. Natural analogues of bleached sandstones in exhumed hydrocarbon reservoirs reflect reaction of Fe oxides with methane or oil.

ULTimateCO2 will test these predictions through a combination of investigations in natural systems where such process are believed to have taken place in Europe and in the US., and through supporting experiments and geochemical modelling to identify the predominant conditions necessary for such reactions to take place.

Today, available thermodynamic databases commonly used by widely-distributed geochemical simulators are based on data sets that are valid only for limited pressure, temperature and salinity ranges as they were mostly derived from lower pT and less saline applications (e.g. shallower groundwater studies). Despite increasing efforts to improve geochemical data bases (e.g. in the “Yucca Mountain Project”; cf. Wolery et al. [18], or in the “Thermoddem” project; http://thermoddem.brgm.fr), there is still a great need to evaluate data quality, validity ranges, and inconsistencies. ULTimateCO2 will identify the parameters which contribute the most significant uncertainties within geochemical simulations and will apply quality criteria to geochemical databases, providing recommendations on acceptable parameter value ranges.

1.3. Long term sealing integrity of faulted and fractured caprock systems

Subsurface storage of CO2 is only meaningful if the long-term mechanical integrity of the caprock, preventing leakage of CO2 to the surface, can be guaranteed (e.g. Hawkes et al., [19]). Analysis of caprock integrity is therefore an important part in the evaluation of storage sites (e.g. Rutqvist et al. [20]; Vidal-Gilbert et al. [21], Orlic et al. [22]). Caprocks may contain pre-existing fractures as a result of mechanical loading during tectonic processes. Change of the stress state can potentially trigger the development of new fracture networks and reactivate existing faults in the caprock. Therefore, fractures may be induced or faults may be partially reactivated during gas extraction or CO2 injection in the case of

storage in depleted gas fields or during CO2 injection in case of storage in deep saline formations. CO2 injection and dissolution in the brines present 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 slow (Hangx et al. [23] [24]), a positive feedback between reactive flow of CO2-rich fluids and fracture propagation or fault reactivation may significantly alter caprock integrity in the long term, especially in the case of depleted gas reservoirs compartmentalised by sealed faults like K12B in the North Sea for instance (van der Meer et al. [25]; Audigane et al. [26]). Most studies focus on the mechanical integrity of initially intact caprock at timescales of similar order as the injection phase (Rutqvist and Tsang [27]; Hawkes et al. [19]; Rutqvist et al. [20]; Busch et al. [28]; Orlic et al. [22]). Accordingly, for assessment of the long-term sealing integrity of 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.

ULTimateCO2 will investigate the long-term sealing integrity of faulted and fractured caprock systems by a unique combination of data from petroleum field analogues, outcrop studies, experiments, and numerical modelling.

1.4. Near-well leakage characterisation and chemical processes

Wells drilled through low-permeable caprock create potential connections between the CO2 storage reservoir and sensitive targets such as overlying and superficial aquifers. Long-term well sealing integrity is therefore essential for fluid confinement. Cement reactivity is particularly of primary concern and a significant amount of studies have been carried out to characterize these interactions (Kutchko et al. [29]; Duguid and Scherer, [30]; Wigand et al. [31]). Integrity can also be decreased due to operations. During drilling, the caprock can be damaged leading to the formation of an excavation damaged zone; the quality and placement of the cement during the completion is also essential for a suitable bounding. All these steps may lead to the creation of annular pathways within the compartments and at the interfaces (i.e. caprock – cement sheet; cement sheet – casing; casing – cement plug), (Gasda et al. [32]). The migration of fluids through these paths may lead to geochemical processes possibly enhancing the lack of sealing integrity (Carey et al. [33]). Understanding the nearwell sealing integrity therefore requires studying the potential pathways and associated migration via altered well compartments, but also along interfaces with deficient bounding: it implies the study of the well environment as a whole. So far, this issue has only been investigated using synthetic interfaces (e.g. Bachu and Bennion, [34]; Carey et al. [33]) and simulating the flow of CO2 and brine in the laboratory.
To go beyond these limits, UltimateCO2 proposes an integrated framework comprising field experiments, laboratory experiments and modelling efforts in the aim of evaluating the conditions of a good well-sealing integrity on the long-term scale. To this aim, UltimateCO2 will drill a wellbore in a caprock-like formation from the Underground Rock Laboratory of Mont Terri (Switzerland), and then investigate the consequences of the contact between the wellbore features and a CO2 stream containing impurities in caprock-representative conditions (Manceau et al., [35]).

1.5. Uncertainty assessment in the long-term modelling of CO2 storage

Due to the complexity of the chemical and geo-mechanical processes that affect the long term fate of CO2, it has been recognized that a careful modelling of uncertainties is required together with the estimation of their impact onto the simulation results. The first step is to assess the sources of uncertainty. As far as large scale geological systems are concerns two specific features have to be addressed, namely the small amount of data and the spatial variability aspects. When assessing the effects of sources of

uncertainty onto predictions ("propagation" of uncertainty through the simulators), the third specific feature of geological models is the computational cost: it is important to use state-of-the-art methods for uncertainty propagation that are parsimonious in terms of runs of the simulators: to this aim surrogate models shall be built.

When dealing with uncertainty, it is important to recognise two basic kinds that are fundamentally different from each other: natural and epistemic uncertainty (Apostolakis, [36]). Whereas the former is described as arising from inherent variability or randomness in the studied systems, the latter stem from sparse, incomplete and imprecise information such as expert's beliefs about some unknown parameter. This distinction is useful in pragmatic terms, because if uncertainty is due to variability, concrete action must be taken to circumvent the potential dangerous effects of such variability, whereas if uncertainty is due to incomplete information, the best action is gaining more information.

Given that the results of the long term process studies (WP3, 4, 5) will be integrated at the basin scale (WP2), the second issue to be tackled is the representation of the uncertainty introduced by the spatialization (i.e. upscaling) of the input parameters at the scale of the sedimentary basin (extending over several tens of kms). When data is available in sufficient amount, especially the number of wells, the spatial uncertainty is classified as spatial variability and can be modelled using geostatistics (Chilès & Delfiner, [37]) and random field techniques (Ghanem and Spanos, [38]). However, in the context of scarce data, such an issue will require the development of specific methods combining spatial variability representation and lack of knowledge representation, for instance based on modern uncertainty theories (Loquin and Dubois, [39]).

Due to the computational cost of a simulator at the reservoir or the basin scale, it is crucial to develop uncertainty propagation methods that are parsimonious in terms of runs of the model. Brute-force methods such as Monte-Carlo simulation which may require thousands of runs are thus excluded. Recently various methods have been proposed in order to build surrogate models (also called emulators) that are almost costless-to-evaluate analytical functions that mimic the original simulator. Among others, kriging surrogate (Santner et al., [40]) and polynomial chaos expansions (Blatman and Sudret, [41], [42]) have proven efficiency in the domain of structural and fluid mechanics, among others.

ULTimateCO2 will integrate uncertainty assessment by (i) performing a literature review on relevant methods of uncertainty and sensitivity analysis for CO2 simulation models, (ii) identifying sources of uncertainty using either classic statistical methods or expert judgement through workshop discussion, and (iii) adopting a method of uncertainty propagation using epistemic uncertainty approach and surrogate models to improve interpretation of long-term predictions in consultation with modellers during workshops. The implementation of the methodology will be assessed during dynamic modelling to estimate the impact on long term trapping mechanisms evolution.

The ULTimateCO2 work programme contains seven work packages to address all these specific issues (Fig 3).

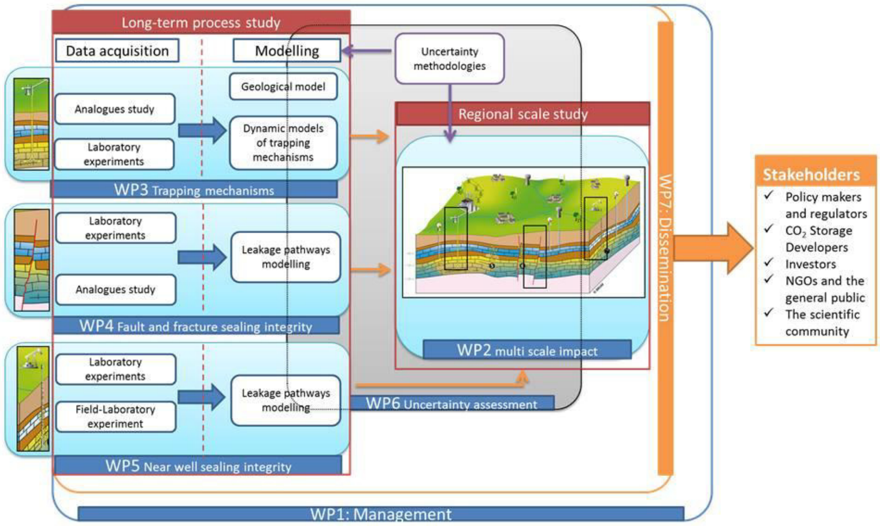

Fig. 3. The work package structure for ULTimateCO2 project

4. Conclusion and perspectives

The ULTimateCO2 project started in December 2011 and will last for 4 years. ULTimateCO2 will assess the long-term CO2 storage behaviour in terms of efficiency and security. The project is dedicated to studying the main physical processes needed to develop a better, quantitative understanding of the long-term geological storage of CO2, namely: (i) reservoir trapping mechanisms, (ii) sealing integrity of fractured and faulted caprock, and (iii) leakage through interfaces in the well vicinity. The research programme will comprise laboratory experiments, numerical modelling application and development, field data implementation and review of natural and industrial analogue evidence. Close collaboration with the NER300 candidates and EEPR demonstration sites will underpin all investigation with relevant supply of data industrial context. ULTimateCO2 will define a set of recommendations that will enable both regulators and operators to demonstrate that site specific long-term site performance will lead to permanent and safe CO2 containment. This will enable robust storage and allow clear conditions to be established for post-closure liability transfer. Web site: http://www.ultimateco2.eu

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