

New insights from 3D geological models at analogue CO₂ storage sites in Lincolnshire and eastern Scotland, UK.

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SUMMARY: Subsurface 3D geological models of aquifer and seal rock systems from two contrasting analogue sites have been created as the first step in an investigation into methodologies for geological storage of carbon dioxide in saline aquifers. Development of the models illustrates the utility of an integrated approach using digital techniques and expert geological knowledge to further geological understanding. The models visualize a faulted, gently dipping Permo-Triassic succession in Lincolnshire and a complex faulted and folded Devonian-Carboniferous succession in eastern Scotland. The Permo-Triassic is present in the Lincolnshire model to depths of -2 km OD, and includes the aquifers of the Sherwood Sandstone and Rotliegendes groups. Model-derived thickness maps test and refine Permian palaeogeography, such as the location of a carbonate reef and its associated seaward slope, and the identification of aeolian dunes. Analysis of borehole core samples established average 2D porosity values for the Rotliegendes (16%) and Sherwood Sandstone (20%) groups, and the Zechstein (5%) and Mercia Mudstone (<10%) groups, which are favourable for aquifer and seal units respectively. Core sample analysis has revealed a complex but well understood diagenetic history. Re-interpretation of newly reprocessed seismic data in eastern Scotland has significantly reduced interpretative uncertainty of aquifer and seal units

at depths of up to -6 km OD in a complex faulted and folded Devonian-Carboniferous succession. Synthesis of diverse data in the 3D geological model defines a set of growth folds and faults indicative of active Viséan to Westphalian dextral-strike slip, with no major changes in structural style throughout the Carboniferous, in contrast to some published tectonic models. Average 2D porosity values are 14-17% in aquifer units and <2% in the seal unit, with a ferroan dolomite cement occluding porosity at depth.

Low-carbon use of fossil fuels could be achieved by capture of CO₂ at power stations and storage in the pore space of rock units deep below ground. Volumetrically, CO₂ can be most efficiently stored underground because it undergoes a sharp reduction in volume with increasing pressure and temperature as it is injected deep into the subsurface, associated with a phase change from gas to a liquid or supercritical fluid. The conditions required are generally reached at depths of between 500 and 1000 m, dependent on the geothermal gradient. Thus the basic requirements for the subsurface storage of CO₂ are the identification of porous candidate aquifer formations in the vicinity of power stations, a sufficient volume of rock to accommodate the CO₂, and suitable seal rocks and structural traps to contain it. Best-practice criteria are a homogeneous aquifer sandstone buried at depths between 1 and 2.5 km, with porosity greater than 20%, permeability greater than 500 mD, and a thickness of greater than 50 m, capped by a greater than 100 m thick mudstone seal with very low porosity and permeability (see Chadwick *et al.* 2008 for more information). However, a lower porosity of greater than 10%, an aquifer sandstone greater than 20 m thick, or a seal rock greater than 20 m thick could be acceptable.

Commonplace in the hydrocarbons industry using good quality well and seismic data since the 1990s (see examples in Davies *et al.* 2004, 2005), digital 3D geological modelling is increasingly being used in a much wider range of geological applications as a mechanism to integrate diverse spatial data and geological understanding into a consistent representation of the subsurface (Turner 1992; Turner & Gable 2007). Such framework models make explicit the distribution, geometry and structure of key stratigraphical units, providing a basis for a refined understanding of the geological record and the discovery of hitherto unknown aspects

of the subsurface (Ford *et al.* 2010; Smith *et al.* 2011). Combining framework models with information on the physical properties of the intervening strata allows the subsurface to be increasingly well characterized, and for attributed models to be employed in a variety of applications ranging from engineering to natural resource management, including supporting the sustainable use of the subsurface as both a source and a sink (Culshaw 2005 Lelliot *et al.* 2006; Kemp 2007; Royse *et al.* 2010; Chadwick *et al.* 2010). In this paper, key seismic, well, borehole, mine plan and outcrop data have been interpreted and integrated for two sites in order to define the geometry and characteristics of aquifer and seal rocks buried at depths greater than 800 m. The subsurface 3D geological models were an important component of the CO₂ Aquifer Storage Site Evaluation and Monitoring (CASSEM) project, which studied aspects of the Carbon Capture and Storage (CCS) chain, including transport of CO₂ from coal-fired power plant to carbon storage and monitoring in saline aquifers (Smith *et al.* 2011). The methodology developed for these onshore and nearshore analogue sites described here is a pathway for characterizing CO₂ storage sites in offshore saline aquifers (Smith *et al.* 2011). It is emphasized that the sites described here are not considered as actual CO₂ storage localities, and there are no plans to inject CO₂ into either of them. This paper describes specific geological outcomes from the 3D geological modelling and summarizes the results of this initial geological analysis with respect to suitability criteria for CO₂ storage such as depth, porosity, permeability and heterogeneity (e.g. Chadwick *et al.* 2008, p.15) at a broad site evaluation scale. Although the models were built to study CO₂ storage methodologies and were subsequently used for numerical flow simulations of CO₂ injection (Jin *et al.* 2010; Smith *et al.* 2011, ch. 4), it is the particular significant improvements in regional geological understanding that are described here.

Two initial areas of interest were chosen: within a 100 km radius of the Ferrybridge Power Plant in Yorkshire, England, and within a 75 km radius of Longannet Power Plant in central Scotland (Figs 1a, b).

After initial geological evaluation, an area extending from Saltfleetby on the Lincolnshire coast to Lincoln in the west (Fig. 1a; Ford *et al.* 2008) was chosen to create a 3D geological model of the primary Triassic aquifer (Sherwood Sandstone Group) and the underlying secondary Permian aquifer (Rotliegendes Group). These units are onshore equivalents of the targets for

potential CCS storage in the Southern North Sea (Bunter Sandstone Formation of the Bacton Group and the Rotliegendes Group respectively; Johnson *et al.* 1994). The geology of this area is relatively simple (e.g. Kent 1980; Institute of Geological Sciences 1980), with a good coverage of modern 3D seismic data and geophysical wells (Fig. 2).

The area within 75 km of Longannet Power Plant extends around the Firth of Forth from west to east Fife and Edinburgh to East Lothian in eastern Scotland, the 'Forth area' (Fig. 1b; Monaghan *et al.* 2008). This site is an example of a relatively complex faulted and folded sequence of uppermost Devonian - Lower Carboniferous aquifer rocks, with a limited coverage of 1950s - 1980s 2D seismic data and sparse well data (Fig. 3).

By selecting sites with contrasting geological settings and data availability, the CASSEM study aimed to develop generic methodologies for geological modelling in CO₂ storage (Ford *et al.* 2009; Smith *et al.* 2011).

1. METHODOLOGY

1.1 Data collation and interpretation

Prior to modelling, a review of data availability and quality for each area was undertaken in a Geographical Information System. In a data-poor region such as the Forth area, all available datasets were utilized (Fig. 3). In a relatively data-rich area such as Lincolnshire, the baseline datasets producing the highest confidence interpretation were used. In Lincolnshire, 2D and 3D seismic data, tied to geophysical wells, are the most important datasets for defining the subsurface geometry of key stratigraphical levels (Fig. 2). Where available, borehole records held by the British Geological Survey (BGS) National Geoscience Data Centre, depth data from coal mine abandonment plans (Fig. 3), and outcrop lines from BGS digital maps provided additional constraining data points. Integrated interpretation of the datasets was undertaken by geologists with regional knowledge to create files of 3D point data representing key horizons and fault contacts. These data were collated to form the basis for 3D geological

modelling. Data points and modelled surfaces are in metres or kilometres relative to Ordnance Datum (m OD or km OD).

1.2 3D geological modelling

The 3D geological model was constructed using the Geological Object Computer Aided Design (GOCAD® Paradigm™) 3D modelling software. This application facilitates the construction of digital faulted surfaces based on a combination of datasets such as seismic picks, borehole/well data points, mining data, map outcrop data and geologist-interpreted data. The workflow can be briefly described as importing and collating 2D and 3D data, importing fault pattern information and constructing appropriate fault geometries, and application of the GOCAD Structural Modelling Workflow. This is followed by multiple manual iterations involving visual inspection, derivation of thickness models to highlight areas where surfaces differ from the conceptual geological model, and obtaining additional geological information, including expert advice, to better constrain the model in these areas. Uncertainty maps were created for each modelled surface and more comprehensive risk and uncertainty analysis was subsequently undertaken (Polson & Curtis 2010; Smith *et al.* 2011).

1.3 Rock sample analysis

Borehole core material held by the BGS National Geoscience Data Centre from within or close to the geological model areas was assessed, with preference given to the deepest available core material representing the principal lithologies of the analogue aquifers and seal rocks. Over 90 polished thin sections were taken from samples in the vertical plane, approximately perpendicular to bedding.

After brief examination by optical petrographic microscope, detailed mineralogical and petrographic observations were made of the polished thin sections using backscattered scanning electron microscopy (BSEM) coupled with energy-dispersive x-ray microanalysis (EDXA). Modal mineralogical analysis was carried out by image analysis of digital EDXA elemental maps. Two-dimensional (2D) porosity data were obtained by petrographic image analysis (PIA) of BSEM images, using the Olympus AnalySIS Auto (v.5) PIA software

package. Pore area, elongation and equivalent circular diameter (ECD) were measured, with resultant total porosity values and quantification and characterization of the macropores. A mesopore / macropore cut-off of 15 μm ECD was used.

2. THE PERMO-TRIASSIC AQUIFER SYSTEM, LINCOLNSHIRE, ENGLAND

In Lincolnshire, the primary analogue aquifer is the Sherwood Sandstone Group and the corresponding seal is the Mercia Mudstone Group (Fig. 4), both of Triassic age. A secondary analogue aquifer/seal pair exist at greater depth, comprising the sandstone-dominated Permian Rotliegendes Group sealed by the Marl Slate, Cadeby and succeeding evaporite-rich formations of the Zechstein Group (Fig. 4). In the southern North Sea, these rocks host major oil and gas reservoirs with substantial saline aquifer potential (DTI 2006).

The geological model is based on an extensive interpretation of third-party 2D and 3D seismic data, geological borehole/well data and existing BGS geological mapping (Fig. 2). Additional resources were incorporated, including published information on the regional geological framework and tacit geological knowledge provided through regional expertise.

Construction of the Lincolnshire 3D geological model used c. 400 line km of 2D seismic data and c. 540 km^2 of 3D seismic data, provided under licence by the UK Onshore Geophysical Library and interpreted in the Geographix® Seisvision 3D and 2D software. These datasets range in quality from poor to very good (Figs 2, 5). In the eastern 'Lincolnshire Wolds' 3D survey, there is a marked contrast in data quality (reflection amplitude, reflection continuity and well-tie) between the western (poor) and eastern (moderate to good) parts of the region of study (Fig. 2). As a consequence, 3D data were replaced in the western area by sparser but better quality 2D lines to build the geological model there. The seismic picks were controlled using well data and mapped surface outcrop. Eighteen wells (Fig. 2) were used to convert geological horizons and faults to depth. The majority of wells penetrated the entire Permo-Triassic succession to terminate in underlying Carboniferous strata, so picks for most of the modelled horizons exist in most of the wells shown on Figure 2. The exception is the Yellow Sands Formation (Rotliegendes Group), which was not recognized in a small number

of wells, typically in areas where this aeolian dune-sand dominated unit is interpreted to be thin or presumed to be absent.

The c. 975 km² Lincolnshire 3D geological model was created according to BGS standard procedures using the GOCAD software application (see above). It was constructed around six stratigraphic horizons; in ascending order these are the base Permian (i.e. top Carboniferous), top Rotliegendes Group, top Cadeby Formation, top Brotherton Formation, top Roxby Formation, top Sherwood Sandstone Group, top Mercia Mudstone Group and top Lincolnshire Limestone Formation (Fig. 4). These do not represent all the subdivisions of the sequence, but key horizons that are widely enough separated, or that form significant lithological boundaries, to enable the modelling to be undertaken. For descriptive purposes, the sequence between the top Rotliegendes Group and top Cadeby Formation is referred to as Cadeby Equivalents, and that between the top Cadeby Formation and top Brotherton Formation as the Edlington Equivalents. The sequence between the top Brotherton Formation and top Roxby Formation is referred to as the Roxby Equivalents (Fig. 4). Each modelled horizon is defined in 3D as a semi-continuous surface, constrained where appropriate by 1:50,000 scale geological map linework at outcrop and at depth by a combination of borehole, 2D- and 3D-seismic data. The modelled stratigraphical horizons are affected by faulting that expresses itself in the modelled surfaces as elongate fault-gaps with oblique offsets. The 26 faults included in the model are represented by continuous surfaces, constrained in 3D by their corresponding intersection with the stratigraphical horizons, as identified by seismic data interpretation. The top primary aquifer reaches depths of -480 to -1215 m OD, and the top secondary aquifer reaches depths of -830 to -1880 m OD within the studied area (Figs 6, 7a). The well-constrained 3D geological model constructed for the area allows the structure and thickness between each modelled geological unit to be readily assessed, and to test a seminal palaeogeographical hypothesis (Smith 1989).

The modelled succession in the study area generally dips at about 1 degree towards the east-northeast (Figs 6, 8). This regional dip is recognized throughout the Lincolnshire/Humberside district, and is largely related to subsidence in the North Sea area and tectonic movements that occurred during the Mesozoic and Cenozoic. These movements are inferred to be related to crustal extension that occurred synchronously with the opening of the Atlantic

Ocean (Smith *et al.* 2005). The dip of individual horizons is greatest for the base Permian at 1.1 degrees and reduces to 0.9 and approximately 0.7 degrees for the top Permian and the top Sherwood Sandstone Group respectively. This change in dip is accommodated by a 350 m increase in the modelled thickness of the Permian and Sherwood Sandstone Group strata over a distance of 50 km from west to east, which is commensurate with differential thermal subsidence on the western margin of the evolving Zechstein Basin. The dip of 0.7 degrees at the top Mercia Mudstone Group and top Lincolnshire Limestone Formation surfaces is similar to that at the base of the Mercia Mudstone, indicating that subsidence was relatively even across the whole area following deposition of the Sherwood Sandstone Group and until at least the Late Jurassic.

In contrast to the Forth geological model described below, the Lincolnshire model reveals evenly dipping stratigraphical surfaces that are largely devoid of major fold structures. No significant anticlinal structure was proved, but minor folding is present in the form of very gentle, laterally impersistent folds with an alignment broadly parallel to that of the modelled faults (Fig. 9). The amplitude of these minor structures generally increases with depth, from about 5 m at the level of the Lincolnshire Limestone Formation to about 20 m at the level of the top Cadeby Formation, the increase in size reflecting upwards propagating fault-tip folding above reactivated faults in the underlying Carboniferous strata. Although the scale of these structures is close to the maximum effective resolution of the seismic data, their recognition on multiple adjacent seismic lines gives confidence to their interpretation. In addition to the minor folding, disturbance directly associated with faulting has resulted in the formation of more pronounced localized fold structures, as shown in Figure 8 for the top Sherwood Sandstone Group surface.

2.1 Permian Palaeogeography

Palaeogeographic reconstruction and associated facies determination is a key aspect of modelling the geological potential for CO₂ storage, and contributes to the characterization of aquifer (e.g. Rotliegendes Group) and seal (e.g. Zechstein Group) properties, including porosity and permeability. Modelling significant changes in Permian facies in the Lincolnshire

area provides an onshore analogue to inform studies of storage potential in equivalent offshore formations in the Southern North Sea Basin. The early Permian palaeogeography of the modelled area was interpreted by Smith (1989) as an enclosed post-Variscan basin with deposits that include piedmont conglomerates, aeolian sandstones and siltstones. In keeping with the rest of the basin, these onshore deposits are now included in the Rotliegendes Group (British Geological Survey 2006). Reconstructions of the Permian palaeogeography of eastern England by Smith (1989) provide a valuable framework, but the area of the Lincolnshire 3D geological model is data-poor and this new work, incorporating a range of recent data, presents a significant refinement.

The 3D geological model shows three broad zones of contrasting sediment thickness and distribution for the Rotliegendes Group (Fig. 10a). In the west there is a patchy zone of thin deposits that are usually less than 30 m thick. The central zone is characterized by variable sediment thickness, with several discrete circular to elongate areas of thick sedimentation that reach up to about 90 m in thickness. The eastern zone shows a general coalescence of features and thickening of the succession to between approximately 50 and 90 m.

The western zone corresponds approximately to the area of thinly developed piedmont gravels, patchy blown sand and bare rock recognized by Smith (1989). This interpretation is supported by corresponding borehole records that describe Zechstein Group deposits resting directly on Carboniferous strata (e.g. Spridlington 1 Borehole [TF 01830 83813]) or the presence of thinly developed aeolian Yellow Sands Formation (e.g. 6 m of "basal" sand recorded in the Dunholme 1 Borehole [TF 00853 79195]). The central zone represents most of the modelled area, and is broadly coincident with the region characterized by Smith (1989) as wind-blown sand on gravel interdigitating southwards with piedmont and fluvial fan deposits. This association is confirmed by the Apley Borehole [TF 10147 75104], which proved 8 m of quartzose, well-sorted sand over 15 m of lithic, angular conglomerate. The thickness changes, morphology and lithology of the central zone suggest the existence of large-scale aeolian dunes, with a width of 4 to 6 km. These are comparable in extent and thickness to those identified through borehole interpretation at an equivalent level in the Harrogate district of Yorkshire (Cooper & Burgess 1993) and through a combination of borehole and outcrop evidence in north-east England (Steele 1983). The model indicates a

roughly NW-SE elongation to these features, similar to the WNW-ESE orientation proposed for the Yorkshire region by Versey (1925), based largely on interpreted borehole information, which contrasts to the SW-NE trend suggested by Cooper & Burgess (1993) for the Harrogate district. The interpretation for the Lincolnshire area may indicate a change in dune style and orientation in the south, to one that accords with the orientations that Glennie (1982, 1983) found for the area to the east of here based on thickness and sedimentological data from boreholes.

The eastern zone of the Rotliegendes Group is interpreted as a south-east extension to the area of thicker, continuous wind blown sand shown by Smith (1989) to the north of the modelled area. Evidence for its presence is from boreholes, including Saltfleetby 1 [TF 41450 90883], which proved over 60 m of medium- to fine-grained 'frosted' sand.

The contact between the Rotliegendes Group and the overlying Zechstein Group is unconformable, with the Zechstein Group largely burying the Rotliegendes Group sand dune topography. It marks a rapid flooding event that transformed the Zechstein Basin from a desert below sea level into an enclosed evaporitic sea (Smith 1989; Tucker 1991). The first deposits of the Zechstein Group sequence are the thin (1-3 m) euxinic mudstones of the Marl Slate Formation that are the British equivalent of the Kupferschiefer mudstones recognized widely beneath the North Sea and on the European mainland. The succeeding Zechstein Group succession is cyclic, with repetitions of carbonate/dolomite, sulphate and various salt phases with periodic terrestrial input. Smith (1989) interpreted it as a stack of five progressively evaporitic cycles, while Tucker (1991) recognized seven sequence stratigraphical cycles related to highstands for the carbonate ramps and lowstands for the flanking evaporite deposits. This latter interpretation has now gained wide acceptance in the UK (Ruffell *et al.* 2006), while elsewhere in the Zechstein Basin slight variants of the sequence stratigraphy have been proposed (Kaiser *et al.* 2003; Becker & Bechstädt 2006).

The thin Marl Slate Formation mudstones are included with the overlying Cadeby Formation in the Cadeby Equivalents. This unit is shown to increase gradually in thickness from the south-west to the north-east by about 100 m over 20 km, becoming thickest along a broad WNW-ESE trending ridge across the centre of the modelled area. This feature was recognized by Taylor & Coulter (1975) and elaborated by Smith (1989); it includes the early

carbonate phases of the Zechstein Group and is interpreted as a carbonate ramp fringed by a belt of patch reefs and shoals (Fig. 11). North-eastward dipping clinofolds associated with this ramp have been mapped on the seismic data (Pharaoh *et al.*, 2011). From the reef-edge high eastwards, the north-east flank of the formation thins rapidly. At its steepest in the south, it thins by 100 m over 2 km, but north of this throughout most of the area it thins typically by around 90 m over 5 km (Figs 6, 8, 11). This zone of rapid thinning in the south is of similar dimensions to that shown by Smith (1989) for the Durham area, and is best interpreted as the margin of a shelf-edge reef with a steep front edge descending into deeper water (Smith & Francis 1967).

The rapid eastward thinning of the Cadeby Equivalents, shown by the 3D geological model to the east of the inferred contemporary reef, corresponds with a complementary rapid thickening of the Edlington Equivalents (Figs 6, 8, 10b, 11). The Edlington Equivalents considered here include the largely evaporitic units shown in Figure 4. This relationship has been recognized by Smith (1989) and Tucker (1991), Tucker interpreting it as highstand carbonate deposits flanked by lowstand evaporite deposits. The initial thickness increase is about 100 m across 4 km of the seaward slope of the Cadeby Equivalents, but there is also a gradual thickening towards the northeast, attributed to the basinward deposition of later, extensive carbonate and evaporite deposits, including the Hayton Anhydrite and Kirkham Abbey formations (Smith 1989; Tucker 1991). On the shoreward side of this rapid increase in thickness of the Edlington Equivalents, there is a clearly defined, 2.5 km wide corridor where a reduced thickness is present. This depression is interpreted as a roughly N-S aligned lowstand channel feature, emanating from the hinterland to the south (Fig. 10b), which was subsequently filled by Roxby Equivalents strata (Fig 10c). The inferred channel may be associated with an ephemeral river course related to those postulated by Smith (1989, fig. 6) to have been present during the deposition of the Cadeby Formation. The channel alignment is similar to those proposed by Ford *et al.* (2010) for the Cadeby and Edlington formations, based on a lithofacies analysis of the area directly to the west of the Lincolnshire 3D geological model.

The model also shows an overall increase in the thickness of the Roxby Equivalents towards the north-east, with the greatest change occurring along a zone that broadly follows the

postulated western margin of the Billingham Anhydrite Formation (Smith 1989) (Fig. 10c). Local irregularities in the edge of this zone, including an embayment similar in proportion to that identified in the western limit by Smith (1989) in the Doncaster area, suggests a similarly convolute limit to the Billingham Anhydrite Formation in the modelled area. The reduced thickness of the Roxby Equivalents in the north-west and south-central parts of the model is consistent with shoaling towards the contemporary shoreline proposed by Smith (1989) for this part of the sequence.

2.2 Faulting

Geological faulting is clearly visible in selected seismic profiles and faults with a throw in excess of approximately 10 m are expected to be resolved (e.g. Fig. 5). The scale of geological faulting in this area is relatively minor in comparison with other parts of the UK, and specifically with the Forth model. The faults trend NW to WNW, most commonly dipping at high angles to the NE to ENE, with vertical throws typically of 20 to 30 m and a maximum of 50 m in the case of the Nocton Fault (Fig. 9) in the west of the model (throws on the top Sherwood Sandstone surface). These structures and the corresponding half-graben are broadly coincident with the western edge of the Carboniferous Humber Basin as shown by Evans & Allsop (1987) and Pharaoh *et al.* (2011) (Fig. 9). Graben structures are also revealed by the model, most notably in the west, where opposing faults suggest an easterly expression of deeper-seated structures associated with the Gainsborough Trough (Evans and Allsop 1987; Pharaoh *et al.* 2011; Fig. 9). This is a common fault pattern for the late Palaeozoic-Mesozoic succession of eastern England and is believed to be related to the reactivation of Caledonian and Variscan fault structures in the Palaeozoic basement (Smith *et al.* 2005). The nature of individual faults and fractures, which may be sealed at depth (i.e. presenting a barrier to fluid migration) or open at depth (i.e. presenting a potential pathway), was not studied and could be assessed by future work.

In most cases, faults that have been identified in the seismic interpretation, up to and including the level of the Lincolnshire Limestone Formation, are not recognized at the ground surface. These structures are interpreted to terminate within the primary overburden. This

interpretation is consistent with the lack of faults recorded at surface on published 1:250,000 and 1:50,000 scale BGS geological maps (Fig. 9) and the diminishing magnitude of minor folding with proximity to the ground surface, and represents a new structural model for the area.

2.3 Model limitations and uncertainty

The Lincolnshire model is appropriate for a scale of use between 1:50,000 and 1: 250,000. Misinterpretation of the seismic picks on the seismic data is a potentially significant source of uncertainty. However, the seismic data used in the region of study are generally of good to very good quality, both laterally and with increasing depth, and most of the horizons are associated with a distinctive pattern of reflections. Limitations of the seismic data are most clearly evident in the east of the model, where the processed 3D data contains SW-NE trending ridges and troughs with an amplitude of about 8 m and a wavelength of around 1500 m. The results of this effect are shown in Figure 10a, where the gross thickness variation in the Rotliegendes Group is overprinted by a linear fabric due to this seismic data artefact. Additional uncertainties may be introduced into the depth-converted seismic picks by potential errors in the velocity model. It is difficult to quantify the uncertainty that the depth conversion introduces, and this has not been attempted. Uncertainty maps were prepared for each modelled/seismically picked horizon, using expert judgement and based on seismic data quality and distance from well tie (e.g. Figure 7b), and the maximum uncertainty on any modelled surface has been interpreted as ± 30 m, which is considered to be a good resolution for major aquifer and seal rock units buried at -700 to -2000 m OD. Further work on sensitivity analysis of geological uncertainty, expert elicitation and risking was undertaken (Smith *et al.* 2011, ch. 6), with aquifer permeability, thickness and relative permeability being the most influential input parameters, and a low modelled probability of CO₂ leakage from seal rock.

2.4 Rock characteristics and properties

A description of the rock mass between the subsurface geometries defined by the 3D geological model is a critical part of the geological framework required to understand any application to CO₂ storage. Rock samples from borehole core were used to observe the pore space characteristics, together with borehole and field observations on the lithological heterogeneity of the strata. For the Lincolnshire area, borehole core samples came largely from the BGS Cleethorpes No.1 Borehole [TA 30237 07090] (Fig. 2) where the primary aquifer and secondary aquifer/seal were at depths from 1100 – 1190 m. Additional core material, including that from the primary seal, was only available from boreholes of shallower depths to the west of the modelled area (Fig. 1).

2.4.1 Cretaceous, Jurassic and Triassic overburden

The Triassic Penarth Group is a 10 – 20 m thick, largely argillaceous unit composed of black, fissile shales interbedded with thin sandy limestones and overlain by weakly calcareous and dolomitic mudstones. The lithological character of the group suggests that it could be considered as a vertical extension of the primary seal (Fig. 4). Strata of Jurassic and Cretaceous age represent most of the primary overburden. Up to approximately 660 m of Jurassic strata and a maximum of approximately 200 m of Cretaceous strata are recorded in the east of the region of study. The lower part of the Jurassic succession, represented by the marine Lias Group, is dominated by mudstones and silty mudstones with subordinate limestones, siltstones, sandstones and ironstones. The Middle Jurassic is a complex package of limestones, marine sandstones, shales and ironstones. The marine Upper Jurassic comprises a mudstone-dominated succession with minor sandstones, limestones and siltstones. The Lower Cretaceous is a package of marine sandstones, mudstones, ironstones and chalk. The upper part of the Cretaceous succession comprises the Chalk Group, a marine succession dominated by chalk, with minor marly-chalk, limestone and flint that occurs as nodules or laterally continuous layers (Fig. 4). The rock characteristics and properties of the overburden have not been investigated in detail in this study.

2.4.2 Primary seal – Mercia Mudstone Group

The Mercia Mudstone Group comprises the primary seal (Fig. 4). It consists predominantly of red mudstones with subordinate siltstones and sandstones (Fig. 12). Thin, fine-grained dolomitic limestones and beds of gypsum or anhydrite are widespread throughout the group. The thickness of the Mercia Mudstone Group in the region of study ranges from a minimum of approximately 200 m in the north and west to over 300 m in the south and east, but it is difficult to subdivide into formations. However, a siltstone-rich basal succession (Fig. 12), reaching up to 80 m thick, may be correlated with the Tarporley Siltstone Formation. The latter is characterized by interlaminated and interbedded gypsum-cemented sandstones, siltstones and mudstones in approximately equal proportions.

2D porosity values for the Mercia Mudstone Group are generally low (<10% total porosity; Fig. 13). Much of this is microporosity, but a significant amount of macroporosity is present in the basal Tarporley Siltstone Formation, where total porosities may be as high as 30%.

Examination of core at shallow depths from boreholes in the west of the modelled area, showed that the Mercia Mudstone Group is strongly affected by the hydration of anhydrite to gypsum. Gypsification results in the disruption of the mudstone fabric, and is accompanied by expansive disruption, due to increased volume as anhydrite hydrates to gypsum, accompanied by fracturing and the development of displacive gypsum veining, and dissolution and collapse. This alteration proceeds as a result of groundwater penetrating from the surface downwards, and upwards from the underlying Sherwood Sandstone aquifer to the base of the Mercia Mudstone Group (similar to that observed in shallow Zechstein anhydrite deposits, Bath *et al.* 1987). Disruptive gypsification and alteration are likely to be of less importance in the deeper sequence, where groundwater is very saline and pressure and temperature are higher (Mossop & Shearman 1973; Zambak & Arthur 1986). Ten samples of mudstone and siltstone, largely unaffected by gypsification and anhydrite dissolution, were chosen from borehole core between 82 and 364 m drilled depth, as no deeper samples were available. These rocks have no significant interconnected macroporosity, and the Mercia Mudstone Group may be a very good seal at depth within the target area. Mineralogically clean sandstones within the basal part of the Mercia Mudstone Group are similar to those of the Sherwood Sandstone Group. Muddier, poorly sorted sandstones and siltstone layers

comprise a tightly packed fabric of detrital quartz with minor K-feldspar, muscovite, biotite and chlorite in a matrix of illitic silt and clay. More argillaceous strata contain laminae of dolomicrite and discontinuous layers of anhydrite.

2.4.3 Primary aquifer – Sherwood Sandstone Group

The Sherwood Sandstone Group is the primary analogue aquifer (Fig. 4), comprising mainly fine- to coarse-grained, reddish brown, fluvial sandstones with occasional thin and laterally discontinuous marl seams. The sandstones are commonly cross stratified and contain channel structures and sporadic layers of mudstone clasts (Ford & Monaghan 2009). The thickness of the Sherwood Sandstone Group in the region of study ranges from a minimum of approximately 170 m in the south-west to over 380 m in the north-east. Component formations of the Sherwood Sandstone Group are not readily distinguishable in the region, and for the purpose of this study, this unit is considered at group level.

Twenty-seven samples of the Sherwood Sandstone Group, from borehole core ranging from 213 m to 1317 m drilled depth, were chosen to avoid the shallow unconfined aquifer, with 24 samples coming from the saline aquifer in the BGS Cleethorpes No. 1 Borehole. The samples have the highest mean total 2D porosities and mean 2D macropore sizes of this study. Mean 2D porosity is about 20% but some values exceed 40% (Fig. 13). Mean permeabilities ranging from 106 to 2166 mD have been measured previously from the Cleethorpes No. 1 Borehole (Downing *et al.* 1985).

Most sandstones examined are subfeldspathic arenites with some feldspathic arenites and sublithic arenites (Fig. 14). Primary detrital components include dominant quartz with subordinate to minor K-feldspar, albite, lithic clasts, minor to trace muscovite, biotite and chlorite and accessory heavy minerals.

Porosity and permeability in the Sherwood Sandstone Group and the basal Permian sandstones are strongly influenced by diagenetic modification, observations similar to those described in earlier studies (Bath *et al.* 1987; Milodowski *et al.* 1987). Burial compaction has reduced the primary intergranular porosity. Clean, well-sorted, quartz-rich sandstones show less compaction than muddier sandstones or sandstones with a high proportion of plastic

lithic clasts. Sandstones with a large quantity of mudstone clasts often have the intergranular pores filled by clay pseudomatrix produced by compactional deformation of those clasts. Illitic clay coats grain surfaces and an early diagenetic dolomite (dolomite or dolomitized calcite) cement is an important phase in most sandstones. Anhydrite may be a significant cement and trace cements of sylvite and halite were also observed. Authigenic kaolinite is common, microporous and largely replaces detrital framework grains. Many of the sandstones display evidence for the development of significant secondary porosity (e.g. Fig. 15). The main processes that generate secondary porosity are dissolution of: 1) anhydrite (and/or gypsum), halite and sylvite cement; 2) dolomite cement; 3) detrital feldspars and lithic grains (framework grain dissolution). In the Sherwood Sandstone Group, the extent of mineral dissolution increases from the east towards outcrop and the groundwater recharge area in the west (Bath *et al.* 1987; Milodowski *et al.* 1987). Anhydrite, sylvite and halite cements are observed in sandstones in the deep North Sea reservoirs, but are absent in the shallow aquifer.

Fibrous illite is encountered in the Rotliegendes Group of the southern North Sea, where published studies have concluded that it is generally restricted to sandstones that have undergone deep burial (Marie 1975; Glennie *et al.* 1978). However, its presence in Sherwood Sandstone Group sandstones (Fig. 16) at shallower depths than offshore from the Cleethorpes No.1 Borehole indicates that it may have a more widespread distribution than previously thought. Extensive, well-developed authigenic fibrous illite was observed on SEM images of pore surfaces in Sherwood Sandstone Group samples preserved in formation-brine (Fig. 16). It nucleates on pore walls and forms a meshwork of fibres growing across and restricting the intergranular pores. This may significantly decrease permeability, even though the illite is volumetrically small and has little overall effect on the total porosity.

2.4.4 Secondary seal/overburden – Zechstein Group

The variable lithologies of the Roxby, Brotherton, Edlington, Cadeby and Marl Slate formations of the late Permian Zechstein Group comprise the primary analogue bottom seal, secondary seal and overburden (Fig. 4).

Two Marl Slate Formation BSEM samples were obtained from the Cleethorpes No.1 Borehole and comprise tightly compacted mudstone and siltstones, with no significant macroporosity, giving an average 2D porosity of approximately 5% (Milodowski & Rushton 2008; Fig. 13). Samples of the Roxby Formation from relatively shallow depths from boreholes outside the modelled area (262 and 310 m drilled depth) are silty mudstones with anhydrite. They have been affected by gypsification, but the unaltered siltstone and mudstone matrix has negligible porosity. Similarly, a sample of the Sherburn Anhydrite from 316 m drilled depth comprises dense crystalline anhydrite with no obvious porosity. As discussed above, gypsification and alteration are likely to be less significant in the deeper sequence where groundwater is very saline, and pressure and temperature are higher. Zechstein Group carbonate lithologies were not analysed, but for the purpose of this study it is assumed that any potential fracture or grain porosity is infilled by evaporite cementation. Therefore, based on these very limited observations, it seems likely these Zechstein Group lithologies have good potential to be seal rocks where they are present at greater depth in the modelled area.

2.4.5 Secondary aquifer – Rotliegendes Group

The 0 - 94 m thick Rotliegendes Group of early Permian age is the secondary analogue aquifer. The Rotliegendes Group is modelled at group level but comprises two formations: the Permian Basal Breccia overlain by the Yellow Sands Formation (Fig. 4). The Permian Basal Breccia is characterized by a matrix-supported conglomerate, including rounded to angular clasts of mudstone, sandstone, ironstone, limestone and less common igneous and metamorphic rocks; the matrix comprises grey-brown, dolomitic or calcareous sandstone. Borehole information indicates that the Permian Basal Breccia is largely absent from the region of study, and where present rests directly on Carboniferous strata. The Yellow Sands Formation is characterized by generally uncemented or weakly cemented, mainly medium- and fine-grained sand or sandstone. This unit was deposited by aeolian processes and represents a relict desert dune field, as discussed previously.

Thirteen samples from the Cleethorpes No. 1 Borehole were examined. The Yellow Sands Formation has an average 2D porosity of 16% (Fig. 13) with a maximum of about 25%,

although this value varies considerably in response to localized dolomitic cementation. The porosity of argillaceous conglomerates within the Permian Basal Breccia is approximately 7% (Milodowski & Rushton 2008). The mineralogy of the Rotliegendes Group samples is similar to the Sherwood Sandstone Group, but with a smaller proportion of albite, which may in part be due to diagenetic dissolution of albite and its replacement by authigenic kaolinite. The porosity and permeability of the Rotliegendes Group samples are influenced by very similar diagenetic factors to those described for the Sherwood Sandstone Group.

2.4.6 Carboniferous underburden

The basal surface of the Rotliegendes Group is characterized by a sharp, angular contact on Carboniferous strata. Comprising the Pennine Coal Measures Group, the underburden consists of an alternating succession of sandstone, siltstone and mudstone with frequent coal seams. Pressure connectivity may exist between the Carboniferous succession and overlying sandstones of the Rotliegendes Group.

2.5 Summary

In the context of an analogue site for CO₂ storage, the 3D geological model for the Lincolnshire area defines substantial thicknesses of analogue aquifer and seal rocks at depths greater than -800 m OD. The 2D porosities, lithological variability and diagenetic history are favourable and relatively well understood at depth. With no major structural traps for CO₂ storage, residual CO₂ saturation and any effect on the up-dip potable aquifer have been studied by work on subsequent fluid flow modelling and physical property analysis (Jin *et al.* 2010; Smith *et al.* 2011).

3. THE DEVONO-CARBONIFEROUS AQUIFER SYSTEM, FORTH AREA, EASTERN SCOTLAND

In the Forth area of eastern Scotland, the primary analogue aquifer comprises the fluvial and aeolian sandstones of the Upper Devonian-lowermost Carboniferous Knox Pulpit Sandstone

and Kinnesswood formations (Fig. 17). The analogue seal rock is the Carboniferous Ballagan Formation. Minor aquifers and seals also occur throughout the Carboniferous overburden (Fig. 17). Eleven surfaces have been modelled, including the top and base seal, top, base and a unit within the potential aquifer, and six stratigraphic horizons within the overburden. The area has known anticlinal structural traps (e.g. Underhill *et al.* 2008). Aquifer rocks have low to medium porosity (up to 20%), very low primary permeability and likely low secondary fracture permeability at the depths studied here (e.g. British Geological Survey 1988; Brereton *et al.* 1988; Cawley *et al.* 2005). Data quality and availability are poor to moderate (Fig. 3).

The Forth 3D geological model is based on an interpretation of third-party 2D seismic data, hundreds of borehole records, tens of downhole geophysical well records, significant amounts of subsurface coal mining data and BGS 1:50,000 scale outcrop mapping (Fig. 3). Additional resources were incorporated, including published information concerning the regional geological framework and tacit information provided through regional geological expertise.

The c. 1420 line km of 1970s - 1980s 2D seismic data used are of variable quality, from very poor (e.g. Midlothian) to moderately good (e.g. Conoco 1987 survey in the Firth of Forth; Fig. 3). They were interpreted using Landmark™ SeisWorks 2D software. The seismic picks were controlled and depth-converted using 5 geophysical wells. None of the wells penetrates as deep as the potential aquifer and seal rocks; they terminate in Strathclyde Group strata (Visean) down to around 2 km subsurface. Estimated thicknesses using regional geological knowledge were used to pick interpreted seismic horizons beneath the well-data control points.

The c. 3645 km² 3D geological model was created according to BGS standard procedures using the GOCAD software (see above). The eleven modelled surfaces define in 3D a succession folded into a series of anticlines and synclines and cut by faults of varying orientations and throws. The top primary aquifer is interpreted to reach depths of c. -2000 to -3000 m OD over the anticlines (Figs 18, 19). The combination of several digital data types in three dimensions, with geological expertise, has resulted in a regionally extensive and kilometres-deep definition of the subsurface geometry, including that in data-poor areas away from seismic data that would not usually be made explicit via contour maps.

3.1 Re-processing and re-interpretation of seismic data

Construction of the Forth 3D geological model was carried out in two phases. An initial interpretation for this study of the existing, publically available seismic data over the offshore Midlothian-Leven Syncline resulted in multiple pinching out of units at the aquifer/seal rock level in an area of poor data quality. In addition, the irregular, discontinuous nature of some of the key stratigraphic horizons around the Forth Anticline, in an area of poor data quality, was interpreted as due to faulting.

To improve data quality and the resulting data interpretation and geological model, reprocessing of a grid of offshore 2D seismic data (Conoco 1987) was carried out by WesternGeco for Schlumberger Water and Carbon Services as part of the CASSEM project. The technical details, described in Sansom (2009), involved pre-stack noise attenuation, pre-stack demultiplex, offset migration and post-stack processing. Interpretation of the reprocessed data (McInroy & Hulbert 2010) revealed that areas with incoherent reflectors in the original dataset, often interpreted to be faults, were coherent, steeply dipping and tightly folded reflectors (Fig. 20). As a consequence, several faults were removed from the original interpretation. Better imaging in the trough of the Midlothian-Leven Syncline led to re-interpretation of the seismic picks, from lateral pinch-outs to through-going, subparallel, synformally folded layers at aquifer/seal level (Fig. 20). There was also a change in the depth of key picks over the Forth Anticline (up to 200 m upwards) and the Midlothian-Leven Syncline (up to 1000 m downwards), and many of the deep reflections, thought to be artefacts, were removed.

3.2 Geological structure and faulting

The modelled horizons very clearly show the regional structure of NNE-trending anticlines and synclines (Figs 18, 19). The most prominent feature is the c.14 km wide Midlothian-Leven Syncline, which reaches an interpreted depth of c. -6100 m OD on the Base Carboniferous horizon. To the east of the Midlothian-Leven Syncline is the smaller, c. 1.6 km wide (at closure) Forth Anticline in the Firth of Forth and the c. 500 m wide (at closure)

D'Arcy-Cousland Anticline in Midlothian. To the west of the Midlothian-Leven Syncline is the Earl's Seat Anticline and the c. 1 km wide (at closure) Burntisland Anticline (Fig. 19). Much farther west, strata deepen towards the Clackmannan syncline of the Kincardine Basin.

Many differing tectono-stratigraphic models have been published for the Carboniferous Midland Valley of Scotland, involving north-south extension (Leeder 1982), east-west tension (Stedman 1988), strike- or oblique-slip movements (Read 1988), and multiphase extension and strike-slip movements on differing orientations of faults (Rippon *et al.* 1996; Ritchie *et al.* 2003). More recent work on the eastern Midland Valley proposed that the Midlothian-Leven Syncline and its flanking Burntisland and D'Arcy-Cousland anticlines developed as major growth folds during the Late Palaeozoic under a predominantly dextral strike-slip regime (Underhill *et al.* 2008). In contrast, the Earl's Seat Anticline and Thornton-Balgonie Syncline were proposed to have formed after the Namurian, wholly as a result of post-depositional (Variscan) compressional deformation.

In the reprocessed Firth of Forth seismic data, continuous, steeply dipping and tightly folded reflectors superimposed upon the broader Forth Anticline are particularly well imaged above one second two-way travel time (TWTT, approximately -1.8 km OD; Fig. 20). The folds appear to become increasingly tight upwards. Folding is interpreted to continue to aquifer/seal rock depths at around 1.5 seconds TWTT (approximately -2.5 km OD). A single fault is interpreted at depth beneath the base Upper Devonian reflector at the hinge zone between the Forth Anticline and Midlothian-Leven Syncline. Rarely, on some lines, the tight folds on the south-eastern edge of the Forth Anticline appear broken by high angle, small offset reversed faults above about 0.5 seconds TWTT (approximately -1.1 km OD). This geometry could be interpreted as a pop-up flower structure, which would sit above the fault interpreted at depth at the hinge zone between the Forth Anticline and Midlothian-Leven Syncline.

Importantly, interpretation of the reprocessed seismic data on the Firth of Forth reveals no major changes in structural style throughout the Carboniferous, as would be expected if a multiphase tectonic history on differing orientations of faults was applicable. Deposition of Upper Devonian- lowermost Carboniferous (to Top Ballagan Formation) strata was followed by a Lower-Mid Carboniferous (Strathclyde Group) wedge of clastic sedimentary strata,

thickening to the northeast. This Strathclyde Group thickening is consistent with field observations along the Fife coast where a westerly prograding wedge of fluvio-deltaic sediments built out into a lacustrine environment characterized by oil-shales (Greensmith 1962, 1965). Stratal thickening, indicating growth into an active Midlothian-Leven Syncline, and thinning onto an adjacent Forth Anticline can be observed from Visean (near top Strathclyde Group) to Westphalian (Scottish Coal Measures Group) or younger strata, and is particularly marked in the Westphalian strata. Inversion/strike-slip with further development of the Forth Anticline structure and associated folds is interpreted in the Late Carboniferous, consistent with post-Westphalian (post-Scottish Coal Measures Group) reversed movement on the Pentland Fault (Peach *et al.* 1910; British Geological Survey 2003; Underhill *et al.* 2008).

Faults at several different scales were incorporated into the 3D geological model (e.g. Figs 18, 19). Over the whole area, seven of the largest regional scale faults were modelled: the Pentland, Ochil (East and West), Dura Den, Archerfield, Dunbar-Gifford, Lammermuir and Southern Upland faults. These have a predominant NE to E trend, and surface traces of tens of kilometres and throws of hundred of metres. A second set of faults was modelled, based on data exported from seismic interpretation. Many of these faults are interpreted entirely in the subsurface, though some are likely to extend to rockhead. They trend in several orientations, but most commonly trend NE and vary between 1 and 10 km in length. The final set of modelled faults comprises smaller, surface-mapped structures included in the model over areas with seismic data coverage. They have traces of a few to tens of kilometres, throws of tens of metres and commonly trend E or NE.

The West and East Ochil Faults were modelled as one continuous 'Ochil Fault', though in reality they likely have differing kinematic histories. This large fault structure has a vertical offset of up to c. 2800 m OD on the Base Carboniferous horizon (Figs 19, 21). The East Ochil Fault is critical because it separates the outcrop area of the main aquifer units and subsurface tie-point of the BGS Glenrothes Borehole [NO 25617 03144], in the north, from areas of the model in the south where the aquifer units are at significant depths and constrained only by seismic data beneath well tie depths. Previous studies have highlighted uplift and tilting of the footwall block of the East Ochil Fault, noted thicker upper Carboniferous strata in the

hangingwall (Browne & Woodhall 1999), and proposed Namurian and end-Carboniferous, right-lateral, strike-slip on the structure (Read 1989). The model defines large thickness variations, particularly in the Visean Strathclyde Group (Fig. 21), for which there is well control on seismic picks. For example, the vertical offset on the fault at the base Limestone Coal Formation is around 500 m, whereas at base Pittenweem Formation it is around 1.5 km (Fig 21). Clearly, the East Ochil Fault existed as an active feature during Visean and Namurian development of the Midlothian-Leven Syncline and associated growth folds. Rippon *et al.* (1996) described an active West Ochil Fault from Lower Devonian to Namurian times. In the light of recent work documenting less than 30 km of post-Early Devonian lateral movement on the Highland Boundary Fault (Tanner 2008), the East and West Ochil faults possibly played a more significant role in the Carboniferous dextral strike-slip evolution of the eastern Midland Valley than previously thought, linked to the development of associated growth folds.

Taking all the coeval syn-depositional faults and folds together in and around the Forth area, this interpretation is consistent with a model of early to late Carboniferous (Visean-Westphalian) growth folds under dextral strike slip (Fig 19b) and Late Carboniferous basin inversion suggested by Underhill *et al.* (2008). It is inconsistent with a Late Devonian-Lower Carboniferous N-S syn-depositional normal fault in the Midlothian-Leven Syncline area (Ritchie *et al.* 2003) and changes in structural style though the Carboniferous.

3.3 Model limitations and uncertainty

The Forth model is appropriate for a scale of use between 1:100,000 and 1: 250,000. Over the areas of the 3D geological model constrained by seismic data, misinterpretation of the seismic picks is the main source of uncertainty. Large areas of the model, particularly at the potential aquifer/seal depths are poorly constrained by seismic data, borehole or mining data points and have a large component of expert geological interpretation. Modelled surfaces in these areas have large uncertainties of hundreds of metres, highlighted by uncertainty maps for each modelled surface (e.g. Figure 19d), qualitatively drawn using expert judgement and taking into account data density, quality and geological complexity. Further work on sensitivity analysis of geological uncertainty, expert elicitation and risking (Smith *et al.*, 2011,

ch. 6) confirmed a greater uncertainty for a riskier Forth site. The models are a simplification of the known geology; for example, they do not include the full structural complexity and are not dissected by known igneous intrusions and vents, both of which could compartmentalize the aquifer and compromise the seal. Outcrop observations indicate that analogue aquifer, seal and overburden strata are very likely to be faulted and fractured; future work could examine whether faults and fractures are likely to be sealed at depth. A key assumption is that the main aquifer aeolian facies (Knox Pulpit Sandstone Formation) is present for at least c. 16 km to the south of the East Ochil Fault, over the Forth and Burntisland anticlines and Midlothian-Leven Syncline. As the Knox Pulpit Sandstone Formation is not observed in Edinburgh and Lothians, a simplistic abrupt southerly extent has been modelled. Modelled units show significant variation in thickness with the most certainty close to the original data points.

3.4 Rock characteristics and properties

The rock mass physical properties and lithological heterogeneity data came from borehole core, outcrop and existing records within the 3D geological model area. Borehole core samples came largely from the BGS Glenrothes Borehole where the primary aquifer and seal were at drilled depths >200 m. Additional primary aquifer/seal material was collected from shallow depth core (<70 m) and outcrop; additional material representing minor aquifers/seals in the overburden was collected from borehole core with drilled depths >200 m (Fig. 3).

3.4.1 Carboniferous overburden

The Carboniferous succession overlying the potential aquifer and seal reaches up to c. 5.7 km in thickness in the centre of the Midlothian-Leven Syncline and is of variable thickness elsewhere, depending on the level of erosion and geological structure. The character of the succession is laterally and vertically variable, dominated by alternations of sandstone, siltstone, mudstone, limestone and coal, representing non-marine, deltaic and shallow marine depositional environments. Sandstones within the overburden are generally less than 20 m in thickness and typically are laterally discontinuous over a kilometre scale or

less. Seal rocks occur throughout the overburden; normally these are silty claystones varying in thickness from metre-scale up to 40 m or more.

A range of lithologies was sampled, representing both potential minor aquifer and seal rocks in the overburden (11 samples). Mineralogically, the sandstones are commonly subfeldspathic to sublithic arenites with detrital quartz and minor K-feldspar, albite, muscovite, biotite and chlorite (Fig. 14). Mudstones and siltstones are commonly composed of illitic clay with minor quartz, muscovite, biotite and chlorite. 2D porosities ranged from negligible in finely laminated, tightly compacted siltstones and mudstones, were commonly between 6% and 13%, but up to 18% in sandstones from greater than 200 m drilled depth, and 21% in outcrop sample sandstones (Milodowski & Rushton 2008; Fig. 22). Relatively low mean macropore sizes were observed in the deeper sandstone samples, suggesting that interconnectivities are limited. Broadly similar processes influence the porosity of the sandstones. The primary intergranular porosity has been reduced by a closely compacted grain fabric and a patchy dolomite cement. Significant secondary porosity is present as a result of framework grain dissolution after feldspars and possibly some lithic clasts. Some samples show major authigenic chlorite and others have authigenic interstitial grain-replacive and pore-filling kaolinite. Pore size and interconnectivity are highest in coarser grained sandstones with significant grain dissolution. However, overall the sandstones represent poor to moderate quality, potential minor aquifer units.

3.4.2 Primary potential seal – Ballagan Formation

The Ballagan Formation is over 150 m thick in the BGS Glenrothes Borehole, up to about 900 m in West Lothian, and is likely to be present across the study area, apart from where it is locally absent by unconformity in the Lomond Hills north of the East Ochil Fault. It is characterized by generally grey mudstones and siltstones, with nodules and beds of ferroan dolostone (cementstone); the beds are usually less than 0.3 m thick (Browne *et al.* 1999; Fig. 23). Gypsum, anhydrite and pseudomorphs after halite occur. Thin sandstones are present in many areas, and thick localized sandstones are also included in the formation in the Edinburgh area.

The Ballagan Formation core rock samples (4 samples from the BGS Glenrothes Borehole) were finely laminated siltstone and mudstone, micaceous sandstone and dolomicrite (Fig. 24) to dolomicritic mudstone. They are highly compacted, and plastic lithic grains such as mudstone clasts and clay pellets have been intensely deformed to form an intergranular pseudomatrix. The total 2D porosity is very low (mean <2%) and represented by microporosity with negligible macroporosity (e.g. Figs 22, 24). The Ballagan Formation appears to represent a potentially good seal rock. However, fractures observed in borehole core require further investigation.

3.4.3 Primary potential aquifer - Knox Pulpit Sandstone and Kinnesswood formations

The Upper Devonian Knox Pulpit Sandstone Formation has been mapped in Fife to reach thicknesses of 130 - 180 m and it is likely to be present at depth within the Firth of Forth (Browne *et al.* 1987), but it has been proven to be absent by borehole drilling in Edinburgh where the Kinnesswood Formation rests directly on the Devonian Pentland Hills Volcanic Formation. Correlative interbedded aeolian and fluvial Upper Devonian strata are seen at Pease Bay to the south-east of the modelled area (Browne & Barclay 2005).

The Knox Pulpit Sandstone Formation in Fife comprises soft, weakly cemented, white and cream-coloured, very fine- to coarse-grained feldspathic sandstones with characteristic pin-stripe lamination of aeolian origin (Browne *et al.* 1999). The rarity of pebbles is a distinctive feature with small masses of ochreous decomposed calcrete (cornstone) near the top of the formation and greenish grey silty claystone near the base (Fig. 23). Analysis of borehole logs shows 99 - 100% of the unit to be of sandstone.

The characteristics of the Knox Pulpit Sandstone Formation are known only down to depths of 584 m from the BGS Glenrothes Borehole. In the nine samples analysed, the sandstones are subfeldspathic arenites composed of detrital quartz with subordinate K-feldspar, muscovite and rare heavy minerals and lithic fragments (Fig. 14). Intergranular clay is produced by the compactional deformation of mudstone clasts or clay pellets. Ferroan dolomite and ankerite are major cements, along with minor quartz and K-feldspar overgrowths. Authigenic kaolinite replacing detrital framework grains is common. The mean 2D porosity is 14% but ranges

from 3% to 26% with relatively high mean macropore sizes (Milodowski & Rushton 2008; Fig. 22), Brereton *et al.* (1988) reported a mean horizontal permeability from the BGS Glenrothes Borehole of between 60 and 70 mD, but with some permeabilities > 1000 mD.

The overlying Carboniferous Kinnesswood Formation also forms part of the potential aquifer volume. It is commonly 100 - 200 m thick, but reaches up to 640 m in the Edinburgh area. The Kinnesswood Formation is interpreted as being present across the whole of the area, probably interfingering with the top of the Knox Pulpit Sandstone Formation. The Kinnesswood Formation consists predominantly of purple-red, yellow, white and grey-purple, fine- to coarse-grained sandstones, which are mostly cross bedded and arranged in upward-fining units (Browne *et al.* 1999). Fine-grained, planar or poorly bedded sandstones, red mudstones and thin beds and nodules of calcrete (pedogenic concretionary limestone) also occur. The percentage of sandstone within the Kinnesswood Formation in boreholes in Fife varies from 82 - 86%, with up to 10% pedogenic limestone and up to 6 - 8% mudstone/siltstone.

The six sandstones examined are mineralogically similar to those of the Knox Pulpit Sandstone Formation. In the BGS Glenrothes Borehole, the Kinnesswood Formation yielded a mean 2D porosity of 17% with a range from about 7 to 22% (Milodowski & Rushton 2008; Fig. 22). Permeabilities in this borehole ranged from 0.1 to over 400 mD (Brereton *et al.* 1988).

In outcrop and shallow aquifer samples from the Kinnesswood and Knox Pulpit Sandstone formations, compaction has reduced the primary intergranular porosity considerably. Much of the present porosity in these rocks is secondary, and dominated by the dissolution of feldspar or lithic clast framework grains, which produced large oversized pores. Some of these framework grain dissolution sites are partially filled by microporous authigenic kaolinite (Fig. 25). Porosity has been enhanced by the removal of ferroan dolomite cement. In samples from hundreds of metres depth in the BGS Glenrothes Borehole, ferroan dolomite cement has not been removed, preserving an uncompacted sandstone fabric (Fig. 25), and resulting in lower 2D porosities (4-13%).

The fluvial, Upper Devonian Glenvale Sandstone Formation, which is laterally equivalent to the Knox Pulpit Sandstone Formation at its top, and the underlying Burnside Sandstone Formation, could also form part of the potential aquifer (Fig. 23). Together, the Glenvale Sandstone and Burnside Sandstone formations are up to 500 m thick and consist predominantly of fine- to very coarse-grained sandstones with pebbles and beds of conglomerate (Browne *et al.* 2004). The two core rock samples from the Burnside Sandstone Formation represent tightly compacted and poorly sorted, muddy sublitharenite with wackestone or packstone grain fabrics. Virtually all primary porosity has been lost in these samples through the greater compaction of these rocks.

3.5 Summary

In the context of an analogue site for CO₂ storage, the 3D geological model for the Forth area defines analogue aquifer and seal rocks folded into anticlinal trap structures at depths greater than 1 km OD. The properties of the analogue aquifer appear of moderate quality, with a key uncertainty being the regional extent of the Knox Pulpit Sandstone Formation and its porosity, permeability and fracturing at depths greater than 600 m. The properties of the Ballagan Formation suggest that it could be a good seal rock, though fracturing needs to be further investigated. The Carboniferous overburden contains discontinuous sandstone bodies with low to moderate 2D porosity and siltstones/mudstones with low 2D porosity, suggesting that it could enhance sealing capacity. Fluid flow modelling, structural analysis and additional physical property analysis were undertaken on this analogue storage site (Jin *et al.* 2010, Smith *et al.* 2011).

4. CONCLUSIONS

Two contrasting 3D geological models illustrate the utility of an integrated approach using digital techniques and expert geological knowledge. By defining the subsurface geometries and faulting of key stratigraphic horizons and combining these with rock properties, the geological frameworks for two analogue CO₂ storage sites have been built. The study was undertaken to establish methodologies; the sites have not been considered as real candidate CO₂ storage sites.

The Lincolnshire model of Permo-Triassic aquifers and seals has proven favourable depth, thickness and rock properties for initial geological screening of a CO₂ analogue storage site, though no significant structural trap exists. The certainty of the model is high due to good data quality and coverage. The succession dips between 0.7° and 1.1° to the ENE, reaching a depth of -1500 m OD on the top Sherwood Sandstone Group at the Lincolnshire coast. High angle normal faults with throws of 20-30 m exhibit a NW and WNW trend, consistent with regional structure (Evans & Allsop 1987; Pharaoh *et al.* 2011). Thickness modelling combined with lithological information from boreholes has tested and refined the Permian palaeogeographical maps of Smith (1989). Of particular note are the interpretation of large-scale NW-SE oriented Rotliegendes Group aeolian dunes, and the identification of a Cadeby Formation reef edge and seaward slope together with complementary Edlington Formation thickening. Mineralogy and 2D porosity data for 55 Lincolnshire samples favourable for a CO₂ analogue storage site have been described, with a diagenetic history and well known lithological character. However, samples preserved in formation brine from the Sherwood Sandstone Group contained fibrous illite, which may significantly decrease permeability.

The 3D geological model of the Forth area of Devonian-Carboniferous strata defines potential aquifers and seals buried at depths >1000 m OD with anticlinal structural traps. However, due to limited data availability and quality, certainty in the model at aquifer and seal depths is low. Together with the poor to moderate 2D porosity and permeability values and the lithological heterogeneity of the potential aquifer strata, this degree of uncertainty makes the Forth area a less favourable analogue CO₂ storage site than the Lincolnshire area at an initial geological screening stage.

The Forth model makes explicit regionally extensive and kilometres-deep surfaces and faults, synthesizing variable data coverage. As long as the model constraints and uncertainty are understood, it forms a valuable tool in understanding the regional geological evolution. For example, the subsurface modelling of anticlines, synclines and faults up to 6 km depth and into the Upper Devonian supports and extends previous work on the structural and stratigraphic evolution of the area (e.g. Read 1989; Underhill *et al.* 2008). Reprocessing of a key seismic dataset has resulted in greater certainty in interpretation of tight folds superimposed upon the Forth Anticline, with a single fault interpreted at depth beneath the

Upper Devonian in the hinge zone between the Forth Anticline and Midlothian-Leven Syncline. The geometry of the modelled horizons implies no major changes in structural style from the Upper Devonian and throughout the Carboniferous. The pattern of coeval E-W and NNE faulting on major, reactivated faults and smaller intrabasinal structures, and NNE-trending growth folding is consistent with Visean - Westphalian dextral strike-slip followed by Late Carboniferous basin inversion. Large throws on the East and West Ochil faults have been modelled, with significant growth in the Visean and Namurian concomitant with growth folding. The mineralogy, 2D porosity and diagenetic history of 42 rock samples establish a mean of <2% porosities in potential seal rocks. Intact ferroan dolomite cement in the deepest potential aquifer sandstone samples preserves an uncompacted sandstone fabric with lower 2D porosities (4-13%) than shallow aquifer samples (up to 26%).

Reprocessing of 2D seismic data from the Forth area has highlighted the potential for the relatively cheap re-use of older datasets before committing to more expensive 3D seismic datasets or new seismic surveys. Smith *et al.* (2011) describe how these 3D geological models and framework were further evaluated as analogue sites for CO₂ storage.

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REFERENCES

- BATH, A.H., MILODOWSKI, A.E. & SPIRO, B. 1987. Diagenesis of carbonate cements in Permian-Triassic sandstones in the Wessex and East Yorkshire-Lincolnshire basins, UK: a stable isotope study. *In*: MARSHALL, J.D. (ed). Diagenesis of Sedimentary Sequences. *Geological Society Special Publication*, **36**, 173-190.
- BECKER, F. & BECHSTÄDT, T. 2006. Sequence stratigraphy of a carbonate-evaporite succession (Zechstein 1, Hessian Basin, Germany). *Sedimentology*, **53**, 1083–1120.
- BRERETON, R., BROWNE, M.A.E., CRIPPS, A.C., GEBSKI, J.S., BIRD, M., HALLEY, D.N. & McMILLAN, A.A. 1988. *Glenrothes Borehole: geological well completion report*. British Geological Survey Report, Investigation of the Geothermal Potential of the U.K.
- BRITISH GEOLOGICAL SURVEY. 1988. *Geothermal energy in the United Kingdom: review of the British Geological Survey's Programme 1984 - 1987*. Investigation of the geothermal potential of the UK.
- BRITISH GEOLOGICAL SURVEY, 2003. Edinburgh. Scotland Sheet 32E. Bedrock. 1:50 000. (Southampton: Ordnance Survey for British Geological Survey)

- BRITISH GEOLOGICAL SURVEY. 2006. Rotliegendes Group. Available: <http://www.bgs.ac.uk/Lexicon/lexicon.cfm?pub=RLG>. Last accessed 4th Nov 2010.
- BROWNE, M.A.E., ROBINS, N.S., EVANS, R.B., MONRO, S.K. & ROBSON, P.G. 1987. *The Upper Devonian and Carboniferous sandstones of the Midland Valley of Scotland*. Investigation of the Geothermal Potential of the UK, British Geological Survey.
- BROWNE, M.A.E., DEAN, M.T., HALL, I.H.S., MCADAM, A.D., MONRO, S.K. & CHISHOLM, J.I. 1999. *A lithostratigraphical framework for the Carboniferous rocks of the Midland Valley of Scotland*. British Geological Survey Research Report, RR/99/07.
- BROWNE, M. A. E. & WOODHALL, D. G. 1999. Geology of the Kirkcaldy district - a brief explanation of the geological map. *Sheet Explanation of the British Geological Survey*, 1:50 000 Series. Sheet 40E (Scotland).
- BROWNE, M.A.E. SMITH, R.A & AITKEN, A.M. 2004. *Stratigraphical framework for the Devonian (Old Red Sandstone) rocks of Scotland south of a line from Fort William to Aberdeen*: British Geological Survey Research Report RR/01/004.
- BROWNE, M. A. E., & BARCLAY W. J. 2005. Siccar Point to Hawk's Heugh, Scottish Borders. In *The Old Red Sandstone of Great Britain* (W. J. BARCLAY, M. A. E. BROWNE, A. A. McMILLAN, E. A. PICKETT, P. STONE AND P. R. WILBY) Geological Conservation Review Series, No 31, Joint Nature Conservation Committee, Peterborough, 181-186.
- CAWLEY, S. SAUNDERS, M.R., LE GALLO, Y., CARPENTIER, B., HOLLOWAY, S., KIRBY, G.A., BENNISON, T., WICKENS, L., WICKRAMARATNA, R, BIDSTRUP, T., ARKLEY, S.L.B., BROWNE, M.A.E. & KETZER, J.M. 2005. The NGCAS project - Assessing the potential for EOR and CO₂ sequestration at the Forties oilfield, offshore UK. In THOMAS, D.C. & BENSON, S.M. (eds) *Carbon dioxide storage in deep geologic formations*, Volume 2, Elsevier Sciences, 713-750.
- CHADWICK, R.A., ARTS, R., BERNSTONE, C., MAY, F., THIBEAU, S. & ZWEIGEL, P. 2008. *Best practice for the storage of CO₂ in saline aquifers*. Keyworth, Nottingham, British Geological Survey Occasional Publication no 14. ISBN 978-0-85272-610-5.

- CHADWICK, A., CLOCHARD, V., DELEPINE, N., LABAT, K., STURTON, S., BUDDENSIEK, M. L., DILLEN, M., NICKEL, M., LIMA, A.L., WILLIAMS, G., NEELE, F., ARTS, R. & ROSSI, G. 2010 Quantitative analysis of time-lapse seismic monitoring at the Sleipner CO₂ storage operation. *The Leading Edge*, **29**, 170-177.
- COOPER, A.H. & BURGESS, I.C. 1993. *Geology of the country around Harrogate*. Memoir of the British Geological Survey, Sheet 62 (England and Wales).
- CULSHAW, M. G. 2005. From concept towards reality: developing the attributed 3D geological model of the shallow subsurface. *Quarterly Journal of Engineering Geology & Hydrogeology*, **38**, 231-284.
- DAVIES, R. J., CARTWRIGHT, J. A., STEWART, S. A., LAPPIN, M. & UNDERHILL, J. R. (eds) 2004. *3D Seismic Technology: Application to the Exploration of Sedimentary Basins*. Geological Society, London, Memoirs, 29, The Geological Society of London.
- DAVIES, R. J., GRAS, R. & PAYRE, X. 2005. A vision for 3D seismic technology and visualization. In: DORE, A. G. & VINING, B. A. (eds) *Petroleum Geology: North-West Europe and Global Perspectives—Proceedings of the 6th Petroleum Geology Conference*, 1483–1486. Petroleum Geology Conferences Ltd. Published by the Geological Society, London
- DOWNING, R. A., ALLEN, D. J., BIRD, M. J., GALE, I. N., KAY, R. L. F. & SMITH, I. F. 1985. Cleethorpes No.1 Geothermal Well – a preliminary assessment of the resource. *Investigation of the Geothermal Potential of the UK. WJ/GE/85. British Geological Survey Report*.
- DTI. 2006. *Industrial Carbon Dioxide Emissions and Carbon Dioxide Storage Potential in the UK* Report COAL R308 DTI/Pub URN 06/2027.
- EVANS, C. J & ALLSOP, J. M. 1987. Some geophysical aspects of the deep geology of eastern England. *Proceedings of the Yorkshire Geological Society*, **46**, 321-333.
- FORD, J.R., PHARAOH, T.C., HULBERT, A.G., VINCENT, C.J. & COOPER, A.H. 2008. *CASSEM Work Package One : British East Midlands and Lincolnshire geological modelling*. British Geological Survey Report, CR/08/152.

- FORD, J.R. & MONAGHAN, A.A. 2009. *Lithological heterogeneity of the Mercia Mudstone and Sherwood Sandstone Groups in the Yorkshire-Lincolnshire region, and Knox Pulpit Sandstone, Kinnesswood and Ballagan Formations in the Forth region : additional information for CASSEM Work Package One*. British Geological Survey Report, CR/09/053.
- FORD, J.R., MONAGHAN, A.A., MILODOWSKI, A.E. & KIRK, K. L. 2009. *CASSEM Work Package One – Summary methodological report for 3D geological framework and rock sample mineralogy*. British Geological Survey Report, CR/09/009.
- FORD, J.R., MATHERS, S.J., ROYSE, K. R., ALDISS, D.T. & MORGAN, D.J.R. 2010. Geological 3D modelling: scientific discovery and enhanced understanding of the subsurface, with examples from the UK. *Zeitschrift der Deutschen Gesellschaft für Geowissenschaften*, **161**, 205-218.
- GLENNIE, K. W. 1982. Early Permian (Rotliegendes) palaeowinds of the North Sea. *Sedimentary Geology*, **34**, 245-265.
- GLENNIE, K W. 1983. Lower Permian Rotliegend desert sedimentation in the North Sea area. in BROOKFIELD, M. E. & AHLBRANDT, T. S. (Eds). *Eolian Sediments and Processes*. Developments in Sedimentology, **No. 38**, 521-541 (Amsterdam: Elsevier, 660 pp)
- GLENNIE, K.W., MUDD, G.C. & NAGTEGAAL, P.J.C. 1978. Depositional environment and diagenesis of Permian Rotliegendes sandstones in Leman Bank and Sole Pit areas of the UK Southern North Sea. *Journal of the Geological Society of London*. **135**, 25-34.
- GREENSMITH, J. T., 1962. Rhythmic deposition in the Carboniferous oil- shale group of Scotland. *Journal of Geology* **70**, 355–364.
- GREENSMITH, J. T., 1965. Calciferous Sandstone Series sedimentation at the eastern end of the Midland Valley of Scotland. *Journal of Sedimentary Research* **35**, 223–242.
- INSTITUTE OF GEOLOGICAL SCIENCES, 1980. Louth. England and Wales Sheet 103. Solid and Drift, 1:50 000. (Southampton: Ordnance Survey for Institute of Geological Sciences)
- JIN, M., PICKUP, G.E., MACKAY, E.J., TODD, A.C., MONAGHAN. A, AND NAYLOR, M, 2010. Static and Dynamic Estimates of CO₂ Storage Capacity in Two Saline Formations in the UK.

Paper no. 131609, Society of Petroleum Engineers EUROPEC/EAGE Annual Conference and Exhibition, June 2010.

JOHNSON, H., WARRINGTON, G. & STOKER, J.J. 1994. Permian and Triassic of the Southern North Sea. In: KNOX, R.W. & CORDEY, W.G. (Eds) *Lithostratigraphic nomenclature of the UK North Sea*. British Geological Survey, Nottingham.

KAISER, R., NOTH, S. & RICKEN, W. 2003. Sequence stratigraphy with emphasis on platform-related parasequences of the Zechstein 2 carbonate (Ca₂) – the northern platform margin of the Southern Permian Basin (NE Germany). *International Journal of Earth Sciences (Geol Rundsch)*. **92**, 54-67.

KEMP, E A DE. 2007. 3D Geological Modelling Supporting Mineral Exploration. In: GOODFELLOW, W. D. (Ed), *Mineral Deposits of Canada: A Synthesis of Major Deposit Types, District Metallogeny, the Evolution of Geological Provinces, and Exploration Methods*: Geological Association of Canada, Mineral Deposits Division, Special Publication 5, 1051-1061.

KENT, P. (ed.). 1980. British regional geology: Eastern England from the Tees to The Wash, (2nd edition). (London: HMSO for the British Geological Survey).

LEEDER, M.R., 1982. Upper Palaeozoic basins of the British Isles- Caledonian inheritance versus Hercynian plate marginal processes. *Journal of the Geological Society of London* **139**, 479–491

LELLIOTT, M. R., BRIDGE, D. MCC., KESSLER, H., PRICE, S. J. & SEYMOUR, K. J. 2006. The application of 3D geological modelling to aquifer recharge assessments in an urban environment. *Quarterly Journal of Engineering Geology and Hydrogeology*, **39**, 293-302;

MARIE, J.P.P. 1975. Rotliegendes stratigraphy and diagenesis. In: WOODLAND, A.W. (Ed) *Petroleum and the Continental Shelf of North West Europe. 1. Geology*. Applied Science Publishers, Barking, Essex, UK.

MCINROY, D.B & HULBERT, A. 2010. *CASSEM: Interpretation of the reprocessed Conoco 87 Firth of Forth Seismic Survey, and subsequent modifications to the 3D geological model*. British Geological Survey Report, CR/10/026

- MILODOWSKI, A.E., STRONG, G.E., WILSON, K.S., HOLLOWAY, S. & BATH, A.H. 1987. Diagenetic influences on the aquifer properties of the Permo-Triassic sandstones in the East Yorkshire and Lincolnshire Basin. *Investigation of the Geothermal Potential of the UK. British Geological Survey.*
- MILODOWSKI, A E & RUSHTON, J E. 2008. Mineralogical and porosity characterisation of potential aquifer and seal units for carbon capture and storage methodologies for the CASSEM Project. *British Geological Survey Report, CR/08/153.*
- MONAGHAN, A.A., MCINROY, D.B., BROWNE, M.A.E. & NAPIER, B.R. 2008. CASSEM Work Package One - Forth Geological Modelling. *British Geological Survey Report, CR/08/151.* 99pp.
- MOSSOP, G.D. & SHEARMAN, D.J. 1973. Origins of secondary gypsum rocks. *Transactions of the Institute of Mining and Metallurgy*, **82**, B147-B154.
- PEACH, B N, CLOUGH, C T, HINXMAN, L W, GRANT WILSON, J.S., CRAMPTON, C.B., MAUFE, H.B., BAILEY, E.B., 1910. The Geology of the Neighbourhood of Edinburgh, Second edition, *Memoir of Geological Survey.*
- PETTIJOHN, F.J., POTTER, O.E. & SEIVER, R. 1987. *Sand and Sandstone*. New York: Springer.
- PHARAOH, T. C., VINCENT, C. J., BENTHAM, M. S., HULBERT, A. G., WATERS, C. N. & SMITH, N. J. 2011. Structure and evolution of the East Midlands region of the Pennine Basin. *Subsurface Memoir of the British Geological Survey*
- POLSON D. & CURTIS A. 2010. Dynamics of uncertainty in geological interpretation. *Journal of the Geological Society of London*, **167**, 5-10.
- READ, W.A., 1988. Controls on Silesian sedimentation in the Midland Valley of Scotland. In: BESLY, B.M., KELLING, G. (EDS.), 222–241 in *Sedimentation in a synorogenic basin complex: the Upper Carboniferous of northwest Europe*. Blackie and Son, Glasgow.
- READ, W.A. 1989 Sedimentological evidence for a major subsurface fracture system linking the eastern Campsie and the eastern Ochil faults. *Scottish Journal of Geology*, **25**, 187-200.
- RIPPON, J., READ, W. A. & PARK, R. G. 1996. The Ochil Fault and the Kincardine basin: key

- structures in the tectonic evolution of the Midland Valley of Scotland. *Journal of the Geological Society, London*, **153**, 573-587.
- RITCHIE, J. D., JOHNSON H., BROWNE M. A. E. & MONAGHAN A. A. 2003. Late Devonian-Carboniferous tectonic evolution within the Firth of Forth, Midland Valley, as revealed from 2D seismic reflection data. *Scottish Journal of Geology*, **39**, 121-134
- ROYSE, K. R. KESSLER, H., ROBINS, N. S., HUGHES, A. G. & MATHERS, S. J. 2010. The use of 3D geological models in the development of the conceptual groundwater model. *Zeitschrift der Deutschen Gesellschaft für Geowissenschaften*, **161**, 237-249.
- RUFFELL, A.H., HOLLIDAY, D.W. & SMITH, D.B. 2006. Permian: arid basins and hypersaline seas.. in BRENCHLEY, P.J. & RAWSON, P.F. (eds) *The Geology of England and Wales*. The Geological Society, London, 269-293.
- SANSOM, J. 2009. Data Processing Report for CASSEM Reprocessing Project, Firth of Forth, for Schlumberger Water and Carbon Services. *WG Contract Number: C180*.
- SMITH, D B & FRANCIS, E A. 1967. *Geology of the Country Between Durham and West Hartlepool*. Memoirs of the Geological Survey of Great Britain. No. 27 (England and Wales).
- SMITH, D. B. 1989. The late Permian palaeogeography of north-east England. *Proceedings of the Yorkshire Geological Society*, **47**, 285-312.
- SMITH M. CAMPBELL, D., MACKAY E. & POLSON D. (EDS). 2011. *CO₂ Aquifer Storage Site Evaluation and Monitoring (CASSEM)*. Heriot-Watt University, Edinburgh. ISBN 978-0-9571031-0-8
- SMITH, N. J. P, KIRBY, G. A., & PHARAOH, T. C. 2005. *Structure and evolution of the south-west Pennine Basin and adjacent area*. Subsurface memoir of the British Geological Survey.
- STEDMAN, C., 1988. Namurian E1 tectonics and sedimentation in the Midland Valley of Scotland: rifting versus strike-slip influence. In: BESLY, B.M., KELLING, G. (EDS.), *Sedimentation in a Synorogenic Basin Complex: the Upper Carboniferous of Northwest Europe*. Blackie & Son, Glasgow, pp. 242–254.

- STEELE, R. P. 1983. Longitudinal drag in the Permian Yellow Sands of northeast England. in BROOKFIELD, M. E. & AHLBRANDT, T. S. (Editors). *Eolian sediments and processes. Developments in sedimentology. No. 38*, 543-550. (Amsterdam: Elsevier 660pp).
- TANNER, G. 2008. Tectonic significance of the Highland Boundary Fault, Scotland. *Journal of the Geological Society*, London. **165**, 915 – 921.
- TAYLOR, J. C. M. & COULTER, V. S. 1975. Zechstein of the English Sector of the southern North Sea basin. 249-263 in WOODLAND, A W (Editor). *Petroleum and the continental shelf of north-west Europe, Vol. 1 Geology*. (Barking, England: Applied Sci. Publishers Ltd.) 501pp.
- TUCKER, M. E. 1991. Sequence stratigraphy of carbonate-evaporite basins: models and application to the Upper Permian (Zechstein) of northeast England and adjoining North Sea. *Journal of the Geological Society, London*, **148**, 1019-1036.
- TURNER, A K (ED). 1992. Three-Dimensional Modelling with Geoscientific Information Systems. North Atlantic Treaty Organisation ASI Series C: Mathematical and Physical Sciences, 354, Kluwer, Dordrecht (1991) 443p.
- TURNER, A. K. & GABLE, C. W. 2007. A review of geological modelling. In: Three-Dimensional Geologic Mapping for Groundwater Applications. In: THORLEIFSON, L. H., BERG, R. C. & RUSSELL, H. A. J. (Eds). *Three-dimensional geologic mapping for groundwater applications*. Minnesota Geological Survey, Open-File Report 07-4, 90 p.
- UNDERHILL, J.R., MONAGHAN, A.A. & BROWNE, M.A.E. 2008. Controls on structural styles, basin development and petroleum prospectivity in the Midland Valley of Scotland. *Journal of Marine and Petroleum Geology*, **25**, 1000-1022.
- VERSEY, H. C. 1925. The beds underlying the Magnesian Limestone in Yorkshire. *Proceedings of the Yorkshire Geological Society*, **20**, 200-214.
- ZANBAK, C. & ARTHUR, R. 1986. Geochemical and engineering aspects of anhydrite/gypsum phase transitions. *Bulletin of the Association of Engineering Geologists*, **23**, 419-433.

FIGURES

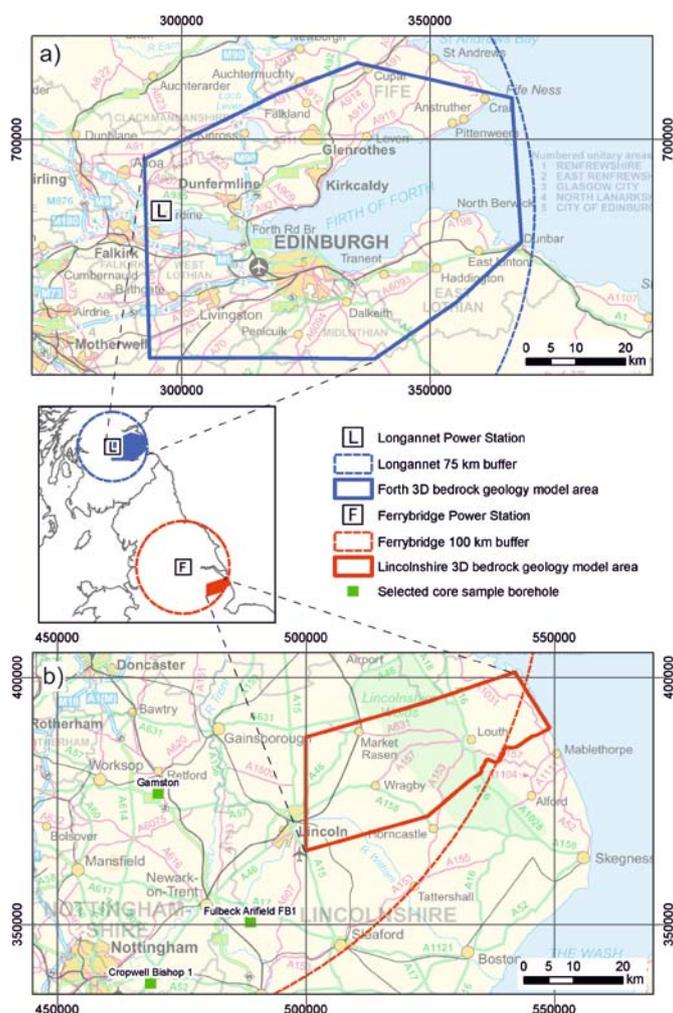


Fig. 1. Location maps showing the areas of study surrounding a) Longannet Power Plant (Forth area) and b) Ferrybridge Power Plant (Yorkshire/Lincolnshire area), including the location of selected borehole samples (see also Fig. 2). OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved.

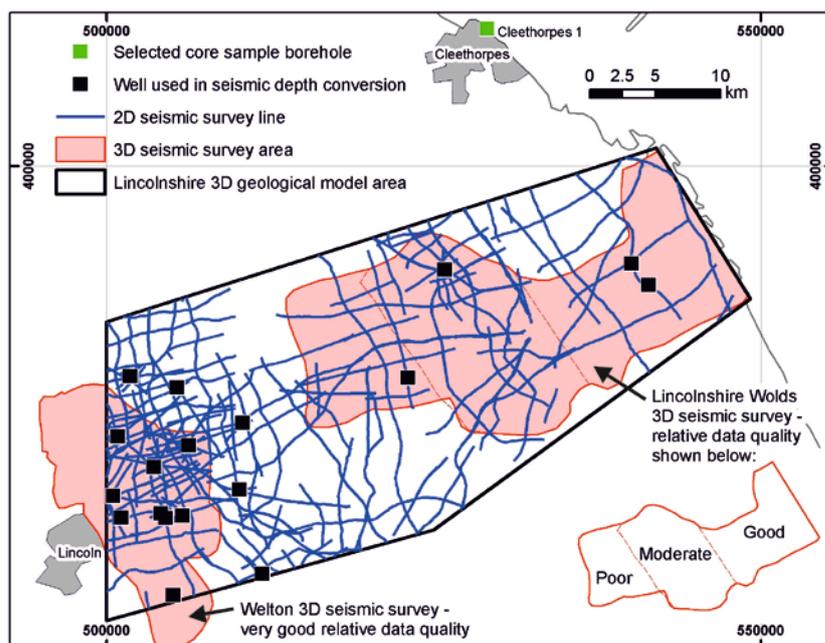


Fig. 2. Distribution of seismic data, wells and the Cleethorpes No. 1 Borehole considered in the Lincolnshire 3D geological model and corresponding rock sample analysis (see also Fig. 1). NB. areas of “low” and “moderate” quality 3D seismic survey data were selectively substituted by better quality 2D data. OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved. Location of seismic lines from UK Onshore Geophysical Library.

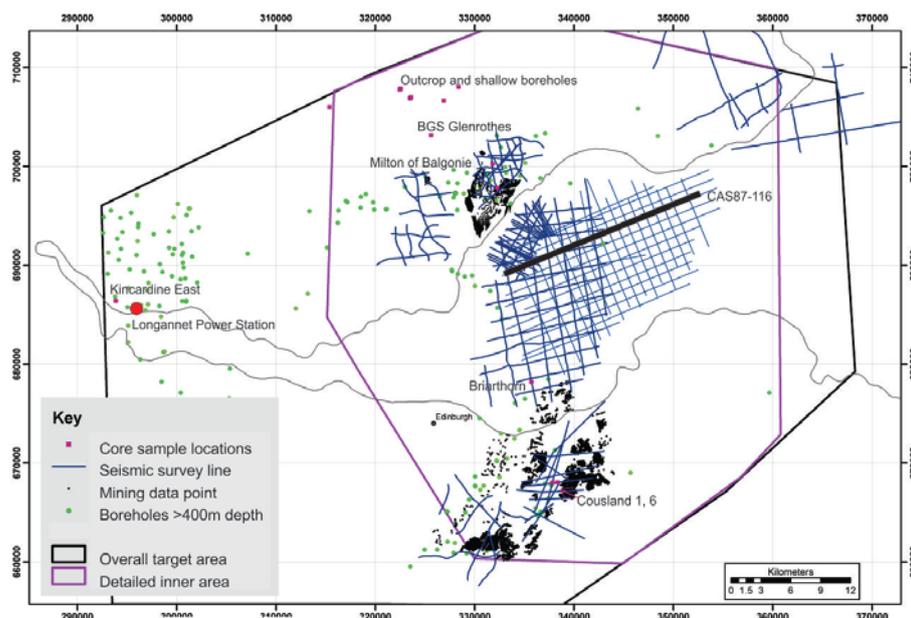


Fig. 3. Distribution of seismic data, boreholes, and mining data used in the Forth 3D geological model and corresponding rock sample analysis. OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved. Location of seismic lines from UK Onshore Geophysical Library (onshore) and reproduced under sub-licence from Phoenix Data Solutions Ltd. (offshore). The location of seismic line CAS87-116 (Figure 20) is shown.

	Group/Sub-Period	Formations	Dominant lithology	Status and Thickness(m)	
CRETACEOUS	Chalk Group (Upper Cretaceous)	Undivided	Chalk and marly-chalk, flint as nodules and persistent horizons	Primary Overburden Approx. 200 m	
	Lower Cretaceous	Undivided	Sandstone, mudstone, ironstone and chalk		
JURASSIC	Upper Jurassic	Undivided (Inc. Lincs. Limestone Formation —)	Mudstone with minor sandstone, limestone and siltstone	Primary Overburden Approx. 660 m	
	Middle Jurassic	Undivided	Limestone, sandstone, mudstone and ironstone		
	Lias Group (Lower Jurassic)	Undivided	Mudstone with subordinate limestone, siltstone, sandstone and ironstone		
TRIASSIC	Penarth Group	Not fully divisible in area	Grey and greenish grey calcareous mudstone	Primary Overburden Approx. 10 - 20 m	
	Mercia Mudstone Group	Not fully divisible in area	Red-brown calcareous mudstone and siltstone with anhydrite and gypsum	Primary Seal Approx. 200 - 300 m	
	Sherwood Sandstone Group	Not fully divisible in area	Red-brown sandstone with calcareous mudstone and mud-flake conglomerate.	Primary Aquifer Approx. 170 - 380 m	
PERMIAN	Zechstein Group	Roxby Equivalents	Roxby Formation (including Littlebeck Anhydrite Formation)	Red-brown calcareous and anhydritic or gypsiferous mudstone	Primary Bottom Seal Approx. 4 - 120 m
			Anhydrite with minor gypsum	Red-brown calcareous and anhydritic or gypsiferous mudstone	
			Sherburn (Anhydrite) Formation	Grey and red-brown anhydrite, minor gypsum and mudstone	
			Roxby Formation (part)	Red-brown calcareous and anhydritic or gypsiferous mudstone	
			Boulby Halite Formation	Salt	
			Billingham Anhydrite Formation	Grey anhydrite with minor gypsum	
	Edlington Equivalents	Brotherton Formation	Light grey fine-grained dolomitic limestone	Secondary Overburden Approx. 15 - 50 m	
		Edlington Formation (including Grauer Salztun and Fordon Evaporite fms)	Salt and mudstone	Secondary Overburden Approx. 10- 175 m	
			Red-brown calcareous and anhydritic mudstone with minor gypsum		
		Kirkham Abbey Formation	Grey dolostone		
		Hayton Anhydrite Formation	Grey anhydrite with minor gypsum		
	Cadeby Equiv's	Cadeby Formation	Grey and light yellowish brown dolostone	Secondary Seal Approx. 5 - 132 m (Cadeby), 1 - 2 m (Marl Slate)	
		Marl Slate Formation	Dark grey laminated dolomitic pyritic mudstone		
	Rotliegendes Group	Yellow Sands Formation	Grey fine-grained aeolian sand	Secondary Aquifer 0 - 94 m	
Permian Basal Breccia		Sandstones and matrix supported conglomerate			

Fig. 4. Lithological summary of the bedrock succession considered in the Lincolnshire area and position of the modelled horizons highlighted in red. The secondary bottom seal or underburden (alternating sandstone, siltstone and mudstone of the Carboniferous Pennine Coal Measures Group) was not studied and is not shown.

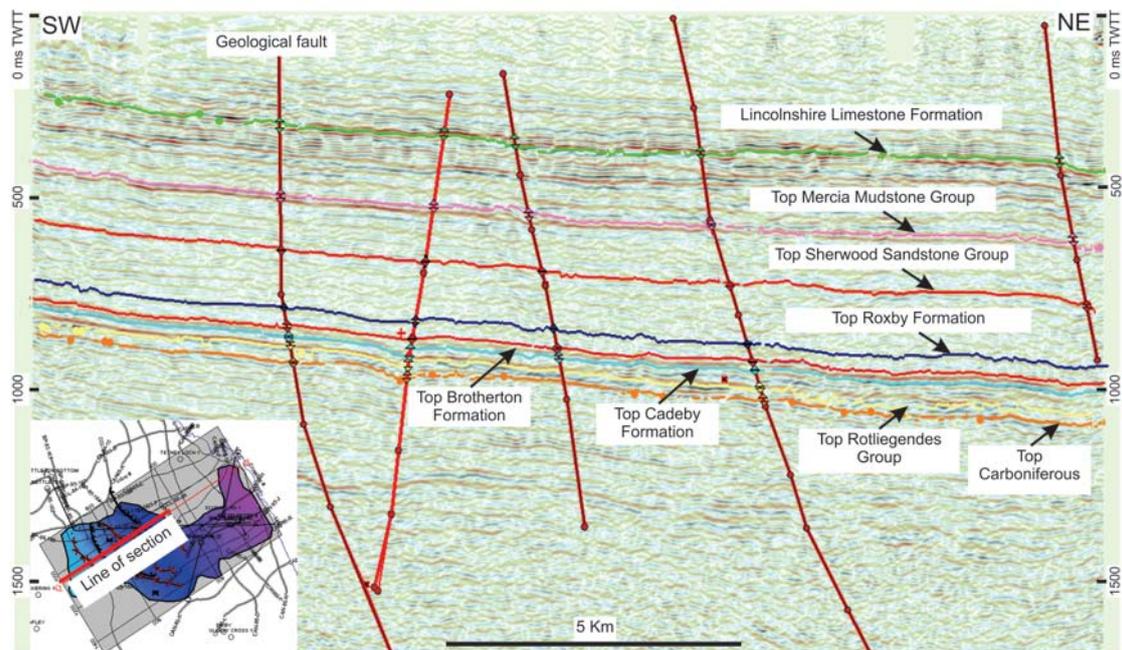


Fig. 5. Example line of section showing 3D seismic data and surface interpretation including geological faults in the Lincolnshire 3D bedrock geology model area. Shown with permission of the UK Onshore Geophysical Library.

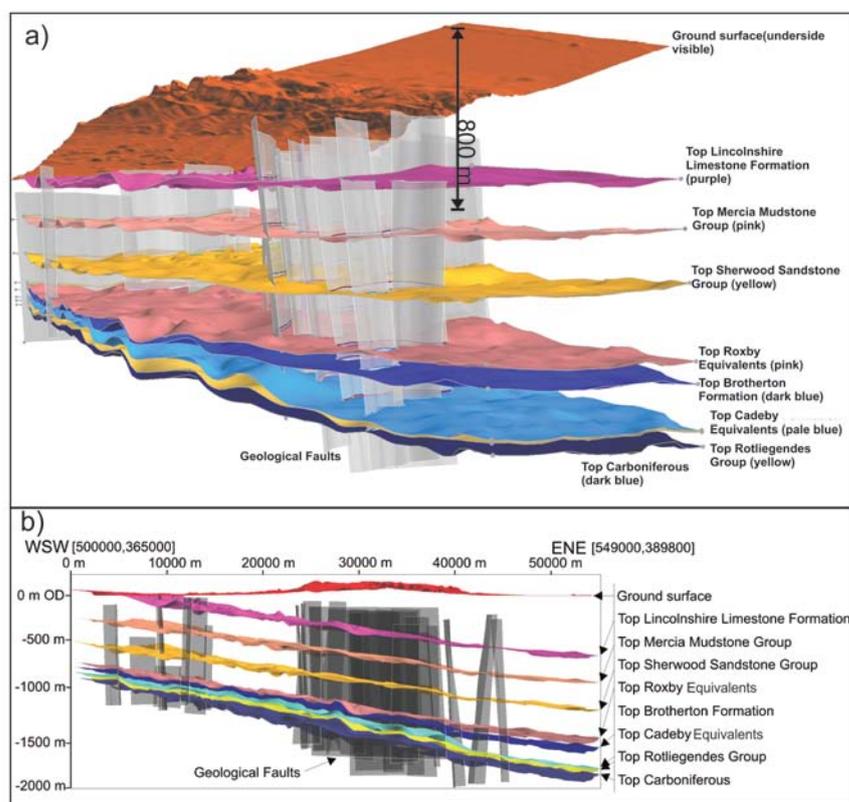


Fig. 6. (a) Vertically exaggerated (15 times) isometric view of the Lincolnshire 3D geology model viewed from the south-east, looking north-west. (b) Vertically exaggerated (10 times) view of the Lincolnshire 3D geological model viewed from the SSE, looking along strike. Based on interpreted seismic data, the majority of the faults are shown to terminate upwards within the succession above the Lincolnshire Limestone. The lower termination of the faulting beneath the top Carboniferous surface is based on an arbitrary cut-off. Ground surface based on NEXTMap Britain elevation data from Intermap Technologies.

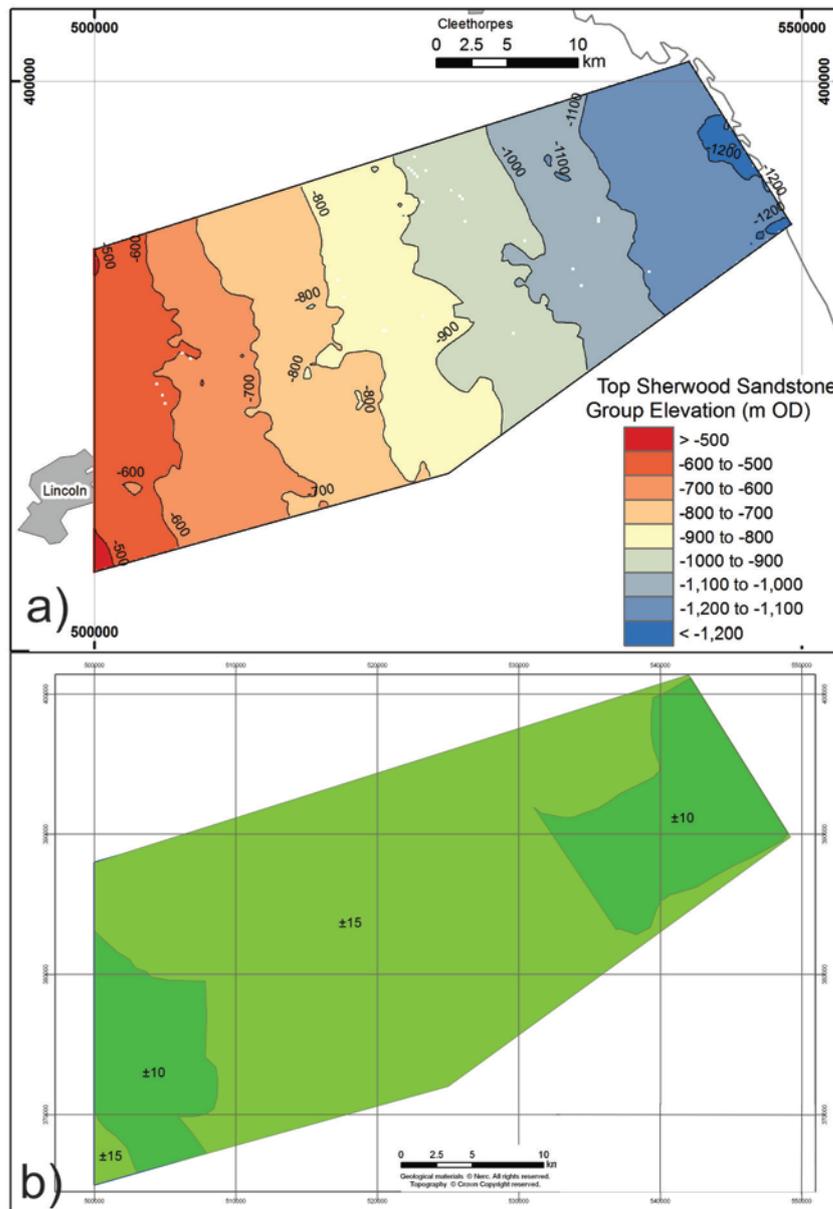


Fig. 7. a) Elevation map for the top Sherwood Sandstone Group (primary aquifer), derived from the Lincolnshire 3D geological model. b) Corresponding map of model uncertainty on top Sherwood Sandstone Group, values in metres

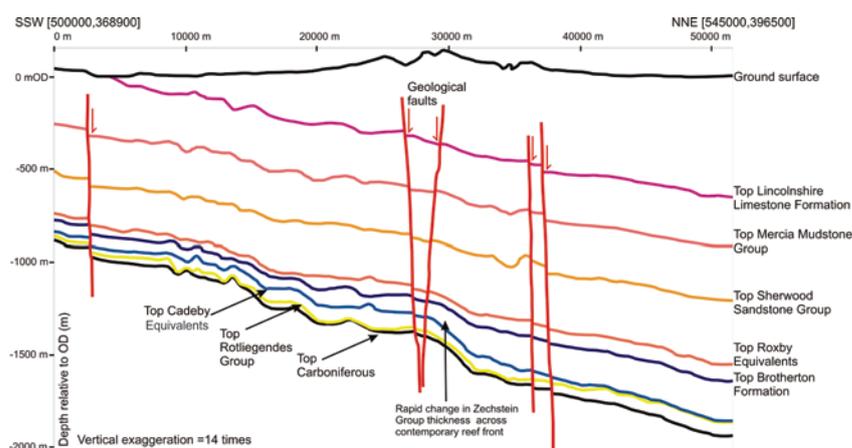


Fig. 8. Cross-section derived from the Lincolnshire 3D geological model running SSW–ENE approximately parallel to the direction of maximum dip (a vertical exaggeration of 14 times is used). The relatively simple gross structure and gradual thickening of the succession towards the ENE is shown. Thickness variation in the Permian associated with the contemporary reef front are highlighted. Ground surface based on NEXTMap Britain elevation data from Intermap Technologies.

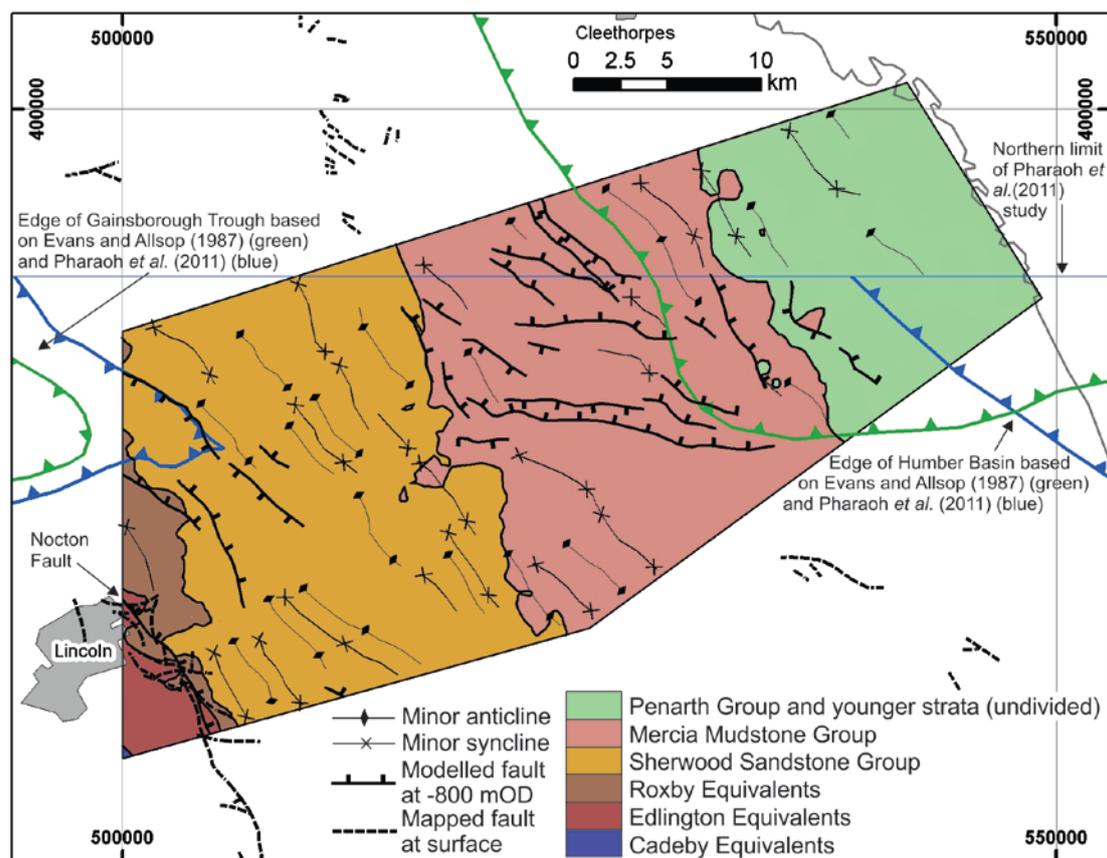


Fig. 9. Concealed faulting, minor folding and bedrock geology derived from the Lincolnshire 3D geological model at a level of 800 m below OD, shown together with surface faulting generalized from 1:50 000 and 1:250 000 scale geological maps, major Carboniferous graben basins from Evans and Allsop (1987) and Pharaoh *et al.* (2011) OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved.

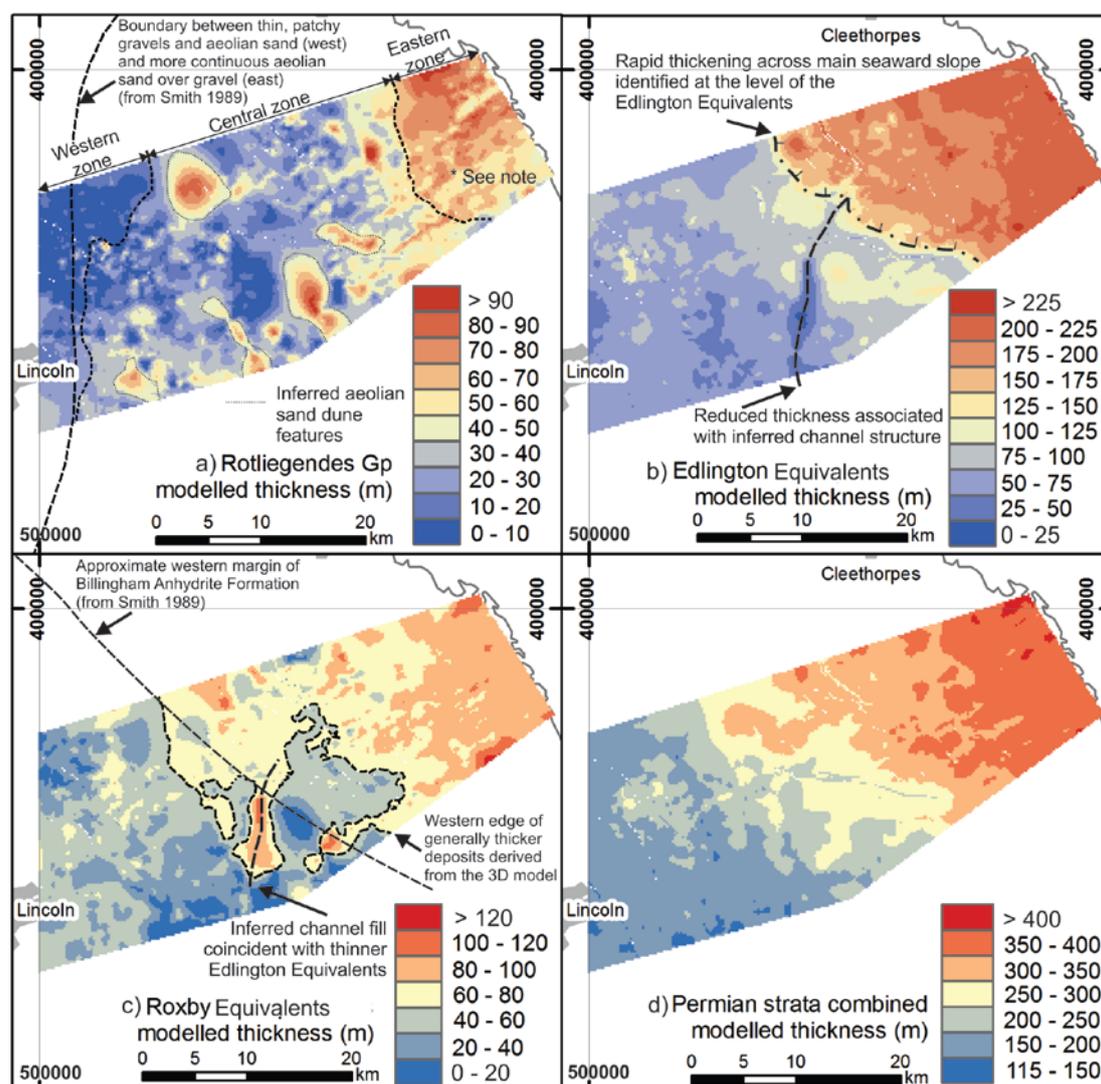


Fig. 10. Thickness for selected Permian units derived from the Lincolnshire 3D geological model: (a) Rotliegendes Group showing zones of contrasting thickness and morphology, including inferred aeolian dune features (* localized SW-NE linear fabric due to seismic data artefact); (b) Edlington Equivalents showing inferred roughly N-S aligned channel structure and rapid thickening across contemporary reef front; (c) Roxby Equivalents showing increased thickness inferred as channel fill; (d) Permian strata combined. Details of unit composition are given in the text. For Cadeby Equivalents thickness variation, see Figure 11. OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved.

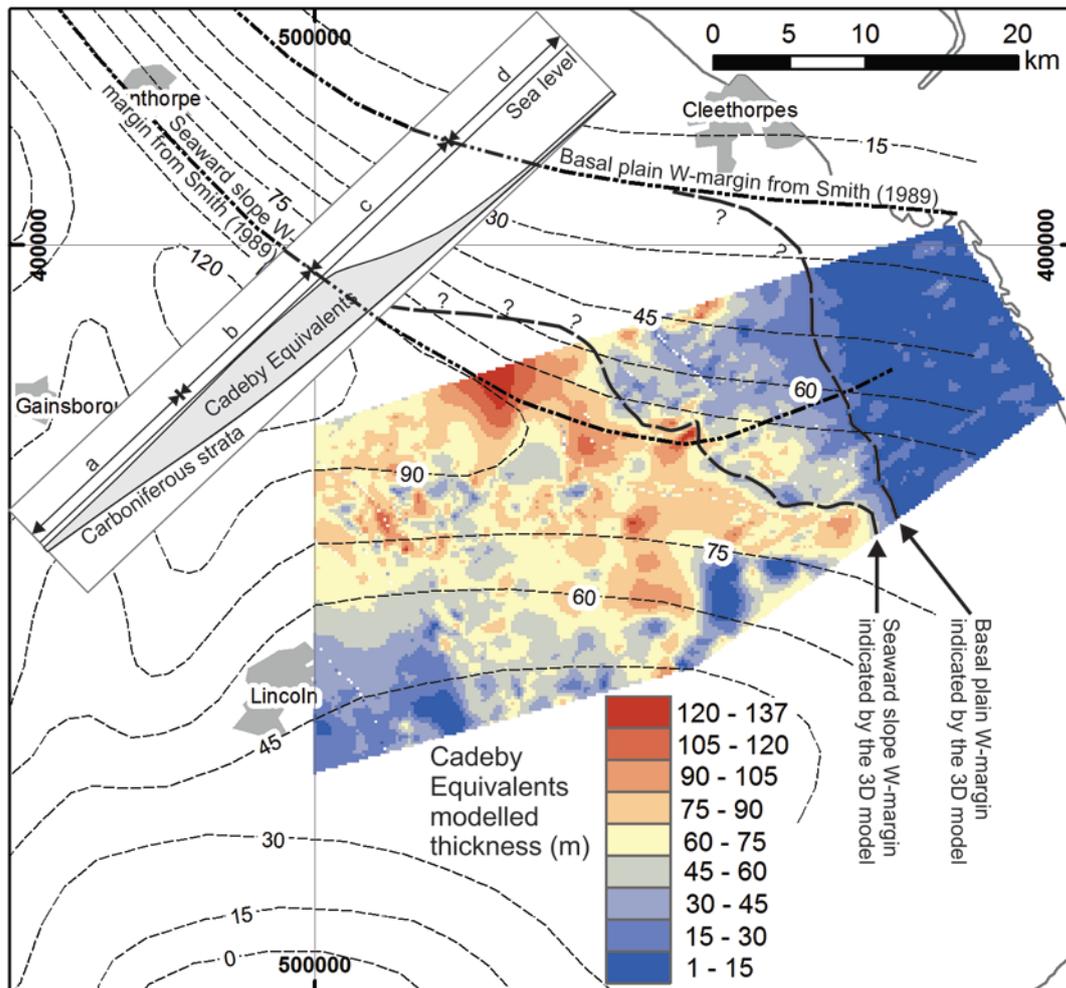


Fig. 11. Cadeby Equivalents (Cadeby Formation and Marl Slate Formation) thickness grid derived from the Lincolnshire 3D geological model shown with Cadeby Formation (carbonate rocks) isopachytes in metres, facies belts and corresponding schematic section in metres from Smith (1989). Facies belts shown in schematic cross section are: a) littoral belt and inner shelf; b) belt of patch reef and shoals plus open outer shelf; c) main seaward slope of outer shelf; d) basal plain. OS Topography © Crown Copyright BGS100017897/2011. All Rights Reserved.

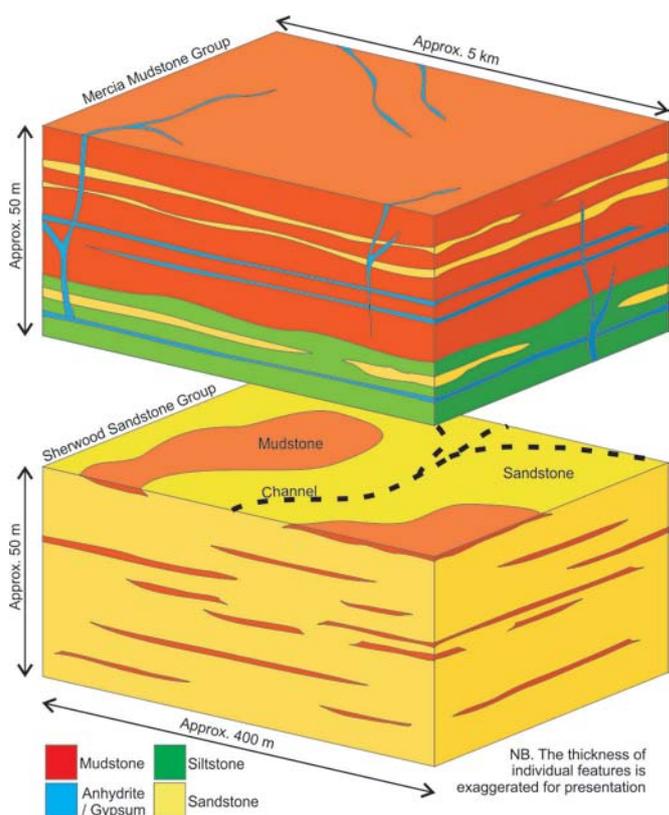


Fig. 12. Schematic block diagram showing: expected distribution of lithological heterogeneity within the Mercia Mudstone Group (primary seal, this block represents the lower part of the unit within the Lincolnshire 3D geological model area) and expected distribution of mudstone horizons within the Sherwood Sandstone Group (primary aquifer, this block represents an arbitrary position within the vertical succession). Note the differing horizontal scale on each block.

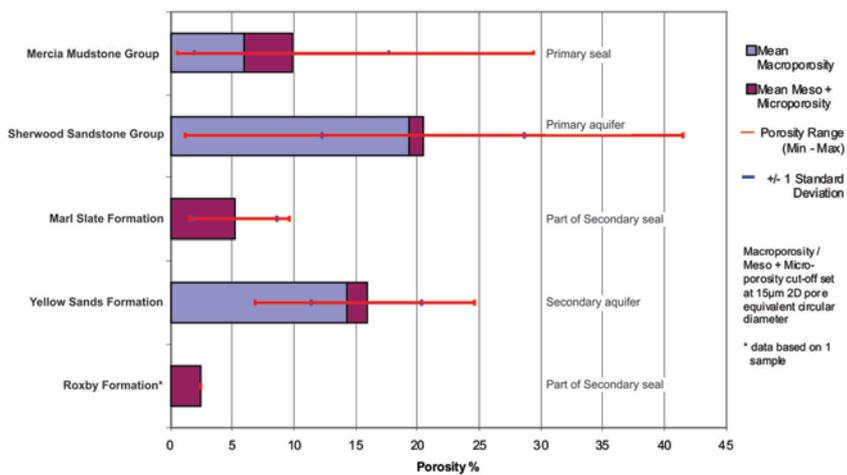


Fig. 13. Summary of 2D porosity data by unit from the Lincolnshire 3D geological model area.

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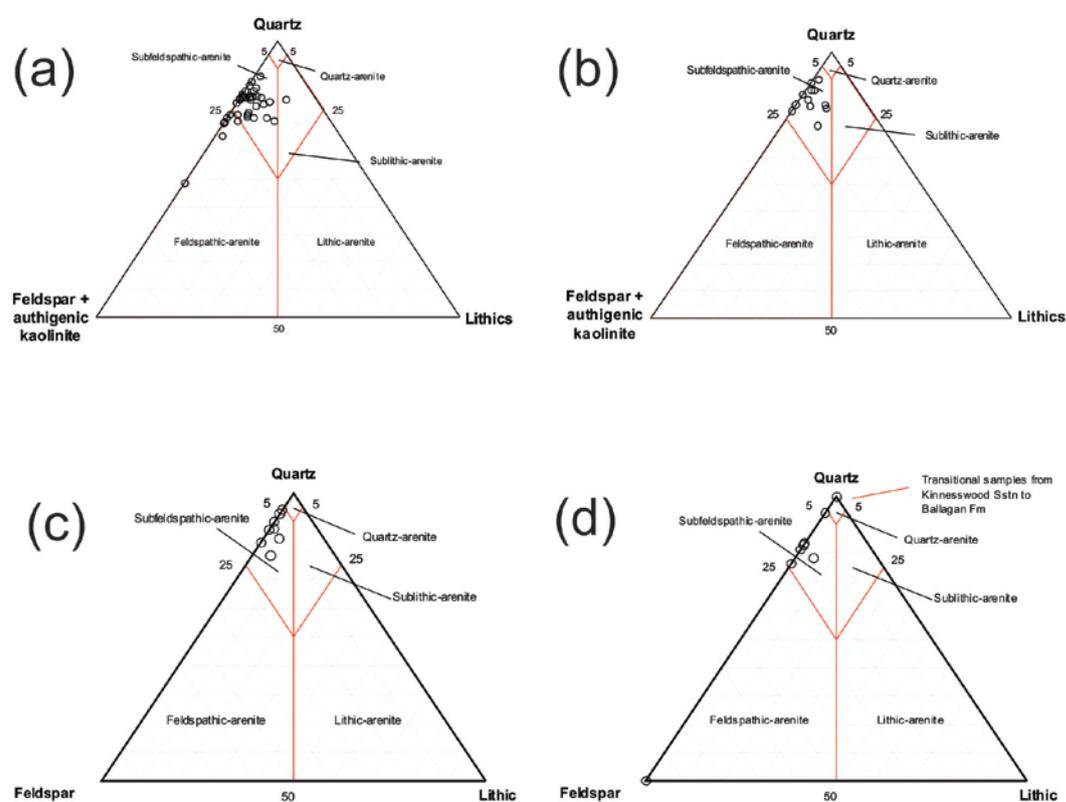


Fig. 14. (a) Classification of sandstone samples from the Sherwood Sandstone Group on the basis of estimated original proportions of quartz, feldspar and lithic clasts after accounting for authigenic kaolinite replacement of feldspars. (b) Classification of sandstone samples from the Basal Permian aquifer on the basis of estimated original proportions of quartz, feldspar and lithic clasts after accounting for authigenic kaolinite replacement of feldspars. (c) Classification of sandstone samples from the Knox Pulpit Sandstone Formation on the basis of measured proportions of quartz, feldspar and lithic clasts. (d) Classification of sandstone samples from the Kinnesswood Formation on the basis of measured proportions of quartz, feldspar and lithic clasts. All classifications after Pettijohn *et al.* (1987).

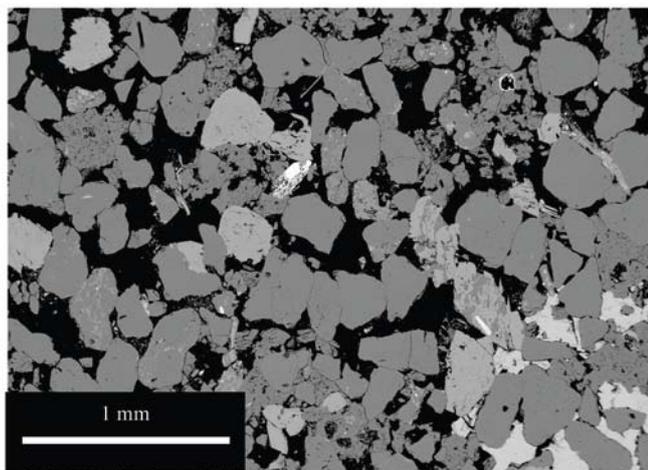


Fig. 15. BSEM image of Sherwood Sandstone Group, showing heterogeneously-packed grain fabric with locally tightly-packed detrital grains and areas with open uncompacted grains and oversized intergranular pores. Patchy or micronodular dolomite (dull grey) can be seen cementing areas of uncompacted (expanded fabric) sandstone (bottom centre) and pore-filling anhydrite cement (white) is also present (bottom right). Sample CLSH7, 1116.31 m, BGS Cleethorpes No.1 Borehole, Lincolnshire.

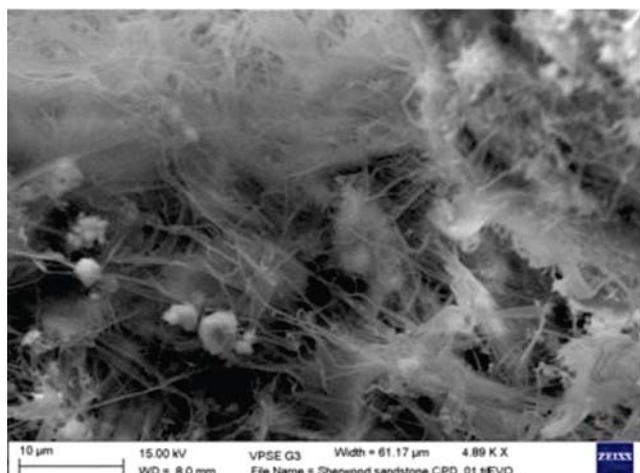


Fig. 16. Environmental SEM photomicrograph of authigenic fibrous illite lining pore surfaces in sandstone sample prepared by CO₂ critical point drying of core samples preserved in formation brine immediately after recovery from the Sherwood Sandstone Group, BGS Cleethorpes No.1 Borehole, Lincolnshire.

Period	Group	Formations – West Lothian	Formations – East Lothian	Formations - Fife	Status
CARBONIFEROUS	Scottish Coal Measures Group	Scottish Upper Coal Measures Formation Cyclical sandstone, siltstone, mudstone with minor coal, >1200 m			Overburden
		Scottish Middle Coal Measures Formation Cyclical sandstone, siltstone, mudstone, seatrock and coal, 350 m			
		Scottish Lower Coal Measures Formation Cyclical sandstone, siltstone, mudstone, seatrock and coal, 240 m			
	Clack-mannan Group	Passage Formation Sandstone, conglomerate and claystone with minor coal, limestone and ironstone, 380 m			
		Upper Limestone Formation Cyclical limestone, mudstone, siltstone and sandstone, seatrock and coal, >600 m			
		Limestone Coal Formation Cyclical sandstone, siltstone and mudstone, seatrock and coal, >550 m			
		Lower Limestone Formation Cyclical limestone, mudstone, siltstone and sandstone with minor seatrock and coal, 240 m			
	Strathclyde Group	West Lothian Oil-Shale Formation Cyclical oil-shale, sandstone, siltstone and mudstone with minor coal, limestone and ironstone, >1120 m	Aberlady Formation Cyclical sandstone, siltstone and mudstone with minor coal, seatrock, limestone and ironstone, 140 m	Pathhead Formation Mudstone and siltstone with limestone and dolomite and minor sandstone, coal and ironstone, 220 m	
				Sandy Craig Formation Mudstone and siltstone with minor oil-shale, limestone, sandstone and coal, 670 m	
		Gullane Formation Cyclical sandstone, mudstone and siltstone with minor coal, seatrock, limestone and ironstone, 560 m		Pittenweem Formation Mudstone and siltstone with minor limestone, oil-shale and sandstone, >260 m	
		Anstruther Formation Mudstone, siltstone and sandstone with minor limestone, oil-shale and coal, >810m			
Inverclyde Group	Clyde Sandstone Formation Sandstone with minor mudstone and pedogenic limestone, > 300 m			Seal	
	Ballagan Formation Mudstone, siltstone and dolostone with sandstone in the Edinburgh area, 900 m				
	Kinnesswood Formation Cross-bedded sandstone with minor mudstone and pedogenic limestone, 640 m				
DEVONIAN	Stratheden Group	Knox Pulpit Sandstone Formation Aeolian laminated sandstone with minor calcrete and claystone, 180 m			Aquifer
		Glenvale Sandstone Formation Sandstone with minor siltstone and claystone, 350 m			Possibly aquifer
	Burnside Sandstone Formation Sandstone with minor conglomerate, siltstone and mudstone, 160 m				
Lanark/Arbuthnott-Garvock Groups	Pentland Hills Volcanic Formation Igenous rocks		Ochil Volcanic Formation Igneous rocks	Underburden	

Fig. 17. Lithostratigraphical summary of the succession considered in the Forth 3D geological model and position of the modelled horizons highlighted in red. Maximum thicknesses are given in metres. Igneous rocks present within the Carboniferous succession are not shown.

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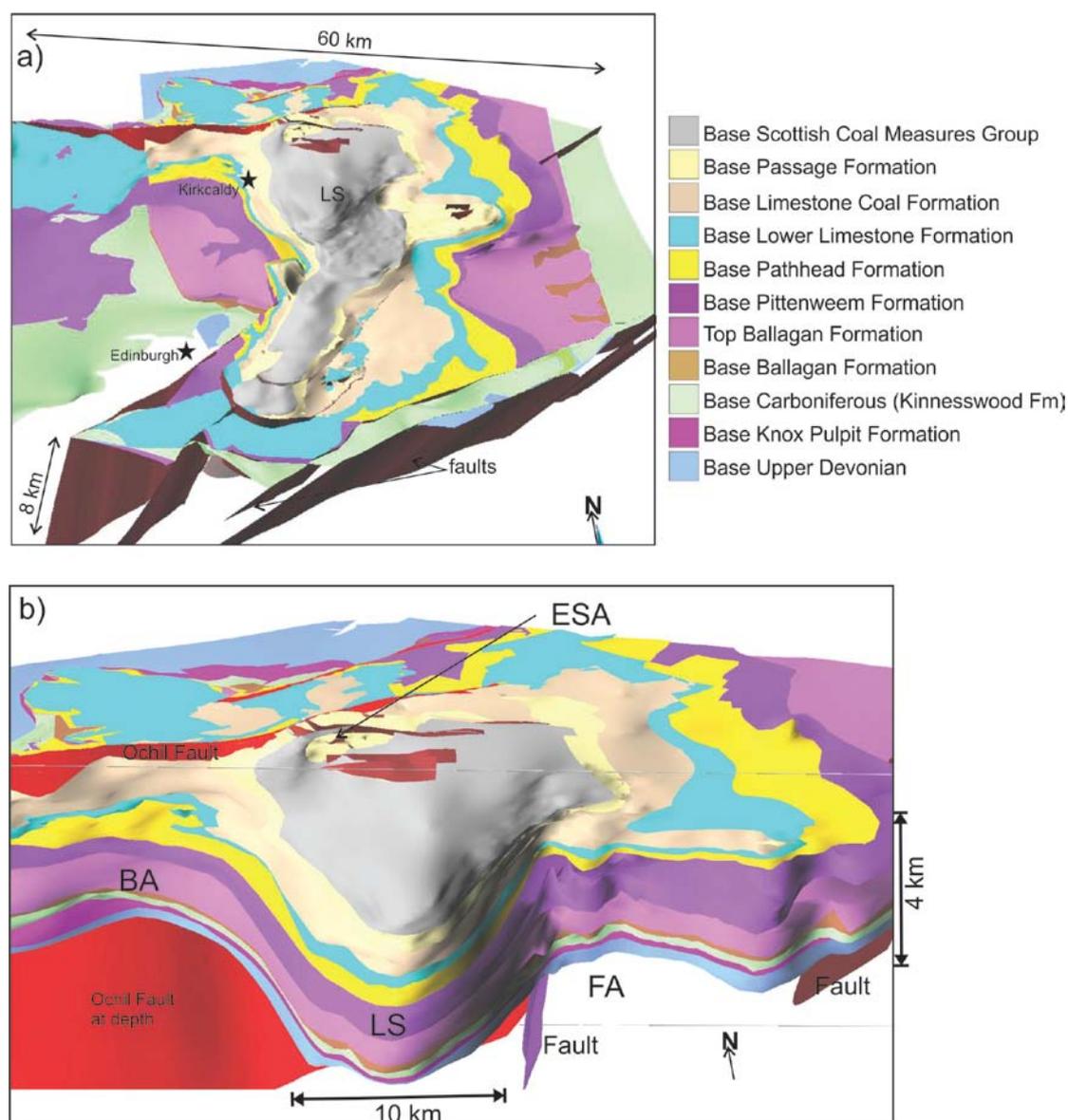


Fig. 18. (a) Overview of the Forth 3D geological model, looking north from above, vertical exaggeration x2. Each modelled stratigraphic surface is represented by a coloured XYZ mesh cut by faults (in red) and stacked vertically. A more traditional elevation map plot of two of the surfaces is shown in Figure 19. The Midlothian-Leven Syncline (LS) is the most prominent feature highlighted by the grey Coal Measures Group surface. Note the straight edges to some modelled surfaces (e.g. Top Ballagan Formation) running north-south represent the modelled extent for those surfaces, rather than an outcrop trace (b) Sliced Forth geological model looking north, vertical exaggeration x2. From west to east across the Firth of Forth the fold structures are the Burntisland Anticline (BA), Earl's Seat Anticline

(ESA), Midlothian-Leven Syncline (LS), Forth Anticline (FA). Igneous intrusions are not represented.

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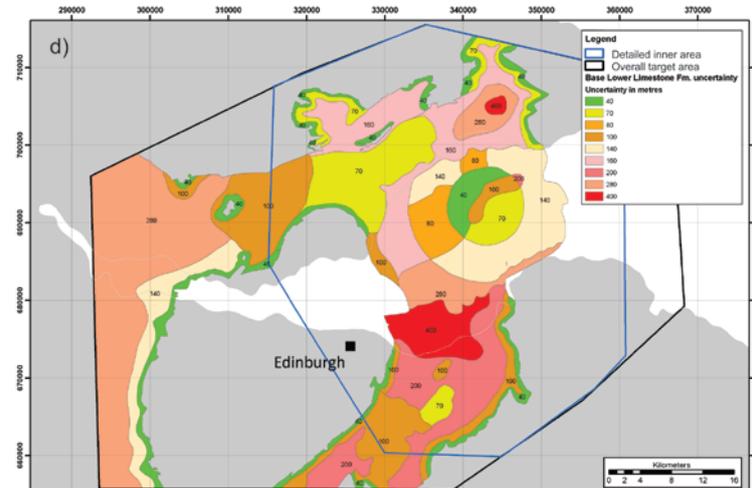
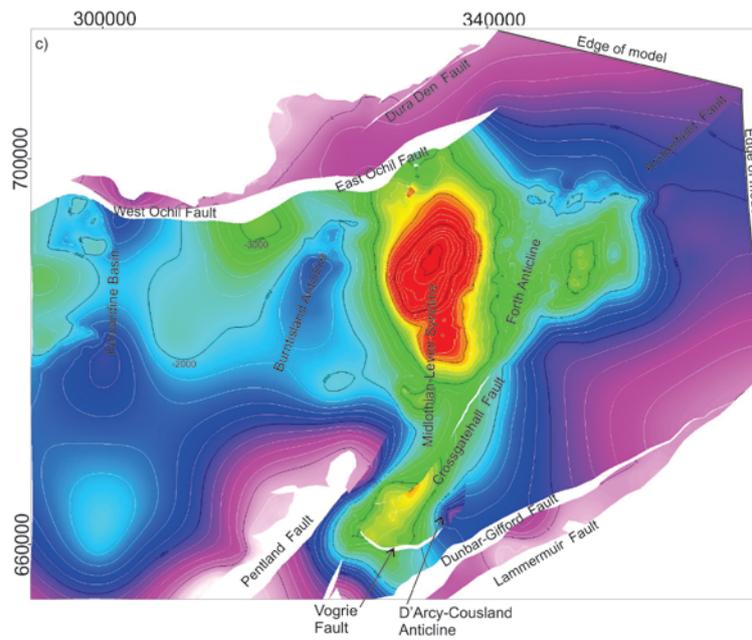
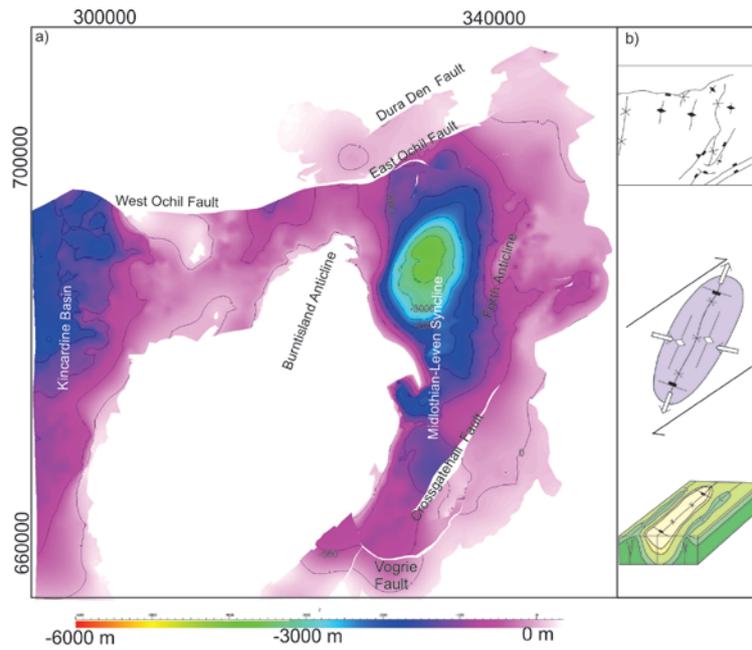


Fig. 19. Elevation map plots in metres relative to Ordnance Datum of (a) base Lower Limestone Formation and (c) base Carboniferous (equivalent to the base Kinnesswood Formation, within the aquifer strata) derived from the Forth 3D geological model. The Midlothian-Leven Syncline, Forth and Burntisland anticlines and many of the modelled faults can be seen. Note that white gaps in the model are fault polygons and the uneven edges to the model are where the horizon crops out at the surface. (b) is a summary of the major modelled structures, a theoretical dextral strike-slip strain ellipse, and a model of growth folds applicable to this area after Underhill *et al.* (2008). (d) Map of model uncertainty on base Lower Limestone Formation (Contour map a), values in metres.

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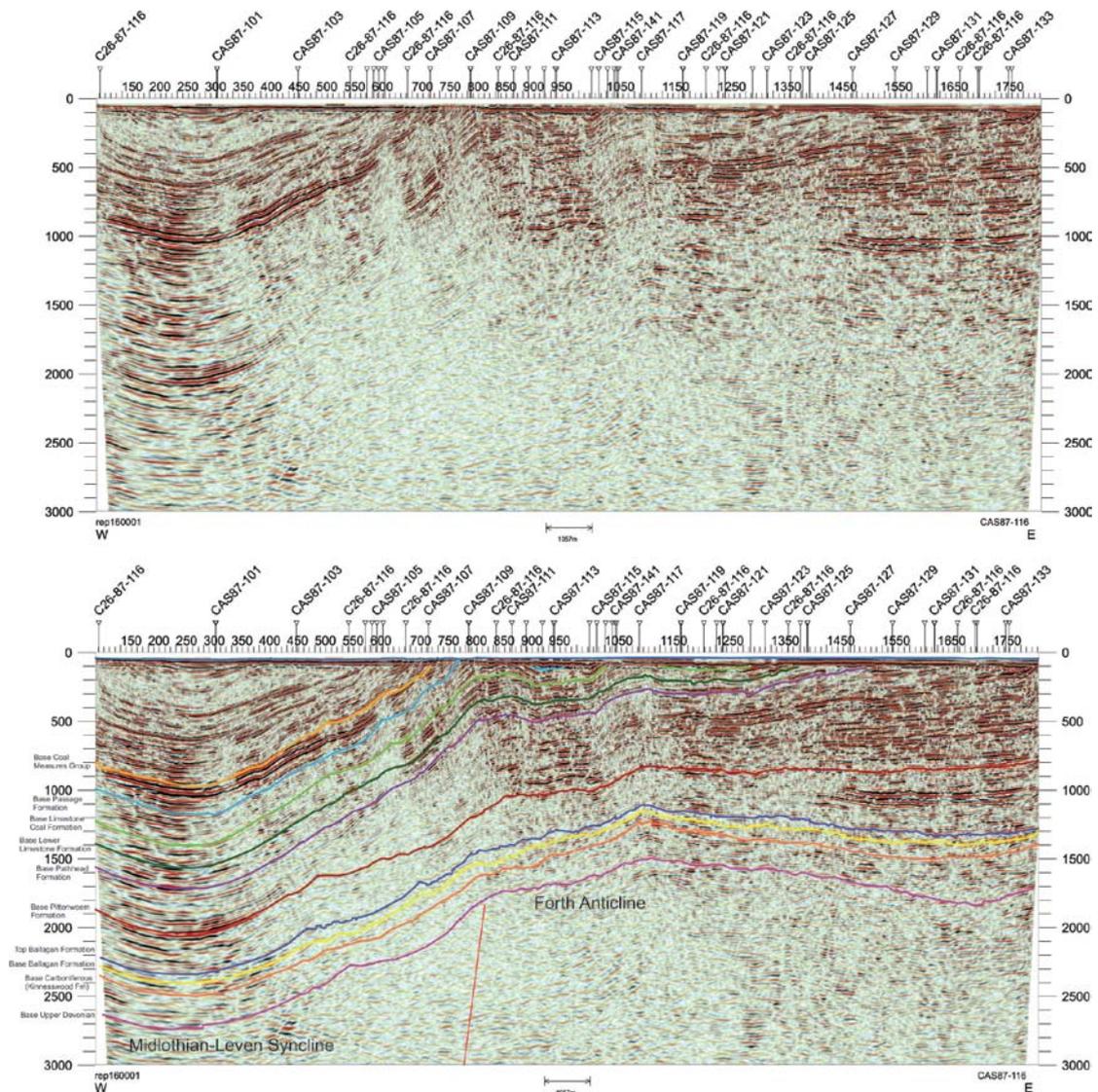


Fig. 20. Example of the reprocessed and re-interpreted seismic data from the Firth of Forth . Line CAS87_116 oriented SW-NE to the southern end of the Forth Anticline structure, see Figure 3 for location and text for discussion, depth axis is two-way travel time in milliseconds. Seismic data reprocessed by WesternGeco for Schlumberger Water and Carbon Services, and reproduced under sub-licence from Phoenix Data Solutions Ltd.

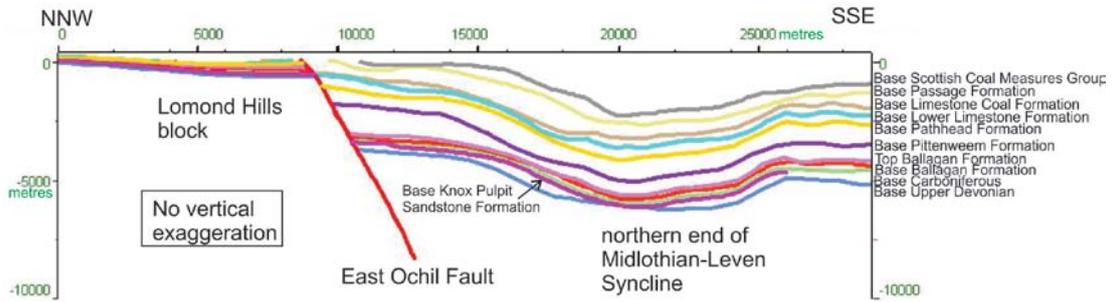


Fig. 21. Representative cross-section derived from the northern part of the Forth geological model showing the large offset and syn-depositional growth on the East Ochil Fault.

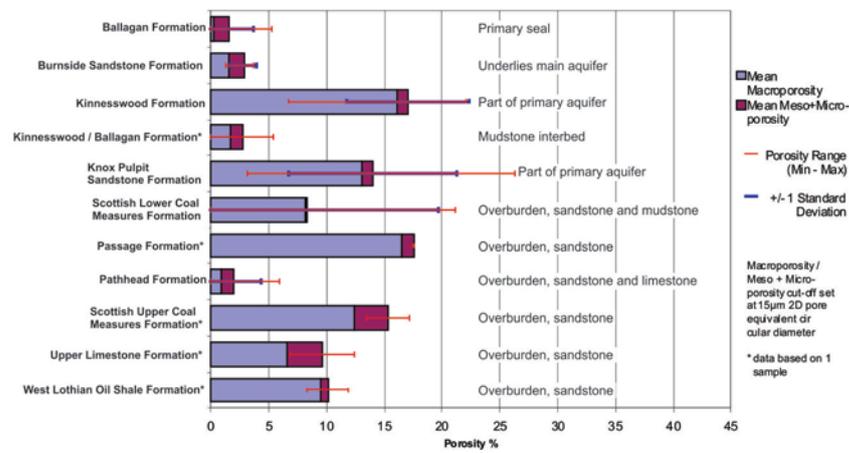


Fig. 22. Summary of 2D porosity data by formation from the Forth geological model area

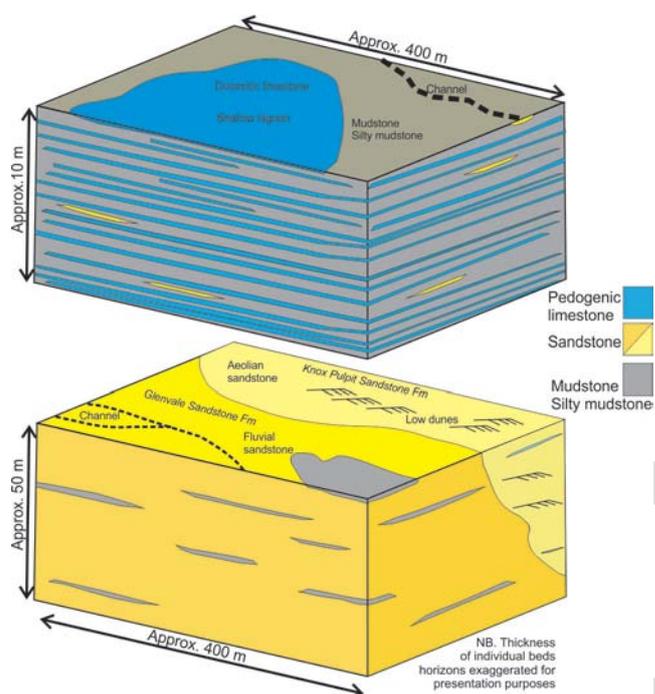


Fig. 23. Schematic block diagram showing expected distribution of mudstone and pedogenic limestone horizons within, and interpreted depositional setting of, the Knox Pulpit Sandstone and Glenvale Sandstone formations, and the lithological heterogeneity in overlying Ballagan Formation strata. Note that the intervening Kinnesswood Formation sandstones are not shown. These blocks represent an arbitrary position within the vertical succession of the Forth 3D geological model, and are subject to a vertical exaggeration. The passage laterally between the two sandstone units has been drawn much simplified.

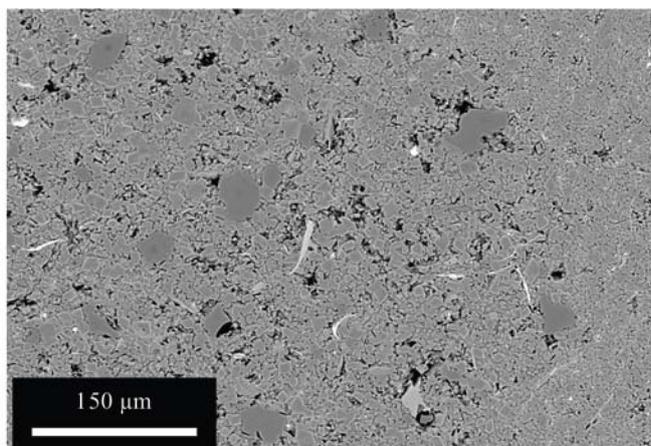


Fig. 24. BSEM image of recrystallised dolomicrite (microdolosparrite) showing tight, matrix of intergrown fine ferroan dolomite crystals, with scattered quartz silt and very sparse mica grains. No macroporosity is present. Sample SSK2540, Ballagan Formation, 335.15 m, BGS Glenrothes Borehole, Forth area.

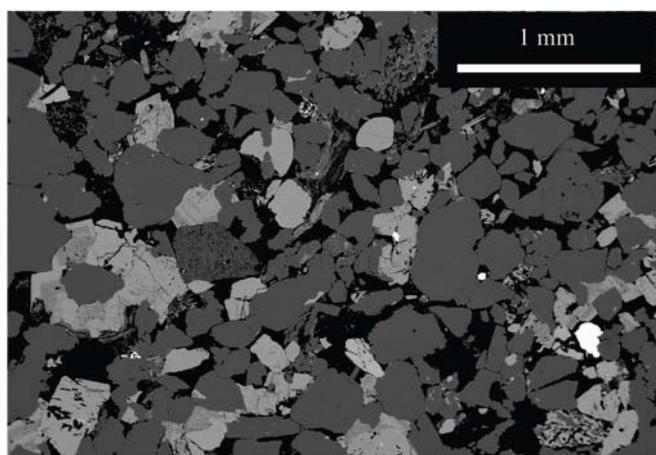


Fig. 25. BSEM image of clean, fine to medium sandstone composed of major detrital quartz (dull grey) and minor K-feldspar (light grey), with patches of ferroan dolomite cement (zoned and patchy mid grey). The rock has a compacted grain fabric with rounded to subrounded coarser quartz grains and more angular finer sand grains. Oversized pores are present and may contain authigenic kaolinite. Euhedral crystal faces on some quartz grains represent authigenic quartz overgrowth cement. Detrital muscovite is exfoliated and replaced by

kaolinite along cleavage. Sample SSK2526, Knox Pulpit Sandstone Formation, 584.38 m, BGS Glenrothes Borehole, Forth area.

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