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Thermal Modelling in the Midland Valley of Scotland using BasinMod™ and HotPot

DGSM Midland Valley

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Thermal Modelling in the Midland Valley of Scotland using BasinMod™ and HotPot

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Foreword

This report is the published product of a study by the British Geological Survey (BGS). The models are based on current understanding and knowledge of the complex geology of the Midland Valley of Scotland (MVS). This report considers the Eastern part of the Midland Valley around the Firth of Forth from the late Visean to the present day.

Two different modelling techniques were used to model the study area in the east of the MVS around the Firth of Forth. Thermal models of three boreholes were produced using BasinMod 7.61 (Platte River software). BasinMod was used to model compaction and temperature through burial over geological time based on stratigraphic and maturity data. Maximum depths of burial were evaluated at several boreholes across the eastern Midland Valley, in order to map eroded overburden over the study area. These results were used with surface-contour data from an earlier phase of the study as input to HotPot (BGS Software), which was used to construct maps of the predicted maximum depth of burial and temperature. The HotPot results were compared to those obtained from using BasinMod.

This study forms part of a multidisciplinary study of the Midland Valley to contribute to the Digital Geoscientific Spatial Model (DGSM), created to hold the data that reflects the current understanding of the 3D structure and composition of the UK.

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Summary

The Midland Valley of Scotland (MVS) has a complex geological history. The overall structure of the basin is that of a fault bounded, late Palaeozoic sedimentary basin. Volcanic intrusions and lavas are also present. It is generally believed that Dinantian extension tectonics resulted in mantle thinning, high heat flow and basaltic magmas. This regime is thought to have continued until the late Namurian when active extension appeared to give way to post-extensional thermal subsidence (Stephenson et al 2003). Westphalian volcanism was more limited and strike-slip tectonics was probably dominant. The majority of rocks at the surface are of Devonian to Carboniferous age. A few younger deposits are found in the MVS terrane suggesting that Mesozoic rocks probably covered the MVS before the latest period of uplift and erosion that is believed to have begun in the Palaeogene.

This report concentrates on the eastern Midland Valley around the Firth of Forth. Three boreholes with suitably detailed stratigraphy and maturity (vitrinite reflectance) data were chosen and modelled using BasinMod™ (Platte River Software). The palaeo-heat flow curve was based on the assumption that extension would have caused high heat flow through the Carboniferous and into the Namurian. Given the lack of thermal maturity data, it was assumed that the heat flow would then gradually decrease to its present day level.

The boreholes selected for use with BasinMod were successfully modelled using 420-660m Variscan (end-Carboniferous) erosion and 1300-1900m Palaeogene-Quaternary erosion. From using BasinMod to model maturity, high heat flow (up to 83mW/m^2) resulting from tectonic activity appeared to have caused the most rapid increase on the maturity of the coals as indicated by their vitrinite reflectance. Maximum depth of burial for the base of the Silesian Limestone Coal Formation was 2900m and maximum temperature reached was 115°C during the Tertiary. Igneous intrusions were seen to have a very localised heating effect on the surrounding rocks.

The HotPot model concentrates across a larger area of the eastern Midland Valley. A number of boreholes and several Earthvision grids were used to perform backstripping calculations and to construct the basin depositional history. The thermal history of the basin was then developed using a generalised model, based on high heat flow during the Carboniferous extensional phase of tectonics, decreasing slowly to the present day levels.

The HotPot modelling results are given in section 4 of this report, and are compared with the BasinMod results in section 5. Using these two modelling packages in the Midland Valley allows comparison of two contrasting modelling techniques; the BasinMod model is based on thermal maturity data (vitrinite reflectance) and the HotPot model is based on mechanical compaction. Some conclusions drawn from the authors' experience of using these two packages are presented in section 6. Finally, section 7 outlines products from these modelling packages that may be added to the DGSM GLOS.

1 Introduction

The objectives of this study were to model the Firth of Forth basin, in the eastern Midland Valley of Scotland, using both the HotPot and the BasinMod software, to compare the results, to calibrate the two methods against each other and to produce guidelines for use of these basin modelling techniques in future studies. This basin was considered suitable for such a study, as there is a good selection of well data, from both oil and coal exploration, ideal for BasinMod work, and earlier phases of the project have produced a well-constrained Earthvision model from which HotPot input data could be obtained.

BasinMod is a modelling software package distributed by Platte River Software. BasinMod 1D (v.7.61) was used to model the geological history of three boreholes across the study area. Borehole stratigraphy and rock properties were used to model compaction and temperature through burial over geological time. The modelled maturity and maturity data were then compared graphically and used to develop the model until a good fit to the data was achieved. Plots of the maturity and temperature vs. depth and time were produced.

The HotPot basin modelling software is designed for producing pseudo-3D depositional and thermal history models of sedimentary basins using a layer-based approach. The primary input data to HotPot is a stack of surface depth grids, such as those produced from mapping programs like Earthvision or GOCAD, and its primary output results are grids used to map predicted layer thicknesses and temperatures at key stages during basin development. This approach is the counterpoint to that used in standard commercial oil-industry basin modelling software, such as BasinMod, which use vertical modelling methods, either at well-bores (1D) or along cross-sections (2D).

The BasinMod and HotPot studies and the comparison of the two techniques are described in separate sections of this report. Guidelines for using the HotPot and BasinMod techniques are summarised here but described in detail in ‘best practice’ documents.

2 Geological History of the Midland Valley

The Midland Valley (MVS) has a complex and often disputed geological history which is difficult to define due to later overprinting and erosion. It is bounded by the Highland Boundary Fault to the north and the Southern Upland Fault to the south. The overall structure of the basin is that of a fault bounded, late Palaeozoic sedimentary basin. The central and eastern areas are folded into NNE-SSW trending synclines and anticlines. Volcanic intrusions and lavas are also present across the MVS region. The majority rocks at the surface are of Devonian to Carboniferous age (Figure 1). The oldest rocks at outcrop are of Ordovician and Silurian age. A few deposits of Lias and Cretaceous are found on Arran and Northern Ireland, and a few outliers of Triassic and Cretaceous age occur in the Forth Approaches, suggesting that Mesozoic rocks probably also covered the Midland Valley. The latest period of uplift and erosion and shaping of the landscape is generally believed to have started in the Palaeogene (related to magmatism or underplating). Figure 2 shows the timescale and stratigraphy of the Midland Valley (after Read et al 2002 and Browne et al 1999).

2.1 DEVONIAN-WESTPHALIAN STRUCTURAL EVOLUTION OF THE MVS

A number of hypotheses have been put forward to explain the structural origin of the MVS. The main ones are discussed here.

1) North-south extension. Leeder (1982) discussed the hypothesis that the MVS was formed as a Caledonide fore-arc basin (Leggett 1980) under north-south closure of the Iapetus Ocean. Large-scale subsidence during the Silurian-Ordovician could then be explained by the presence of thin oceanic or transitional continental crust underlying the fore-arc basin (Dickinson and Seeley 1979). Based on extensive calc-alkaline volcanism, Leeder (1982) concluded that the MVS remained an active fore-arc basin during the late Silurian to early Devonian with during- and post-subduction plutonism and volcanism. Molasse sediments were then fed into this basin from landmasses to the north and south. Leeder (1982) believed that during the mid Devonian transcurrent motion occurred causing folding (it was unclear to Leeder from evidence if this was dextral or sinistral). Leeder also proposed that from the upper Devonian to Westphalian times the MVS continued as a remnant fore-arc sedimentary basin, though he found it difficult to therefore explain the recurrence of massive mantle melting in Dinantian times which produced alkaline volcanism. Leeder (1982) concluded that the Carboniferous lithosphere north of St Georges land was subject to a north-south tension from late Devonian to the end of the Carboniferous.

2) Read (1988) concentrated on Silesian sedimentation patterns as deduced from available borehole information, he proposed that the controlling structural features of the late Namurian and Westphalian differed from those in the early Namurian. Read (1988) believed that most sediment input was from the north, with some contribution from the south, and that the Silesian sedimentation patterns indicated subsidence of a single depositional basin, with some local cycles (e.g. progradation of delta fronts). Overall Read (1988) believed that the borehole evidence supported the theory that early Devonian lithospheric stretching and crustal rifting was followed by late Devonian and Carboniferous thermal sag and dextral strike-slip faulting along the major NORTH-EAST-orientated basin-bounding faults (Dewey 1982). Read (1988) identified four main sets of structural features believed to have been active during the Silesian; from the trends of these structural features, Read (1988) supported the hypothesis of dextral strike-slip movement during the Silesian.

3) Coward (1993) discussed the wider tectonic evolution of northwest Europe. During the closure of the Iapetus, Caledonide structures in northwest Europe formed through accretion of continental fragments and magmatic arcs mainly from the south-east onto a North Atlantic Craton, causing basin formation and inversion, thrusts and large strike-slip north-west–south-east fault formation. Coward then compared the Late Caledonide (Devonian and early Carboniferous) expulsion of the English North Sea Baltic wedge by an Acadian indentor to the present-day collision of the Himalayas. The approximately triangular wedge was bounded by the Ural ocean to the east, the sinistral Great Glen – Midland Valley – North Atlantic shear systems to the north-west and the dextral English Channel – South Polish Trough shear systems (in Devonian times) and the South Wales – Southern North Sea – Polish Trough shear zone (early Carboniferous times) to the south (Coward 1993). During the early Carboniferous the block expanded north-west–south-east as it was released from the indentor into space created by back-arc extension related to Variscan subduction. Pull-apart basins formed along the shear systems. During the Late Carboniferous, closure of the Ural Ocean reversed the sense of shear along the block margins and the block was pushed back between the Acadian collision zones. Basin inversion resulted from the reversed shear stresses.

4) Rippon et al. (1996) and Ritchie et al. (2003) subdivided the tectonic evolution into late Devonian–Dinantian fault controlled subsidence, Dinantian sinistral fault movement, basin-wide Silesian subsidence, late Silesian dextral transtensional and transpressional strike-slip faulting. Late Devonian to early Carboniferous controlled depocentres in the hangingwall blocks of two large north-north-east–north-east trending faults were identified from seismic data as described in Ritchie et al (2003). In this paper, Ritchie et al proposed the formation mechanism to be either east-west extension or sinistral movement along major north-east-trending strike-slip faults with depocentres forming between en-echelon segments. During the Silesian, Ritchie et al 2003 believed the evidence from the seismic data supported the hypothesis that the eastern part of the MVS was dominated by basin-wide fault controlled subsidence, followed by local inversion. Strike-slip motion reversed to dextral movement along these major north-east-trending faults, with transpression causing inversion of Dinantian depocentres and evidence of transtensional strike-slip faulting. North-north-east-trending anticlines show stratigraphic thinning of beds of Namurian A to late Westphalian age. Ritchie et al (2003) felt that the observations given in this paper supported the structural model of Coward (1993) and believed that the Leeder (1982) model of north-south Dinantian extension followed by Silesian post-rift subsidence and minor strike-slip fault movement would not have produced the observed major north-north-east-trending Late Devonian to Dinantian initiated faults or large north-north-east trending synsedimentary Silesian growth folds. Ritchie et al felt that the major strike-slip faults played a far greater role in the structural evolution of the MVS than accounted for by Leeder (1982).

To summarise, the structural model assumed for the basin models in this report is as follows: Closure of the Iapetus in the Caledonian orogeny caused accretion of continental fragments and arcs onto the North Atlantic craton (Coward 1993). During the Late Caledonian (Devonian and Dinantian), a triangular block, bounded to the East by the Ural Ocean, by the sinistral Great Glen – MVS – North Atlantic shear zones in the north-west, and the dextral English Channel – South Polish Trough shear zone (Devonian) and South Wales – Southern North Sea – Polish Trough shear zone (early Carboniferous) to the south, was pushed out by an Acadian indentor and expanded north-west–south-east into space created by back-arc extension related to Variscan subduction (Coward 1993). Fault-controlled subsidence dominated during the Devonian-early Carboniferous (Ritchie et al 2003). Pull-apart basins formed along the sinistral shear systems. During the Silesian, closure of the Ural Ocean to the east of the block reversed the sense of shear along the block margins, inverting Dinantian depocentres and forming new Silesian depocentres. Large, north-north-east trending synsedimentary folds formed during the Silesian (Coward 1993, Ritchie et al 2003). Rapid basin subsidence and volcanism continued until the mid-Namurian, implying active rifting and extension continued (Stephenson et al 2003). In the late Namurian, active extension appeared to give way to post-extensional thermal subsidence, and widespread marine transgressions caused the basins to lose their separate identities (Stephenson et al 2003). There is evidence of erosion of Carboniferous strata before deposition of Permian sediments. Late-Carboniferous intrusions imply a brief period of north-south extension during this time, possibly a result of laterally transported magmas from a mantle plume beneath Scandinavia (Wilson et al 2004).

This study concentrates on the eastern Midland Valley. North-north-east trending anticlines and synclines, west-north-west trending faults, north-north-east extensional faults accommodating oversteepened fault limbs and some north-north-east high angle reversed faults formed into flower structures are taken as evidence for Visean-Westphalian dextral strike-slip (Underhill et al 2002). Further tightening of the folds is likely to have resulted from transpressional deformation across the Variscan foreland and the continuing effects of dextral shear (Underhill et al 2002).

2.2 IGNEOUS ACTIVITY IN THE MVS

Dinantian extension resulted in mantle thinning, high heat flow and basaltic magmas. The earliest volcanics identified in the MVS are of Tournasian age, but were relatively localised. In the Visean epoch, large quantities of alkali basaltic magmas erupted in the Midland Valley (e.g. Clyde Plateau Volcanic Formation, Arthurs Seat Volcanic Formation, Garleton Hills Volcanic Formation). These volcanic piles then formed topographic highs, separating sedimentary basins to the east and west. Stephenson et al (2003) believed that the rapid onset of widespread and voluminous igneous activity at the time of subsidence and sedimentation indicated lithospheric stretching with passive rifting and diapirism from the upper mantle. In the western and central parts of the Midland Valley, basin development was controlled by north-east–south-west orientated Caledonide faults, and volcanism was concentrated along north-east trending lineaments. In the eastern MVS, towards the end of the Visean, north-south orientated basins began to develop and the margins of these became the focus of volcanism. During early-mid Namurian, active extension continued and volcanism was controlled by north-north-east trending fault blocks in the central and west MVS. In the east MVS, volcanism concentrated along hinge areas between highs and basins. The Midlothian and east Fife basins were separated from the central basins by an amalgamation of volcanic piles that now form the Bathgate Hills (Dinantian-Namurian), the Burntisland area (Dinantian) and the Pentland Hills (Silurian-Devonian) (Stephenson et al 2003). Westphalian volcanism was more limited in extent, being concentrated in the Firth of Forth and around Fife. Tholeiitic dykes of Stephanian age were intruded with a general east-west trend from the Atlantic margin to the Central Graben of the North Sea (Cameron & Stephenson 1985).

2.3 SEDIMENTATION AND SEDIMENTARY ROCKS IN THE MVS

Ordovician and Silurian

The oldest rocks exposed in the Midland Valley are of Ordovician age, however, Cameron and Stephenson (1985) commented on indirect evidence for Pre-Palaeozoic metamorphic basement from seismic reflection profiles. The Ordovician rocks in the MVS include three inliers of conglomerate containing pebbles of Arenig igneous material. The Silurian is represented by Llandovery to Ludlow or even Downtonian strata (Rolfe, 1973) on the southern margin of the MVS. The Silurian sediments show a gradual progression from the marine Llandovery sediments, through the red, fossil fish bearing Wenlock and Ludlow strata to the continental deposits of the Lower Devonian.

Devonian

The Lower Devonian rocks are molasse deposits, sourced by rapid erosion of the upland regions and deposited in a continental basin on folded and eroded Lower Palaeozoic rocks (Cameron & Stephenson 1985). Cameron and Stephenson (1985) indicated that there was evidence for deposition in palaeo-braided rivers and alluvial fans. Andesitic, basaltic and occasionally rhyolitic lavas are intercalated with the Lower Devonian sediments (Cameron & Stephenson 1985). The MVS around the Firth of Forth consists mainly of andesitic and basaltic lavas (with volcanic conglomerates) and lacustrine flagstones with fish fossils (Arbuthnott Group), sandstone, siltstone and mudstone, conglomerates of igneous and metamorphic material, basaltic and andesitic lavas and a thin, concretionary limestone layer (Garvock Group), mudstone and siltstone overlain by arenaceous sandstones (Strathmore Group) (Cameron and Stephenson 1985). Middle Devonian strata are not evident on the MVS, Upper Devonian strata were deposited on a folded and eroded surface of older rocks. The Upper Devonian is fragmented and not well correlated laterally. The majority of the sediments around the Firth of Forth are cross-bedded sandstones, breccia, conglomerates and cornstones. Around Edinburgh, the maximum thickness of the Upper Devonian is around 600m, in Ayrshire the maximum thickness is about 300-400m. The strata thin to the south-west and north-west (Cameron & Stephenson 1985). The Upper Devonian consists of an upward fining and maturing, mainly alluvial sequence.

Carboniferous

Movement along large north-east–south-west orientated faults associated with Visean-Westphalian dextral shear stresses and differential subsidence caused a great variation in thickness of Carboniferous deposits. The depositional environment changed from the arid terrestrial conditions of the Devonian to a more humid fluvio-deltaic system with marine transgressions. Large quantities of organic material suggest a warm and wet or tropical environment and palaeomagnetic data implies that England and Scotland were at equatorial latitudes (Cameron & Stephenson 1985). Most of the Carboniferous sediments were deposited in cycles of marine limestone or mudstone, non-marine mudstone and sandstone, seat-earth or coal, then back to marine sediments. The cycles are usually about 10m thick, but can be up to 30m thick (Cameron & Stephenson 1985).

Carboniferous - Dinantian; Tournaisian Inverclyde Group

The oldest Dinantian rocks identified in the MVS are of the Kinnesswood Formation and were mainly deposited in meandering rivers. They consist largely of calcretes in overbank siltstones or claystones and channel margin sandstones (Read et al 2002). The Kinnesswood Formation can be up to 600m thick around Edinburgh (Cameron & Stephenson 1985). This Formation is then transitionally overlain by the Ballagan Formation which is mainly a lacustrine-lagoonal deposit of mudstone and thin dolostones. Periodic desiccation produced local evaporites. Marine incursions were also noted (Read et al 2002). The thickness of the Ballagan Formation is variable up to 380m (Cameron & Stephenson 1985). Fault-controlled subsidence dominated during the Devonian-early Carboniferous (Ritchie et al 2003). During this time, north-west–south-east extension dominated the triangular block.

Carboniferous - Dinantian; Visean Strathclyde Group

In the eastern MVS, the Ballagan Formation is overlain by basaltic volcanism (e.g. Arthurs Seat) or the Gullane Formation (transitional boundary). Deposition of the Gullane Formation fluvial and lacustrine sediments continued after this phase of volcanic activity in the eastern MVS. The Gullane Formation is then conformably overlain by the West Lothian Oil Shale Formation; fluvial-lacustrine deposits deposited in deep lakes. In East Lothian the Gullane Formation is overlain by the Aberlady Formation, consisting of fluvio-deltaic sediments deposited into lakes or marine embayments. The Bathgate Group lavas are found in the succession from just above the Two Foot Coal in the Strathclyde Group to the Passage Formation in the Namurian. Extensive basaltic volcanism occurred in the MVS during deposition of the Strathclyde Group. (Browne et al 1999).

Carboniferous - Dinantian; Visean Lower Limestone Formation

In the eastern MVS, the Lower Limestone Formation was deposited conformably on the Strathclyde Group sediments. The sediments show cycles of deposition in a marine to fluvio-deltaic environment (Read et al 2002). The Lower Limestone Formation shows its greatest thickness of around 220m in the Midlothian-east Fife area (Cameron & Stephenson 1985). The main rock types in the Lower Limestone Formation are sandstone, mudstone, limestone and coal with root beds.

Carboniferous - Silesian; Namurian Limestone Coal Formation

During the Silesian, closure of the Ural Ocean caused inversion of Dinantian depocentres and formation of large synsedimentary folds. (Coward 1993, Ritchie et al 2003). Dextral strike-slip along major north-east trending basin-bounding faults occurred. The Limestone Coal Formation was deposited in a fluvio-deltaic environment and is characterised by the presence of numerous thin coal seams. Coals are rarely more than 2m thick and show considerable lateral variation, this and seam splitting makes correlation between coalfields difficult. The thickness of the Limestone Coal Formation is highly variable, from 30m in parts of Ayrshire, to 550m in the northern part of the central coalfield (Cameron & Stephenson 1985). The strata consist of sandstones, siltstones and mudstones with coals and seat-earths. Two marine bands indicate transgressions across much of the region, one in the lower part of the succession, one in the middle. A further marine assemblage is present in the western MVS. These marine and fluvio-deltaic deposits can be seen to thin over anticline highs and thicken into basins such as the Kincardine Basin. In Fife, contemporaneous pyroclastic rocks and a few lavas exist and in the West Lothian area near Bathgate, a sequence of basaltic lavas replaces most of the Limestone Coal sediments.

Carboniferous - Silesian; Namurian Upper Limestone Formation

The upper Limestone Formation represents a return to shallow marine conditions with cyclic deposition of thick limestones, marine fossil-bearing mudstones and thick fluvial sandstones. The majority of the Formation consists of thick sandstone beds. Coals are generally poorly developed in comparison with the underlying Limestone Coal Formation. The Upper Limestone Formation attains a maximum thickness of about 590m in the Kincardine Basin. There is noticeable thinning over anticlines such as the Burntisland Anticline (to around 210m) and thickening in basins, e.g. 500m near Leven in east Fife. In Midlothian, the Formation reaches a maximum thickness of around 330m on the west margin of the syncline near Loanhead (Cameron & Stephenson 1985). In the late Namurian, active extension appeared to give way to post-extensional thermal subsidence, and widespread marine transgressions caused the basins to lose their separate identities (Stephenson et al 2003).

Carboniferous - Silesian; Namurian Passage Formation

The Passage Formation also shows cycles between fluvial deposition and marine transgressions. The lower part of the Passage Formation was deposited on an erosive surface by meandering rivers (Read et al 2002). The main rock type in the Passage Formation is thick coarse-medium grained fluvial sandstone. Many sandstone beds were deposited on an eroded surface. The thickest occurrence of the Passage Formation is around 335m in the Kincardine Basin (Cameron & Stephenson 1985). In Midlothian, the Passage Formation is about 240m thick and consists mainly of arenaceous sandstone with fewer marine bands than in the Kincardine Basin (Cameron

& Stephenson 1985). An unconformity cuts through the middle of the Passage Formation. This mid-Carboniferous break affected much of Europe and North America (Read et al 2002). The upper part of the Passage Formation consists mainly of fluvial sandstones deposited in braided rivers with rare marine incursions (Read et al 2002). During the upper part of the Passage Formation, basaltic lavas were erupted into East Fife and in Ayrshire. The volcanism in East Fife persisted into the mid-Westphalian. Late Carboniferous-Permian dextral shear movement along north-east–south-west trending faults caused basin inversion and new depocentre formation in the MVS region (Ritchie et al. 2003).

Carboniferous - Silesian; Westphalian Lower Coal Measures

Basinwide thermal subsidence continued in the Westphalian. The Lower Coal Measures (LCMS) are dominated by fluvio-deltaic deposits with frequent coal bands. The non-marine sediments are usually part of a cycle with mudstone at the base, sandstone, siltstone and mudstone in the middle and coal and a root bed at the top of the cycle. Marine bands are found near the base of the sequence. Generally, the LCMS rests conformably on the Passage Formation; a notable exception to this is in north Ayrshire where the Passage Formation contains volcanic rocks (Cameron & Stephenson 1985). Thickness variation over anticlines such as the Burntisland Anticline is much less apparent in the LCMS and Upper Coal Measures (UCMS) compared to the underlying older Carboniferous strata. The LCMS reaches a thickness of about 150m in the axis of the Leven Syncline around Clackmannan (Cameron & Stephenson 1985). In the Central Coalfield, the LCMS is around 190m thick and thins to the west to around 100m thick near Glasgow. At Westfield in Fife, the LCMS is around 275m thick (Cameron & Stephenson 1985). Basaltic volcanic activity continued around the Firth of Forth and Kirkcaldy.

Carboniferous - Silesian; Westphalian Middle Coal Measures

The base of the Middle Coal Measures (MCMS) is marked by the Europe-wide Vanderbeckei Marine Band. The Middle Coal Measures show similar strata to the Lower Coal Measures and also contain numerous workable coal seams. The MCMS is around 150m thick in the axis of the Leven Syncline near Clackmannan. In the Central Coalfield, the MCMS is around 190 thick. At Westfield in Fife, the MCMS are around 200m thick (Cameron & Stephenson 1985).

Carboniferous - Silesian; Westphalian Upper Coal Measures

The base of the UCMS is marked by the Europe-wide Aegiranum Marine Band. The UCMS is believed to be initially fluvio-deltaic, progressing to purely fluvial. No marine bands are found in the later succession (Cameron & Stephenson 1985). The strata are mainly sandstones, discoloured red by oxidation near the overlying Variscan Unconformity. Coals in the UCMS tend to be poorly developed and laterally inconsistent and there is evidence that oxidation caused alteration or destruction of many of the coal seams. The maximum thickness of the UCMS is recorded in Ayrshire at around 465m, the thickness around Fife and Midlothian and the Central Coalfield is around 270m (Cameron and Stephenson 1985).

The northward advancement of the Variscan Front at the end of the Carboniferous caused a hiatus in deposition. Compressional tectonics began to dominate (Stephenson et al 2003).

Permian and Triassic

Red mudstones and wind-deposited sandstones of Permian and Triassic age indicate these sediments were deposited in arid conditions in contrast to the humid, tropical Carboniferous environment. The sandstones have limited outcrop with the Permian present in the Mauchline Basin (south-west Midland Valley), Arran, offshore in the Firth of Clyde and Forth Approaches. The Mauchline lavas are interbedded with Permian sandstones in Ayrshire. Volcanic necks, and subvolcanic intrusions thought to be of Permian age are found associated with the Mauchline lavas, east Fife and possibly East Lothian (Cameron & Stephenson 1985). The Permian rocks in the west of Scotland are terrestrial, whereas the Upper Permian deposits in the Forth approaches are marine and deposited directly on Devonian and Carboniferous rocks through evaporitic deposition from the hypersaline Zechstein Sea. Red sandstones of Triassic age are found in outcrop in south Arran and in the Firth of Clyde.

2.4 LEVEN SYNCLINE

The study area for this report covers the Leven Syncline, a north-north-east trending synsedimentary fold developed during the Silesian. Figure 1 shows the location of some of the deepest boreholes in the eastern MVS, including those used in BasinMod. Firth of Forth Tower 1 borehole and Milton of Balgonie borehole are both on the western limb of the Leven Syncline, Eskmouth borehole is very close to the axial trace (Figure 3). The Leven Syncline is part of a series of roughly parallel folds, offset dextrally into en echelon segments. It is asymmetric with a steeper-dipping western limb and plunges northwards, apparently dying out in Fife (Ritchie et al 2003). It runs through the Midlothian Coalfield through the Firth of Forth to Fife. The Leven Syncline is cut by a number of east to east-north-east trending fault zones. During the Upper Devonian-Carboniferous, the Leven Syncline represented a major sedimentary depocentre, resulting in some of the greatest thicknesses of Devonian and Carboniferous rocks seen in this part of the MVS.

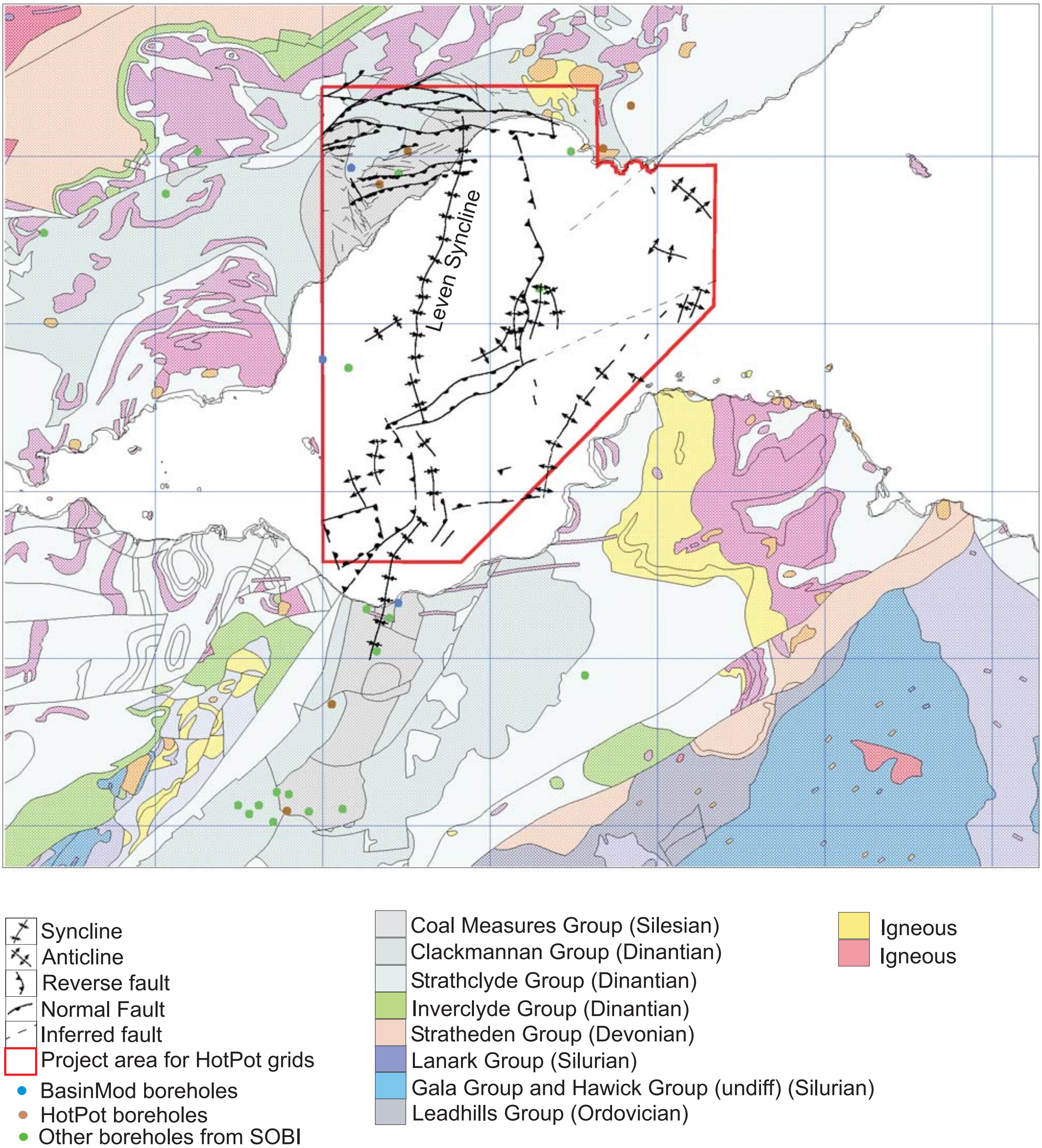


Figure 1: Geological map of the Midland Valley from the BGS GDI and Ritchie et al (2003).

Period	Subsystem	Series	Stage	Group	Formations (Fife Region)
Carboniferous	Silesian	Westphalian C	Bolsolvian	Coal Measures	Upper Coal Measures
		Westphalian B	Duckmantian		Middle Coal Measures
		Westphalian A	Langsettian		Lower Coal Measures
		Namurian	Chokerian-Yeadonian	Clackmannan Group	Passage Formation
			Arnsbergian		Upper Limestone Fm
			Pendleian		Limestone Coal Fm
	Dinantian	Visean	Brigantian		Lower Limestone Fm
				Strathclyde Group	Pathhead Fm
			Asbian		Sandy Craig Fm
					Pittenweem Fm
					Anstruther Fm
			Holkerian-Arundian		Fife Ness Fm
		Tournaisian	Chadian	Inverclyde Group	Ballagan Fm
					Diachronous Transitional base
			Courceyan		Kinnesswood Fm
			Diachronous Transitional base		
Devonian				Stratheden Group	

Figure 2: Carboniferous stratigraphy of the eastern Midland Valley (after Read et al 2002 and Browne et al 1999).

3 Modelling the MVS using BasinMod

3.1 MODEL CONSTRUCTION

BasinMod 7.61 was used to generate models of three boreholes across the region (Figure 3). These boreholes were selected on the following criteria; length of bore; suitable stratigraphic detail and availability of vitrinite reflectance data. BasinMod was used to model the compaction and palaeo-heat flow based on the borehole stratigraphy. This produced a model of the anticipated maturity of organic material in the borehole. This modelled maturity was compared to actual maturity data, in this case, using vitrinite reflectance, to verify that the modelled stratigraphy and heat flow could have produced that maturity. The process of comparing the model results to the data and refining the model is known as 'calibration'. The modelled maturity was calibrated graphically against the maturity data for the boreholes. The slope of the modelled maturity is influenced by the palaeo-heat flow and the actual model maturity values are most affected by the thickness of sediments deposited subsequently. However, vitrinite reflectance data was rarely available in sufficient quantity to reliably calibrate the model so the boreholes which could be used were limited.

The palaeo-heat flow curve was based on the assumption that Late-Devonian-Dinantian back-arc extension of the block and strike-slip along major faults would have caused high heat flow. High heat flow was expected to continue through the Silesian as the sense of shear reversed and large syn-sedimentary folds developed and extension continued into the mid-Namurian. During the mid-Namurian, active rifting is believed to have given way to post-extensional thermal subsidence, and during the Late Carboniferous-Permian, to uplift and inversion of the MVS region, the heat flow would be expected to slowly decline after active rifting and volcanism had ceased. The heat flow was then assumed to decline slowly to the present day level, there is no data in the chosen boreholes after the Carboniferous, to allow more detailed modelling of this time. The current heat flow in Edinburgh is around $53 mW/m^2$ (Rollin et al 2002). Surface temperatures were assumed to be greater during the Carboniferous when this region was near the equator, and assumed to decline to the present day average of around 9°C (Met. Office). For simplicity, it was assumed that any additional Carboniferous sediment deposited before the Variscan that is not seen in the present day stratigraphy was removed by the encroachment of the Variscan Front and Permian deposits were laid down on this erosional surface. Lithology mixes to best approximate the stratigraphy were constructed from borehole records held by BGS Keyworth NGRC, and Murchison House, Edinburgh. Also, sea level was not included in the BasinMod models due to time constraints. Refer to Appendix 1 for more detail on the parameters used during modelling.

3.2 ESKMOUTH BOREHOLE [NT37SW/31 E333250 N670440]

Eskmouth Borehole is located to the South of the project area. There is a good distribution of vitrinite reflectance data. The borehole stratigraphy was divided into Middle Coal Measures, Lower Coal Measures, Passage Formation, Upper Limestone, Limestone Coal and Lower Limestone formation layers. Some of the larger layers were then subdivided based on rock characteristics to refine the model.

Figure 4 illustrates the model results (MCMS – Middle Coal Measures, LCMS – Lower Coal Measures, PGP – Passage Formation, ULGS – Upper Limestone Formation, LSC – Limestone Coal Formation, LLGS – Lower Limestone Formation). Figure 4a shows the comparison of the

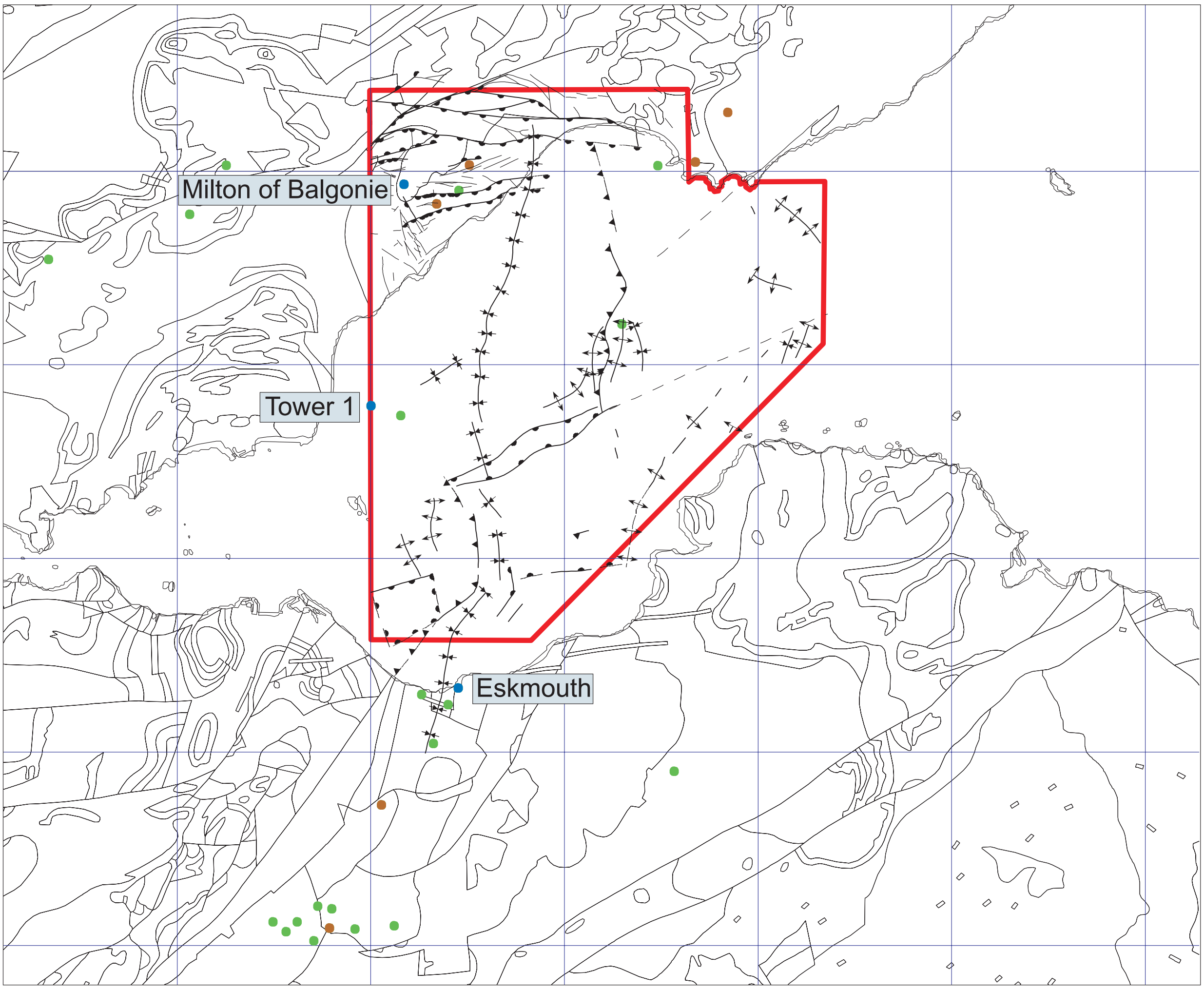


Figure 3: Location of boreholes selected to construct BasinMod 1D models.

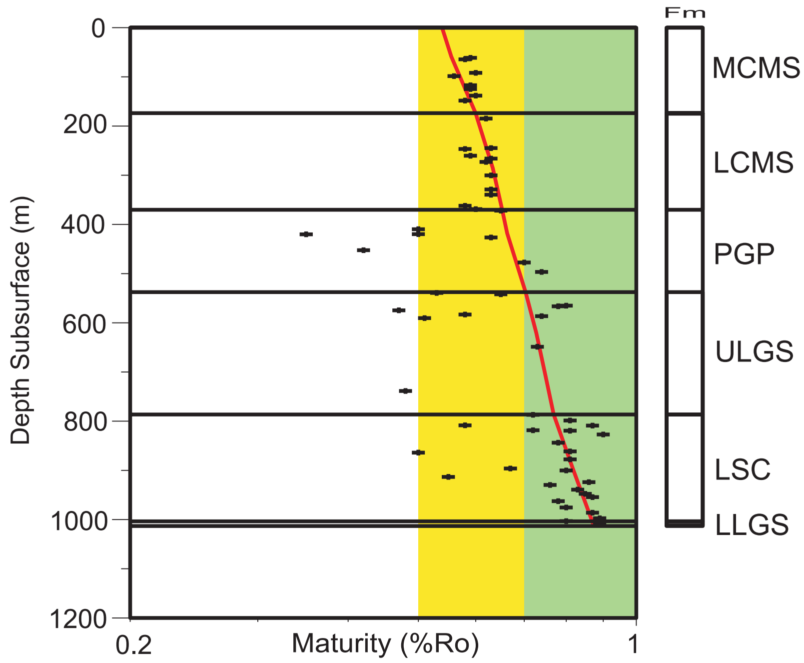
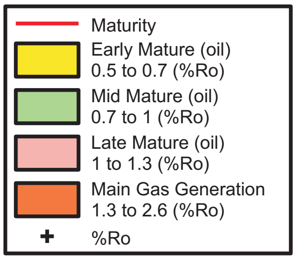


Figure 4a; Eskmouth Borehole Maturity



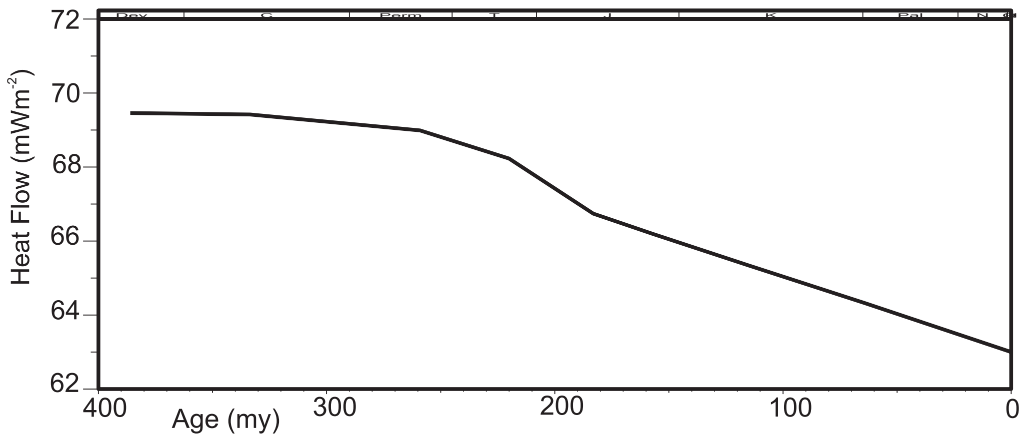
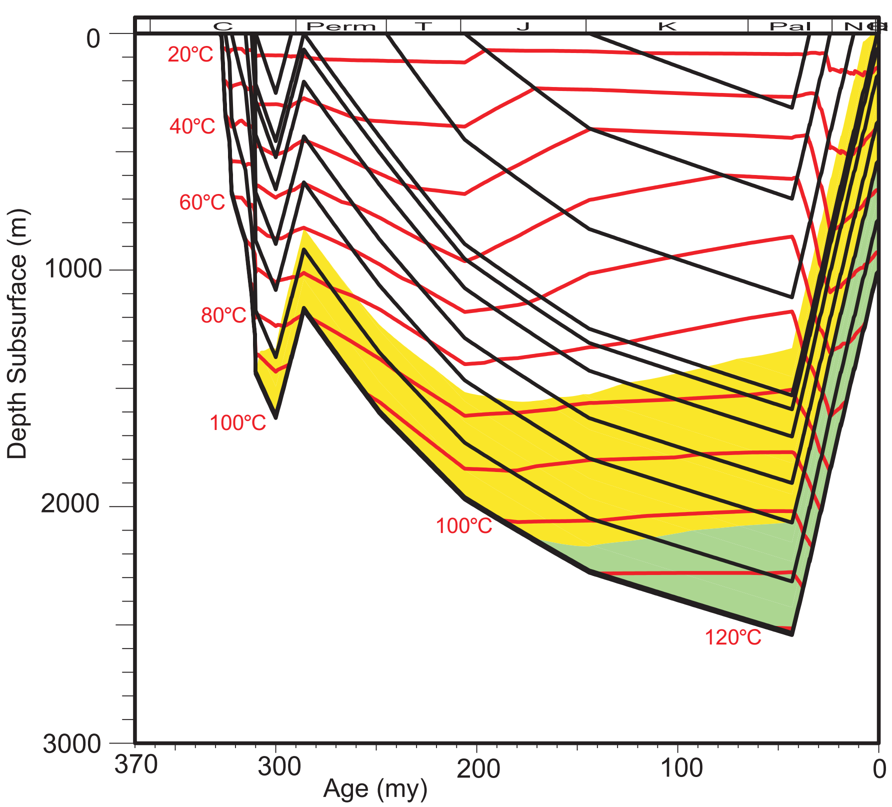


Figure 4b; Eskmouth Palaeo-heat Flow



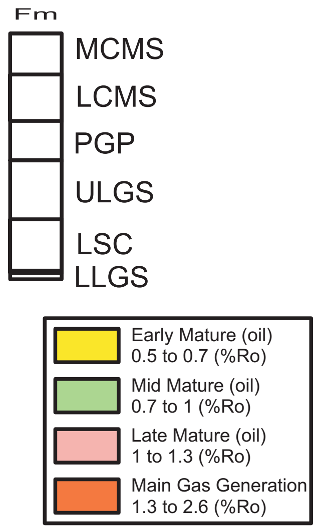


Figure 4c; Eskmouth Burial History

vitrinite reflectance data (black crosses '%Ro') with the modelled maturity (solid red line). Some scatter of the vitrinite reflectance data may be explained by the presence of algal matter, which can cause the coal to look duller under the microscope, resulting in a falsely low reading. Figure 4b illustrates the palaeo-heat flow used for this model. Figure 4c shows the simplified burial history and model isotherms (10ºC spacing). Some layers used in the model are not illustrated here to avoid overcrowding the graphs. The horizontal line across the top of the model indicates the 'surface' beds cut off by this have been eroded before the present day.

The data from the Eskmouth Borehole can be successfully modelled using a maximum heat flow of around $67mWm^{-2}$ in the mid-Carboniferous and deposition of an additional 450m of sediment at the end of the Carboniferous (which was then assumed to have been removed during Variscan tectonic activity) and 1800m sediment deposition through the Permian to Tertiary. This model predicts a maximum depth of burial of 2900m for the top of the Lower Limestone Formation during the Tertiary when the maximum temperature of 115ºC was reached. Figure 4c implies the Lower Limestone and Limestone Coal formations reached the oil window during the mid-late Carboniferous, and that the younger strata up to the mid Upper Coal Measures reached the oil window during deep Tertiary burial.

The borehole stratigraphy was used to calculate approximate sedimentation rates for major formations. The Passage Formation has a relatively low sedimentation rate of 0.03-0.04m/thousand years based on the borehole stratigraphy. The remaining Namurian strata have a sedimentation rate of 0.06-0.25m/thousand years. The Westphalian strata have a sedimentation rate of 0.09-0.16m/thousand years.

3.3 TOWER 1 BOREHOLE [NT38NW/1 E330024 N687894]

Tower 1 Borehole is located in the west of the project area in the Firth of Forth on the margin of the Leven Syncline. The stratigraphy was divided into Lower Coal Measures, Passage Formation, Upper Limestone Formation and Limestone Coal Formation. A thin sill intrudes through this borehole, but does not appear to have affected the available vitrinite reflectance data. Again, the model layers were subdivided based on rock character to refine the model. There is not such a good coverage of vitrinite reflectance data compared to Eskmouth borehole, so the heat flow used for this model was largely based on that used for Eskmouth.

Figure 5 illustrates the model results (LCMS – Lower Coal Measures, PGP – Passage Formation, ULGS – Upper Limestone Formation, LSC – Limestone Coal Formation). Figure 5a shows the comparison of the modelled maturity and maturity (VR) data. Figure 5b shows the heat flow used for this model and Figure 5c shows a simplified burial history with model isotherms (10ºC spacing).

The data from Tower 1 Borehole can be successfully modelled using a maximum heat flow of around $82mWm^{-2}$ in the Carboniferous and deposition of an additional 420m of sediment at the end of the Carboniferous (which was then assumed to have been removed by encroachment of the Variscan front) and 1900m sediment deposition through the Permian to Tertiary. This model predicts a maximum depth of burial of 2900m for the Limestone Coal Formation during the Tertiary when the maximum temperature of around 110ºC was reached. Figure 5c implies that the oil window was reached at a later time than in Eskmouth borehole, with the Limestone Coal Formation entering the oil window during the Permian and the younger strata up to the Lower Coal Measures reaching the oil window during deep Tertiary burial.

The sedimentation rates were again calculated from the borehole stratigraphy. The Passage Formation again appears to have a relatively low sedimentation rate of 0.04-0.07m/thousand years. The remaining Namurian strata have a sedimentation rate of 0.1-0.24m/thousand years.

3.4 MILTON OF BALGONIE BOREHOLE [NT39NW385 E331733 N699335]

Milton of Balgonie borehole is located in the north of the study region on an anticline high on the margins of the Leven Syncline. This borehole cuts through the Midland Valley Sill complex which caused localised heating of the strata in the Lower Limestone Formation. The rock layers were divided into the major stratigraphic groups and then subdivided based on rock characteristics.

Figure 6 illustrates the model results (PGP – Passage Formation, ULGS – Upper Limestone Formation, LSC – Limestone Coal Formation, LLGS – Lower Limestone Formation, SYG – Strathclyde Group, formerly Oil Shale Group). Figure 6a clearly shows the effects of igneous intrusion; the vitrinite reflectance data shows a sharp peak around the sill indicating localised heating. The few points of vitrinite reflectance data in the Oil Shale Group that are considerably higher than the clustered trend are also located near minor intrusions. Figure 6b shows the palaeo-heat flow used to model this borehole and Figure 6c shows a simplified burial history.

The data from Milton of Balgonie Borehole can be successfully modelled using a maximum heat flow of around $68 mWm^{-2}$ in the Carboniferous and deposition of an additional 660m of sediment at the end of the Carboniferous (which was then assumed to have been removed by encroachment of the Variscan front) and 1300m sediment deposition through the Permian to Tertiary. This model predicts a maximum depth of burial of 2300m for the Limestone Coal Formation when the maximum temperature of around 95ºC was reached. The effects of the igneous intrusions were not modelled since the interest here was in the compaction and burial of the rocks in this region. Figure 5c implies that the Strathclyde Group strata reached the oil window during the mid-late Carboniferous and the younger strata up to the Limestone Coal Formation entered the oil window during Tertiary burial.

The sedimentation rates were calculated using the borehole stratigraphy. The Passage Formation again appears to have a relatively low sedimentation rate of 0.05m/thousand years. The remaining Namurian strata have a sedimentation rate of 0.12-0.18m/thousand years. The upper part of the Strathclyde Group has a sedimentation rate varying from 0.03-0.44m/thousand years (upper Dinantian).

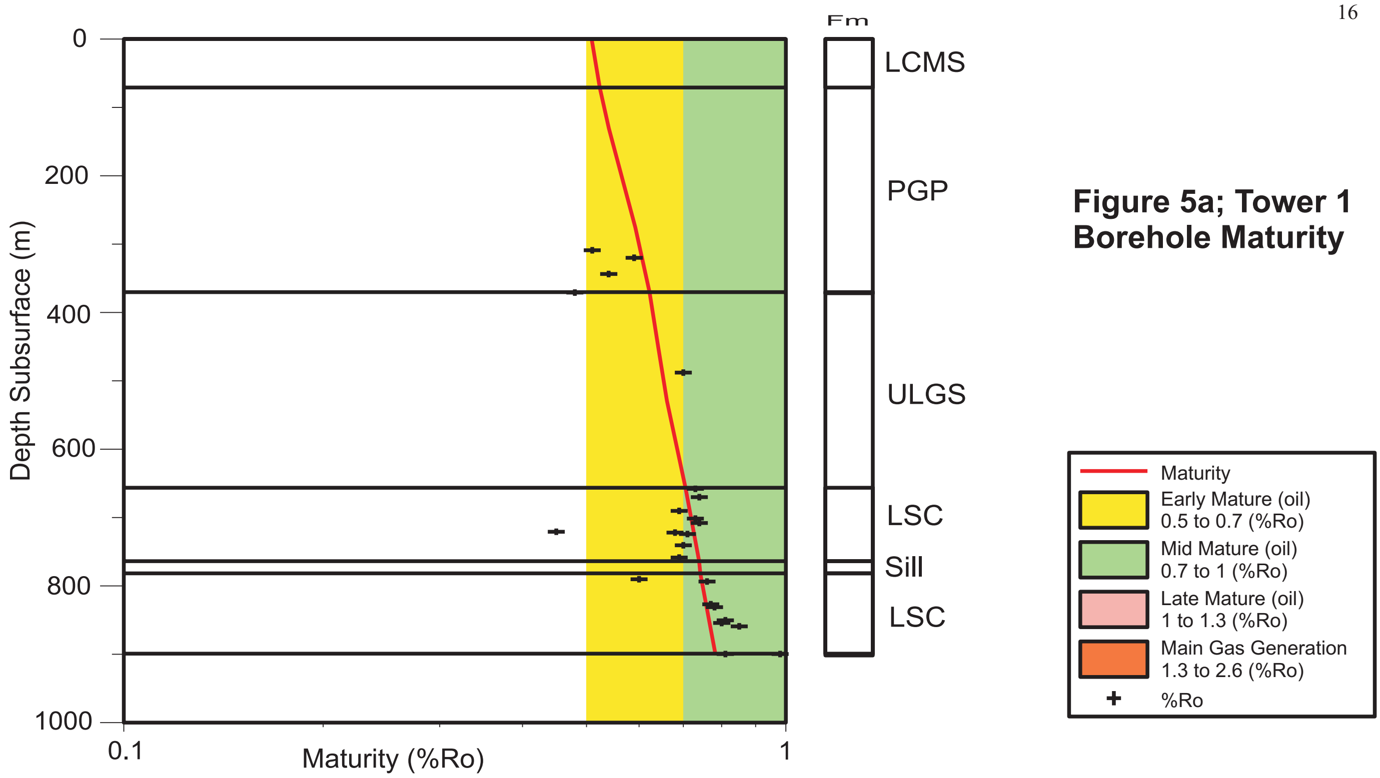


Figure 5a; Tower 1 Borehole Maturity

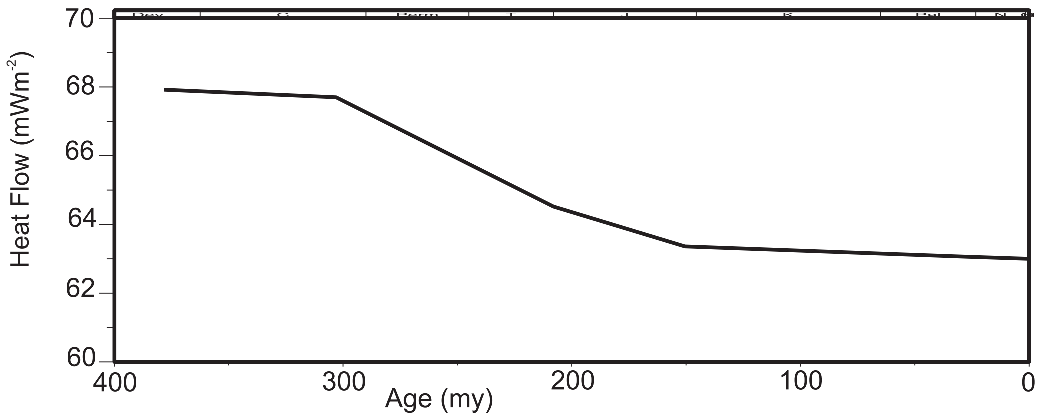


Figure 5b; Tower 1 Palaeo-heat Flow

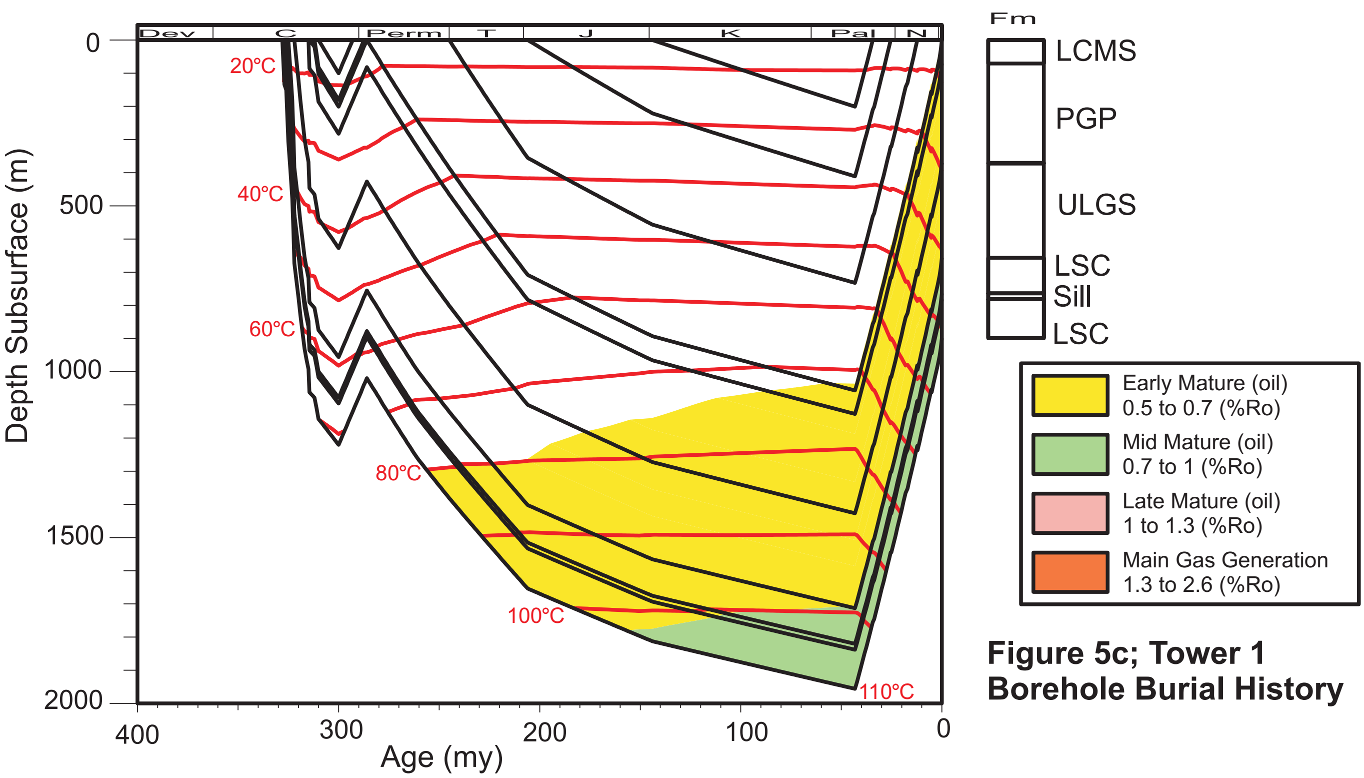


Figure 5c; Tower 1 Borehole Burial History

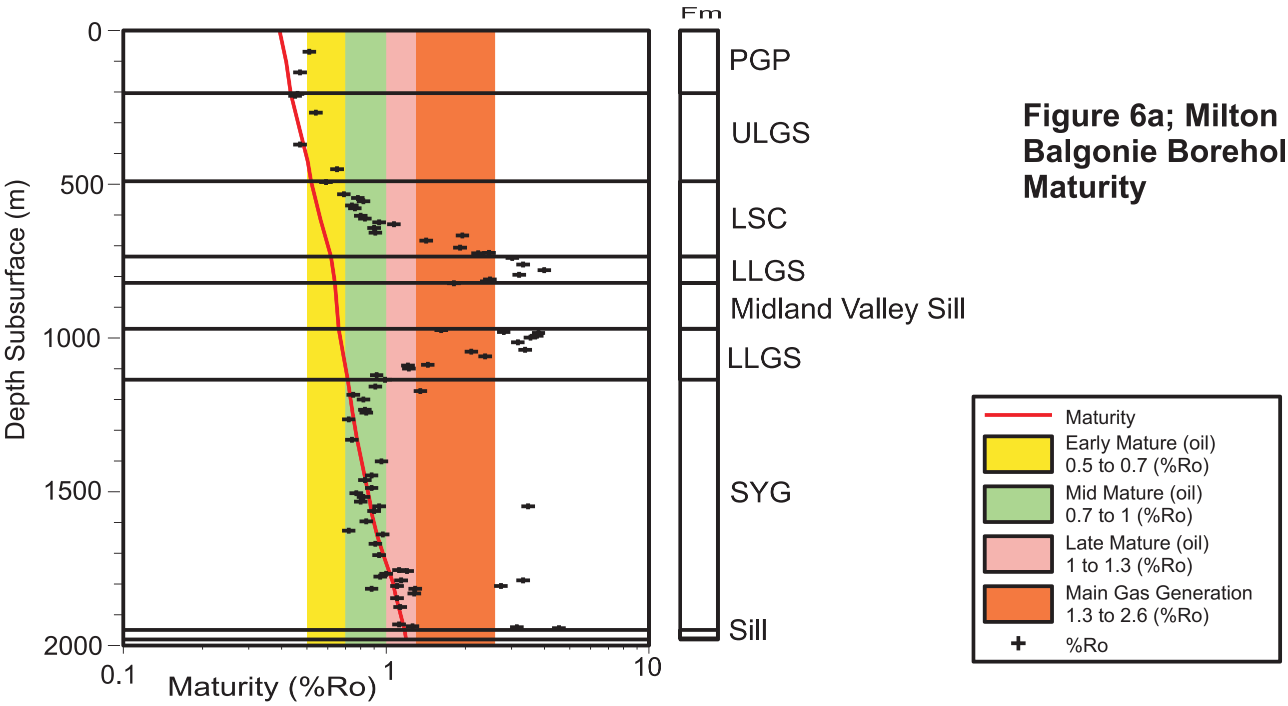


Figure 6a; Milton of Balgonie Borehole Maturity

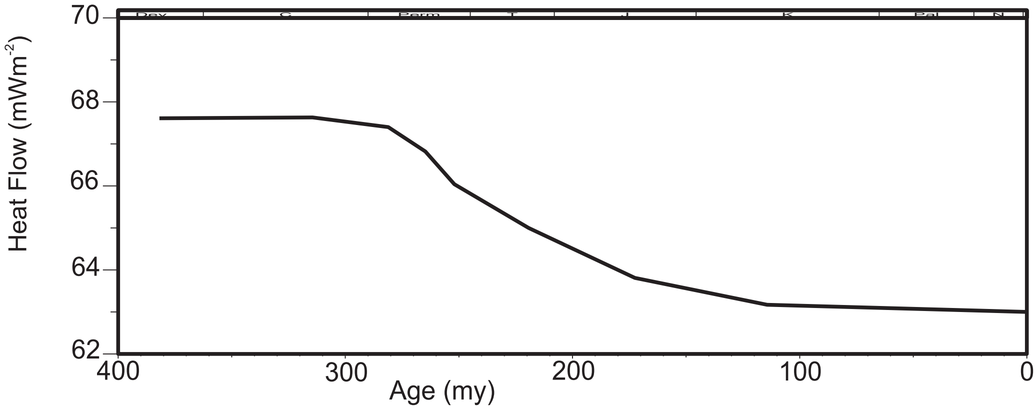


Figure 6b; Milton of Balgonie Palaeo-heat Flow

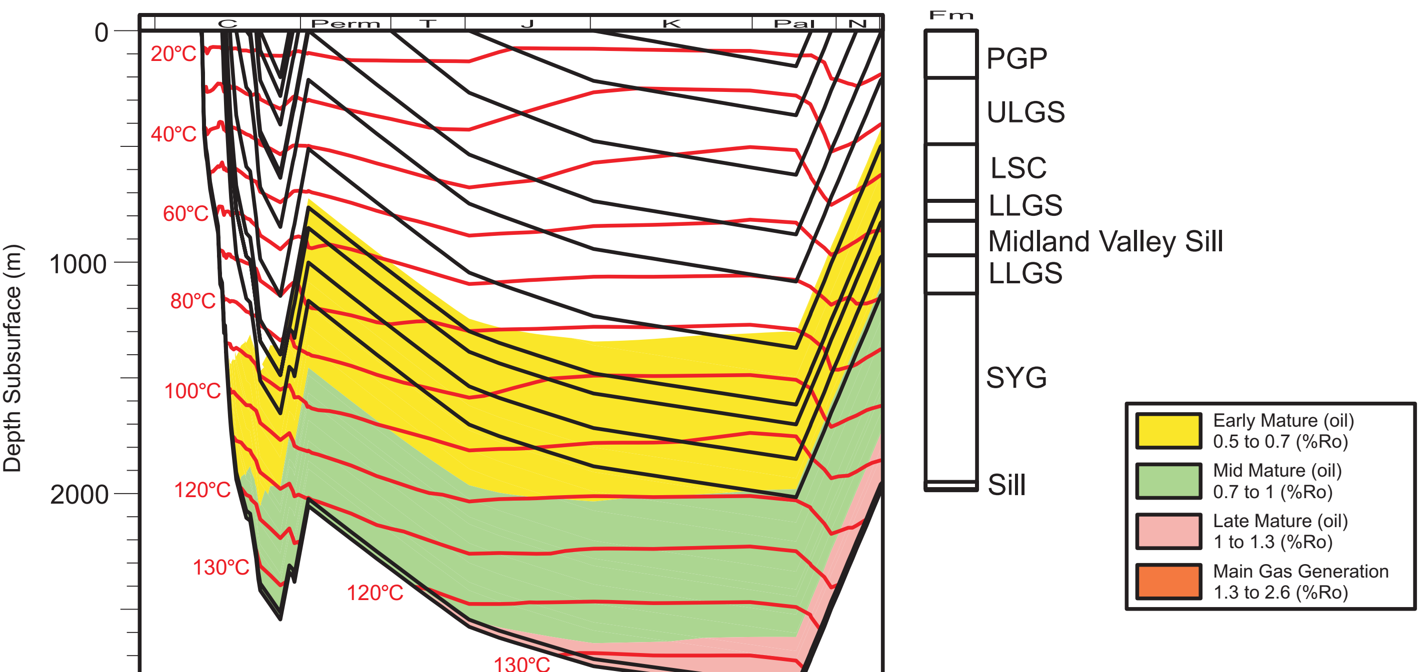


Figure 6c; Milton of Balgonie Burial History

4 Modelling the MVS using HotPot

The BGS basin-modelling program HotPot (Rowley et al. 1993) is used to perform depositional history and thermal history modelling of sedimentary basins. The first stage of this process is to reconstruct the depositional history of a basin, by starting with the present-day basin-fill and successively stripping away one layer at a time, restoring by decompaction the thicknesses of the underlying strata. Where the present-day basin-fill contains unconformities, layers representing the eroded material may be incorporated into this backstripping process. Then the thermal calculation is applied at each stage of the reconstructed depositional history, to synthesise the thermal history of the basin-fill.

The highest strata preserved in the present-day succession in the Firth of Forth basin are of Upper Carboniferous age. It is assumed that the original succession included later Palaeozoic and Mesozoic strata, which have been eroded since Tertiary time. Thus a depth of burial study was carried out to estimate the likely thickness of these eroded strata.

4.1 DEPTH OF BURIAL STUDY

The maximum depth of burial of the succession preserved in the Firth of Forth basin has been estimated using a method that relies on sediment compaction characteristics. As sedimentary deposits are progressively buried their porosity decreases and, consequently, their density increases. This relationship has been demonstrated by laboratory and theoretical work (Sclater & Christie 1980; Baldwin & Butler 1985) and observed in borehole logs (e.g. Lang 1980). Compaction also depends on sediment type; for example, mudstones compact more quickly and to a greater degree than sandstones. Finally, the compaction process is irreversible; sediments do not 'decompact' if their burial depth is reduced by uplift and erosion. Once a set of compaction curves (density vs. depth vs. lithology, Figure 7) have been established, e.g. from a fully preserved sequence, the maximum depth to which a sample, of known lithology and density, was buried is determined by finding the density on the appropriate curve and reading the corresponding depth. An estimate of the thickness of overburden eroded from the sample site is then obtained by subtracting the present depth of the sample from its maximum burial depth.

The reliability of this method depends on the observed sample densities being due solely to sediment compaction. However, other factors may alter the density of sedimentary rocks, such as recrystalisation of limestones or changes in the cement of sandstones. Previous studies (e.g. Marie 1975; Magara 1976) indicate that the best depths of burial estimates are obtained from mudstones.

4.1.1 Compaction curves

The stratigraphic succession in the Firth of Forth basin is not at maximum depth of burial. Since the oldest preserved strata are of late Palaeozoic age, phases of deposition, uplift and erosion during Mesozoic and Tertiary time must be supposed. Therefore, the adopted set of compaction curves (Figure 7) was derived from data used in earlier studies of the Cheshire Basin (Chadwick et al., 1999) and the Wessex Basin (Chadwick 1985) supplemented by theoretical data (Sclater & Christie 1980; Baldwin & Butler 1985) and constant densities for the minerals halite and anhydrite (Cermak & Rybach 1982).

Coal represents a significant lithological component of the Carboniferous strata of the Firth of Forth basin. However, a literature search failed to produce any suitable data regarding the compaction of organic material during burial and coalification and thus it has not been possible to construct a compaction curve for coal.

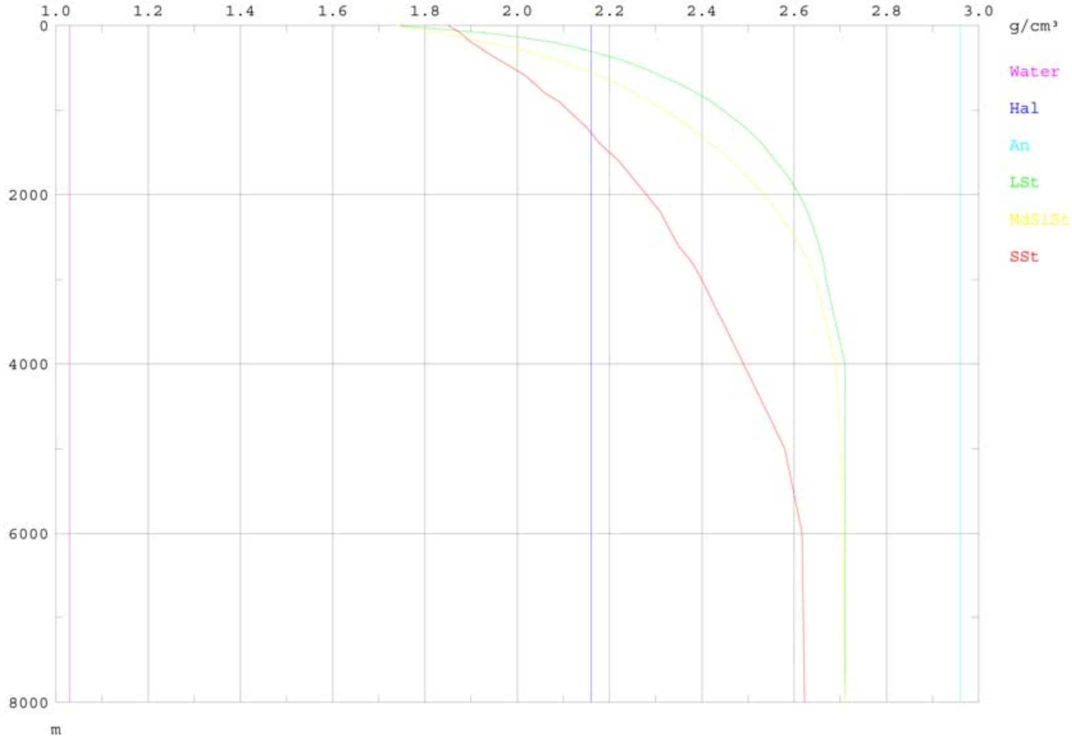


Figure 7: Density vs. depth curves for standard lithological types and minerals, as used for UK basins. Key: Hal = halite, An = Anhydrite, Lst = limestone, MdSlSt = mudstone and siltstone, SSt = sandstone, Water = sea water (average salinity)

4.1.2 Borehole data

The Midland Valley Study GIS was used to identify boreholes in and around the Firth of Forth basin, selecting those with reasonable depth of penetration and having geophysical logs. This yielded 26 oil & gas and coal exploration boreholes. From these, a subset of 14 boreholes having density logs and data availability at BGS Keyworth (either duplicate logs or digitised logs in the Wellog database) was selected. Time did not allow all these boreholes to be analysed for the study; those actually used are shown in Table 1 and their locations in Figure 1 (brown markers).

The best depths of burial estimates are obtained from mudstones. For each borehole, the gamma-ray log was used to define a shale-line and so indicate mudstone-dominated intervals. Such intervals were rejected if the calliper log indicated significant amounts of caving. Density log amplitudes were then averaged over the remaining shaly intervals to give density vs. depth readings.

In the Gartlove 2 borehole a Schlumberger CORIBAND log was available. This provides a lithological composition computed from the responses of a suite of logging tools. The CORIBAND log was compared with the gamma-ray shale-line method and found in broad agreement (it is assumed that part of the CORIBAND algorithm effectively fits a shale-line to the GR log curve).

The Wellsgreen borehole had logs annotated with lithological ‘picks’ by the site geologist. This was also found to be in broad agreement with the GR shale-line method.

The most recent density logs were compensated for borehole diameter, but some of the older data required manual compensation. This step is a likely source of error, as the compensation charts, used in conjunction with the calliper log, are logarithmic and difficult to estimate from.

A significant source of uncertainty, however, is log calibration. Density logs are relative-value tools. That is, if a density log indicates a 20% increase in rock density between depths z_1 and z_2 in a borehole, then that change is likely to be found tolerably accurate if compared to laboratory measurements on core samples. Scaling a density log in terms of absolute density values (g cm^{-3}) requires careful calibration of the density-logging tool. Even then, there are likely to be slight differences on successive runs in a borehole using the same tool and calibration 'source'. Different tools and calibration sources can yield significantly different results on runs in the same borehole. This is illustrated by results from Wellsgreen borehole, where both Schlumberger and BPB density logs were run and yielded results that differ in a systematic manner involving a shift and scale change. Such differences can be reliably assessed and allowed for where strata contain pure mineral bands, e.g. the halite layers within the Mercia Mudstone Group; unfortunately, this is not possible in the Carboniferous strata of the Firth of Forth basin.

Data analysis was carried out in an Excel spreadsheet. Figure 8 illustrates this process for the data from the Kilconquhar borehole. The density vs. depth data were tabulated using a separate worksheet for each borehole. A graph was constructed on each worksheet to display the observed values as points overlain on standard compaction curves. The compaction curves used were for mudstone and mudstone with 10% sandstone. The observed data points plot above the curve (Figure 8, upper cluster of points). The thickness of eroded overburden could then be calculated from the vertical (depth) offset between the points and the curve. This was added to the observed depths to produce a second set of points representing maximum depth of burial. These were also overlain on the standard curves to assess goodness of fit (Figure 8, lower cluster of points).

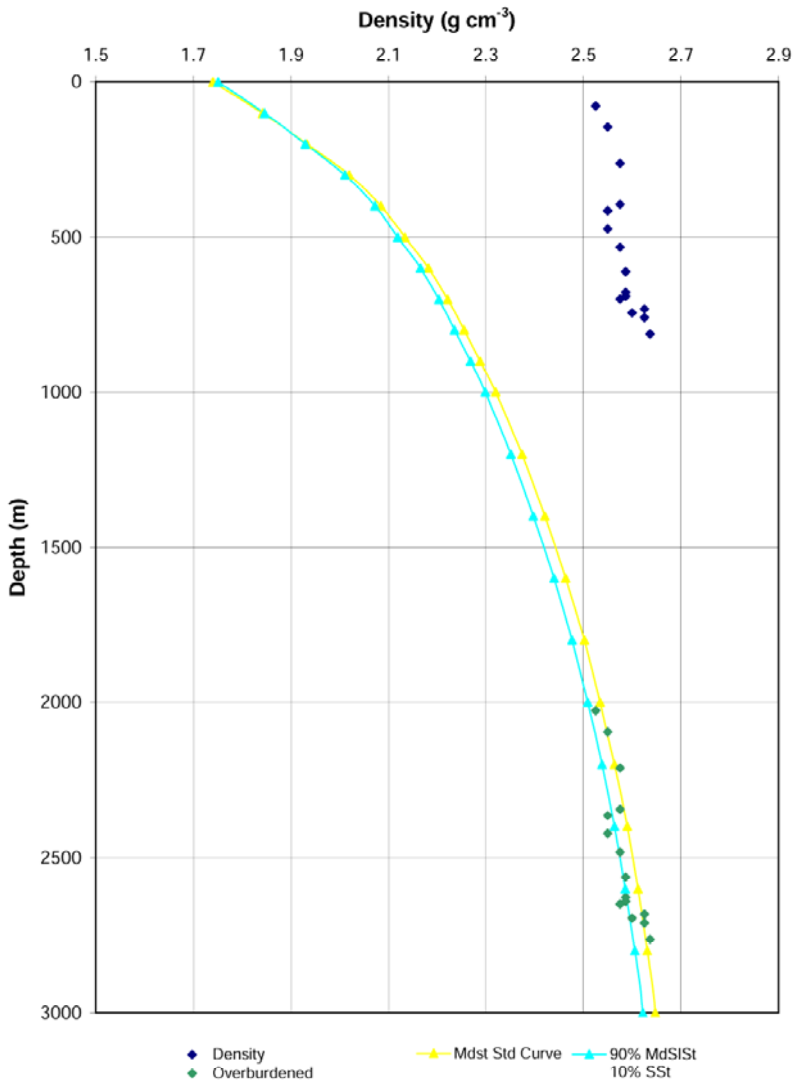


Figure 8: Estimating eroded overburden using compaction curves, Kilconquhar borehole

4.1.3 Estimated eroded overburden

Table 1 summarises the results of the borehole depth of burial study, showing the adopted maximum depth of burial and thickness of eroded overburden at each of the selected borehole locations.

Table 1: Overburden thickness adopted at boreholes

Borehole	Registration	Easting	Northing	Overburden
Gartenkeir 1	NS99SW/290	292665	694860	1250
Gartlove 2	NS99SW/292	294034	692670	2000
Kilconquhar	NO40SE/26	348448	703046	1950
Melville Grange 2	NT36NW/409	330574	667282	1600
Shell Bay	NO40SE/27	346777	700482	1550
Shiells	NT26SE/157	327890	660920	1950
Wellsgreen (BPB)	NT39NW/381	333421	698330	1900
Wellsgreen (Schl)	NT39NW/381	333421	698330	1400
Windygates	NO30SE/195	335101	700337	1300

A common procedure for assessing the reliability of overburden estimates is to add them to the observed depths for a basin-wide stratigraphic horizon. If this produces a smooth surface, then the overburden estimate can be considered consistent. In this case, all but two of the boreholes used in the study lie outside the area for which observed depths were available, so it was not possible to assess reliability quantitatively by this method. Instead, a qualitative assessment was made as part of the overburden mapping.

A contour map of the estimated eroded overburden was produced by Monaghan (pers. comm.), extrapolating from the above borehole values and taking into account the overall structural trends of the Firth of Forth basin. These contours were then digitised and gridded using Earthvision. (Some additional ‘control contours’ had to be introduced to constrain the gridding.) The map produced from the Earthvision grid (Figure 9) was submitted to project geologists for final approval (Monaghan & Browne, pers. comm.).

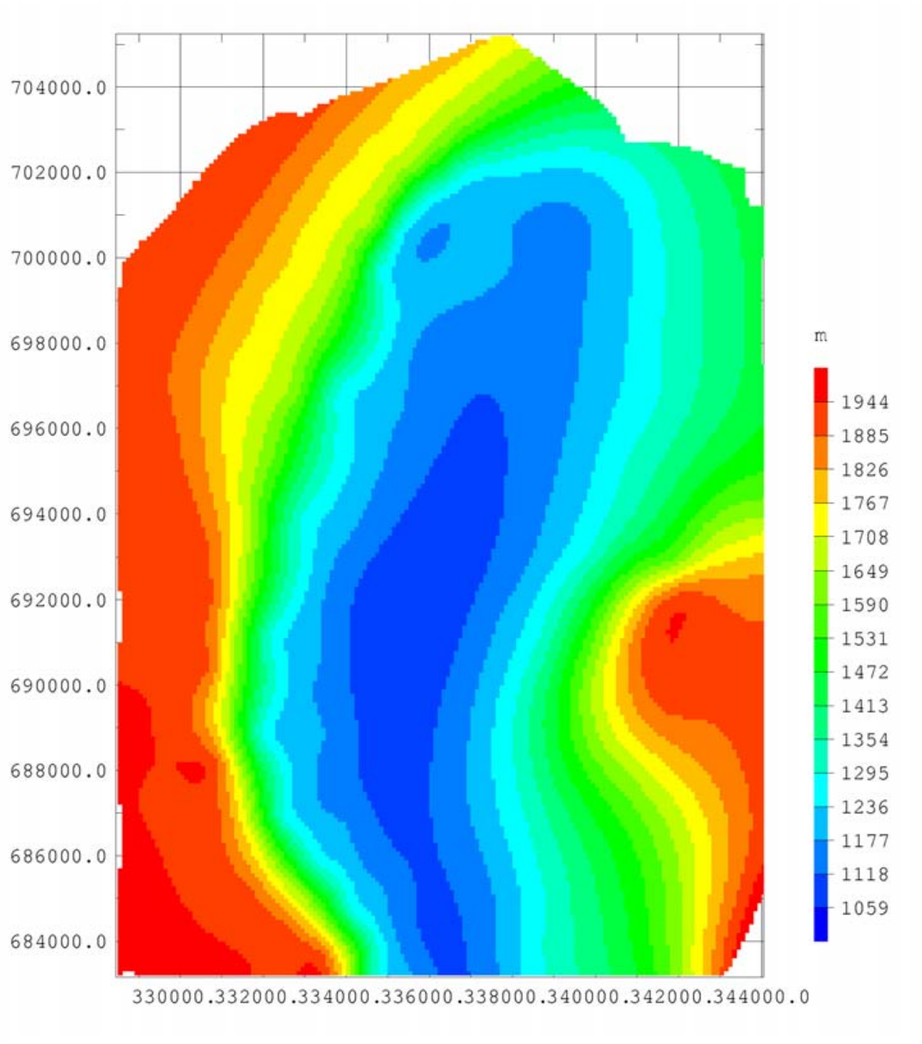


Figure 9: Map of estimated thickness of eroded overburden

The highest preserved strata in the Firth of Forth basin area are of late Palaeozoic age. It is assumed that the eroded overburden contained strata from latest Palaeozoic, through Mesozoic to Tertiary in age. However, it was agreed that there was insufficient evidence to assess reliably how this might have been stratigraphically subdivided, and thus that the eroded overburden would be best considered as a single bulk unit for HotPot modelling. The lithological proportions for this bulk unit were estimated based on preserved Mesozoic and Tertiary strata in basins in England and under the North Sea.

4.2 HOTPOT BURIAL HISTORY MODELLING

The parameters of the eroded overburden layer obtained from the depth of burial study were then merged with the mapped layers of the preserved succession, to form the input to the first, depositional history, stage of HotPot modelling.

4.2.1 Input data

4.2.1.1 AREA OF INTEREST

A HotPot model is constrained in geographic terms by a set of area of interest limits, which also define the spatial resolution of the model. In this case, these were based on previous Earthvision surface modelling of the Firth of Forth basin, from which the layer depth grids were obtained. In this precursor study (Ritchie et al. 2000), the objective had been 2D structural mapping of the surfaces, which had been considered as individual entities in order to produce optimum mapping. As a result, the individual depth grids did not overlay precisely, as required for vertical connection of the grid nodes in HotPot. Therefore, the grids were resampled to a common area of interest, using the following specification based upon their common area of overlap:

Western limit	328450	Southern limit	683150
Eastern limit	344050	Northern limit	705250
East/West spacing	100	North/South spacing	100
No. East/West nodes	157	No. North/South nodes	222

This resampling was done in HotPot, by treating the Earthvision grids as scattered data and using HotPot's internal nearest-neighbour gridding algorithm with a small search-radius to 'snap' the Earthvision grid values to their nearest HotPot grid nodes. Quality control of the resampled grids was performed by visual inspection and comparison to the original Earthvision grid displays.

4.2.1.2 INITIAL STRATIGRAPHY

The stratigraphic table for the model (Table 2) illustrates the main stratigraphy of the Firth of Forth basin and the grouping of the formations for both Earthvision surface modelling and HotPot basin modelling. Supplementary columns show a comparison of formation tops and bases notations for the key boundaries, and their relationship to the surface depth grids produced from Earthvision surface modelling of the basin fill.

Table 2: Model stratigraphy used with HotPot

Formation Tops	Formations	Formation Bases	Grids
DTM		DTM	foffifedtmclip
	Superficial deposits		
Rockhead		Rockhead	foffifetotrh
	Upper Coal Measures Fm Middle Coal Measures Fm		
Barncraig Coal		Barncraig Coal	foffifebarnclip
	Middle Coal Measures Fm Lower Coal Measures Fm		
Dysart Main Coal		Dysart Main Coal	foffifedymaclip
	Passage Formation Upper Limestone Fm Limestone Coal Fm		
Top Hosie Limestone		Base Limestone Coal	foffifetoho200clip
	Lower Limestone Fm Strathclyde & Inverclyde Grps ? Upper Devonian strata		
Top Devonian		Base Carboniferous	devxyz
	Devonian strata		

The following table (Table 3) shows the how the stratigraphical framework of the basin is related to the layer specifications for the HotPot model, and how these are related to the surfaces modelled in Earthvision and used to provide the depth data for the HotPot model.

The table columns represent the following. Deposited: age deposition of layer commenced. Eroded: age erosion of layer commenced. Lithology: percentage-mix of HotPot standard lithologies (mdst = mudstone; sst = sandstone; lst = limestone). File: for non-eroded layers, a grid of depths to base of layer; for eroded layer, a grid of thicknesses of eroded material. (All grid files were made by ASCII export from Earthvision.)

Table 3: Summary of HotPot layer parameters

Layer	Deposited	Eroded	Lithology	File (depth to base)
Superficial deposits	0.5 Ma		80% mdst 20% sst	foffifetotrh.2grd.dat
Eroded overburden	311 Ma	60 Ma	50% mdst 40% sst 10% lst	estover_v4.2grd.dat (thickness)
Middle to Upper Coal Measures	314 Ma		60% mdst 40% sst	foffifebarnclip.2grd.dat
Lower to Middle Coal Measures	316 Ma		70% mdst 30% sst	foffifedymaclip.2grd.dat

Layer	Deposited	Eroded	Lithology	File (depth to base)
Passage Fm to Limestone Coal Fm	327 Ma		40% mdst 40% sst 20% lst	foffifetoho200clip.2grd.dat
Lower Carboniferous strata	355 Ma		50% mdst 30% sst 20% lst	devxyz.2grd.dat

4.2.1.3 DIGITAL TERRAIN MODEL

The 'top' of a HotPot model can be defined by either a planar surface or a topographic surface. A digital terrain model (DTM) had been constructed for the Earthvision mapping of the Firth of Forth basin, and this was used to provide a topographic surface for the HotPot model.

4.2.1.4 COMPACTION CURVES

The set of compaction curves used for the depth of burial study (Figure 7) were used as the reference data for the HotPot decompaction calculations.

4.2.2 Burial history modelling results

Figure 10 shows the results of backstripping the initial stratigraphy. Note that the eroded overburden layer is represented by an unconformity marker in the present-day column and at the top of the 0.5 Ma column, then reconstructed as a deposited layer at the top of the 60 Ma column.

Backstripping produces 48 layer grids (24 density and 24 thickness) together with 21 column summary grids (7 each: bulk density, sediment-loaded thickness and sediment-starved thickness). This gives a grand total 69 possible maps from this model. A representative selection is presented here as colour-fill maps.

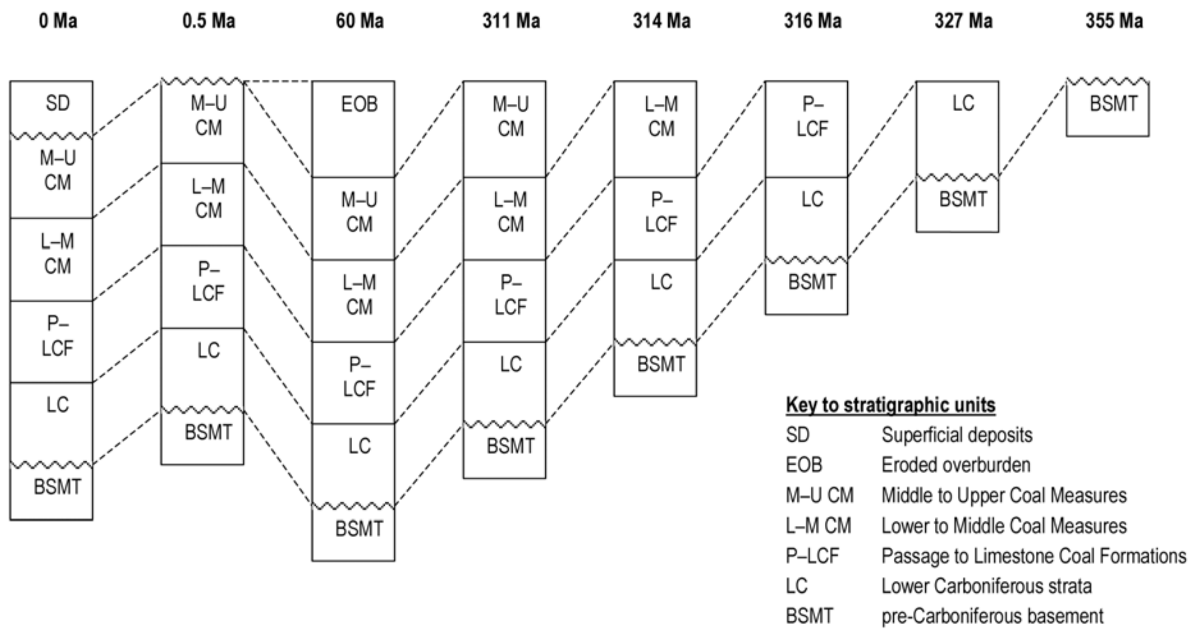


Figure 10: Stratigraphic columns at stages in basin burial history generated by HotPot backstripping process

Figure 11:

A sequence of maps to illustrate the development of the basin. These are taken from the backstripped and decompacted basin burial history produced by HotPot.

A common colour scale is used for all maps, to permit ready comparison.

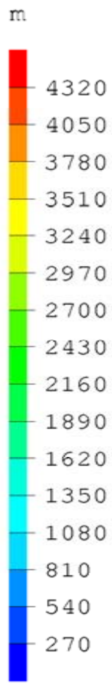
Figure 11a: Thickness of Lower Carboniferous strata immediately after deposition, 327 Ma. *This layer was not interpreted in the north and west of the mapped area. HotPot treats it as zero thickness to allow computations on other layers to proceed.*

Figure 11b: Thickness of the layer representing the Passage – Limestone Coal formations immediately after deposition, 316 Ma.

Figure 11c: Thickness of the layers representing the Lower-Middle Coal Measures and the Passage – Limestone Coal formations, 314 Ma.

Figure 11d: Thickness of the layers from the Middle-Upper Coal Measures to the Passage – Limestone Coal formations, 311 Ma.

Figure 11e: Thickness of the layers from the restored overburden to the Passage – Limestone Coal formations, 60 Ma.



Common colour scale

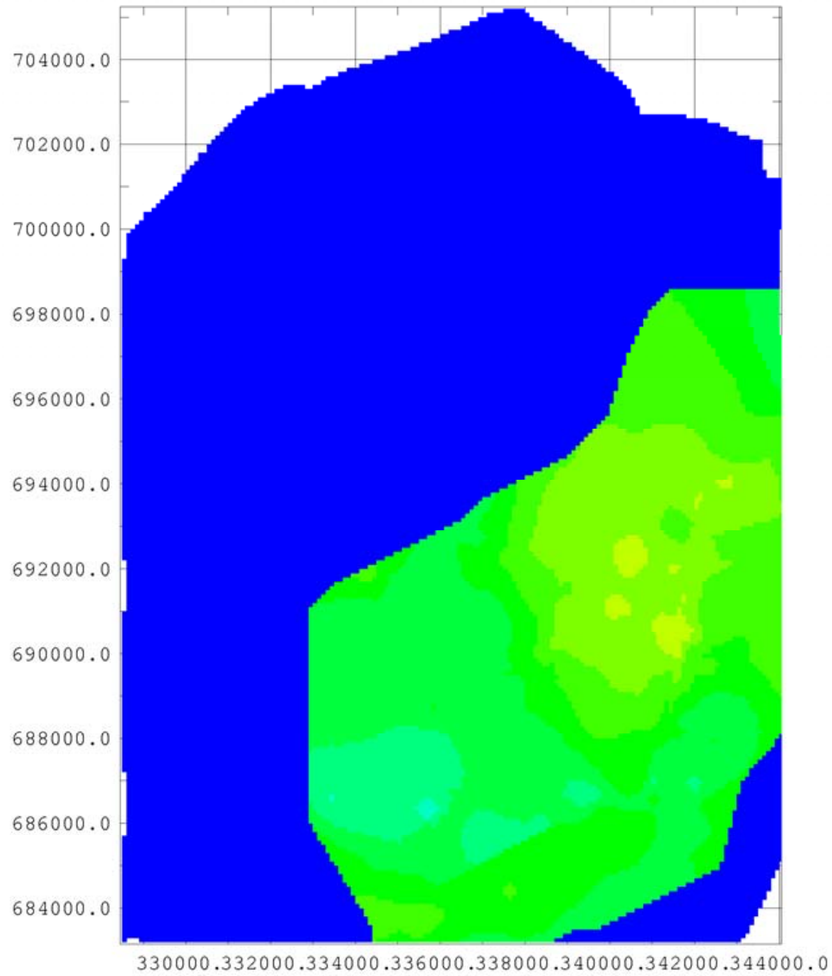


Figure 11a: Sediment load at 327 Ma

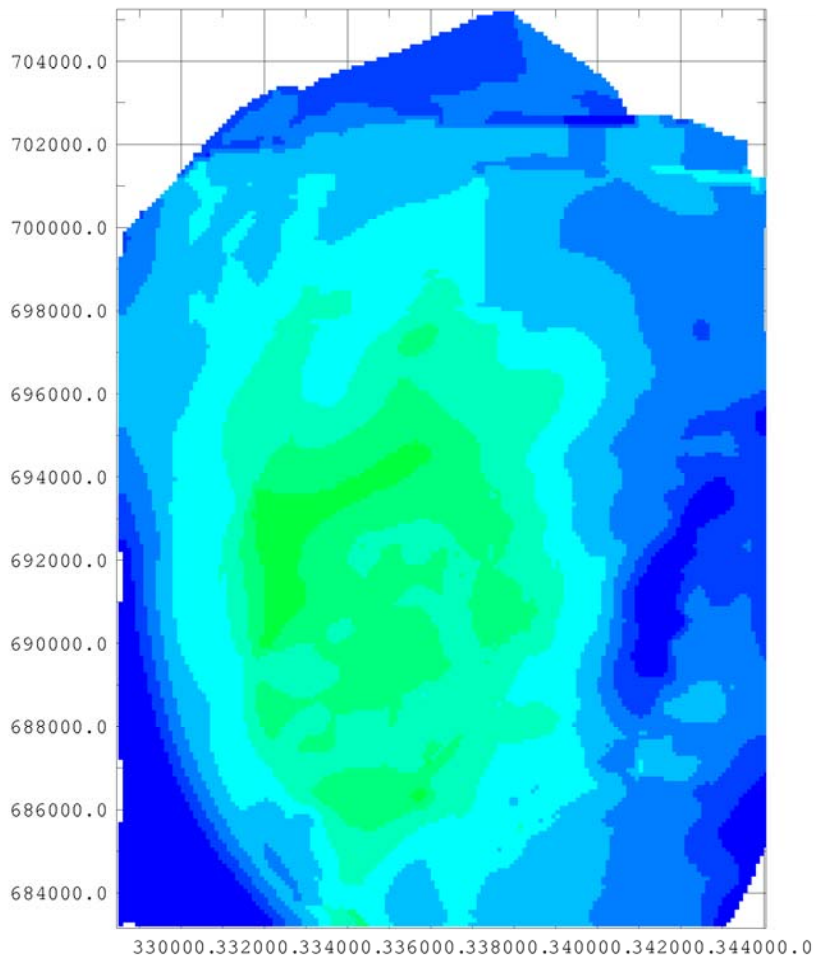


Figure 11b: Sediment load at 316 Ma

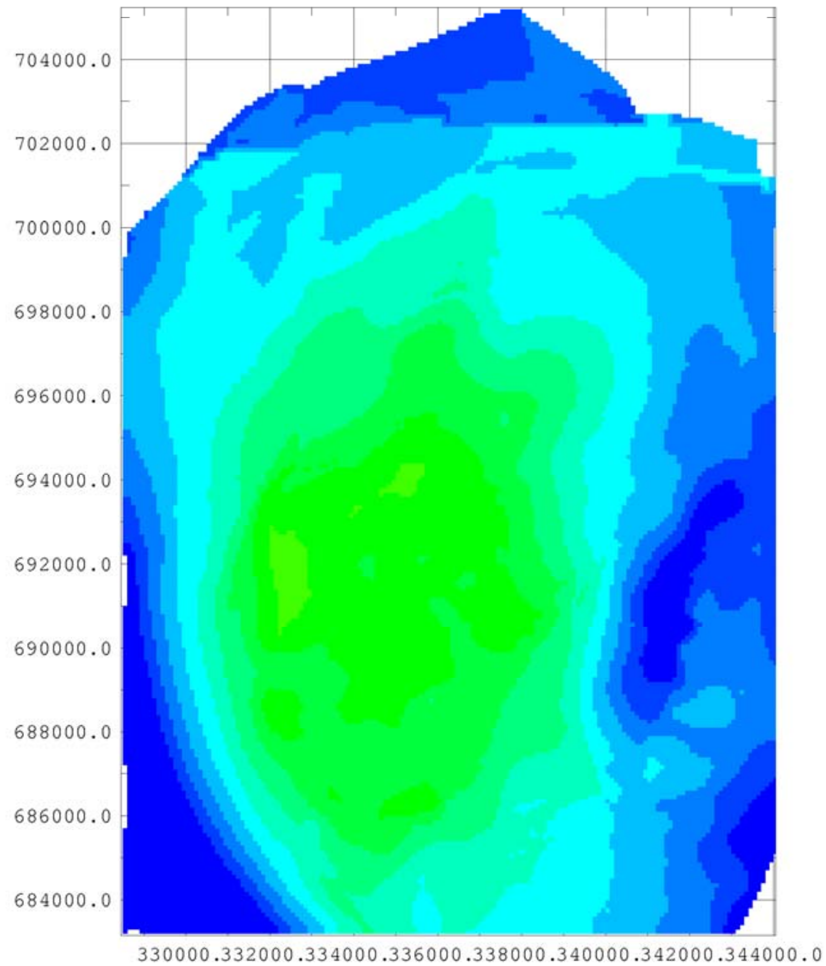


Figure 11c: Sediment load at 314 Ma

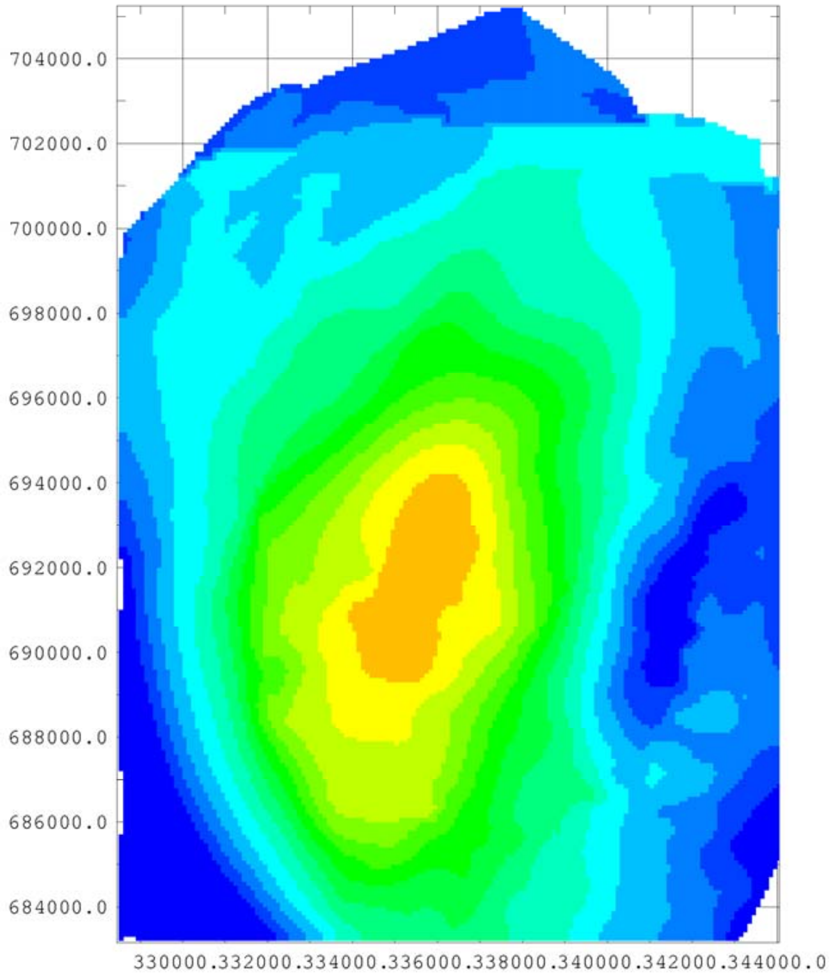


Figure 11d: Sediment load at 311 Ma

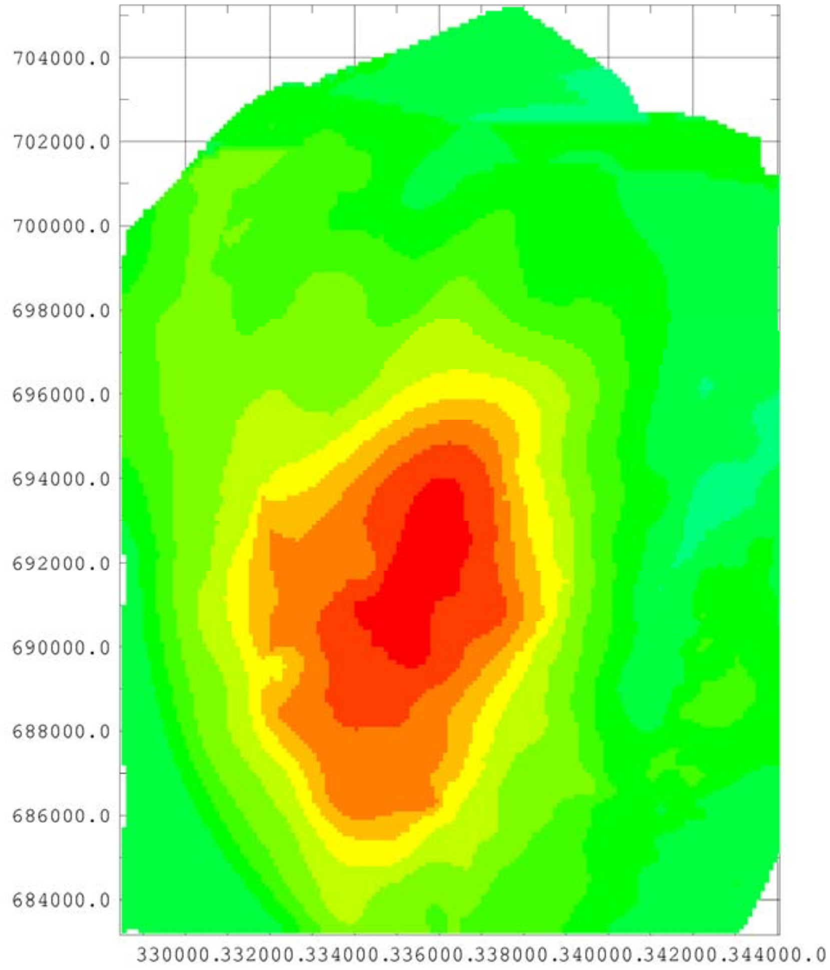


Figure 11e: Sediment load at 60 Ma

4.2.2.1 Sediment loaded thickness maps

Figure 11 shows a selection of backstripped and decompacted sediment thickness maps to illustrate stages in the development of the basin. The maps use a common colour scale for ease of comparison. Figure 11a shows the Lower Carboniferous strata immediately after deposition, at 327 Ma – note that this layer was not interpreted over the north and west of the area; thus, the sharp boundary indicates the limit of interpretation and has no structural significance. The Passage to Limestone Coal formations layer is the lowest unit interpreted over the whole area, so this has been used to illustrate the development of the basin from 316 Ma, when its deposition finished (Figure 11b), through to 60 Ma, when maximum depth of burial was attained (Figure 11e). Each map shows the total sediment load in the basin at a time-point, down to the base of the mapped layer.

When analysing these maps, it must be borne in mind that the data quality was poorer in the lower parts of the seismic sections and that there were no well ties for the lower strata. Interpretation was therefore more uncertain for the Lower Carboniferous layer and the Passage to Limestone Coal formations layer. This may have yielded artefacts in the corresponding surfaces modelled using Earthvision (sections 4.2.1.1 & 4.2.1.2 above). Any artefacts present in the surface data for a layer tend to be amplified by the decompaction computation.

Nevertheless, the development of the basin appears to conform to a typical two-stage scenario, with initial rapid subsidence in small, discrete sub-basins, followed by broad, basin-wide subsidence. Figures 11a & 11b illustrate the initial subsidence phase, with the sub-basins apparent in the central eastern part of the Lower Carboniferous (11a) and the central part of the Passage – Limestone Coal formations (11b). The later, thermal relaxation type, subsidence phase is shown in Figures 11c-e. By the Middle Coal Measures (11c), there is a blanket of sediment forming a single depocentre, and the development of this continues through the Upper Coal Measures (11d) until the maximum depth of burial is reached at 60 Ma (11e).

4.2.2.2 Burial histories at selected locations

Burial history plots were extracted from the stacked HotPot grids at three locations and are shown in Figure 12. Figure 12a shows the burial history at a location near the depocentre of the basin and within the area of the Lower Carboniferous interpretation. Figures 12b,c show the history at the grid nodes nearest the Tower 1 and Milton of Balgonie boreholes used in the BasinMod modelling. These are both near the limits of the basin, where not all layers are present.

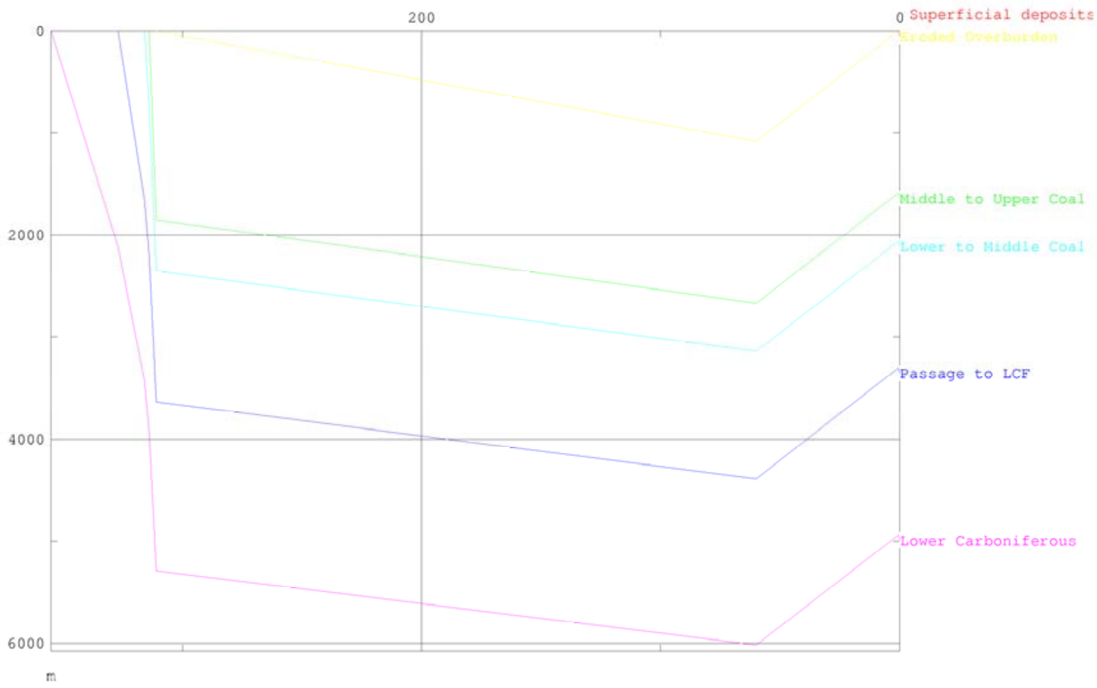


Figure 12a: Burial history in basin depocentre (334950E, 690750N)

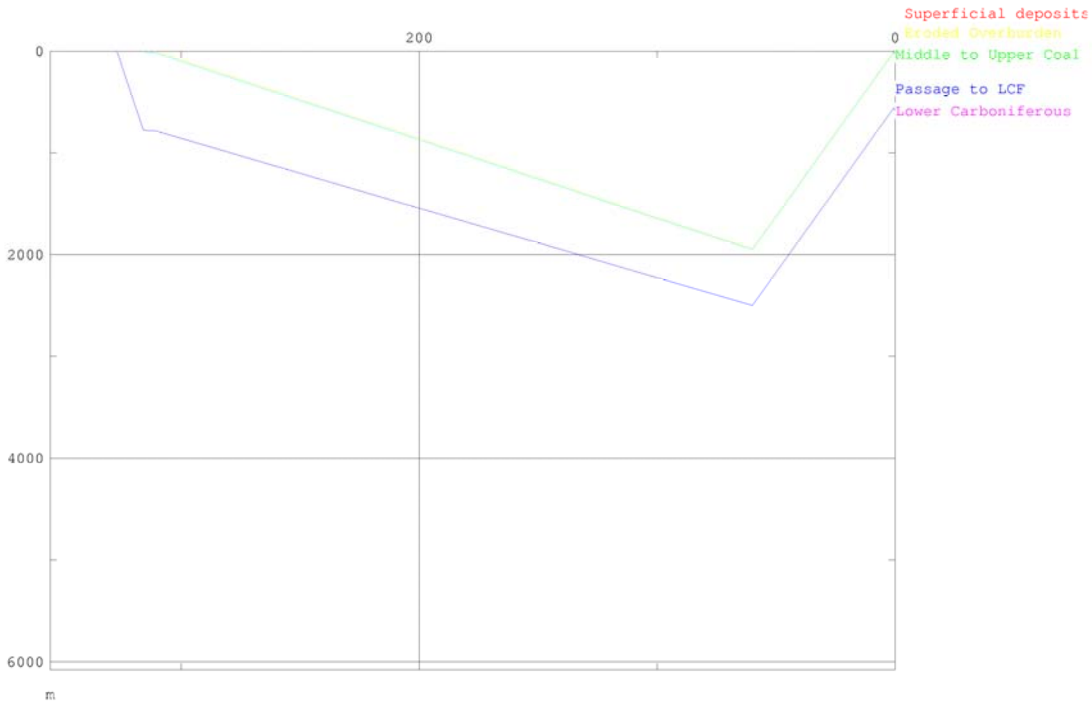


Figure 12b: Burial history near Tower 1 borehole (330050E, 687850N)

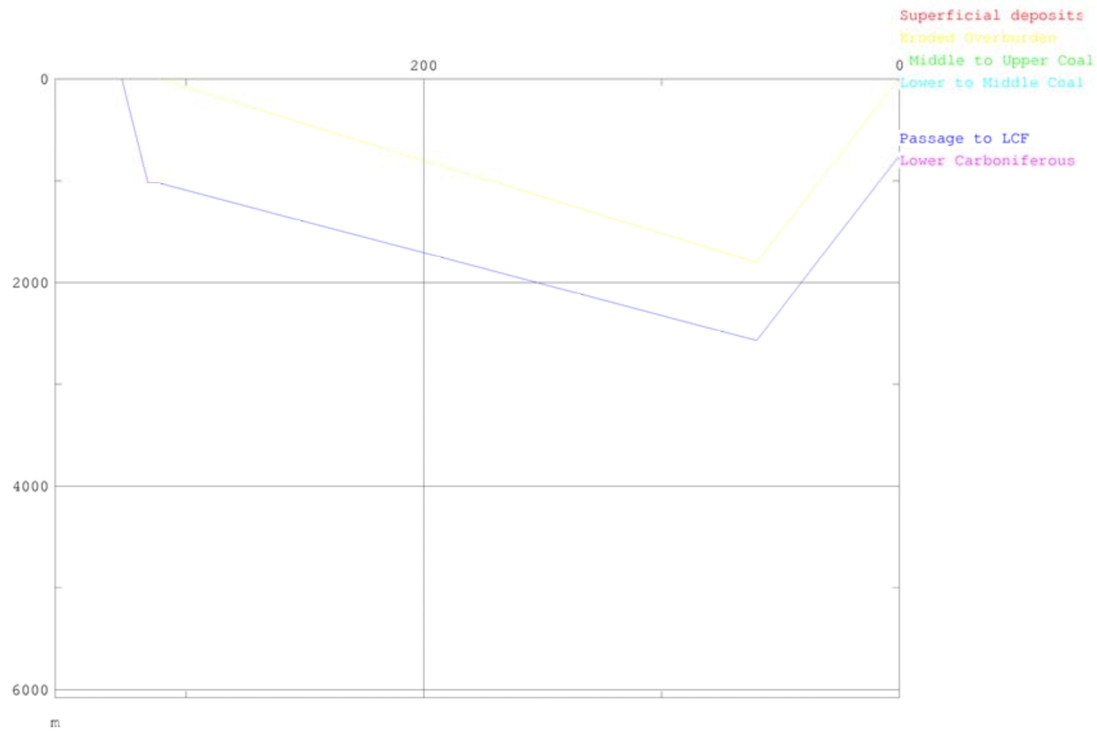


Figure 12c: Burial history near Milton of Balgonie borehole (331750E, 699350N)

4.2.2.3 Rates of deposition

Rates of deposition were estimated for the Carboniferous strata and are shown in Table 4. The estimate for each unit was made using sediment thickness from the backstripped and decompacted grid together with the timing for the start and end of deposition. Values were calculated for the thickness class at the depocentre as seen in the grid.

Table 4: Computed rates of deposition for HotPot model layers

Unit	Start (Ma)	End (Ma)	Duration (Ma)	Thickness (m)	Rate (m Ma^{-1})
Lower Carboniferous	355	327	28	3000	107.14
Passage – Limestone Coal Fm	327	316	11	2000	181.82
Lower – Middle Coal Measures	316	314	2	900	450.00
Middle – Upper Coal Measures	314	311	3	1900	633.33

4.3 HOTPOT THERMAL MODELLING

The second, thermal history modelling stage of HotPot uses a method of 1D vertical heat transfer, which is applied successively to each stack of grid nodes to compute the distribution of temperature at the base of each layer at each stage of the depositional history. The thermal modelling stage requires some inputs additional to the results obtained from the first-stage of depositional history modelling.

4.3.1 Additional input data

4.3.1.1 THERMAL CONDUCTIVITY

The thermal conductivity of rocks varies with both depth and temperature, so the method initialises layer thermal conductivities according to depth of burial, by reference to standard thermal conductivity vs. depth curves, and then iteratively adjusts them for calculated temperature.

The thermal conductivity of sedimentary rocks increases with depth of burial, in a similar manner to density, and is also dependent upon lithology. A set of thermal conductivity vs. depth vs. lithology curves, Figure 13, derived from the observed, near-complete Mesozoic to Neogene sequence in Denmark (Balling et al. 1981) and used in an earlier study of the Cheshire Basin (Chadwick et al., 1999) have been adopted here.

The thermal conductivity of rocks also varies with temperature, although the precise nature of this relationship is not well understood. The consensus (Cermak & Bodri, 1986, Sekiguchi, 1984 and Somerton, 1992) is that, for a given rock type, thermal conductivity decreases with increasing temperature up to about 300°C, where after the change becomes negligible. The method described by Cermak & Bodri, which seems to provide the least dramatic and most consistent variation (see Figures 4 & 5 in Appendix I of Rowley et al. 1993), has been applied to this data set.

4.3.1.2 HEATFLOW ESTIMATION

Heatflow measurements have been made in the Firth of Forth basin area and used in the compilation of the UK Heatflow Map (Figure 2.3 in Rollin et al 1995). Unfortunately, these observations are too sparsely distributed to produce a reliable heatflow map of the area. Therefore, the tabulated value of 53 mW/m^2 for the present-day heatflow at Edinburgh (Rollin et al 2002) has been adopted as a basin-wide value for this modelling. As the Firth of Forth basin is small, and heatflow variation in the south-east of Scotland is gradual, this is believed to be a valid assumption.

Estimating palaeo-heatflow over the period back to the late Devonian or early Carboniferous inception of the basin is problematic. Not least because there are three tectonic models proposed

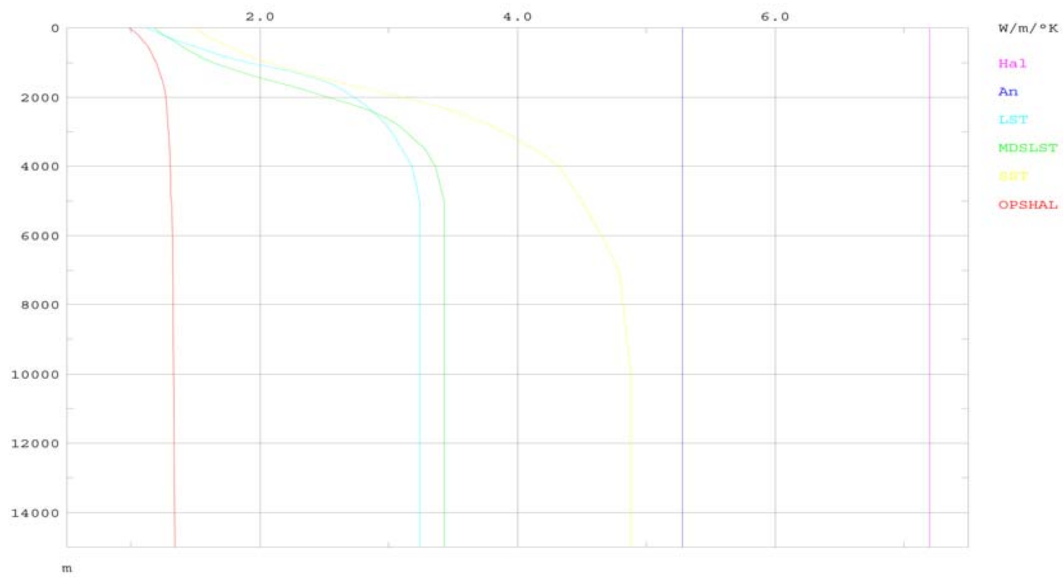


Figure 13: Thermal conductivity vs. depth curves for standard lithological types and minerals, as used for UK basins. Key: Hal = halite, An = Anhydrite, Lst = limestone, MdSlSt = mudstone and siltstone, SSt = sandstone, OPSHAL = overpressured shale

for the development of the basin during the late Palaeozoic: straightforward extension followed by thermal subsidence (Leeder, 1982), dextral strike-slip pull-apart (McCoss 1987, Warr 2000) and sinistral strike-slip pull-apart followed by dextral (Rippon et al. 1996, Ritchie et al. 2003). The latter two, however, can be considered variants on a strike-slip model for estimating heatflow. There is also much discussion over the tectonic regime during the Mesozoic (was it dominantly east–west extensional, cf. the North and Irish Seas?) and in the Tertiary (was it much affected by the Tertiary magmatism centred to the west of Scotland and did this result in a significant pulse of heat input?).

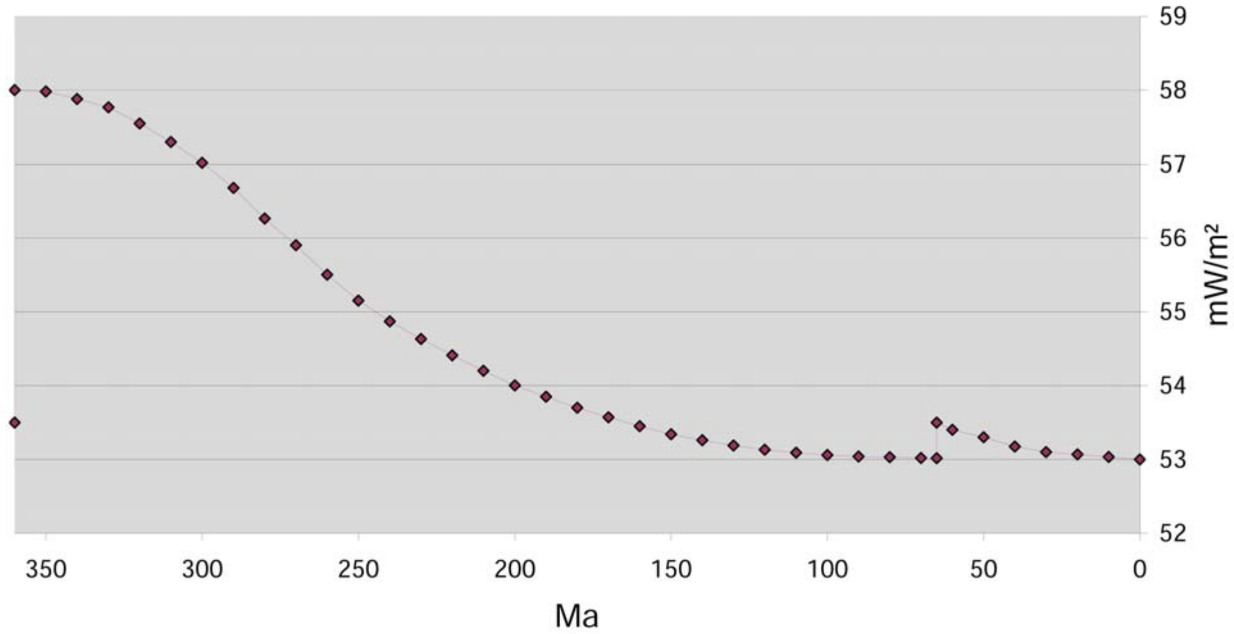


Figure 14: Estimated heatflow profile adopted for HotPot modelling

The model used here assumes that the late Palaeozoic basin development took place in a dominantly extensional regime; that the basin was largely unaffected by Mesozoic extension, which formed basins to east and west of Scotland but seems to have left the mainland as a high; and that there was some heat input during the Tertiary igneous episode. The sediment-starved (tectonic) basin subsidence values obtained from the HotPot burial history modelling indicate initial subsidence was in the range 1200 – 1400 m in the central part of the basin. When the basin reached maximum depth of burial, the tectonic subsidence reached about 2100 m. These are consistent with a McKenzie (1978) extensional model having $\beta \approx 1.5$, and that has been adopted here for construction of the basic heatflow vs. time profile. An instantaneous extension at 360 Ma has been assumed at the start of the curve. A local heatflow pulse incorporated at 65 Ma represents heat input due to Tertiary igneous activity. The baseline of this curve has been shifted to yield the observed present-day heatflow of 53 mW/m^2. The heatflow vs. time profile constructed is shown in Figure 14.

A future alternative model might replace the extensional McKenzie-type curve with one based upon a pull-apart tectonic model.

4.3.1.3 Surface temperatures

The present day average annual surface temperature of the Firth of Forth area is approximately 9°C (Met. Office). This has also been assumed as the likely average surface temperature at 0.5 Ma when deposition of the superficial deposits began.

Estimates of average surface temperatures for earlier periods are poorly constrained. The general view is that the climate of Britain from early Tertiary, through the Mesozoic, to late Palaeozoic was much warmer than the present day, and probably tropical or sub-tropical. Thus, for this study, a constant value of 20°C has been assumed for surface temperatures at all model age-points from 60 Ma to 355 Ma.

4.3.2 Thermal results

The thermal modelling step produces a further 48 data grids, 24 of computed layer thermal conductivity and 24 of predicted temperatures at the bases of the layers throughout the basin's history. A representative selection are presented as colour-fill maps and discussed below.

4.3.2.1 LAYER TEMPERATURE MAPS

Figure 15 shows a selection of the layer temperature maps. A common colour scale is used for ease of comparison. Figures 15a-e illustrate the predicted temperatures at the bases of the layers present when maximum burial was attained, at 60 Ma. Figures 15-h, together with 15d, show the increase in temperature at the base of the Passage to Limestone Coal formations layer, from immediately after its deposition (316 Ma) until maximum burial (60 Ma) – it is useful to compare these with the corresponding sediment thickness maps in Figures 11b-e.

4.3.2.2 THERMAL HISTORIES AT SELECTED LOCATIONS

Thermal history plots were extracted from the stacked HotPot grids at three locations and are shown in Figure 16. Figure 16a shows the thermal history at a location near the depocentre of the basin and within the area of the Lower Carboniferous interpretation. Figures 16b,c show the history at the grid nodes nearest the Tower 1 and Milton of Balgonie boreholes used in the BasinMod modelling. These are both near the limits of the basin, where not all layers are present. These figures may be compared with the corresponding burial history plots in Figure 12.

The burial and thermal histories may be combined to estimate likely geothermal gradients. Table 6 shows some estimates made for a series of grid nodes around the depocentre of the basin and represent the situation at maximum burial, 60 Ma. The total thickness was obtained from the sediment loaded thickness grid and the temperatures are those for the base of the Lower Carboniferous strata. From these, it is estimated that the likely geothermal gradient at 60 Ma was in the approximately 24.5°C per kilometre.

Figure 15:

A sequence of maps to illustrate the thermal history of the basin. Figures 15a-e show the thermal regime at maximum depth of burial (60 Ma). Figures 15f-h with 15d show temperature variation at the base of the Passage to Limestone Coal formations with increasing burial. Compare these with the burial history maps, Figure 12.

A common colour scale is used for all maps, to permit ready comparison.

Figure 15a: Temperature at base of overburden, 60 Ma

Figure 15b: Temperature at base of Middle to Upper Coal Measures, 60 Ma

Figure 15c: Temperature at base of Lower to Middle Coal Measures, 60 Ma

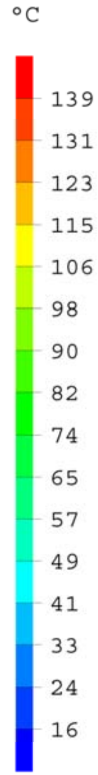
Figure 15d: Temperature at base of Passage to Limestone Coal formations, 60 Ma

Figure 15e: Temperature at base of Lower Carboniferous strata, 60 Ma

Figure 15f: Temperature at base of Passage to Limestone Coal formations, 316 Ma

Figure 15g: Temperature at base of Passage to Limestone Coal formations, 314 Ma

Figure 15h: Temperature at base of Passage to Limestone Coal formations, 311 Ma



Common colour scale

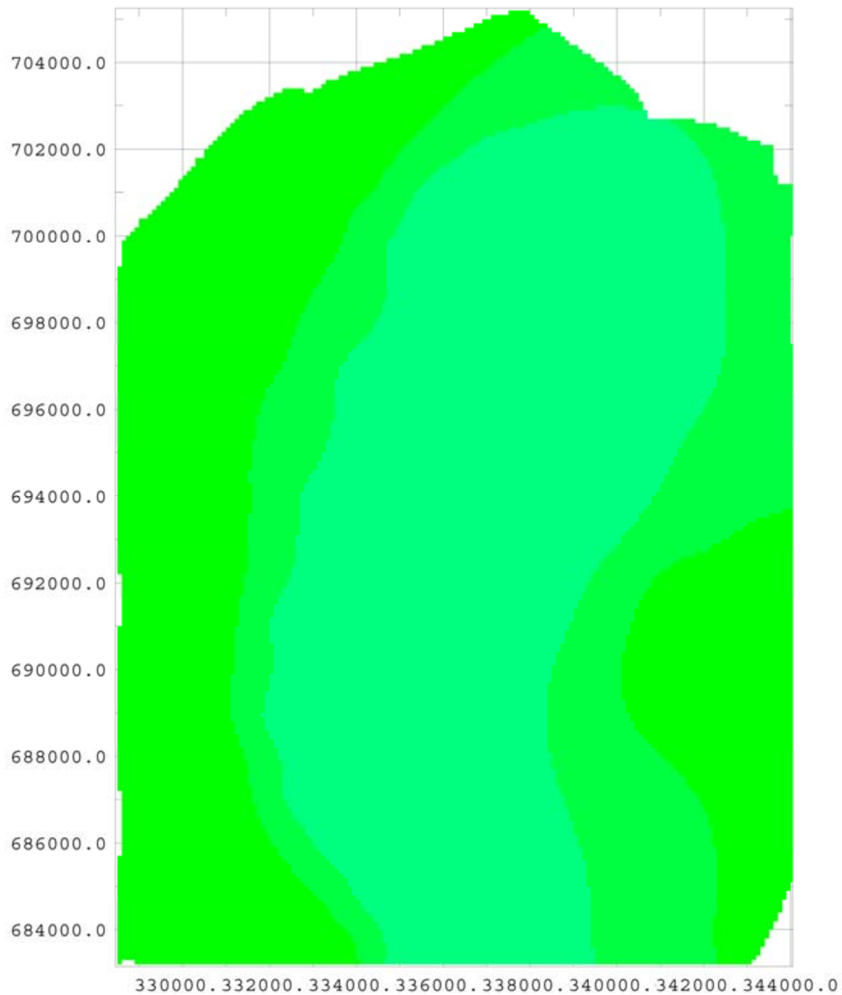


Figure 15a: Temperature at base of overburden, 60 Ma

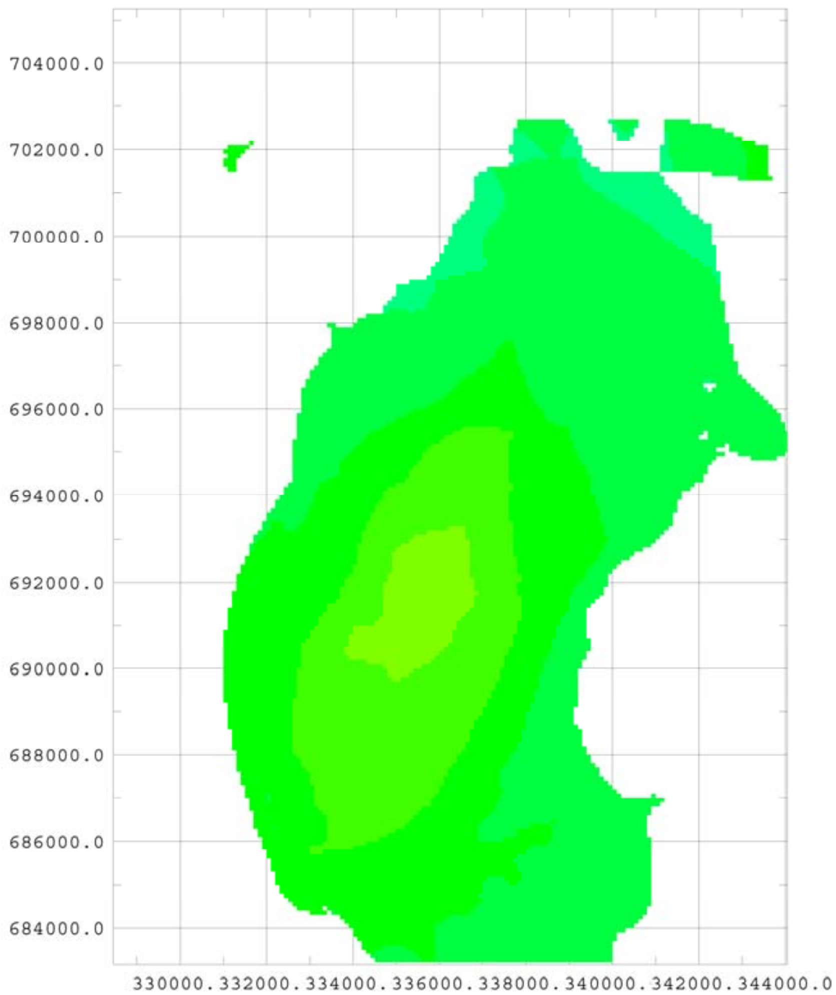


Figure 15b: Temperature at base of Middle - Upper Coal Measures, 60 Ma

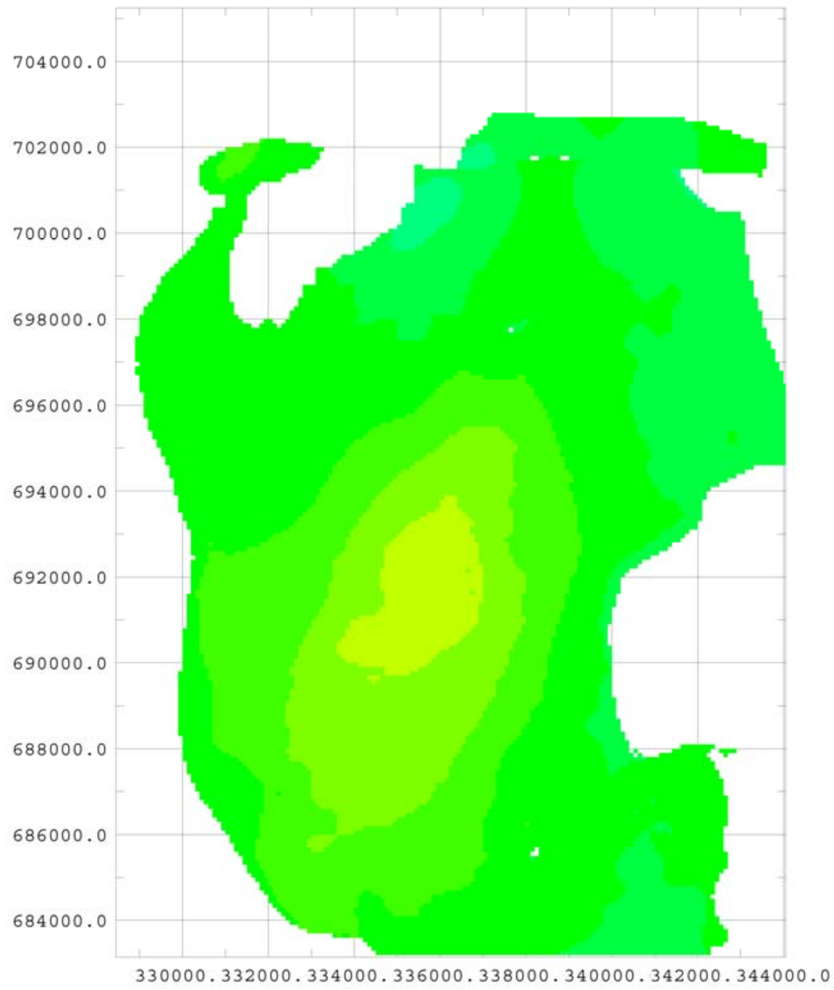


Figure 15c: Temperature at base of Lower - Middle Coal Measures, 60 Ma

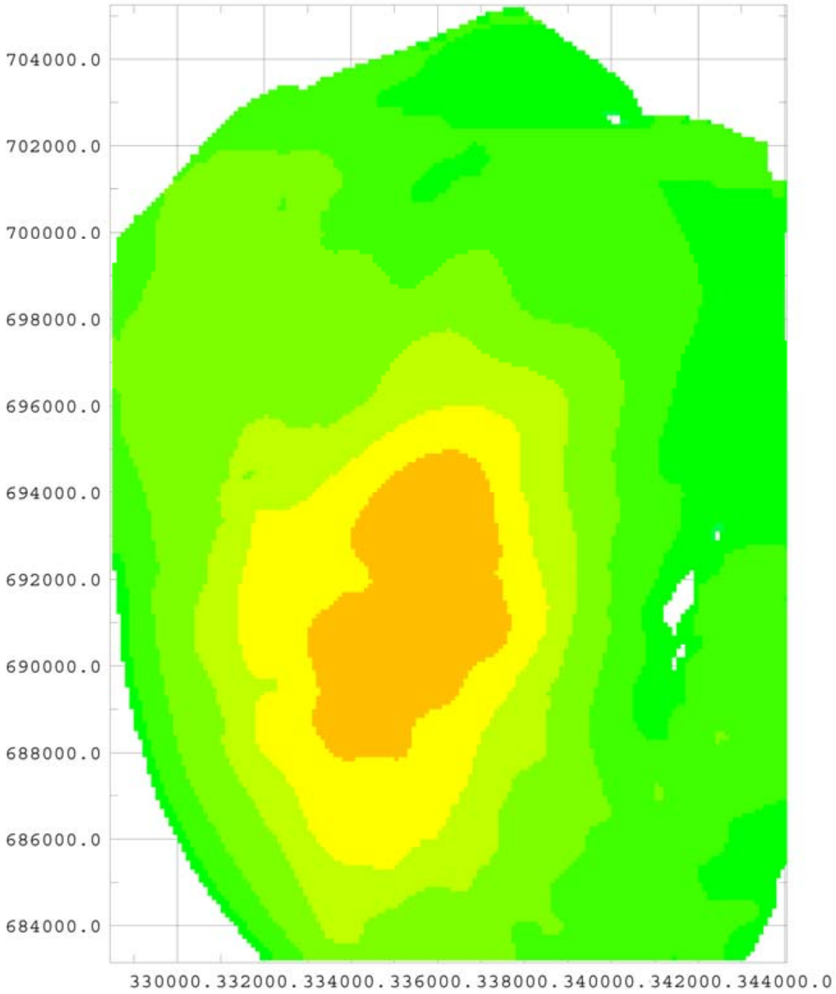


Figure 15d: Temperature at base of Passage - Limestone Coal, 60 Ma

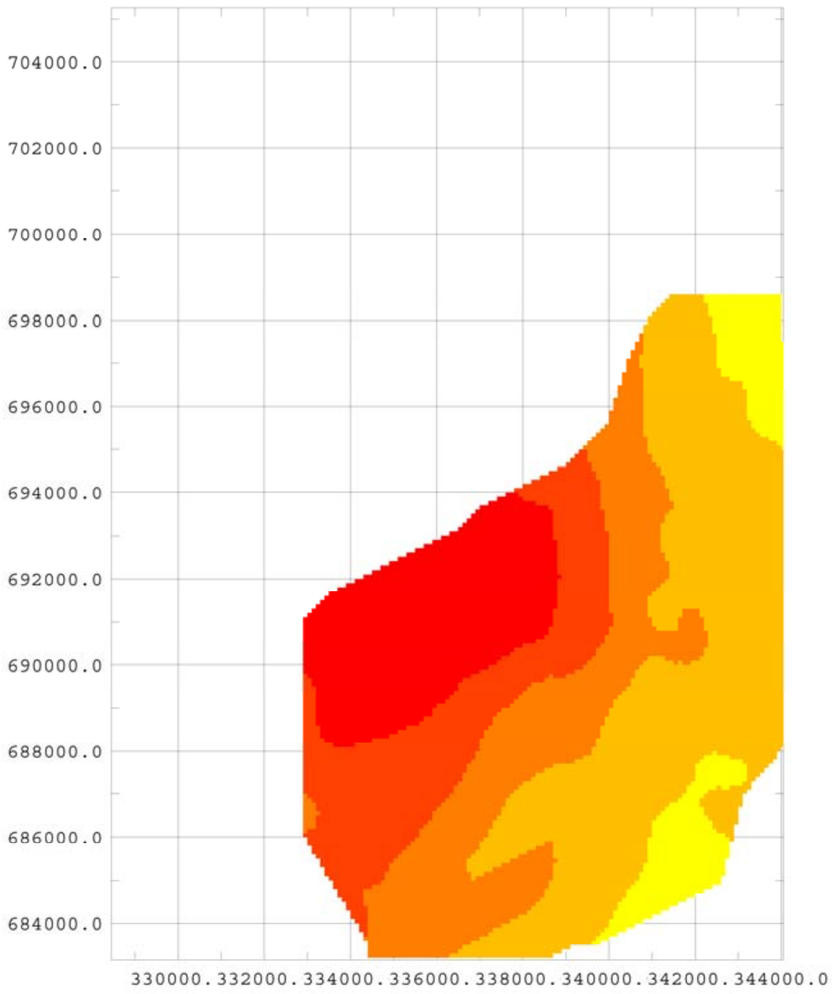


Figure 15e: Temperature at base of Lower Carboniferous strata, 60 Ma

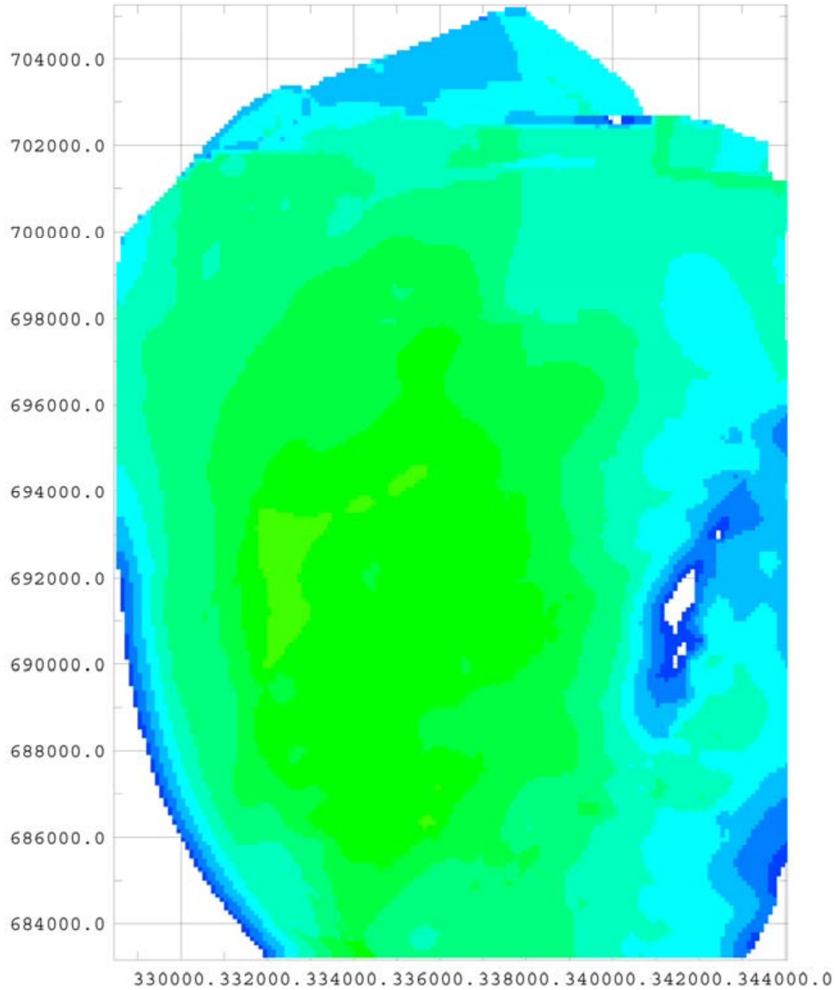


Figure 15f: Temperature at base of Passage - Limestone Coal, 316 Ma

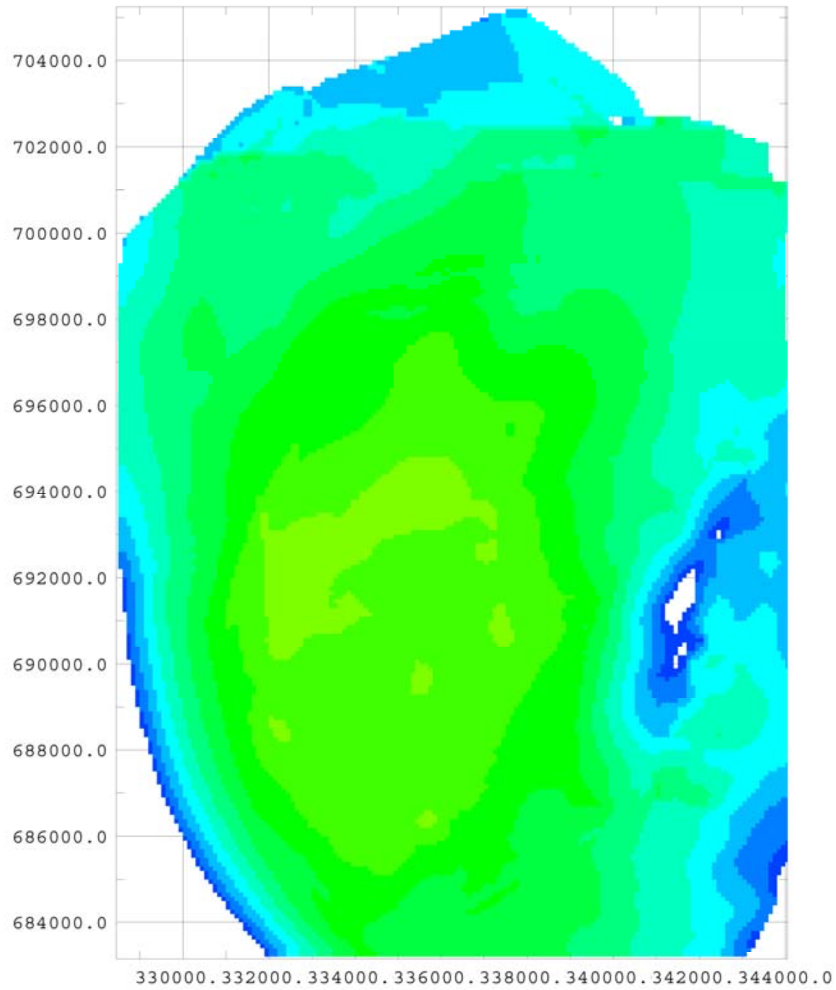


Figure 15g: Temperature at base of Passage - Limestone Coal, 314 Ma

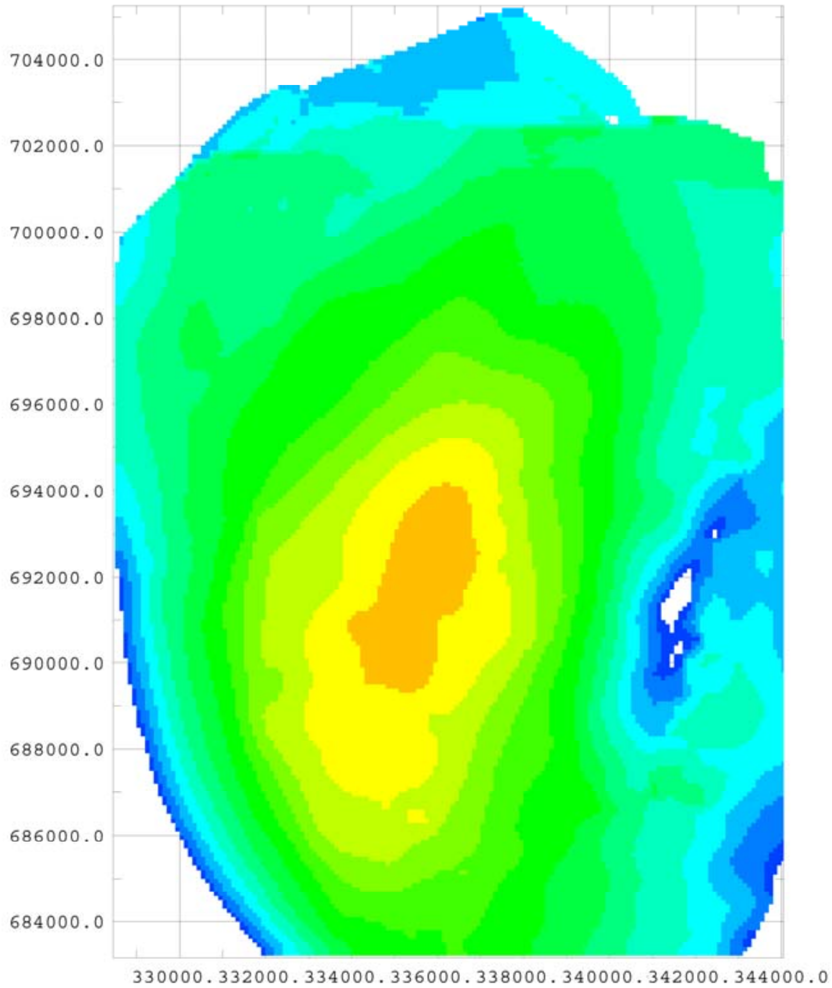


Figure 15h: Temperature at base of Passage - Limestone Coal, 311 Ma

Table 5: Estimated geothermal gradient at 60 Ma

X	Y	Total thickness (m)	Basal temperature (°C)	Geothermal gradient (°C/km)
335750	692350	6049	146.4	24.2
334950	690750	5990	145.5	24.3
338550	690850	5532	139.5	25.2
335050	688750	5647	140.6	24.9
336050	690750	5888	144.1	24.5

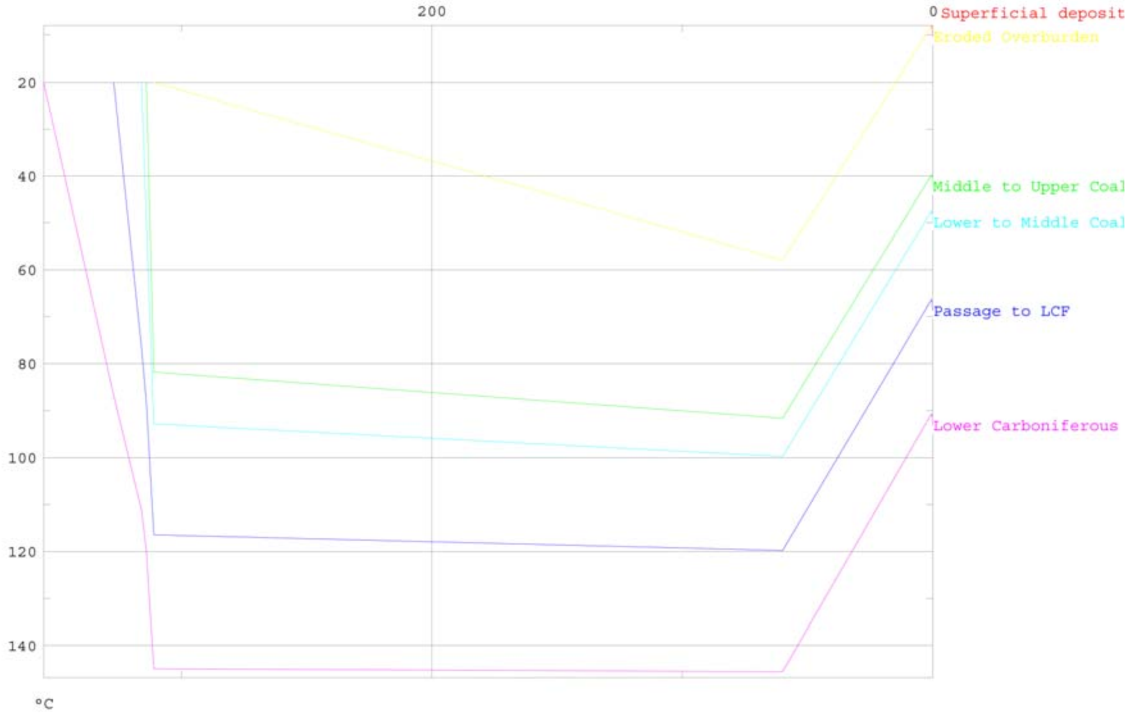


Figure 16a: Thermal history in basin depocentre (334950E, 690750N)

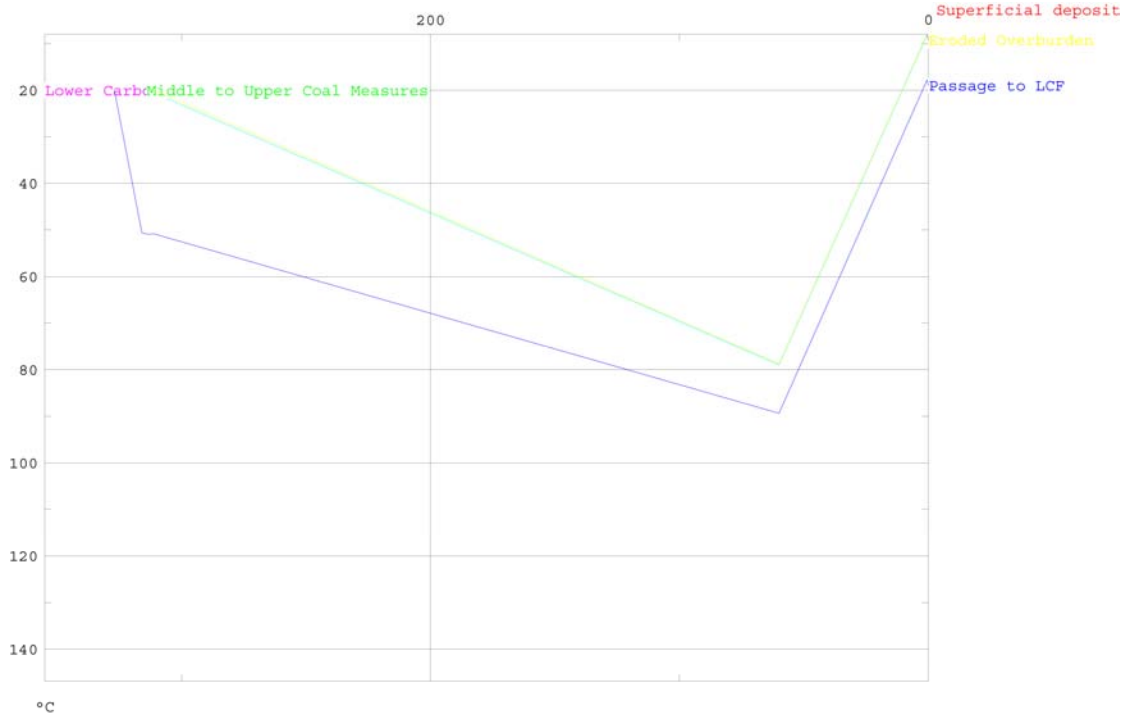


Figure 16b: Thermal history near Tower 1 borehole (330050E, 687850N)

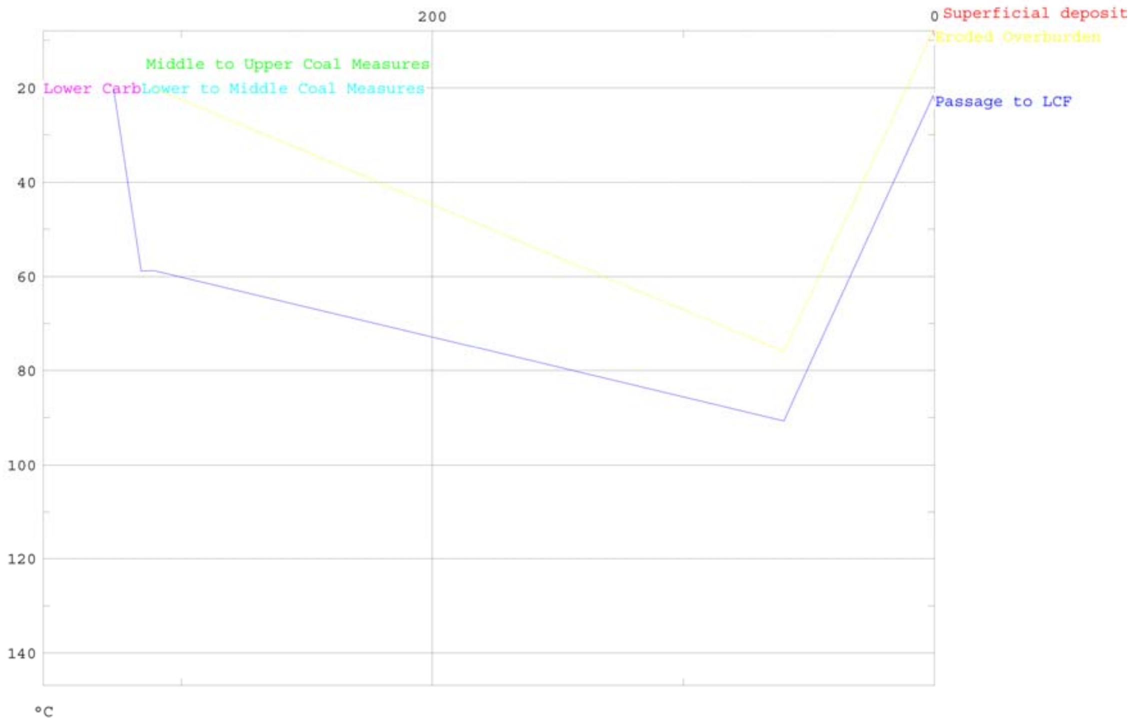


Figure 16c: Thermal history near Milton of Balgonie borehole (331750E, 699350N)

5 Comparison of BasinMod and HotPot Model Results

5.1 DEPOSITIONAL HISTORY

The BasinMod modelling predicts deposition of sediment in the late Carboniferous (younger than that in the preserved strata), erosion of this material following the Variscan uplift, a further, longer period of deposition from Permian to early Tertiary and, finally, relatively rapid erosion of all post-Carboniferous sediment after uplift at about 60 Ma.

A limitation of the compaction-study method of depth of burial analysis used with HotPot is that it cannot detect overprinting. Where preserved strata have been subject to a sequence of events that includes more than one phase of deposition followed by uplift and erosion, this method can predict the maximum depth of burial but not which period of burial it occurred in. Neither can it determine the lesser amount of burial that occurred in the other period. Thus in the Firth of Forth basin, all it can predict is one apparent episode of deposition, stretching from Carboniferous to early Tertiary, followed by the uplift and erosion at 60 Ma.

The calibration of the BasinMod technique allows BasinMod to model the burial and heating that occurred prior to Variscan uplift. This would have been an important episode in the thermal history of the preserved strata, because the regional heatflow was probably then almost at its highest, so any significant burial would have resulted in marked heating and maturation of organic matter. Whereas in the HotPot model this episode is effectively ignored, leading to a possible under-estimate of maturity and an estimation of much later timing for thermal events.

The BasinMod results could be used to introduce the ‘missing’ phase of pre-Variscan deposition and erosion into the HotPot model. However, this would require much more extensive work with BasinMod, to construct models at a similar number of sites to the nine used in the HotPot depth of burial study, so that an isopach map could be constructed to represent the layer of eroded late Carboniferous strata.

5.2 HOTPOT RESULTS AT BASINMOD SITES

A comparison of the maximum burial depths and temperatures obtained from BasinMod and HotPot modelling at the borehole sites used with BasinMod is presented in Table 6. HotPot temperatures and depths of burial are at base of Passage to Limestone Coal formations layer at 60Ma during maximum burial in the Tertiary. BasinMod temperatures and depths of burial are at the base of Limestone Coal Formation during maximum burial in the Tertiary, except for in Tower borehole where the top of the Lower Limestone Formation is not sampled.

Table 6: Comparison of BasinMod and HotPot results

Site	Easting (BNG)	Northing (BNG)	HotPot total thickness (m)	BasinMod depth of burial (m)	HotPot basal temp. (°C)	BasinMod max. temp. (°C)
Eskmouth	334530	673320	Outside HotPot AoI	2900	Outside HotPot AoI	115
Tower 1	330024 [330050]	687894 [687850]	2498	2900	89.4	110
Milton of Balgonie	331733 [331750]	699335 [699350]	2567	2300	90.7	95

In comparison to the HotPot results given above, at the base of the Limestone Coal Formation, the BasinMod models predict that during maximum burial (in the Tertiary) the temperature at the site of Milton of Balgonie borehole is about 95°C with a maximum depth of burial 2300m. The base of the Limestone Coal Formation is not seen in Tower 1 borehole, though around 227m of Limestone Coal strata are observed compared to 244.8m in Milton and 216.9m in Eskmouth, and therefore the maximum depth of burial (2900m) and temperature (110°C) of the lowest strata observed in this borehole are likely to be close to those experienced by the base of the Limestone Coal Formation at this site. The BasinMod model of Eskmouth borehole shows a maximum depth of burial of 2900m and a maximum temperature of 115°C at the base of the Limestone Coal Formation. The BasinMod and HotPot results at the site of Tower borehole and Milton of Balgonie borehole are comparable.

Miall (1999) gives a list of the properties usually associated with back-arc basins including; deep-marine sediment-fill; transition into slope and shelf facies on the continental margin of the basin; little evidence of contemporaneous tectonics except normal faulting. Miall (1999) also gives a list of properties usually associated with basins generated by transcurrent faulting, including: most basins are only a few tens of kilometres across; strata are characterised by numerous local facies changes; movement on individual faults may be local and spasmodic, so that sediments in adjacent basins may have different stratigraphy; syndepositional features; the basin may be cut by later transcurrent faults; sedimentation rates are rapid, commonly exceeding 1m/thousand years.

The sedimentation rates of the Carboniferous strata for the BasinMod models are about 0.03-0.44m/thousand years. Sedimentation rates computed from the HotPot model for this period show sedimentation rates rising from 0.2m/thousand years to 0.6m/thousand years (Table 4, above). The ranges of the sedimentation rate estimations from the two modelling procedures agree, but are lower than the indicative sedimentation rate given by Miall for pull-apart basins. Estimates of Dinantian sedimentation rates are quite high, ranging from 0.03-0.44m/thousand years in Milton of Balgonie borehole to 0.11m/thousand years for the HotPot Lower Carboniferous layer. The Passage Formation was deposited at the beginning of the Namurian, it is believed that during the early Silesian, that closure of the Ural ocean to the east of the triangular block reversed the sense of shear along the block margins, and caused inversion of Dinantian depocentres and synsedimentary folding. The Passage Formation often overlies an unconformity and varies laterally across the MVS. From the BasinMod sedimentation rate estimates, the Passage Group generally appears to have a low sedimentation rate varying from 0.03-0.07m/thousand years for all three boreholes. The Namurian strata deposited after the Passage Group has a higher sedimentation rate in the BasinMod models of 0.06-0.25m/thousand years. The Passage Group to Limestone Coal Formation HotPot layer has a sedimentation rate of 0.18m/thousand years. Stephenson et al believed that rapid basin subsidence and volcanism rapid subsidence, active rifting and extension continued until the mid-Namurian. In the late Namurian, active extension appeared to give way to post-extensional basin-wide thermal subsidence, and widespread marine transgressions caused the basins to lose their separate identities (Stephenson et al 2003) (Figure 11 this report, and Stephenson et al 2003). The Westphalian HotPot layers show a high sedimentation rate estimate of 0.45-0.63m/thousand years. The BasinMod sedimentation rate estimate is lower at 0.09-0.19m/thousand years, though this is only sampled in Eskmouth borehole, south of the HotPot grid area. Also, the HotPot sedimentation rates are given in the main basin depocentre and Eskmouth borehole is south of this region.

Carboniferous strata in the MVS show local variation in thickness and in facies, split coal seams, and a rapid sedimentation rate, supporting the theory of a strong element of transcurrent strike-slip motion on the large, basin-bounding faults. The HotPot model shows strong evidence of extensional style initial synrift deposition in sub-basins followed by broad basin-wide thermal sag subsidence (Figure 11). Taking these factors together, the authors conclude that basin formation included both extensional and strike-slip components; however, it is difficult to conclude which process was dominant.

5.3 THERMAL MATURITY AND THE OIL WINDOW

The BasinMod results imply that in Eskmouth borehole, the rocks of the Limestone Formation and Lower Limestone Formation reached the oil window from the mid Carboniferous onwards (Figure 4c) and the eventually all the strata up to and including the Upper Coal Measures entered the oil window during deep Tertiary burial. Tower borehole shows the oil window being reached much later by the Upper Limestone, Limestone Coal and Upper Limestone formations during the Permian, with the Lower Coal Measures reaching the oil window during deep Tertiary burial (Figure 5c). Strata in Milton of Balgonie Borehole show some of the greatest maturity. In Milton of Balgonie, the Strathclyde Group reached the oil window during the mid Carboniferous and the Lower Limestone Formation following soon after towards the end of the Carboniferous. The Limestone Coal Formation also appears to have reached the oil window during deep Tertiary burial (Figure 6c). Some extremely high maturities are shown by the vitrinite reflectance localised around the Midland Valley Sill.

Unlike BasinMod, HotPot does not perform organic maturity modelling. However, maturity estimates may be obtained from HotPot models by displaying the temperature maps with a pseudo-maturity scale, which shows four colour bands to represent under-mature (lower than 100°C), oil maturation (100°C to 150°C), gas maturation (150°C to 220°C) and over mature (higher than 220°C). These maps are useful in indicating the likely extents of these zones at the various stages in a basin's development. When using HotPot with BasinMod, it should be possible to calibrate these maps in terms of organic maturity from the BasinMod results, but this would require the availability within the mapped area of further borehole sites at which to construct BasiMod models.

The HotPot pseudo-maturity maps indicate that the Lower Carboniferous strata entered the oil window after 327 Ma, by 316 Ma about 50% of the mapped subcrop area was warm enough for oil generation to occur, and by 311 Ma all but a strip on the eastern edge of the subcrop was capable of generating oil (Figure 16a). The Passage to Limestone Coal formations entered the oil window in the period between 314 and 311 Ma, by the end of which about a quarter of the subcrop was in the area above the 100°C isotherm (Figure 16b). The higher Carboniferous strata had not entered the oil window by 311 Ma. The next time reference in the HotPot model is 60 Ma (Figure 10), when maximum burial was reached, and the entire Lower Carboniferous subcrop was within the oil window, as was almost half the Passage–Limestone Coal formations subcrop. However, the HotPot model indicates that at this time only a small area around the depocentre of the Lower–Middle Coal Measures reached maturity, with higher strata remaining under-mature. This is at variance with the BasinMod model, which suggests all Carboniferous strata reached maturity during maximum burial in the Tertiary.

6 Conclusions

BasinMod was used successfully to model three boreholes in the MVS using 420-660m pre-Variscan additional deposition and erosion and 1300-1800m Tertiary-Quaternary additional deposition and erosion. Eskmouth could be successfully modelled using 450m deposited before the Variscan, and then a further 1800m deposited before the Tertiary, Firth of Forth Tower 1 with 420m deposited before the Variscan and 1750m erosion before the Tertiary and Milton of Balgonie with 660m before the Variscan and 1300m erosion before the Tertiary.

BasinMod plots of the maturity vs. time indicate that the high heat flow caused by extension caused the most rapid increase in the maturity of the coals as indicated by vitrinite reflectance. Igneous intrusions were seen to have a localised heating effect on the surrounding rocks.

HotPot was used successfully to produce overburden and palaeo-temperature maps across the eastern Midland Valley. The maximum depth of burial of the Lower Carboniferous rocks (Lower Limestone Coal Formation and older) was calculated to be 5532-6049m resulting in temperatures between 139.9-146.8°C across the basin centre.

In general, agreement between the BasinMod and HotPot models at the two chosen sites was reasonable, however BasinMod tended to predict greater temperatures. The results of BasinMod and HotPot were compared at two sites: Milton of Balgonie borehole and Tower 1 borehole. The BasinMod results at the base of the Limestone Coal Formation were compared to those obtained by HotPot for the Passage Formation to Passage Group layer. HotPot predicted a maximum depth of burial of 2498m, with a temperature of 89.6°C at Milton of Balgonie, compared to a maximum burial of 2300m and 95°C as predicted by BasinMod. HotPot predicted a maximum depth of burial of 2567m with a temperature of 90.9°C at Tower 1 borehole compared to 2900m and 110°C predicted by BasinMod.

The estimates of sedimentation rates are 0.03-0.44m/thousand years from BasinMod and 0.2m/thousand years rising to 0.6m/thousand years from HotPot for the strata from the Lower Carboniferous into the Coal Measures. The sedimentation rate estimates from the two modelling procedures broadly agree, but are lower than the characteristic sedimentation rate given in Miall (1999) for pull-apart basins. Carboniferous strata in the MVS show local variation in facies, split coal seams and at times a fairly rapid sedimentation rate. The HotPot model shows evidence of extensional style initial synrift deposition in sub-basins followed by broad basin-wide thermal sag subsidence. These factors lead the authors to conclude that basin formation was influenced by extensional and strike-slip stresses, however, it is not possible to determine which process was dominant.

Overall, the agreement between the HotPot and BasinMod results is good, implying that the models produced represent a plausible geological history of the MVS. The models are constructed using two contrasting techniques; BasinMod results are obtained using thermal maturity data, the HotPot results are generated based on mechanical compaction. Using HotPot and BasinMod together is a good approach to modelling, because the packages complement each other:

- HotPot provides a basin-wide overview, for example, the subsidence history of smaller individual basins changing to larger-scale subsidence is seen in Figure 11, whereas BasinMod provides analysis on 1D boreholes or 2D sections and is more labour-intensive.
- BasinMod can be used to constrain the palaeo-heat flow more accurately using vitrinite reflectance data for each borehole, the HotPot palaeo-heat flow must be calculated from subsidence rates.

- HotPot is useful for modelling across the basin using grids from structural interpretation, giving a ‘broad-brush’ history and overview. BasinMod allows each borehole to be considered in more detail, for example, the apparent low sedimentation rate in the Passage Formation was noted from the BasinMod results.

BasinMod and HotPot are complementary modelling packages, using results from both can give a more complete view of the sedimentary basin history than either package individually. The results obtained here for the MVS could be improved on further if more time and more maturity data were available to allow further iteration of the model results. In particular, use of BasinMod at additional sites would provide data to enable the single overburden layer used in the HotPot model to be subdivided, and thus allow HotPot modelling of the Permian episode of uplift and erosion.

7 Input to the DGSM

BasinMod plots can be output in a variety of formats, including CGM, then imported into PowerPoint or CorelDraw, amongst other packages. BasinMod stratigraphy, rock properties, maturity data etc, may also be exported as text files or Microsoft Word files which would allow reconstruction of the model using BasinMod or another package.

HotPot produces its results in both printed and digital forms. All layer data can be displayed as colour-coded grid maps. These can be printed directly using any Windows printer driver, or the printer output can be captured into a file (e.g. as PostScript) ready for import into a graphics editing program. Burial and thermal history plots can similarly be displayed and then printed or captured as graphic data. In addition, the gridded layer data may be saved directly as grid files, which are in plain ASCII text, and use either the HotPot grid format or the EarthVision grid export format. Formats of all HotPot data, input and output, are described in the HotPot program documentation (Rowley et al, 1993).

The GLOS (Geological Large Object Store) is held on the BGS UNIX server kwsn. Models are stored within an individual subdirectory in the GLOS. All the models produced for this report would be expected to be held within the Midland Valley subdirectory with metadata files which give details of the format of the files, abstract, model location, scale and detail. The model files and metadata can be retrieved through the DGSM data portal via the BGS intranet.

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Appendix 1: BasinMod model layers and lithology mixes.

Eskmouth					
	Depth to top	**Thickness**	**Age**	**Start Time**	**Composition**
Borehole Data					
recent	0	23.7	recent		
MCM_2	23.7	58.9	Duckmantian	311	81% Sst, 10% SilSt, 9% Shl,
MCM_1	82.6	115.8	Duckmantian	312	63% Sst, 15% SilSt, 16% Shl, 6% Ker
LCM	198.4	197.3	Langsettian	315	59% Sst, 17% SilSt, 15% Shl, 9% Ker
Passage Fm_2	395.7	47.8	Arnsbergian-Langsettian	317	78% Sst, 9% SilSt, 12% Shl, 1% Ker
Passage Fm_1	443.5	119.8	Arnsbergian-Langsettian	322	46% Sst, 6% SilSt, 42% Shl, 6% Ker
U Limestone Fm	563.3	164.6	Arnsbergian	323	41% Sst, 23% SilSt, 31% Shl, 4% Lst, 1% Ker
U Limestone Fm	84	64	Arnsbergian	325	65% Sst, 12% SilSt, 21% Shl, 2% Ker
Limestone Coal Fm	811.9	216.9	Pendleian	327	35% Sst, 25% SilSt, 30% Shl, 10% Ker
L Limestone Fm	1028.8	9.5	Brigantian	327.5	56% Sst, 41% SilSt, 3% Shl,
TD	1038.3				
Model Overburden					
Quaternary		-10		1.12	
Tertiary		-1790		43.2	
Cretaceous		400		144	100% Clk
Jurassic		400		206	100% SilSt
Triassic		500		245	100% Sst
Permian		500		286	100% Sst
Variscan Erosion		-450		300	
UCMS		250	Bolsolvian-Westphalian D	310	80% Sst, 10% SilSt, 10% Shl
MCMS_E		200	Duckmantian	310.3	81% SSt, 10% SilSt, 9% Shl

Sst – sandstone, SilSt – siltstone, Shl – shale, Lst – limestone, Dolo – dolomite, Ker – kerogen (used where coal is present), Clk – chalk, Ig – igneous.

Tower 1					
	Depth to top	**Thickness**	**Age**	**Start Time**	**Composition**
Borehole Data					
recent	0	60.4	recent		
LCMS	60.4	71.2	Langsettian	315	79% Sst, 17% Shl, 4% Ker
Passage Fm	131.6	59.9	Arnsbergian-Langsettian	317	65% Sst, 7% SilSt, 26% Shl, 2% Ker
Passage Fm	191.5	240.5	Arnsbergian-Langsettian	322	70% Sst, 8% SilSt, 21% Shl, 1% Ker
U Limestone Fm	432	159.1	Arnsbergian	323	42% Sst, 27% SilSt, 28% Shl, 1% Lst, 1% Ker
U Limestone Fm	591.1	127.3	Arnsbergian	325	40% Sst, 32% SilSt, 26% Shl, 2% Ker
Limestone Coal Fm_2	718.4	107.4	Pendleian	327	50% Sst, 28% SilSt, 12% Shl, 10% Ker
Sill	825.8	17.8			100% Ig
Limestone Coal Fm_1	843.6	119.9	Pendleian	328	60% Sst, 20% SilSt, 16% Shl, 4%Ker
TD	963.5				
Model Overburden					
Quaternary		-10		1.12	
Tertiary		-1890		43.2	
Cretaceous		450		144	100% Clk
Jurassic		450		206	100% SilSt
Triassic		500		245	100% Sst
Permian		500		286	100% Sst
Variscan Erosion		-420		300	
UCMS		170	Bolsolvian-Westphalian D	310	80% Sst, 10% SilSt, 10% Shl
MCMS_2		130	Duckmantian	311	81% SSt, 10% SilSt, 9% Shl
MCMS_1		100	Duckmantian	312	63% SSt, 15% SilSt, 16% Shl, 6% Ker
LCMS_eroded		20	Langsettian	314	59% SSt, 17% SilSt, 15% Shl, 9% Ker

Milton of Balgonie					
	Depth to top	**Thickness**	**Age**	**Start Time**	**Composition**
Borehole Data					
Glacial till	0	37.5	recent		
Passage Fm	37.5	204.8	Arnsbergian-Langsettian	322	78% Sst, 9% SilSt, 12% Shl, 1% Ker
U Limestone Fm	242.3	223.1	Arnsbergian	323	28% Sst, 40% SilSt, 22% Shl, 7% Lst, 3% Ker
U Limestone Fm	465.4	64	Arnsbergian	325	42% Sst, 28% SilSt, 28% Shl, 2% Ker
Limestone Coal Fm	529.4	244.8	Pendleian	327	34% Sst, 40% SilSt, 17% Shl, 1% Dolo, 8% Ker
L Limestone Fm	774.2	85.3	Brigantian	327.5	42% Sst, 2% SilSt, 50% Shl, 3% Lst, 3% Ker
Midland Valley Sill	859.5	149.4	Stephanian		100%Ig
L Limestone Fm	1008.9	165.1	Brigantian	329	40% Sst, 21% SilSt, 34% Shl, 4% Lst, 1% Ker
Pathhead Beds (Strathclyde Fm)	1174	24.5	Brigantian	330	50% Sst, 30% SilSt, 20% Shl
Pathhead beds	1198.5	165.8	Brigantian	331	1% Sst, 71% SilSt, 21% Shl, 7% Dolo
Pathhead beds	1364.3	129.2	Brigantian	335	26% Sst, 18% SilSt, 53% Shl, 1% Lst, 2% Ker
Sandy Craig beds	1493.5	76.2	Late Asbian	336.5	17% Sst, 39% SilSt, 36% Shl, 8% Dolo
Pittenweem beds	1569.7	31.4	Late Asbian	337	2% SilSt, 98% Ig
Pittenweem beds	1601.1	75.3	Late Asbian	338	30% Sst, 56% SilSt, 12% Shl, 2% Ker
Pittenweem beds	1676.4	152.4	Early Asbian	338.5	27% Sst, 10% SilSt, 51% Shl, 11%Lst
Pittenweem beds	1828.8	35.1	Early Asbian	338.6	29% Shl, 71% Ig
Pittenweem beds (Strathclyde Fm)	1863.9	115.8	Early Asbian	339	24% Sst, 13% SilSt, 58% Shl, 4% Lst, 1% Ker
Sill	1979.7	30.8			5% Shl, 95% Ig
TD	2009.85				
Model Overburden					
Quaternary		-10		1.12	
Tertiary		-1290		43.2	
Cretaceous		200		144	100% Clk
Jurassic		300		206	100% SilSt
Triassic		400		245	100% Sst
Permian		400		286	100% Sst
Variscan Erosion		-660		300	
UCMS		200	Bolsolvian-Westphalian D	310	80% Sst, 10% SilSt, 10% Shl
MCMS_2		100	Duckmantian	311	81% SSt, 10% SilSt, 9% Shl
MCMS_1		140	Duckmantian	312	63% SSt, 15% SilSt, 16% Shl, 6% Ker
LCMS		200	Langsettian	315	59% SSt, 17% SilSt, 15% Shl, 9% Ker
Passage		20	Arnsbergian-Langsettian	317	54% Sst, 19% SilSt, 24% Shl, 3% Ker