Programme Area: Carbon Capture and Storage

Project: Storage Appraisal

Title: Definition of Dynamic Modelling Approach

Abstract:

Use of mathematical modelling to assess dynamic effects on storage of CO2 forms a key part of the UK Storage Appraisal Project methodology. This report reviews potential modelling techniques and identifies the most appropriate approach to be used in UKSAP.

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.

Approach for Dynamic Modelling of CO2 Storage in Deep Saline Aquifers – Summary Report

Prepared for

Energy Technologies Institute

Date: March 2010

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Approach for Dynamic Modelling of CO2 Storage in Deep Saline Aquifers – Summary Report

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1. EXECUTIVE SUMMARY

The purpose of Task 4.1 was to define a common approach for the dynamic modelling. This has been done from an extensive literature review, investigation of modelling software and our own modelling assessments.

The deliverables for Task 4.1 are a short electronic report addressing key issues for the dynamic modelling tasks, with recommendations regarding:

- The physical processes to be represented;
- Under what circumstances;
- Which simulator(s) should be used;
- Common/ standardised parameters;
- Basis for the recommendations
- Task 4 deliverables, acceptance criteria and distribution of activities amongst participants up to the relevant Stage Gate.

The deliverables are provided in this short document, however, support for these recommendations is provided in section 3 and in greater detail in several associated technical reports. Recommended standard input data is provided on the UKSAP Sharepoint website. Recommendations, unless specifically stated, generally refer to the modelling approach for Representative Structures (RS) for Task 4.3, rather than Exemplar Modelling, which is to be covered in Task 4.4. The project plan requires Exemplar Modelling to be specified at the Stage Gate.

The solubility of CO2 in brine and the effect of capillary pressure should be included in RS models. Diffusion and the effect of hysteresis on relative permeabilities and capillary pressure should not normally be included in RS models. Hysteresis effects will be required if it proves necessary to model residual trapping, for example in poorly confined structures. However, it is recommended that hysteresis effects be included as a sensitivity in Exemplar modelling.

The bulk of the RS modelling should be performed isothermally using the industry standard ECLIPSE100™ 'black-oil' simulator. Appropriate standard input data has been placed on the UKSAP SharePoint website. The combination of the ECLIPSE300™ compositional simulator and the CO2STORE module need only be used for checking and sensitivity calculations. The GEM™ simulator should be used for well injectivity and associated thermal, geomechanical and geochemical sensitivity calculations.

The original proposal included a description of how the RS modelling would be undertaken. However, it is essential to prove the applicability of the RS modelling concept before this programme can be successfully implemented. The following issues have been identified which require work to resolve with the initial RS models:

- feasibility of modelling with likely North Sea CO2 injection rates and durations, and consequent model size/ boundary conditions
- the need for a simple and practical but appropriate method of determining CO2 storage efficiency factors from simulations including when to calculate it
- the need to represent the effect of lower permeability rock on likely injection timescales and the simplest effective way to do this.

A programme of work addressing these issues has been specified. The acceptance criterion remains the demonstration of the practicality of implementing the Representative Structure modelling concept.

Conditional on the outcome of some confirmatory studies, it is provisionally recommended that Storage Efficiencies normally be calculated for the RS models at the end of the CO2 injection period. This provides a practical termination point for these simplified models and avoids prohibitively long run times. Except for unconfined sites which depend on residual trapping to store CO2, it is likely that storage efficiencies will be maximal at the end of injection. Since it is the purpose of this study to estimate CO2 storage *potential*, and the Storage Efficiencies derived from RS models need only be sufficient for this purpose, this recommendation is therefore both practical and appropriate. If it transpires that modelling of unconfined sites is required, this might be treated as a special case.

2. INTRODUCTION AND OBJECTIVES

When modelling storage of CO2 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 CO2 in water, vapourisation of water into CO2, varying temperature and/ or salinity etc. Further choices exist with regard to different (but arguably equally valid) input data, including relative permeability functions and CO2 properties (particularly viscosity correlations). The purpose of this Task 4.1, is therefore to define a common approach for the dynamic modelling. This has been done from an extensive literature review, investigation of modelling software and our own modelling assessments. A very relevant study has recently been undertaken by the Energy and Environmental Research Center (EERC) at the University of North Dakota [1] and their conclusions are reviewed here. The EERC study was sponsored by the International Energy Agency Greenhouse Gas Programme (IEAGHG) and the United States Department of Energy (USDOE).

The deliverables for Task 4.1 are a short electronic report addressing key issues for the dynamic modelling tasks, with recommendations regarding:

- The physical processes to be represented;
- Under what circumstances;
- Which simulator(s) should be used;
- Common/ standardised parameters;
- Basis for the recommendations
- Task 4 deliverables, acceptance criteria and distribution of activities amongst participants up to the relevant Stage Gate.

The deliverables are provided in this short document, however, support for these recommendations is provided in section 3 and in greater detail in the following associated technical reports:

- RPS Report ECP1910/150310/1366/V1, Approach for Dynamic Modelling of CO2 Storage in Deep Saline Aquifers – Technical Report, Jeff Masters, Hisham Mamode, David Element, Eugene Balbinski, March 2010.
- Heriot-Watt University Report “Task 4.1 Technical Report”, Prepared for UK CO2 Storage Appraisal Project (UKSAP) for the Energy Technologies Institute (ETI), P.Olden, M.Jin, O.Gundogan, G.Pickup and E.Mackay, March 2010.
- Heriot-Watt University Report “Task 4.1 Geomechanics Report”, Prepared for UK CO2 Storage Appraisal Project (UKSAP) for the Energy Technologies Institute (ETI), P.Olden, March 2010.
- Heriot-Watt University Report “Task 4.1 Geochemistry Report”, Prepared for UK CO2 Storage Appraisal Project (UKSAP) for the Energy Technologies Institute (ETI), O.Gundogan, March 2010.

Recommended standard input data is provided on the UKSAP Sharepoint website. Recommendations generally refer to the modelling approach for Representative Structures (RS) for Task 4.3, rather than Exemplar Modelling which is to be covered in Task 4.4 unless specifically stated. The project plan requires Exemplar Modelling to be specified at the Stage Gate.

Although Task 4.1 was not delayed by the suspension of other tasks, the lack of expected data input from Tasks 1 and 2 has inevitably affected the confidence level in some of our conclusions and the ability to fully specify Tasks 4.2 and 4.3. This input would have informed us about the type and frequency of various UK storage sites. In an effort to minimise project delay the conclusions below represent our best view at this stage but may require revision when this data becomes available.

3. TECHNICAL SUPPORT FOR RECOMMENDATIONS

3.1 Physical Properties and Mechanisms

3.1.1 Gravity

A correct definition of gravity flow will be critical in the appraisal of CO2 sequestration schemes. A significant density difference of the order of 200 kg/m^3 exists between the aqueous and CO2 rich phases. Some important issues are:

- Scoping simulations indicate that storage efficiency is usually dominated by the tendency of the CO2 rich phase to rise within the system.
- The vertical flow of CO2 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 k_v/k_h to define k_z, 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 CO2 at the top of structures.

3.1.2 Capillary Pressure

Scoping simulations with and without capillary pressure utilising the recommended data in section 4.4.2 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.

3.1.3 Residual Trapping

A simulation study by EERC which estimated storage efficiencies at the end of CO2 injection concluded that residual trapping of CO2 due to hysteresis effects only contributed about 1% of the calculated CO2 storage factor. However, we would expect residual trapping and relative permeability hysteresis to become more important subsequently, affecting storage security and long-term fate. It will also be more important for structures which are relatively unconfined. The data needed to model this mechanism is incomplete, see section 4.4.2.

3.1.4 Diffusion

Diffusion coefficients for CO2 in water have been measured and are typically four orders of magnitude smaller than for CO2 in gas.

Analytical calculations and simulation modelling have been used to estimate the rate of dissipation of a CO2 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 CO2 to migrate from the original accumulation. This suggests diffusion is unlikely to be a major consideration for CO2 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 storage efficiency. 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.

3.1.5 Convective Dissolution of CO2

A 2D model was set up to estimate the timescale for dissolution of CO2 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 CO2 sequestration on the injection timescale.

A simulation study by EERC concluded that during CO2 injection, CO2 dissolution only contributed about 3% of the calculated CO2 storage factor.

3.1.6 Thermal Behaviour

The temperature effect due to injecting CO2 at a temperature significantly different to the initial formation temperature extends to approx 1000 m after 50 years of injection. However, the region of maximal temperature change is typically limited to less than 300 m from the well.

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.

A simple TOUGH -2™ simulation model was used to demonstrate that the temperature effect for extended CO2 injection is limited to the near well region and would not significantly affect the storage efficiency factors calculated for a formation or storage site. It is recommended that temperature modelling is only used for near well injectivity or possibly detailed exemplar calculations. However, it may be necessary to consider temperature for geochemical and geomechanical simulation.

3.1.7 Geochemical Behaviour

Geochemistry may impact CO2 storage in two regards. Firstly, the composition of the brine will affect parameters such as the solubility of CO2 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 CCS candidate 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 ECLIPSE 300 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, but adaptations to the commercial software will not be available within the timeframe of this project. RPS has previously studied the effect of nitrogen on Minimum Miscibility Pressures (MMP) which is important for EOR applications, but not for injection into aquifers, which is the main thrust of this study.

It is not considered that mineralization 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.

3.1.8 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 CO2 storage, we should take account 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. We suggest that some geomechanically coupled simulations are performed in both the single well injectivity models and 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.

3.1.9 Key Factors Affecting CO2 Storage Efficiencies

A choice needs to be made in how to obtain CO2 storage efficiencies from simulation results as this can significantly affect values. The EERC study calculated storage efficiencies as the product of Volumetric and Microscopic Displacement Efficiencies and a formation dependent Geological factor. The volumetric efficiency is the ratio of the CO2 plume volume to the 'Minimum Accessible Volume' (MAV). 'Accessible Volume' is defined as the pore volume immediately surrounding the injector which could be filled by CO2. EERC chose to calculate the MAV from the rectangle of minimum area surrounding the plume, translated vertically along the plume height. The microscopic displacement efficiency is the mean CO2 saturation in the MAV. It is a function of the contacted pore volume which can be occupied by CO2 and depends on the irreducible water saturation.

There are potential additional uncertainties introduced depending on how the MAV is defined, through calculating the product of two uncertain factors and because storage efficiencies will vary with time. RPS has done some preliminary work on this, (described in the Technical Report), and has shown that, depending on the MAV definition, storage efficiencies might decline by about ten percentage points in twenty years. EERC only injected CO2 for five years for their heterogeneous cases and typically, just one year, for the homogeneous cases.

The EERC study demonstrated that the degree of confinement afforded by the site structure can strongly influence the storage efficiency. For example, a dome or anticlinal shape may give much higher storage efficiencies than a dipping formation bounded by a fault, which may only have a storage efficiency similar to a flat structure.

If a structure is fully closed the storage efficiency may be much less than if it is well confined, but not pressure isolated. EERC calculate an example for which an 'open' structure stores 25 times more CO2 than an 'equivalent' 'closed' one.

The injection rate may also have a substantial effect on the storage efficiency. EERC has demonstrated that higher rates tend to increase storage efficiencies overall by increasing the pore space contacted. However, we note that the EERC injection rates are substantially lower than would be typical for a North Sea environment, see section 3.2.

The particular depositional environment may not be a key factor affecting storage efficiencies. For example, for nine different clastic depositional environments EERC calculated a relatively narrow range of P50 storage efficiencies compared to other factors, from 4.6% to 6.8%. However, it may still be important to represent the depositional environment adequately in terms of the proportions of different permeability rock. Storage efficiencies calculated from EERC's homogeneous models were typically substantially higher than from their heterogeneous models. For example, a comparable homogeneous case had a storage efficiency of 12%. The reason was that the heterogeneous models all contained significant proportions of low permeability rock which was not accessed for storage on the timescale considered and so reduced the storage efficiency.

3.2 Model Type and Scale

The recent study by EERC gives information about the feasibility of estimating storage efficiency factors using the concept of Representative Structures (RS). A range of generic models were constructed and modelled using a proprietary finite difference reservoir simulator, GEM™. Storage efficiencies were calculated for nine sandstone environments, two limestone and one dolomite. In each case results were provided for each of five open structures.

However, our view is that the practicality of applying the RS modelling concept has only been partially confirmed by the EERC study. This is because their results assume injection at a relatively low rate, 0.18 MMtonne/yr (10 MMscf/d) for only five years. In the North Sea we might typically hope to inject at five times this rate for decades, rather than just a few years. This is important not just because EERC themselves have demonstrated that storage efficiencies increase with rate [see 3.1.9], but also because they may depend significantly on the injection duration.

The EERC study utilised models which were just sufficient to contain the injected CO2, two miles square and 85 ft thick, but with about 200k cells. For example, if injection is increased to say five times higher a rate for 50 years, a model 50 times as large would be required. North Sea formations might be typically hundreds of feet thick, so if site thickness were increased to 340 ft, a model seven miles square would be needed to contain the injected CO2. Although the grid size might be increased as results do not appear sensitive to the particular depositional environment, this could still be a challenge to model with current technology.

Streamline simulation is an alternative simulation technique, ideal for the study of nearly incompressible flows in heterogeneous domains. It could be used to assess what fraction of the reservoir is occupied by CO2 and how far the CO2 migrates. This method may be used for modelling flow in detailed exemplars, as a complement to grid-based simulation. The Imperial College team participating in this project have in-house software that can account for multiphase flow, relative permeability hysteresis, compressible fluids and rate-limited reaction.

3.3 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 CO2 modelling, including a thermal option. As such, it might have provided an inexpensive choice for RS modelling, however, it lacks several features we consider to be essential 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 CO2 injection. ECLIPSE100™ is the 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 CO2 injection into aquifers, though only for isothermal cases and uniform salinity. CO2 may dissolve in the aqueous phase and the water is allowed to vaporise. This requires some care in generating the necessary PVT data entries which can be done, either 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 CO2 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 module, CO2STORE™, which is licensed separately and is designed to facilitate modelling CO2 injection into aquifers. As far as we can check, we believe CO2STORE™ employs reasonable models and correlations to represent the behaviour of CO2. 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 CO2. 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 CO2 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 CO2 storage in saline aquifers. In particular storage efficiencies calculated using both software routes are similar.

The thermal case discussed in 3.1.6 was attempted using both TOUGH-2™and the thermal option of ECLIPSE300™ and CO2STORE™. TOUGH-2™ ran the case easily, but there was an unresolved problem with the ECLIPSE300™ thermal option, in that it ran very slowly and failed to complete.

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 ECLIPSE 300.

PHREEQC is a general purpose geochemical model, but it only allows the user to simulate 1D reactive transport, and so is only of use in validating the geochemical calculations from the 3D 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 CO2 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. Vaporization 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.

4. RECOMMENDATIONS

Recommendations generally refer to the modelling approach for Representative Structures (RS) for Task 4.3, rather than Exemplar Modelling which is to be covered in Task 4.4 unless specifically stated. The project plan requires Exemplar Modelling to be specified at the Stage Gate.

4.1 Physical Properties and Mechanisms

It is recommended that solubility of CO2 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.

It is provisionally recommended that as, for the EERC study, storage efficiencies be calculated for Representative Structures at the end of CO2 injection. This provides a practical termination point for these simplified models and allows hysteresis of relative permeabilities and capillary pressure not to be modelled in these cases, so avoiding prohibitively long run times. Except for unconfined sites which depend on residual trapping to store CO2, it is likely that storage efficiencies will be maximal at the end of injection. Since it is the purpose of this study to estimate CO2 storage *potential*, this definition is therefore appropriate, as well as practical. However, this recommendation is conditional on initial modelling work to define how best and when to calculate storage efficiencies. If it transpires that modelling of unconfined sites is required this might be treated as a special case. It is also recommended that an appropriate Exemplar model be run well beyond the injected period, including the above hysteresis mechanisms, to check the importance of subsequent residual trapping. Storage efficiencies estimated from the RS modelling might then be revised if necessary.

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 Model Type and Scale

It is recommended that isothermal finite difference simulation be used to model the Representative Structures. However, the feasibility of this concept has only been partially demonstrated by the EERC study as yet. In addition, at this point only limited information is available on the nature of potential UK storage sites. It is therefore recommended that the first RS modelling be aimed at verifying the feasibility of this concept on the site scale. Specific recommendations are made in section 5.

There are indications that some of the UK storage potential may be in formations which are not delineated into individual sites. The proportion of storage capacity that may be in this category is as yet unknown and so it is not clear at this stage whether any modelling will be required. We do not therefore recommend any modelling on this scale in the initial phase before the Stage Gate.

4.3 Software

We cannot recommend use of TOUGH -2™ for the standard RS isothermal modelling as it lacks sufficient functionality to specify relative permeability models and adequate input/output interfaces.

It was concluded from 3.3 that ECLIPSE100™ was 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. We are therefore recommending using ECLIPSE100™ for the standard isothermal RS simulations. However, we may still need some access to ECLIPSE300™/CO2STORE™ for checking or sensitivity calculations. The software budget will be reviewed as part of an overall Work Package 4 review, in light of results from Task 4.1

Due to the unresolved problem mentioned in 3.3 we cannot recommend use of the ECLIPSE300™ thermal option for any thermal simulations at this point without further investigation. However, as we are recommending isothermal simulations for the standard RS modelling, this may not be a restriction.

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. Heriot-Watt University has developed expertise in performing these calculations using GEM-GHG and ECLIPSE CO2STORE, and consider that translation between ECLIPSE and GEM datasets will be feasible using the CMG Builder software.

4.4 Standard Dataset

How much data specification is required will depend on the software used. For example, for the combination of ECLIPSE300™ and CO2STORE™ correlations are built in, so less data needs to be specified. Recommended ‘black-oil’ (suitable for ECLIPSE 100) PVT input and relative permeability and capillary pressure data as detailed below have been placed on the UKSAP Sharepoint website. There follows some specific data choices which are independent of software.

4.4.1 Injection composition

For the reasons explained in 3.1.7 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 also for exemplar modelling. The standard injection composition for RS modelling should therefore be pure CO2.

4.4.2 Relative permeabilities and capillary pressure

Although other measurements are available, the most comprehensive set of consistent CO2/brine relative permeability and capillary pressure data is from a Canadian dataset produced by Bennion and Bachu [2]. Other data are available from measurements on Berea sandstone at Stanford [3]. It is recommended that consistent sets of relative permeability and capillary pressure data be used. Our recommendations for various permeability intervals are given below and standard input datasets have been placed on the UKSAP Sharepoint website. 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 4.4.2-1: Relative Permeability and Capillary Pressure Recommendations

5. TASK 4 PLAN TO STAGE GATE

The original proposal included a description of how the RS modelling would be undertaken. However, it is essential to prove the applicability of the RS modelling concept before this programme can be successfully implemented. The acceptance criterion for Task 4.3 up till the Stage Gate should therefore remain as specified in the original proposal, the demonstration of the practicality of implementing the Representative Structure modelling concept. The acceptance criterion for Task 4.2 up to the Stage Gate should also remain the completion of initial Representative Structure export grids, fit for simulation.

The following issues have been identified which require work to resolve with the first RS models:

- feasibility of modelling with likely North Sea CO2 injection rates and durations, and consequent model size/ boundary conditions
- the need for a simple and practical but appropriate method of determining CO2 storage efficiency factors from simulations including when to calculate it
- the need to represent the effect of lower permeability rock on likely injection timescales and the simplest effective way to do this.

It is proposed to start with the following programme of work to address these issues and then continue with the original programme specified in the proposal if still appropriate. At this stage we cannot be more definite about the number and specification of RS models due to the issues listed above and the lack of guiding data on potential UK storage sites from Work Packages 1 and 2. However, we do recommend proceeding with the workshop originally planned in order to choose appropriate RS to model, once sufficient data is available. After this, work can continue as in the original proposal.

It is proposed that the first RS modelling be performed on a simple flat homogeneous structure, but for a single injector at a typical rate of 1 MMt/yr for 50 years on an appropriately large model. This will not only demonstrate the feasibility of the approach, but will also show how storage efficiencies will vary over injection time. The model will also be used to investigate how best to derive storage efficiencies from simulation results. This model should also include explicit modelling of the reservoir seal in order to check in how much detail it needs to be represented. It should also be used to test the effect of alternative boundary conditions, such as extending the grid or attaching analytic aquifers to represent open boundaries.

Another strand of RS modelling will construct heterogeneous models containing a significant fraction of low permeability rock. The EERC results suggest that a simple random distribution might be good enough initially, but if data is available for particular depositional environments, this might also be investigated subsequently. We would then compare not just the magnitude of storage efficiencies compared to the homogeneous case, but also the time taken to converge to a final storage efficiency. Finally, we propose investigating whether the heterogeneous model could be adequately upscaled to provide a more convenient model for running multiple cases.

It is proposed that RPS Energy undertake the work specified above, but that Heriot-Watt University undertake the following supporting studies.

Single and possibly sector well modelling will also be performed to guide representation of injection well performance in the Representative Structure and Exemplar models using the GEM™ simulator as envisaged in the original proposal. As for the RS modelling the following preliminary calculations are proposed while awaiting data from the other parts of the project to define the final parameter range:

- grid resolution and required model size studies for a flat homogeneous model
- rate and well spacing studies in conjunction with the economics task WP3
- separate and combined sensitivity calculations to thermal, geomechanical and geochemical effects.

After the choice of RS models has been made injectivity calculations can then be performed for the appropriate range of parameters.

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