Programme Area: Carbon Capture and Storage

Project: Storage Appraisal

Title: Summary of Dynamic Modelling Scoping Studies

Abstract:

This document is a supporting document to deliverable MS6.1 UK Storage Appraisal Final Report.

Context:

This £4m project produced the UK's first carbon dioxide storage appraisal database enabling more informed decisions on the economics of CO2 storage opportunities. It was delivered by a consortium of partners from across academia and industry - LR Senergy Limited, BGS, the Scottish Centre for Carbon Storage (University of Edinburgh, Heriot-Watt University), Durham University, GeoPressure Technology Ltd, Geospatial Research Ltd, Imperial College London, RPS Energy and Element Energy Ltd. The outputs were licensed to The Crown Estate and the British Geological Survey (BGS) who have hosted and further developed an online database of mapped UK offshore carbon dioxide storage capacity. This is publically available under the name CO2 Stored. It can be accessed via www.co2stored.co.uk.

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Appendix A5.1

Summary of Dynamic Modelling Scoping Studies

Conducted for

The Energy Technologies Institute

By

RPS Energy

Heriot-Watt University

Imperial College

Author	Eugene Balbinski, Eric Mackay, Jeff Masters, Branko Bijeljic
Technical Audit	
Quality Audit	
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Executive Summary

The purpose of this preliminary work was to define a common approach for the dynamic modelling including the physical processes to be represented, modelling tools to be used, the definition of common/standardised parameters and a basis for the recommendations. This was achieved through an extensive literature review, investigation of modelling software and modelling assessments. The following main recommendations were made.

Modelling gravity effects with a sufficiently fine grid where needed is important. The solubility of CO_2 in brine and the effect of capillary pressure should normally be included in dynamic models, but the effect of diffusion is not likely to be significant. The effect of hysteresis on relative permeabilities will be required to model residual trapping as it may be an important trapping mechanism after injection has ceased for poorly confined structures.

It was concluded that the bulk of the dynamic modelling could be performed isothermally with sufficient accuracy using the industry standard finite difference 'black-oil' simulator ECLIPSE100™, and appropriate PVT data input, which was defined. This solution has the advantage of speed over the ECLIPSE300™/CO2STORE module compositional combination. It was proposed that a streamline simulator, such as 3DSL™, be considered for simulation of fine scale models of Exemplar open aquifer units as this would enable greater detail to be modelled due to faster run speeds. Streamline simulation is particularly effective where modelling displacement is more important than pressure changes, as for open aquifers. It was also proposed that a single simulator, GEM™, be used for well injectivity and associated thermal and geomechanical sensitivity calculations.

It was recommended that the most comprehensive set of consistent CO2/brine relative permeability and capillary pressure data available from a Canadian dataset be used for the modelling.

Contents

List of Tables

1 Introduction

When modelling storage of CO_2 in geologic formations, many different and complementary approaches may be taken. Each has its own strengths and weaknesses, and is thus better suited to answering one type of question rather than another. Within any specific group (for example finite difference simulation), there are different software packages capable (or not) of representing various physical processes such as solution of CO_2 in brine, vaporisation of water into CO_2, varying temperature and/ or salinity etc. Further choices exist with regard to different (but arguably equally valid) input data, including relative permeability functions and CO_2 properties (particularly viscosity correlations). The purpose of these scoping studies was therefore to define a common approach for the dynamic modelling. This purpose was achieved from an extensive literature review, investigation of modelling software and modelling assessments. This Appendix is a condensed summary of several more detailed project reports.

2 Physical Properties and Mechanisms

2.1 Gravity

A correct definition of gravity flow will be critical in the appraisal of CO_2 sequestration schemes. A significant density difference of the order of 200 kg/m^3 exists between the aqueous and CO_2 rich phases. Some important issues are:

- Scoping simulations indicate that utilisation of storage volume is usually dominated by the tendency of the CO_2 rich phase to rise within the system.
- The vertical flow of CO_2 can be interrupted by shales or other low permeability material.
- The presence of small shales and other low permeability material cannot be directly modelled within large grid blocks. The usual treatment is to use a suitable value for the ratio of vertical to horizontal permeability in order to define vertical permeability, augmented by inter-cell transmissibility multipliers where appropriate, and possibly pseudo relative permeability.

The main modelling technique is to ensure the grid has sufficient vertical refinement to capture the CO_2 at the top of structures.

2.2 Capillary Pressure

Scoping simulations with and without capillary pressure, utilising the recommended data suggest that, in the absence of heterogeneities with low permeability, the effects of capillary pressure are unlikely to be significant. Such effects may be more significant where there is a possibility of flow between low and higher permeability rock, for example, if modelling the cap rock.

2.3 Residual Trapping

It is expected that residual trapping will tend to become more important after the end of CO_2 injection as relative permeability hysteresis mechanisms come into play, though this may take a considerable time. Residual trapping may therefore be a key factor affecting long-term fate and storage security in stores which are relatively unconfined.

2.4 Diffusion

Diffusion coefficients for CO_2 in water have been measured and are typically four orders of magnitude smaller than for CO_2 in gas.

Analytical calculations and simulation modelling have been used to estimate the rate of dissipation of a CO_2 plume by diffusion through an aqueous phase. The distance travelled was less than 100m after 1000 years. Approximately 100 million years is required for half of the CO_2 to migrate from the original accumulation. This suggests diffusion is unlikely to be a major consideration for CO_2 sequestration on the site or formation scale.

Diffusion is unlikely to be an important process at the field scale though it may be more important when thin, low permeability zones are present, as transverse diffusion into these layers could enhance pore volume utilisation. To effectively model physical dispersion due to heterogeneity it is important to ensure that all significant heterogeneities are adequately represented, preferably by using a fine grid.

2.5 Convective Dissolution of CO_2

A two-dimensional model was set up to estimate the timescale for dissolution of CO_2 promoted by convective mixing. This was estimated to be of the order of hundreds of thousands to millions of years indicating that convective dissolution is unlikely to be a dominant mechanism for CO_2 sequestration on the injection timescale.

There are many simulation studies which support this conclusion, for example, (Gorecki et al, 2009), found that at the end of CO_2 injection, CO_2 dissolution only contributed about 3% to the total CO_2 stored.

2.6 Thermal Behaviour

Scoping studies with an analytical solution indicated that the temperature effect due to injecting CO_2 at a temperature significantly different to the initial formation temperature extends to about 1000 m after 50 years of injection, but the region of maximal temperature change is typically limited to less than 300 m from the well. A simple TOUGH -2™ simulation study also concluded that the temperature effect for extended CO_2 injection is limited to the near well region and would not significantly impact CO_2 storage.

The temperature effect can affect the formation of a solid phase. However, as the water-rich phase is typically vaporised in the near well region regardless of temperature, the solid phase due to an immobile aqueous phase will largely be the same.

It is recommended that temperature modelling is only used for near well injectivity or possibly detailed Exemplar calculations. However, it may be necessary to include temperature effects in geochemical and geomechanical simulation.

2.7 Geochemical Behaviour

Geochemistry may impact CO_2 storage in two regards. Firstly, the composition of the brine will affect parameters such as the solubility of CO_2 in the brine, and the brine density and viscosity, which in turn will affect the displacement process. Secondly, mineral reactions may lead to dissolution of cements in the near injection zone, and precipitation deeper within the formation.

Experimental data for the mineral reactions at temperature, pressure and salinity typical of candidate storage formations are very limited, and hence benchmarking of the numerical tools for modelling these processes is also limited at present. Furthermore, these calculations tend to be computationally very intensive. PHREEQC™, GEM-GHG™, TOUGHREACT™, Reveal™ and ECLIPSE300™/CO2STORE™ were reviewed for extent and accuracy of geochemical calculations, full field fluid transport modelling, and ease of use (data input, error checking, data output and run times).

While injected impurities potentially impact the phase behaviour, none of these models are currently capable of taking all the effects fully into account. Experimental research is currently ongoing at Heriot-Watt University (a project participant), but adaptations to the commercial software will not be available within the timeframe of this project.

It is not considered that mineralisation will be an important factor in determining aquifer storage capacity as this process tends to occur over periods much longer than the injection period. Therefore it is not advised that mineral reactions be included in long term storage calculations. However, dissolution of minerals in the near injection zone may impact integrity of the formation and caprock, and thus calculations should be performed to quantify this. Such calculations should ideally only be performed where formation mineralogy data is available, however, we propose including some simple sensitivity calculations for the well injectivity modelling. Although it is anticipated that all the potential simulation tools will be upgraded over the coming months and years, currently GEM-GHG™ is the tool of preference for these calculations.

2.8 Geomechanical Behaviour

The results from coupled geomechanical and flow simulations can indicate how close a system is to fracturing, or show locations where faults may be reactivated. This is most likely to occur near the injection point, or in the caprock above the injection point. Since the pressure build-up is one of the limiting factors for CO_2 storage, account should be taken of geomechanical effects. On the other hand, when using geomechanical simulations, extra grid cells must be included around the main model region, and this makes the simulation time much longer. It is suggested that some geomechanically coupled simulations are performed in both the single well injectivity models and possibly in the detailed Exemplar models, particularly in the near-well region. Whether to perform such Exemplar calculations will depend on the availability of geomechanical data.

3 Software

TOUGH -2™ and various ECLIPSE™ related options were investigated for finite difference simulation of representative structures. PHREEQC™, GEM-GHG™, TOUGHREACT™, Reveal™ and ECLIPSE™300/CO2STORE™ were reviewed for geochemical calculations, ECLIPSE™/VISAGE™ and GEM-GHG™ for geomechanical modelling.

TOUGH -2™ is an academic research simulator which has good capability in terms of CO_2 modelling, including a thermal option. As such, it might have provided an inexpensive choice for Representative Structure modelling, however, it lacks several features considered essential for this project, including equilibration, industry standard grid definition, tabular relative permeability input and hysteresis, well modelling controls such as pressure limits and input/output interfaces. However, it has been useful in checking and identifying what other codes do, and also in providing a thermal modelling capability.

Schlumberger's ECLIPSE™ reservoir simulators offer a range of industry standard finite difference modelling options for CO_2 injection. ECLIPSE100™ is a standard 'black-oil' simulator, which means it can only model a limited number of components to represent oil, water and gas. For example, it could not model the nitrogen content from injected flue gas. An extended black-oil model can be used to model CO_2 injection into aquifers, though only for isothermal cases and uniform salinity. CO_2 may dissolve in the aqueous phase and the water is allowed to vaporise. This requires some care in generating the necessary PVT data which could be done by coding up data correlations in a spreadsheet or by running the TOUGH -2™ ECO2N module and extracting the required data from its output.

ECLIPSE300™ is a compositional simulator which, for example, allows injected CO_2 and nitrogen to be defined as separate components. However, an appropriate equation of state would need to be defined to do this. ECLIPSE300™ can be used in conjunction with a new Schlemberger module, CO2STORE™, which is licensed separately and is designed to facilitate modelling CO_2 injection into aquifers. It is believed that CO2STORE™ employs reasonable models and correlations to represent the behaviour of CO_2. Use of CO2STORE™ reduces the data entry required, say by comparison with using ECLIPSE100™. However, CO2STORE™ also does not allow modelling of a nitrogen impurity in injected CO_2. If it were desirable to model a nitrogen impurity the ECLIPSE300™ GASWAT option does have this capability, though it has the disadvantage of having a less accurate CO_2 solubility model compared to CO2STORE™.

Comparison of modelling results between the combination of ECLIPSE300™ and CO2STORE™ and ECLIPSE100™ for a range of temperatures and pressures suggest that for isothermal modelling there is no significant loss of accuracy in using ECLIPSE100™ for CO_2 storage in saline aquifers. In particular storage capacities calculated using both software routes are similar.

VISAGE™ may be used to model geomechanical effects using an equivalent material formulation to model the rock mass. The rock behaviour is represented by an intact component and a joint set(s) component. The latter component can be used to model fractures and faults. Within the coupling process the stress/strain state of the geomechanical model can modify the porosity and permeability of the intact component and the permeability of the fractures and faults. VISAGE™ can be coupled with ECLIPSE300™.

PHREEQC™ is a general purpose geochemical model, but it only allows the user to simulate one-dimensional reactive transport, and so is only of use in validating the geochemical calculations from the three-dimensional models.

TOUGHREACT™ is a very versatile model in terms of the potential to perform geochemical calculations. However, it suffers similar limitations to TOUGH-2™ in terms of ability to perform conventional reservoir simulation calculations.

GEM-GHG™ is an equation of state geochemical compositional simulator for modelling CO_2 storage processes. The simulator uses an adaptive implicit discretisation technique to model the component transport in porous media. The oil and gas phases are modelled with an equation of state, the gas solubility in the aqueous phase is modelled with Henry's law. Geochemical reactions, i.e. chemical equilibrium reactions between aqueous components and mineral dissolution and precipitation are available. Vaporisation of water into the gas phase, solid (asphaltene) precipitation, thermal effects and leakage through cap rock and sealing faults are also modelled. GEM-GHG™ also includes a geomechanics module, which allows for simulation of impact of effective stress variations.

Streamline simulation is an alternative simulation technique to traditional finite difference reservoir simulators, ideal for the study of nearly incompressible flows in heterogeneous domains. It is particularly effective where modelling displacement is more important than pressure changes, as for less confined structures or open aquifers. It is proposed that a streamline simulator, (such as 3DSL™, or participant Imperial College's in-house simulator) be considered for simulation of fine scale models of Exemplar open aquifer units, as this would enable greater detail to be modelled due to faster run speeds. The Imperial College in-house simulator can account for multiphase flow, relative permeability hysteresis, compressible fluids and rate-limited reaction.

4 Recommendations

Recommendations generally refer to the modelling approach for Representative Structures (RS), rather than Exemplar Modelling unless specifically stated.

4.1 Physical Properties and Mechanisms

It is recommended that solubility of CO_2 in brine be included as it is modelled relatively easily. Capillary pressure effects might have some significance in the presence of heterogeneities and so should also be included, at least for such cases. As dispersion will be important on the site scale its effects should be accounted for by modelling heterogeneities with sufficiently fine gridding. However, it is recommended that diffusion not be modelled as its effects are unlikely to be significant on the site scale.

Isothermal modelling of Representative Structures (RS) is recommended as sufficient because thermal effects are expected to be localized around injectors on injection timescales. Similarly it should not be necessary to model geomechanical and geochemical effects for RS providing appropriate pressure limits are included. However, thermal, geomechanical and geochemical effects may need to be modelled for well injectivity calculations which will feed into the RS modelling and into detailed exemplar calculations.

4.2 Software

It was concluded in section 3 that ECLIPSE100™ is adequate for isothermal modelling. The combination of ECLIPSE300™ and CO2STORE requires not just licenses for these codes but also for ECLIPSE100™. This combination, though convenient, is relatively expensive compared with the ECLIPSE100™ option. The ECLIPSE100™ option may also have other advantages in that it may require less running time and, in practice, will have more multiple copies available, if many simultaneous simulations are being run. It is therefore recommended that ECLIPSE100™ be used for the standard isothermal RS simulations. However, some access to ECLIPSE300™/CO2STORE™ for checking, sensitivity calculations or Exemplar modelling may still be required.

Simulations requiring coupled geomechanical or geochemical modelling should be carried out using GEM-GHG™. The advantage of this approach is that the functionality of the single code can be used, and there is as high a degree of confidence in the calculations as can reasonably be expected given the lack of experimental data currently available to validate any of the models. Project participant Heriot-Watt University has developed expertise in performing these calculations using GEM-GHG™ and ECLIPSE™/CO2STORE™. Heriot-Watt consider that translation between ECLIPSE™ and GEM™ datasets will be feasible using the CMG Builder software.

4.3 Standard Dataset

How much data specification is required will depend on the software used. For example, for ECLIPSE300™/CO2STORE™ correlations are built in, so less data needs to be specified. Recommended 'black-oil' (e.g. ECLIPSE100™) PVT input, relative permeability and capillary pressure data as identified below have been generated and collated.

It is not appropriate to include geochemical effects in the RS modelling, although some limited geochemical sensitivity calculations will be performed for injectivity modelling and possibly for

Exemplar modelling. The standard injection composition for RS modelling should therefore be pure CO_2.

Although other measurements are available, the most comprehensive set of consistent CO_2/brine relative permeability and capillary pressure data is from a Canadian dataset produced by (Bennion and Bachu, 2008). Other data are available from measurements on Berea sandstone at Stanford (Benson et al, 2008). It is recommended that consistent sets of relative permeability and capillary pressure data be used. Our recommendations for various permeability intervals are given in **Table A5.1** below. All these recommended datasets are from sandstones and have both measured relative permeabilities and capillary pressures, but only some have imbibition and drainage relative permeabilities. There are no imbibition capillary pressure data available.

Formation	**Permeability Range (mD)**	**Measured Imbibition Data Available**
Calmar	< 0.1 mD (shale, caprock)	Yes
Viking 1	0.1 to <10 mD	No
Viking 2	10 mD to 100 mD	Yes
Berea (Stanford)	> 100 mD	No

Table A5.1: Relative Permeability and Capillary Pressure Recommendations

Black oil PVT tables were generated in ECLIPSE100™ format using the TOUGH-2™ ECO2N module (Pruess, 2005).

5 References

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