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3D structural geological model of the Central South Wales Syncline, Great Britain

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1. Model Dimensions

Spatial reference: EPSG Projection 27700 - OSGB 1936 / British National Grid

Axis	Min	Max	Delta
X	261606.80	298207.80	36601.00
Y	182647.50	215448.50	32801.00

Spatial reference: geographic (latitude/ longitude)

Lat	~51°31'N	~51°49'N	~0°18'
Long	~4°00'W	~3°28'W	~0°32'

2. Geological Overview

The 3D structural geological model is implemented for the central part of the South Wales Syncline and its bedrock geology (Figure 1). The geology of South Wales is characterised by a rich variety of formations and rocks of different ages and periods.

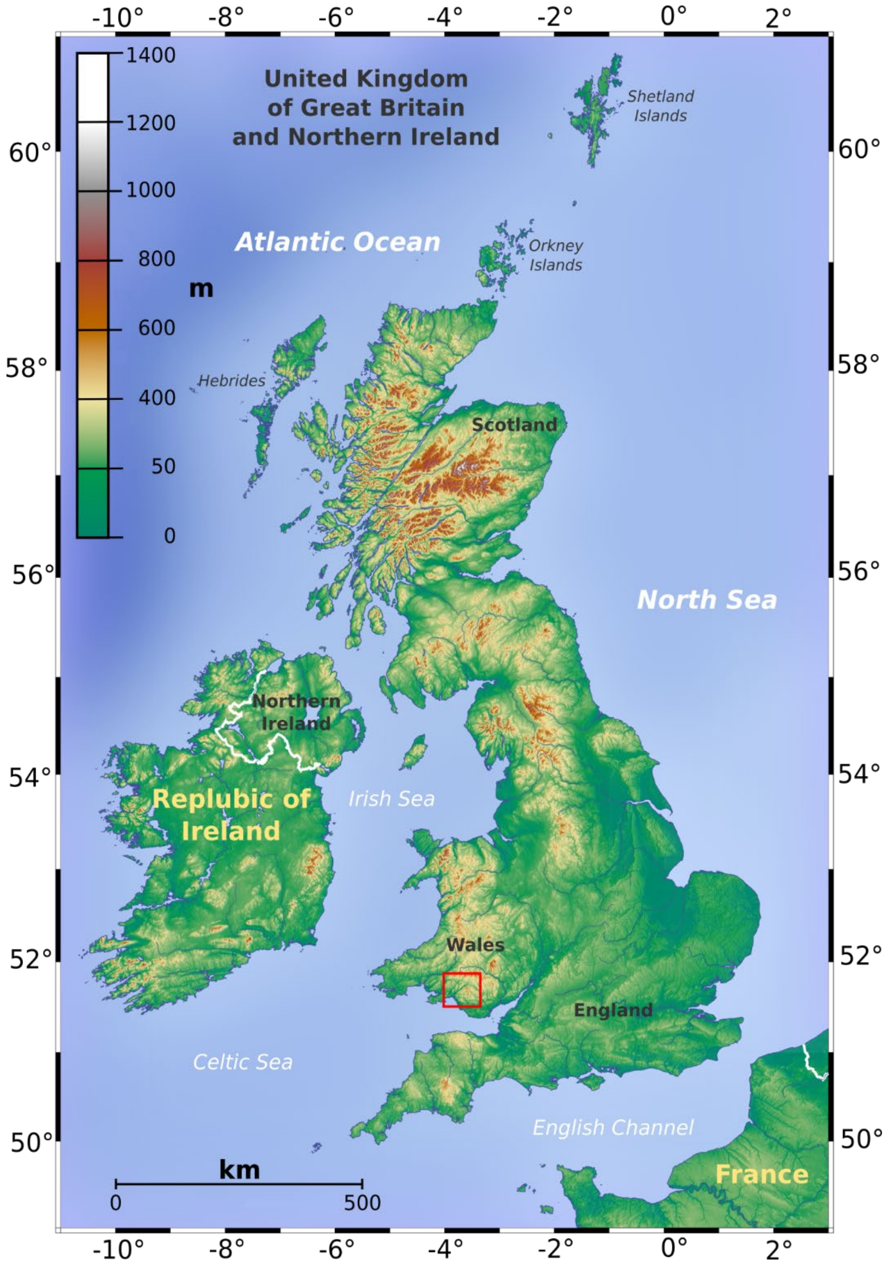


Figure 1. *3D structural geological model of the central South Wales syncline on the relief map of the United Kingdom of Great Britain and Northern Ireland (modified from Maps of Europe, 2014). Red rectangle indicates the approximate location of the 3D structural geological model.*

In its northern part, South Wales has outcrops of Ordovician and Silurian rocks. The oldest rocks that can be observed in the 3D model area, are the rocks from the Pridoli Series from the uppermost Silurian. In South Wales, the series comprises mostly sandstones, siltstones and mudstones characterised by sedimentation patterns that indicate deposition in coastal as well as fluvial and alluvial environments (Howells, 2007). In the early Devonian, marine sedimentation prevailed, evolving in the later stages to a more terrestrial sequence that produced characteristic red sandstones (Howells, 2007). Lower Carboniferous Limestones from the Dinantian Series indicate shallow-marine sedimentation during a major transgression phase, whereas the coarse-grained sandstones from the Millstones Grit Group in the area originate from terrestrial deposition in a fluvial environment at low sea-level stages (Aitkenhead et al., 2002). Devonian formations, Carboniferous Limestones and Millstones formations can be observed mainly in central South Wales, whereas Permian, Triassic and Jurassic rocks are predominantly restricted to the Vale of Glamorgan and surrounding area in the South (Howells, 2007).

Perhaps the most important structural geological feature of South Wales is the large asymmetric syncline extending from east to west over a length of approximately 96 km and 30 km from north to south, respectively. This oval-shaped area covers some 2,700 km^2, with coal-bearing rocks from the Upper Carboniferous (Westphalian Stage) deposited in the central syncline and older rocks outcropping in a peripheral belt around it (Figure 2; Kelling, 1974; Bentley and Siddle 1996; Frodsham and Gayer, 1999; Howells, 2007). The South Wales syncline is part of the Variscan orogenic thrust and fold belt in Central Europe, which extends over a distance of more than 2,000 km from southern Britain through France and Germany to Poland (Ziegler, 1982; Drozdzewski, 1993). Deposition of the Carboniferous occurred on the southern edge of the Wales-London-Brabant Massif and the extensional Pennine Basin north of the massif during the final filling stage of the Variscan Foreland Basin (Dineley, 1992; Howells, 2007).

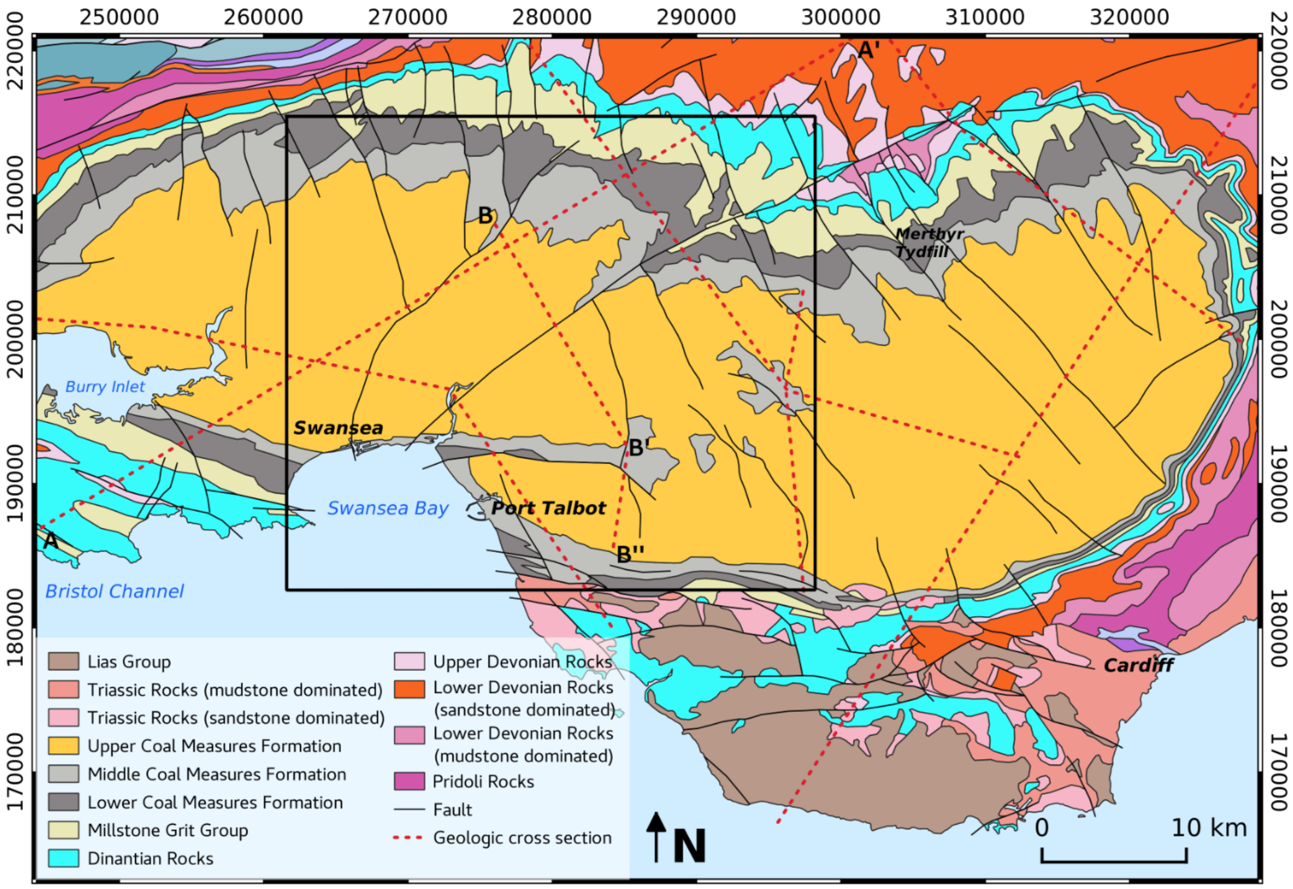


Figure 2. *Bedrock geologic map of South Wales. Geologic cross sections used for model implementation are indicated by red dotted lines. Black rectangle indicates extent of the structural geological 3D model (Bedrock geology and faults based upon BGS Geology 625k, DiGMapGB-625 data set, Contains British Geological Survey materials © UKRI [2019; https://www.bgs.ac.uk/products/digitalmaps/digmapgb_625.html]; Spatial reference: OSGB 1936 / British National Grid, SS; Map created using the Free and Open Source QGIS).*

Today's Carboniferous rocks are a smaller erosional remnant of a once more extensive area of Carboniferous geology with numerous minor folds and a fault pattern that exhibit both extensional, compressional and transcurrent structures (Thomas, 1974; Freshney and Taylor, 1980; Hartley, 1993; Frodsham and Gayer, 1999, Sarhosis et al., 2016). The Variscan orogeny climaxed in the later Carboniferous (Westphalian Stage) and sedimentation likely occurred on a lower to upper delta plain environment. The coal-bearing sequence begins with Namurian grits and shales, overlain by the more productive Lower, Middle and Upper Coal Measures in which coals alternate with mudstones and siltstones, as well as more sandstones-dominated facies in the roof beds (Thomas, 1974; Lewis et al., 1986; Hartley, 1993). Marine bands subdivide the lower, middle and upper units, indicating cyclic sedimentation as a result of temporally unsteady and repeatedly interrupted rise in sea level (Thomas, 1974; Hartley, 1993; Bentley and Siddle, 1996; Hampson et al., 1997; Frodsham and Gayer, 1999). The rise of the water table was accompanied by a decreasing clastic input, which in turn favoured the colonisation of plants and establishment of mires. As a result, coals developed through the accumulation of peat and its later conversion by burial events (Hartley, 1993; Howells, 2007). Later, end-Variscan tectonics progressively inverted, faulted and folded the basin by northward propagating thrusting. This led to bed-parallel shortening, distortion and splitting as well as merging into composite beds (Hartley, 1993; Howells, 2007). Many of the faults in the area, NNW-trending in the western and central parts of the syncline and more north-westerly trending in the eastern parts, developed during folding, whereas others postdate folding (Kelling, 1988, Gayer and Jones, 1989). Today, thicknesses of the basin infill vary enormously across the entire area as the westward inclination of the syncline is associated with a sedimentary succession that is more than 3.5 km thick (Frodsham and Gayer, 1999). The superficial cover of Tertiary and Quaternary sediments is predominantly limited to smaller morphological depressions or deeper U-shaped valleys and riverbeds, as the sediments have been eroded along with the younger Mesozoic rocks (Howells, 2007). Thus, the 3D geological model contains the bedrock, as it is exposed in most parts of the area.

3. Data Sources and Processing

Open access data, mainly from the British Geological Survey (BGS), has been used to implement the 3D South Wales model. In the first instance, the BGS LithoFrame Viewer (Contains British Geological Survey materials © UKRI, 2019; URL: https://www.bgs.ac.uk/services/3dgeology/lithoframe.html), which enables complex 3D geological models of parts in the UK to be viewed and queried, has been used to extract a set of seventeen interconnected 2D geologic cross sections as the main data basis for the 3D South Wales model (Figure 3; Location of cross sections is shown in Figure 2). The BGS LithoFrame viewer is peer-reviewed and captures the national bedrock geology in a unified framework. In addition, a bedrock geologic map with the trend of major regional fault zones (Scale 1:50,000; Figure 2) has been derived from the BGS Geology of Britain viewer, a simple tool aimed at the general public, to explore the geology of the UK (Contains British Geological Survey materials © UKRI, 2019; URL: http://mapapps.bgs.ac.uk/geologyofbritain/home.html).

The 2D geologic cross sections and bedrock geologic map have been used to identify and integrate fault zones and nine geologic units from the Upper Coal Measures Formation (Carboniferous) to the Pridoli rocks (Silurian; as shown in Figure 3) into the 3D South Wales model. Since the 2D geologic cross sections alone represent only a weak data basis for a detailed integration of the surface topography, an ASTER Digital Elevation Model data set (NASA, 2001) provided by the United States Geological Survey has additionally been used. Coordinate transformation and data filtering to 5% of the data size due to the high resolution of the original data set have been performed using the gdal_translate utility (URL: https://www.gdal.org/gdal_translate.html; Figure 4).

The Geology of Britain viewer also offers the possibility to retrieve borehole scans with detailed stratigraphic information. However, there are only a limited number of deep boreholes within the model domain, particularly in the central, and thus deeper parts of the syncline where scans are often confidential and inaccessible. In addition, the layer boundaries of the major geologic units in the area, as derived from the bedrock geologic map and the geologic 2D cross sections are not specifically documented in the borehole scans. Thus, depth adjustment of the individual layers at borehole locations was not feasible.

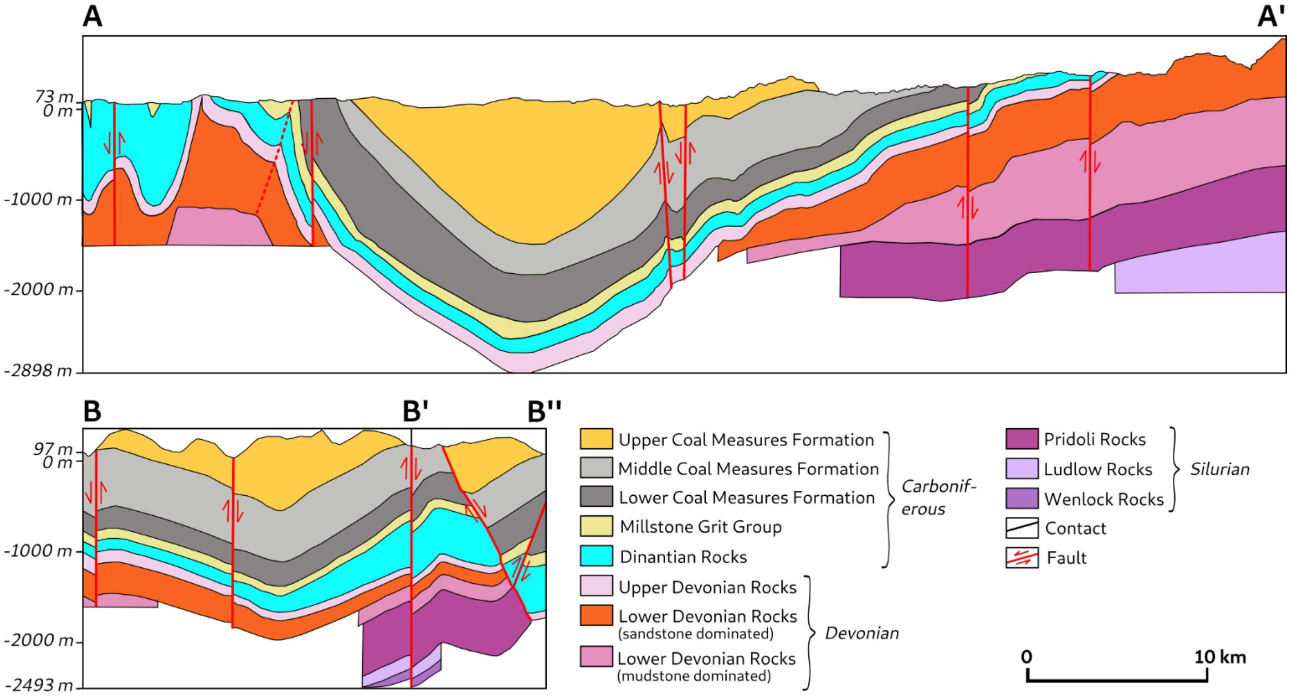


Figure 3. *Example of two geologic cross sections that have been extracted from the BGS LithoFrame Viewer, digitised and used for model implementation (Based upon the National Bedrock Fence Diagram [UK3D LithoFrame model], Contains British Geological Survey materials © UKRI [2019; URL: https://www.bgs.ac.uk/services/3dgeology/lithoframe.html]). Location of cross sections can be derived from Figure 2.*

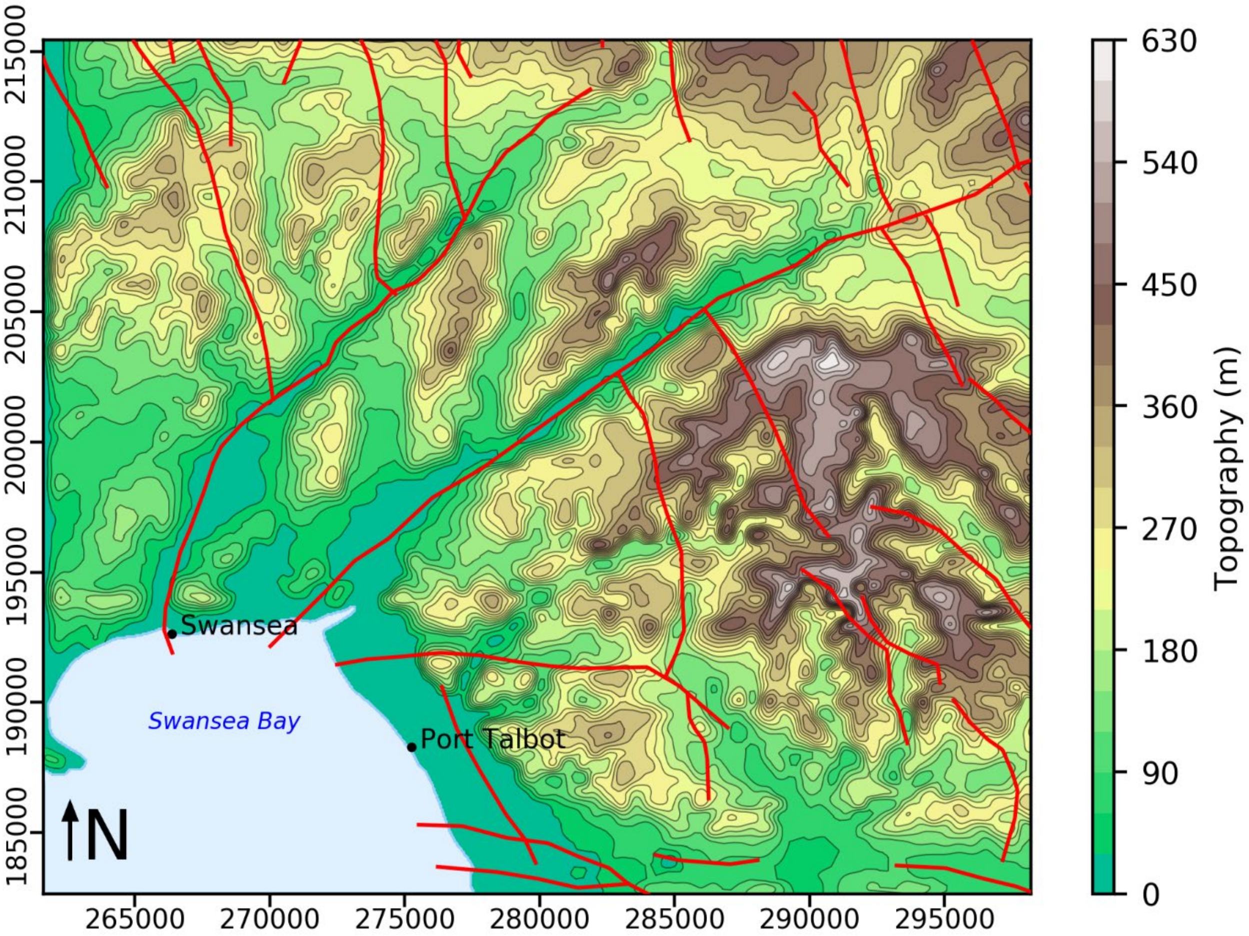


Figure 4. *Topography in the study area. Traces of regional fault zones are shown in red.*

4. Description of the 3D Structural Geological Model

Model implementation started with the processing and georeferencing of the 2D geological cross sections and the bedrock geologic map on the British National Grid (Spatial reference: OSGB 1936 / British National Grid, SS) followed by the digitisation of the individual layer boundaries and fault zones using the Petrel software package (Schlumberger, 2012; Figs. 5 and 6). The derived set of polylines was then used to calculate the elevation depth of the surfaces and to generate the fault zones. For the surface generation, the convergent interpolation algorithm has been used which adapts good to dense and sparse data sets through converging iterations at successively finer grid resolutions. Data trends have been extrapolated, respectively (Basic gridder: Taylor series projection, smoother gridder: Briggs biharmonic, minimum curvature; Schlumberger, 2012). The strike lines of the faults have been digitised from the bedrock geologic map, fault dip and vertical fault trace from the 2D geologic cross sections (Figure 6). The final step involves merging the gridded elevation depth surfaces into a 3D model. The fault surfaces were included in the final 3D model generation process in order to correctly map the throw between adjacent geologic units. Depth values of the strata striking out at the ground surface correspond to the topographic height from this point to receive a good match with the bedrock geology in the study area. For this purpose, it was necessary to work with auxiliary points and/or polylines in areas without any information on layering and distribution of geologic units. Nonetheless, the Swansea Bay remains a great unknown in this respect, as neither bathymetric data nor information on the distribution and spatial relationship of geologic units was available for this specific area. All geologic units within the model domain, with the exception of Lower Devonian and Silurian rocks, are outcropping at the surface (Figs. 2 and 5).

The faults displace the geologic units by several hundred meters in maximum. However, these large displacements along steep to more shallow dipping normal faults are mainly restricted to the southern border of the basin. In the central part of the basin, displacements reach only some tens of meters.

The final 3D structural geological model covers the entire central syncline structure of South Wales and is 32.8 km wide and 36.6 km long. It is implemented with a horizontal grid spacing of 50 m, and a vertical resolution corresponding to the number of integrated layers. The grid dimensions are X_{min} 261606.8, X_{max} 298207.8, Y_{min} 182647.5, Y_{max} 215448.5.

In total, the 3D model includes 21 fault zones and the elevation depth of ten surfaces: (1) Top Upper Coal Measures Formation; (2) Top Middle Coal Measures Formation; (3) Top Lower Coal Measures Formation; (4) Top Millstone Grit Group; (5) Top Dinantian Rocks; (6) Top Upper Devonian Rocks; (7) Top Lower Devonian Rocks (sandstone dominated); (8) Top Lower Devonian Rocks (mudstone dominated); (9) Top Pridoli Rocks; (10) Top Ludlow Rocks (in parts).

The geospatial data sets in comma delimited ASCII format (.csv) contain isoline points stored in an array of (X, Y, Z) values. The first two column entries X and Y are the geographical coordinates measured in metres (X = easting value, Y = northing value). Depending on the data set, the Z-value (last column entry; in m) corresponds to either the elevation depth (top of layers) or the thickness at the respective coordinate. The finite number of data points is derived from the contour lines generated for each surface and varys depending on the extent of the surface (e.g. layer pinchouts and outcropping of units) and the chosen interval (10 m – 50 m). The vertical datum to which the elevation depth refers is the mean sea level (MSL). Thickness values of layers are true vertical thicknesses (TVT) and assumed to be zero for values less than or equal to 0.1. In order to capture the full extent of the fault surfaces and ensure an accurate reconstruction, points along their top and base as well as regularly scattered across their surface with a predominant spacing of 100 m in vertical and 300 m in horizontal directions have been extracted and stored in an array of (X, Y, Z) values. Data sets from the 3D South Wales structural geological model are arranged in chronological order of strata from young to old (from top to bottom in the model):

Elevation depth data	**Thickness data**
1_top_upper_coal_measures.csv	1_thickness_upper_coal_measures.csv
2_top_middle_coal_measures.csv	2_thickness_middle_coal_measures.csv
3_top_lower_coal_measures.csv	3_thickness_lower_coal_measures.csv
4_top_millstone_grit_group.csv	4_thickness_millstone_grit_group.csv
5_top_dinantian.csv	5_thickness_dinantian.csv
6_top_upper_devonian.csv	6_thickness_upper_devonian.csv
7_top_lower_devonian_sand.csv	7_thickness_lower_devonian_sand.csv
8_top_lower_devonian_mud.csv	8_thickness_lower_devonian_mud.csv
9_top_pridoli.csv	9_thickness_pridoli.csv
10_top_ludlow.csv	
In addition, topography can be found in file:	**Fault data**
0_topography.csv	Fault_1-21.csv

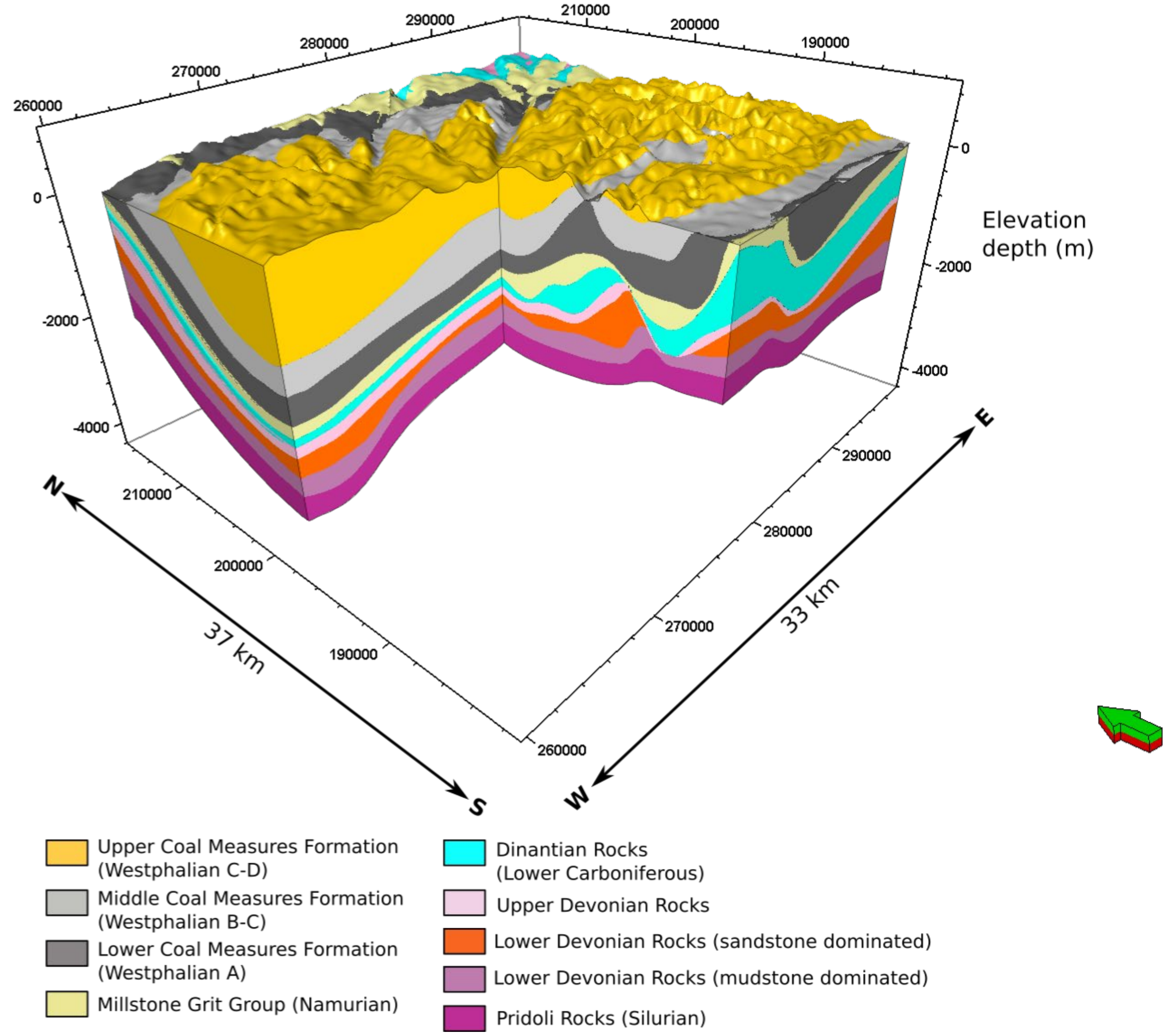


Figure 5. *Direction of view from SSW on the 3D geological model of the central South Wales syncline. Front part of the model is hidden to show the internal geometry of the study area. Vertical exaggeration is 5 times.*

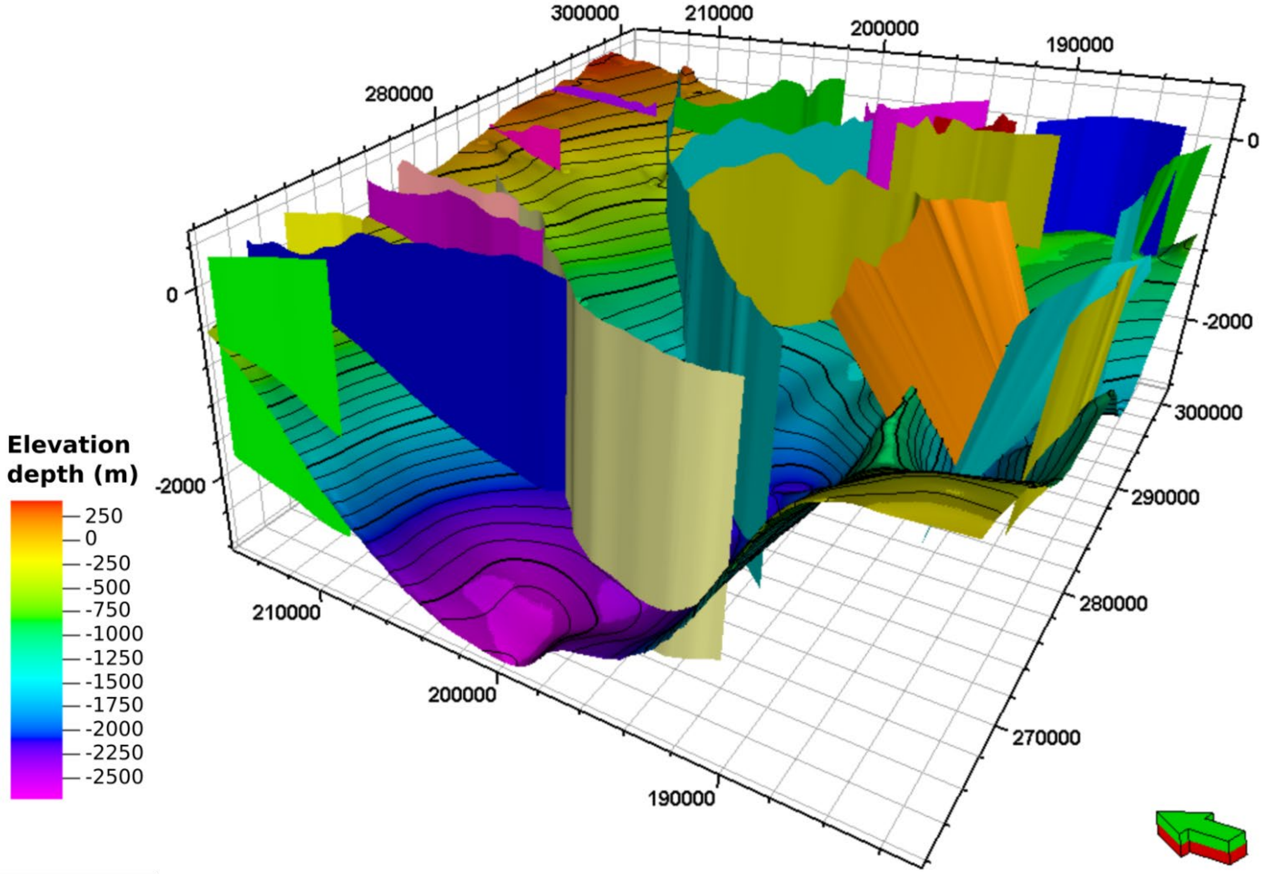
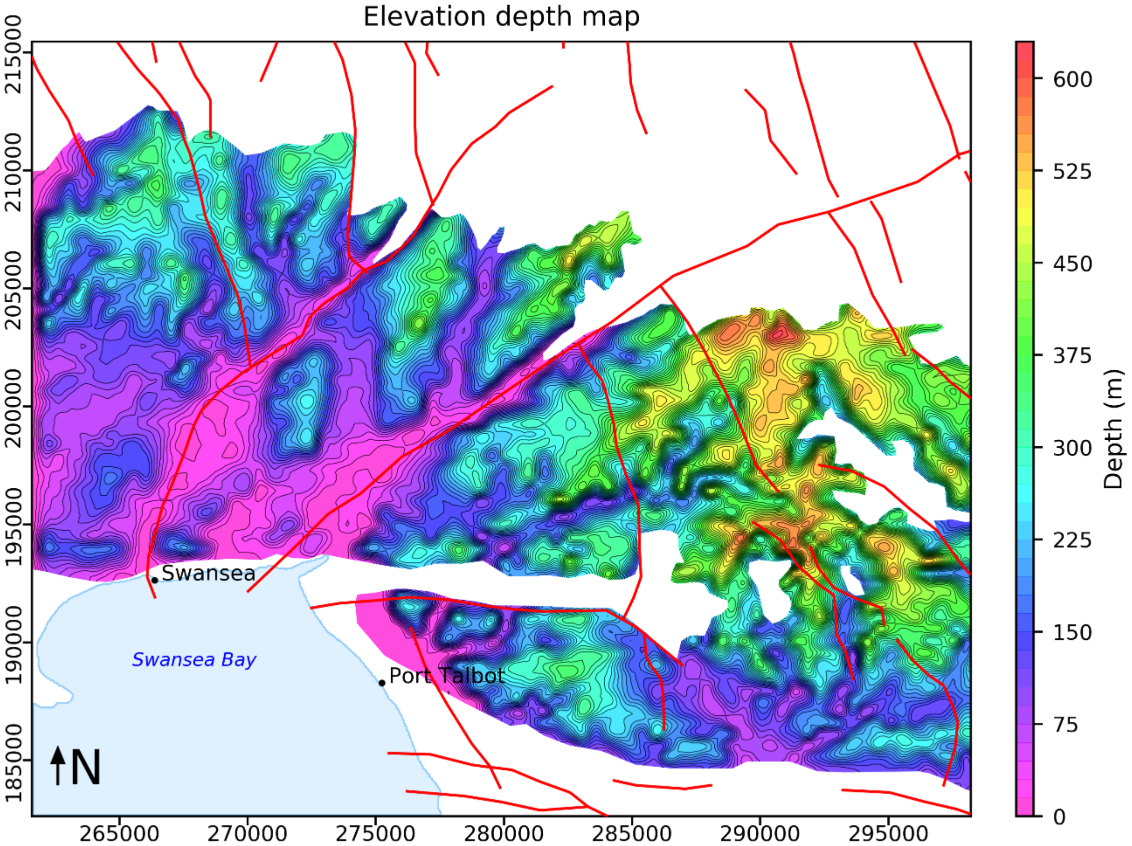


Figure 6. *SSW view on the top surface of the Millstone Grit Group (Namurian) and the 21 implemented fault surfaces. Vertical exaggeration is 5 times.*

Upper Coal Measures Formation (Westphalian C-D, Carboniferous)



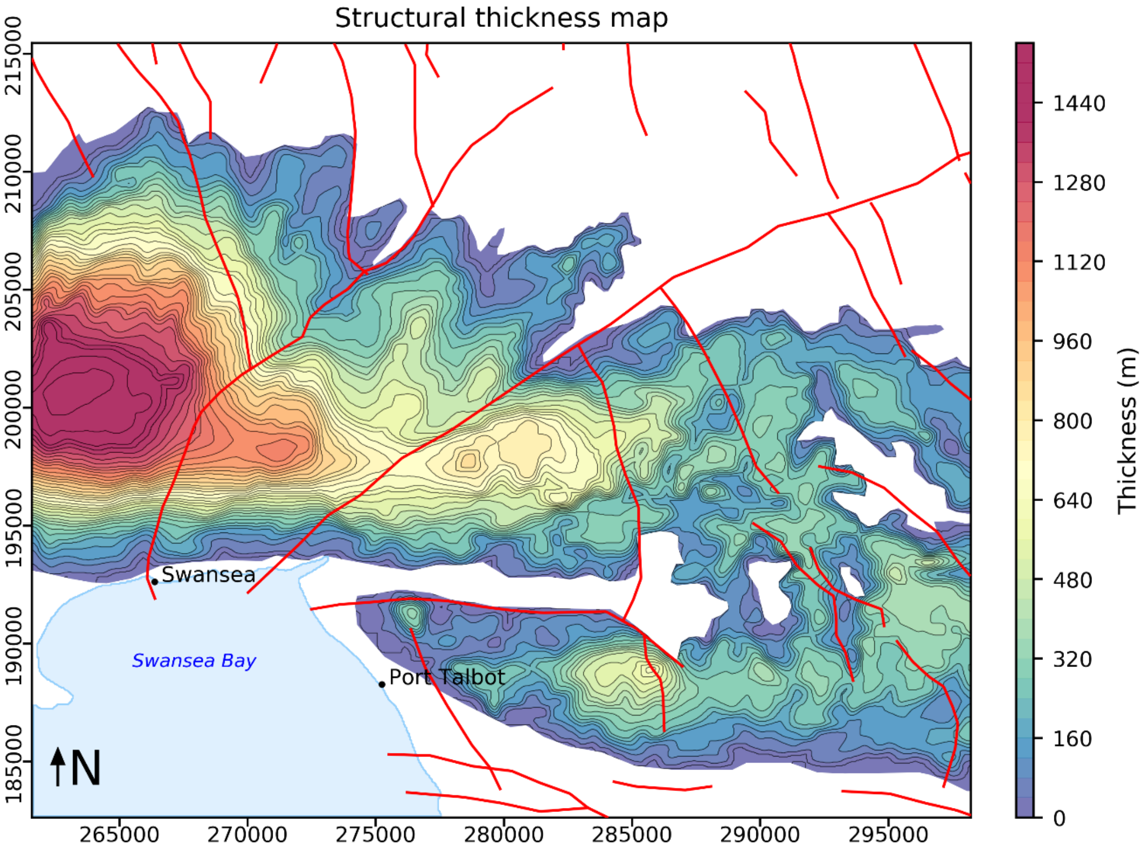
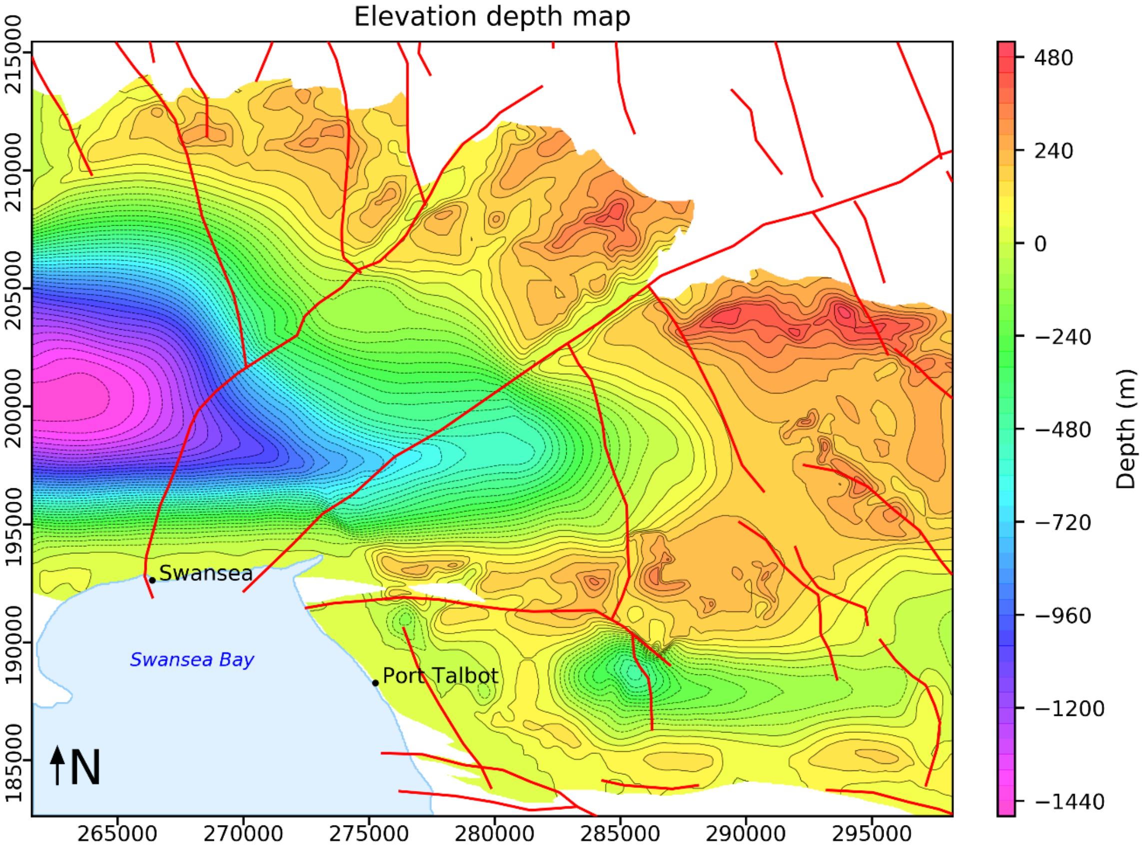


Figure 7. *Layer 1 – Elevation depth map (data file: 1_top_upper_coal_measures.csv) and thickness map (data file: 1_thickness_upper_coal_measures.csv) of the Upper Coal Measures Formation. Traces of regional fault zones are shown in red.*

Middle Coal Measures Formation (Westphalian B-C, Carboniferous)



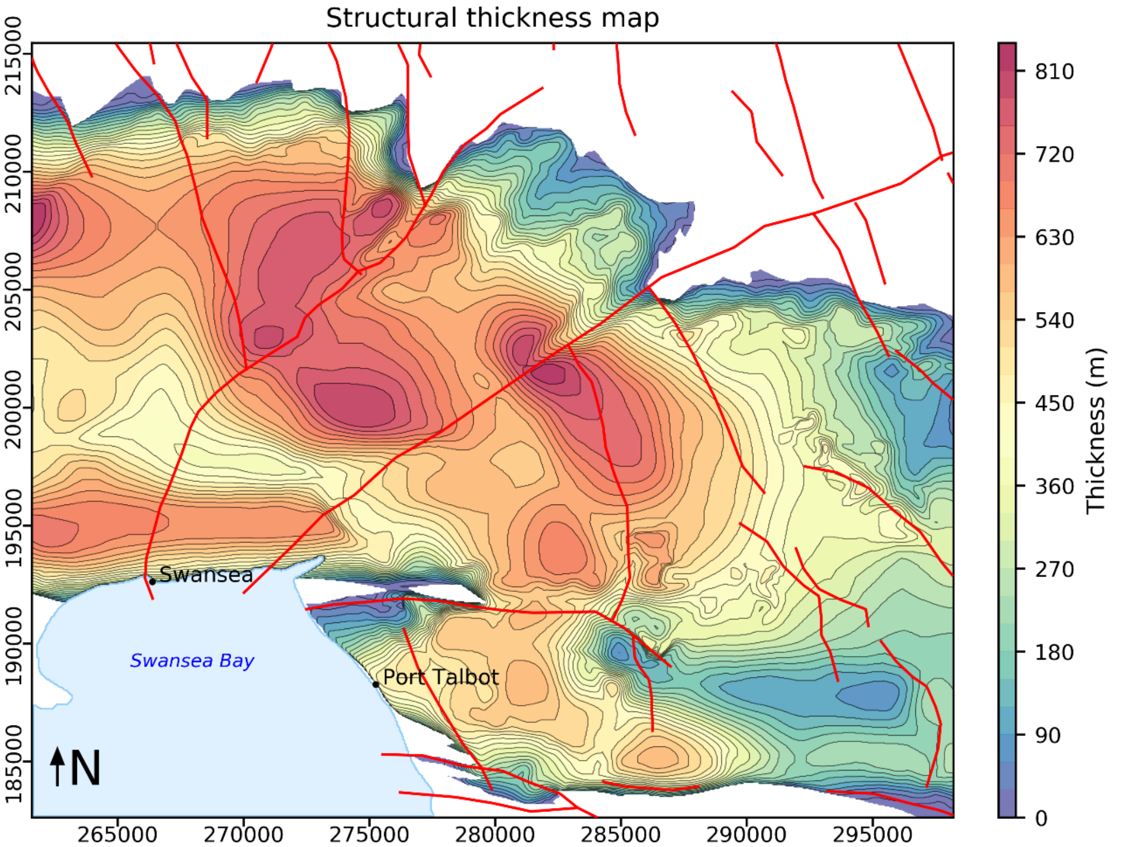
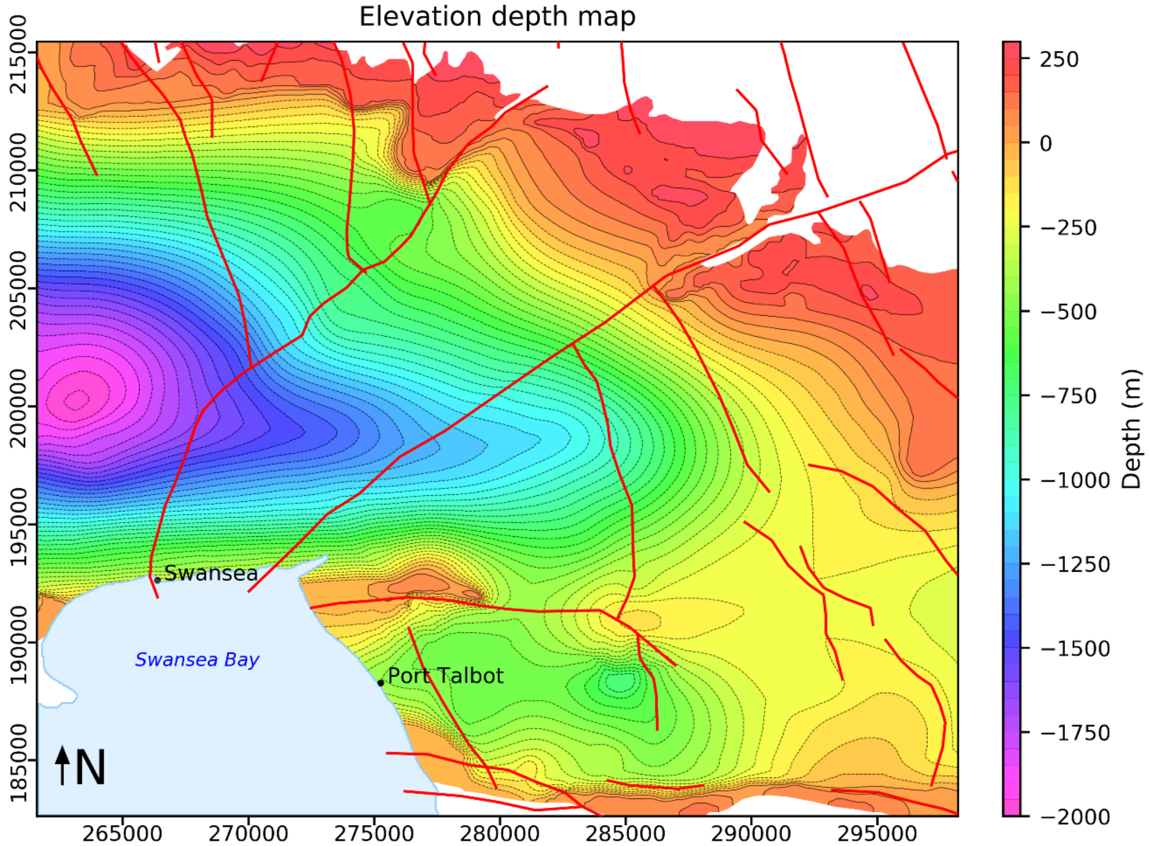


Figure 8. *Layer 2 – Elevation depth map (data file: 2_top_middle_coal_measures.csv) and thickness map (data file: 2_thickness_middle_coal_measures.csv) of the Middle Coal Measures Formation. Traces of regional fault zones are shown in red.*

Lower Coal Measures Formation (Westphalian A, Carboniferous)



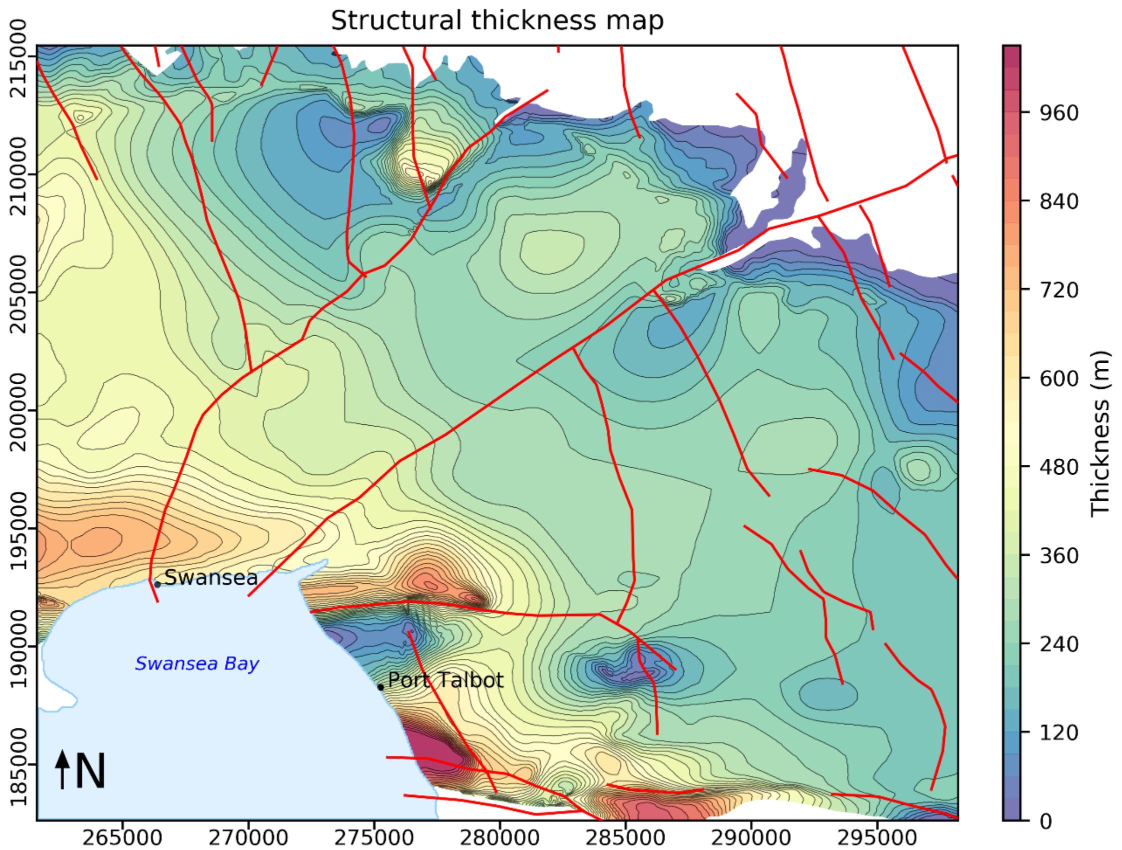


Figure 9. *Layer 3 – Elevation depth map (data file: 3_top_lower_coal_measures.csv) and thickness map (data file: 3_thickness_lower_coal_measures.csv) of the Lower Coal Measures Formation. Traces of regional fault zones are shown in red.*

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Millstone Grit Group (Namurian, Carboniferous)

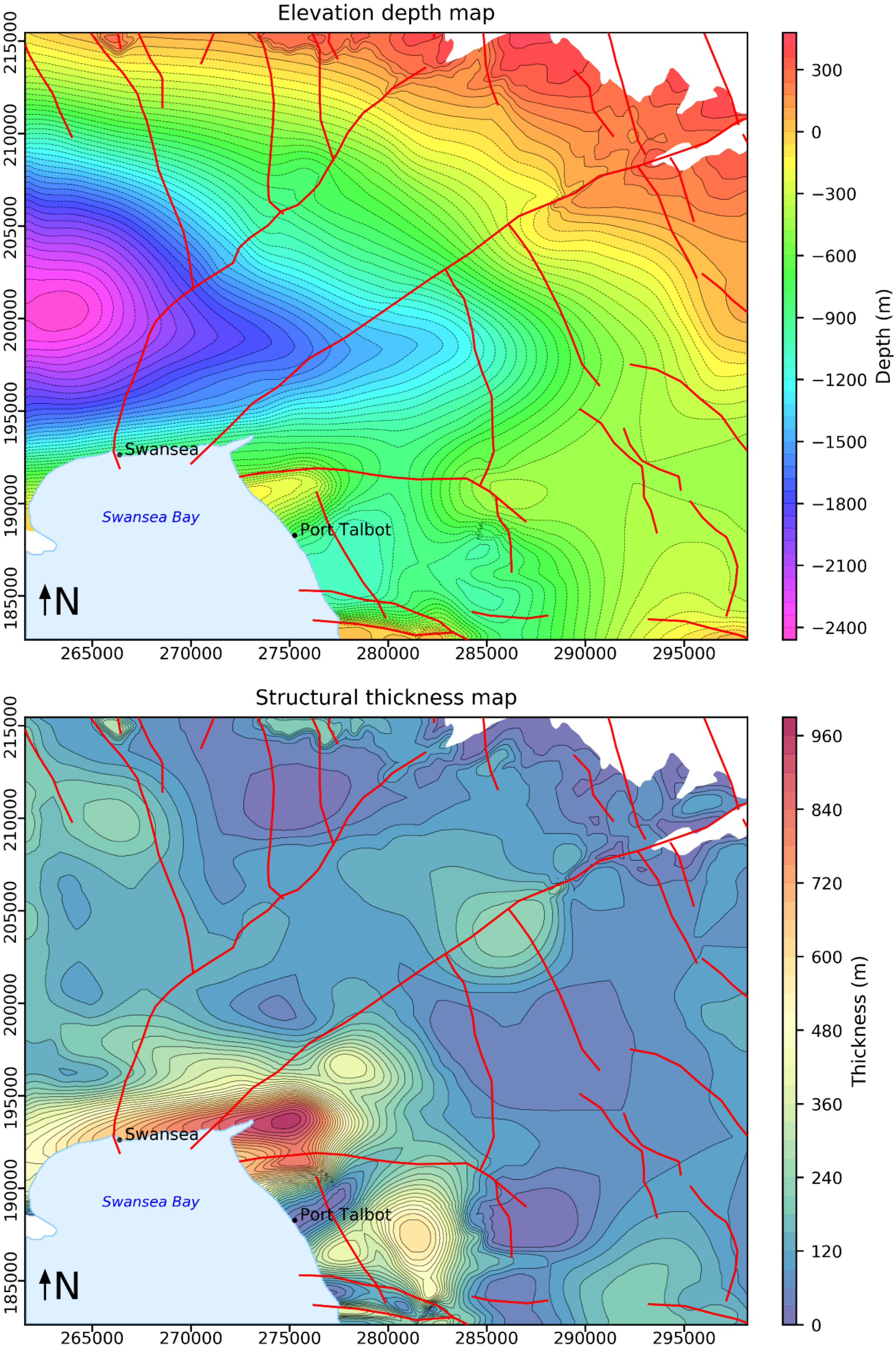

Figure 10. *Layer 4 – Elevation depth map (data file: 4_top_millstone_grit_group.csv) and thickness map (data file: 4_thickness_millstone_grit_group.csv) of the Millstone Grit Group. Traces of regional fault zones are shown in red.*

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Dinantian Rocks (Lower Carboniferous)

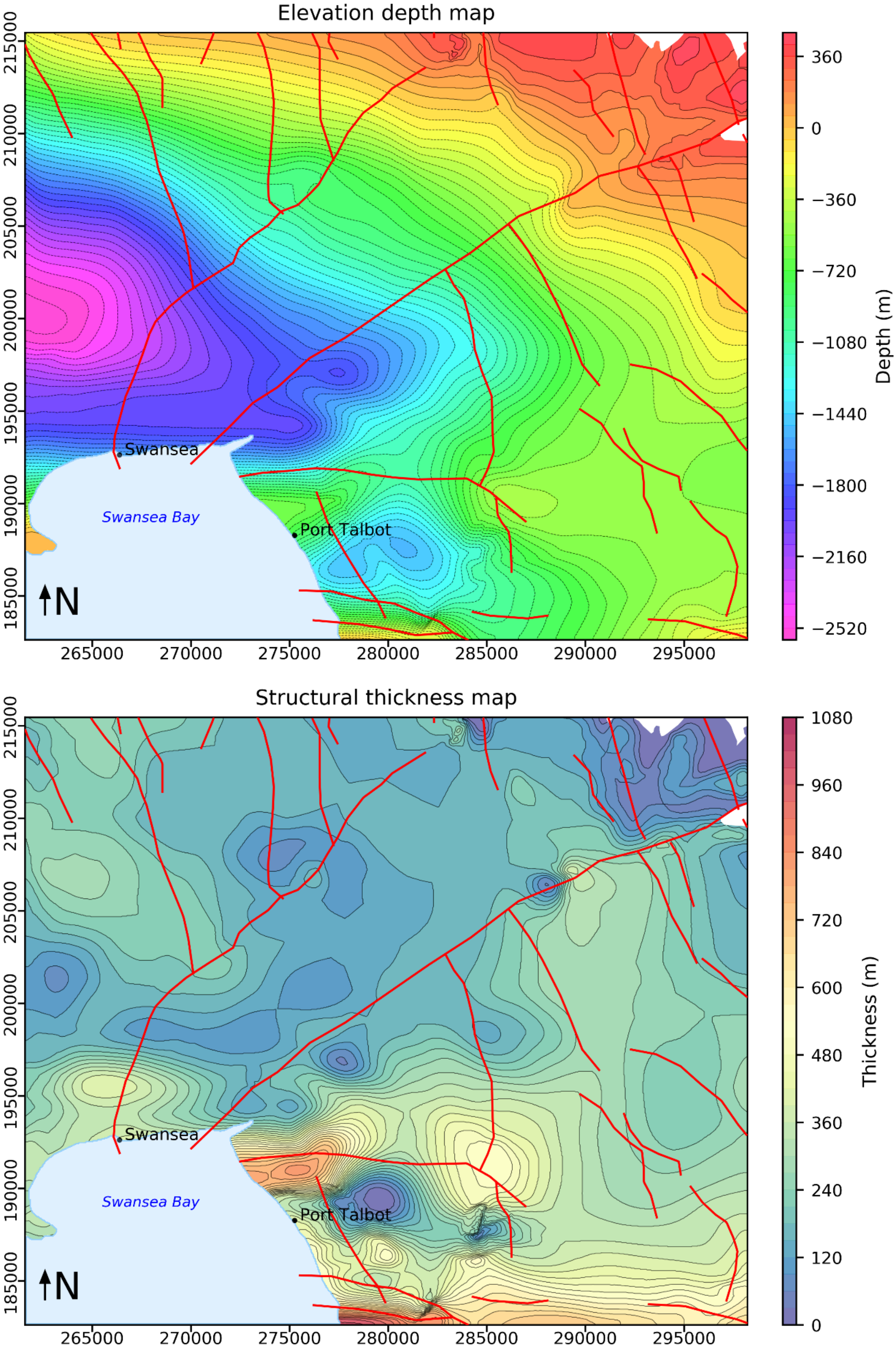


Figure 11. *Layer 5 – Elevation depth map (data file: 5_top_dinantian.csv) and thickness map (data file: 5_thickness_dinantian.csv) of the Dinantian Rocks. Traces of regional fault zones are shown in red.*

Upper Devonian Rocks

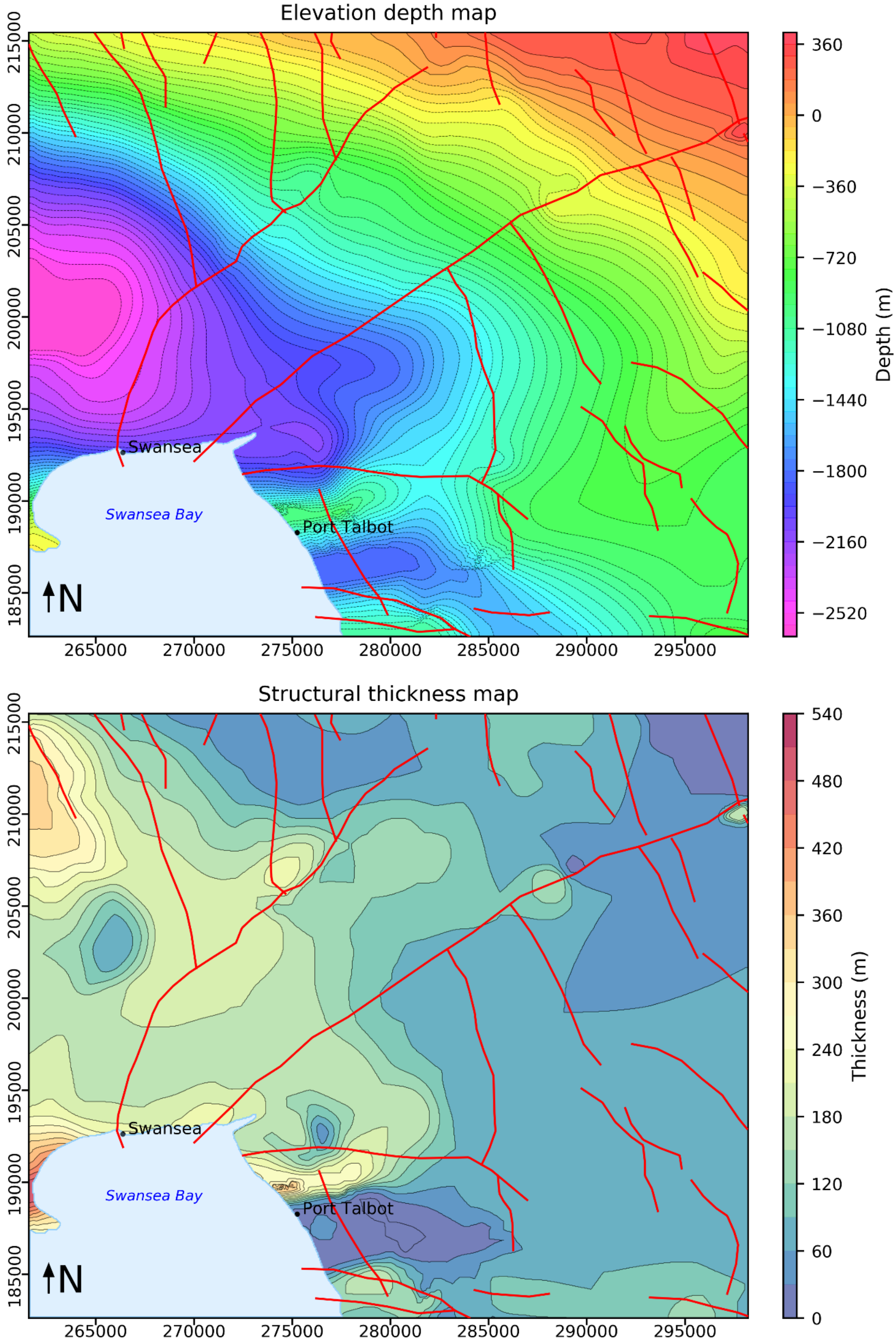
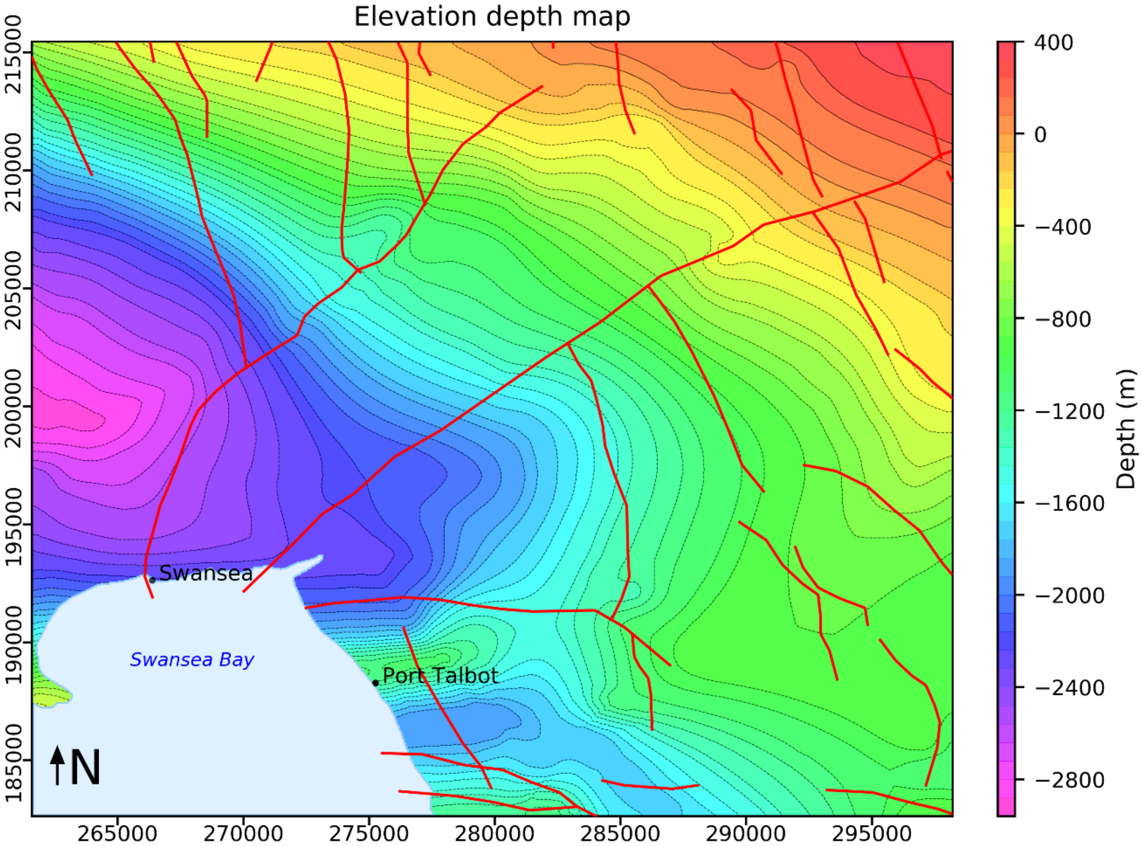


Figure 12. *Layer 6 – Elevation depth map (data file: 6_top_upper_devonian.csv) and thickness map (data file: 6_thickness_upper_devonian.csv) of the Upper Devonian Rocks. Traces of regional fault zones are shown in red.*

Lower Devonian Rocks (sandstone dominated)



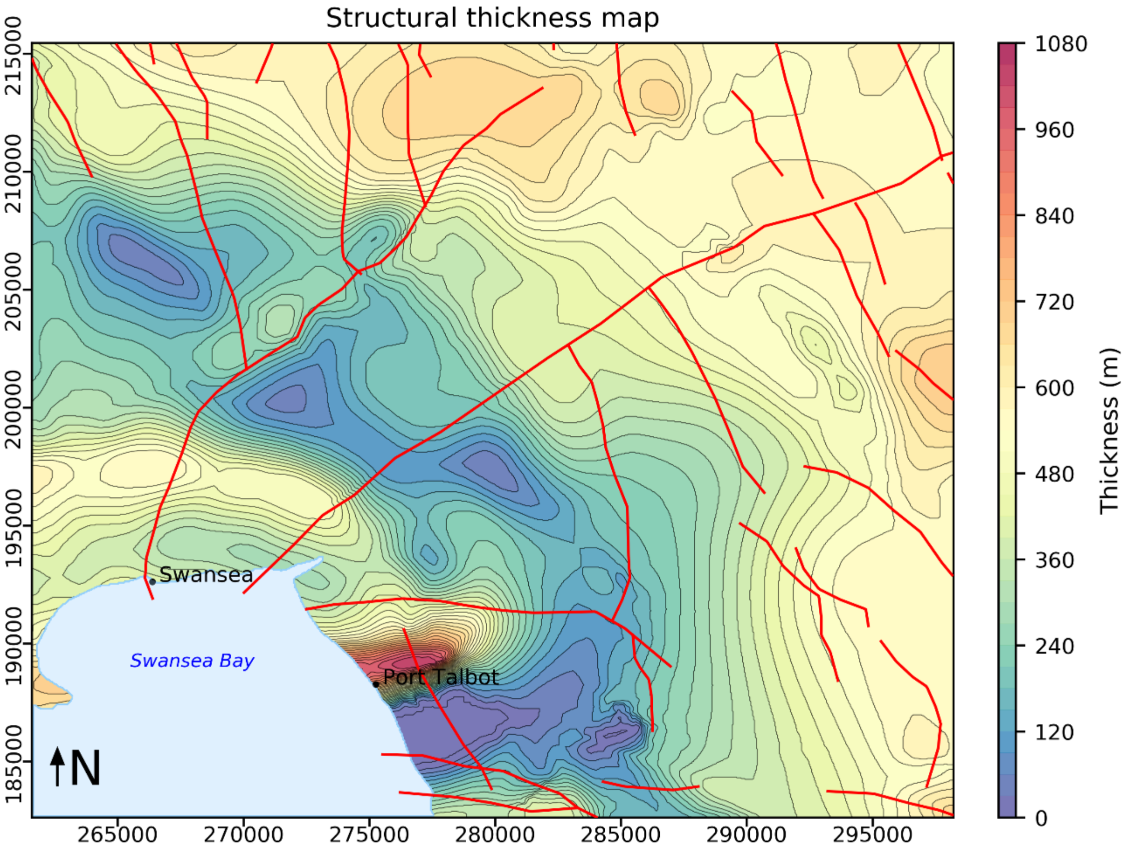


Figure 13. *Layer 7 – Elevation depth map (data file: 7_top_lower_devonian_sand.csv) and thickness map (data file: 7_thickness_lower_devonian_sand.csv) of the sandstone dominated Lower Devonian Rocks. Traces of regional fault zones are shown in red.*

Lower Devonian Rocks (mudstone dominated)

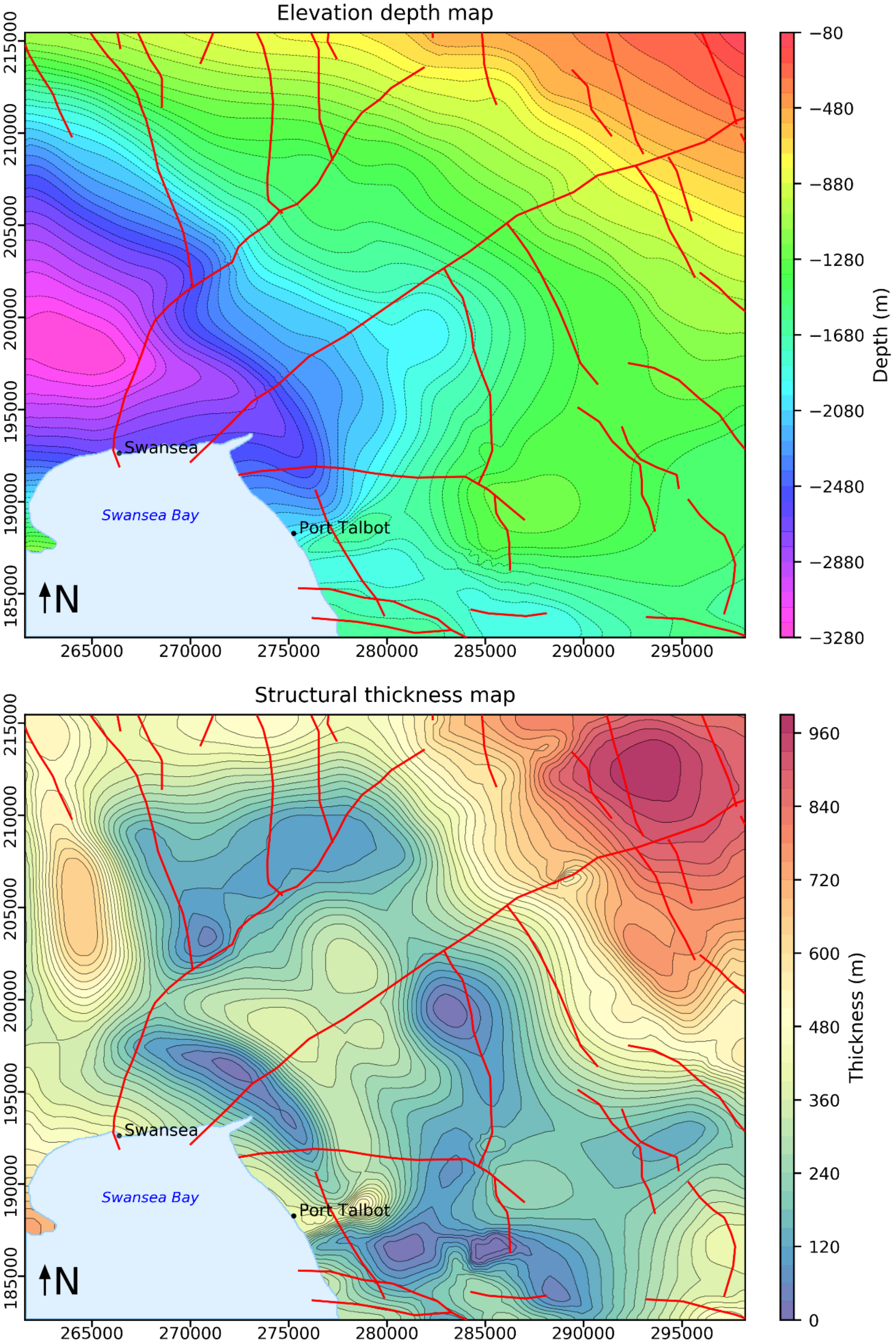
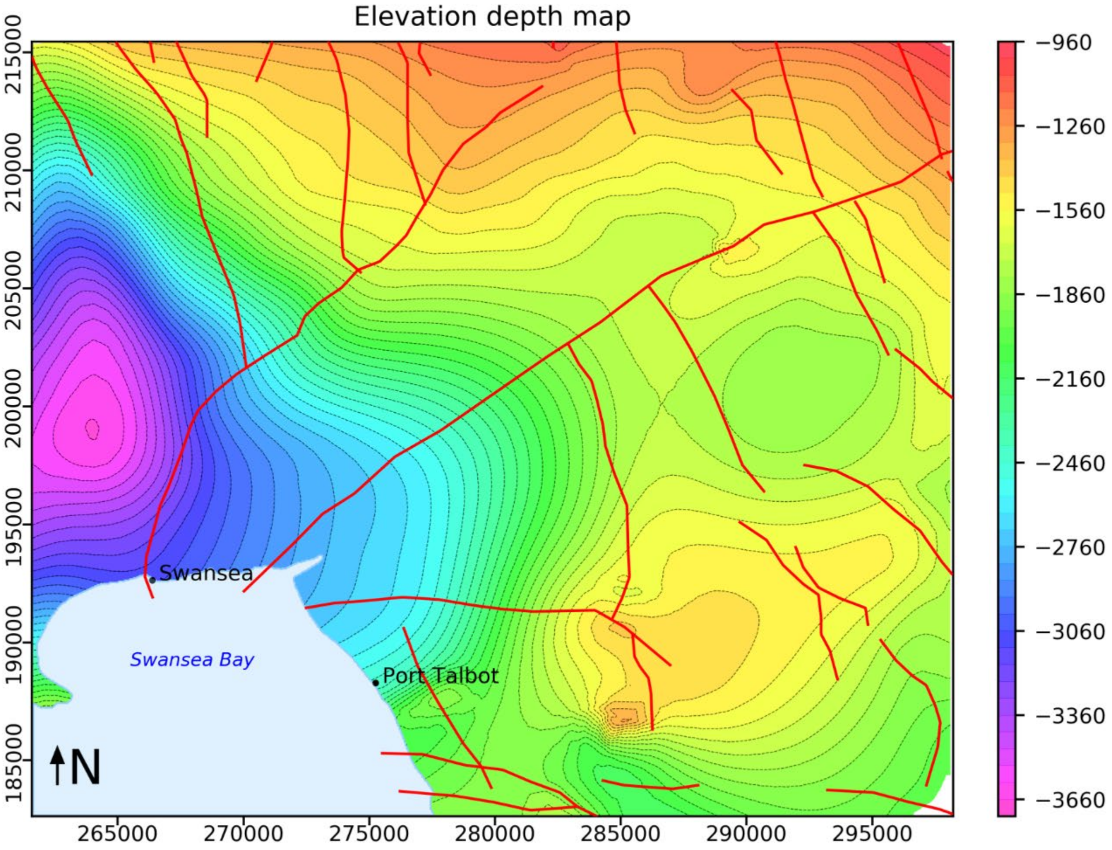


Figure 14. *Layer 8 – Elevation depth map (data file: 8_top_lower_devonian_mud.csv) and thickness map (data file: 8_thickness_lower_devonian_mud.csv) of the mudstone dominated Lower Devonian Rocks. Traces of regional fault zones are shown in red.*

Pridoli Rocks (Upper Silurian)



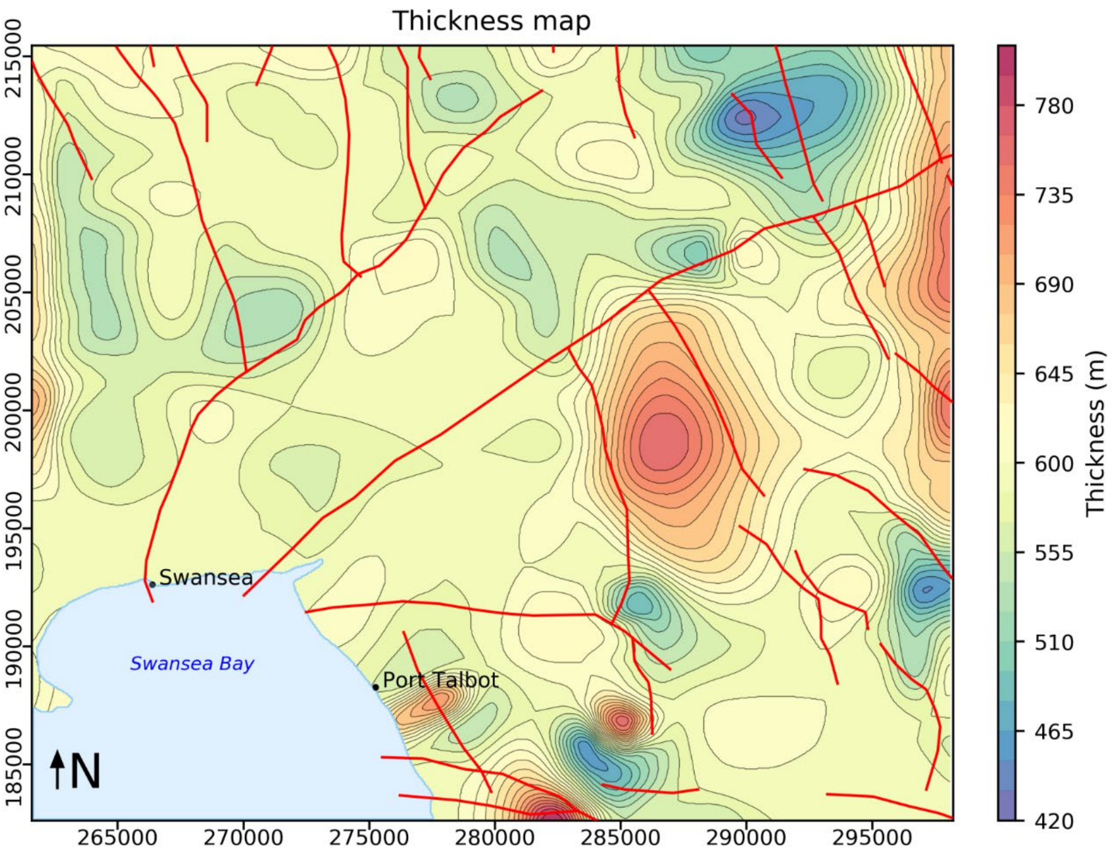


Figure 15. *Layer 9 – Elevation depth map (data file: 9_top_pridoli.csv) and thickness map (data file: 9_thickness_pridoli.csv) of the Pridoli Rocks. Traces of regional fault zones are shown in red.*

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Ludlow Rocks (Upper Silurian)

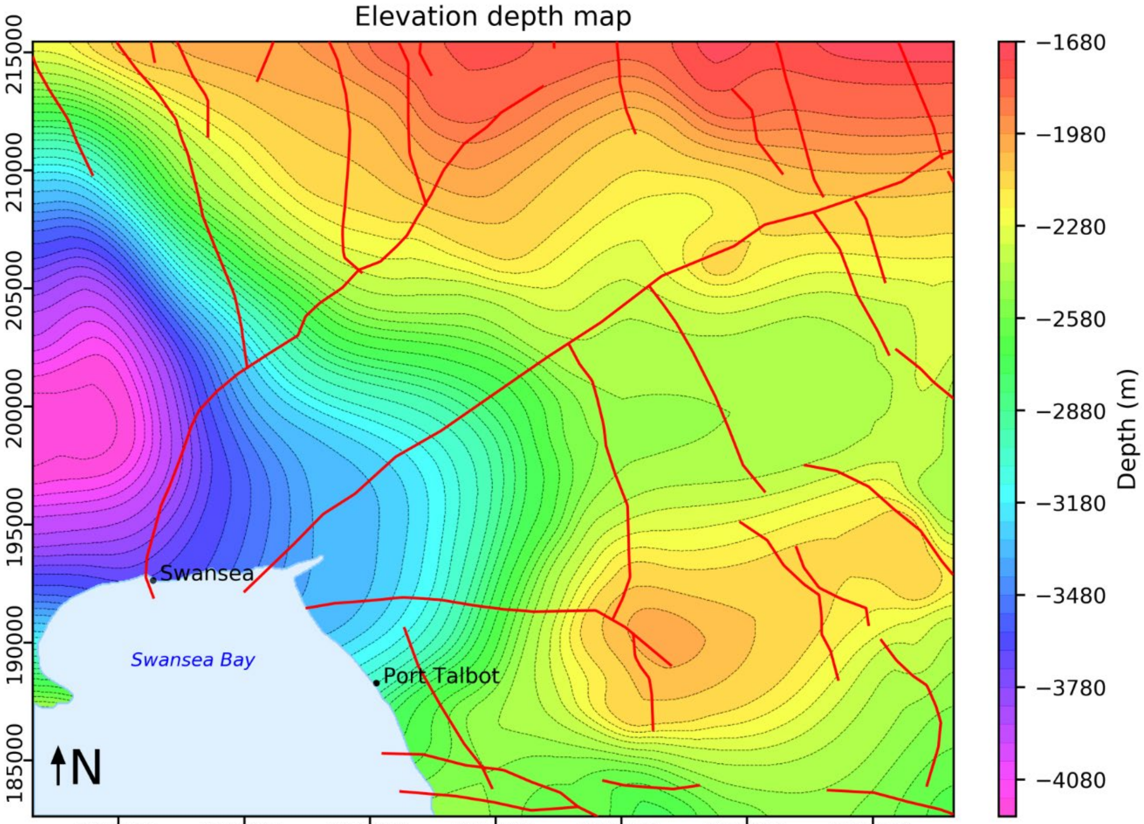

Figure 16. *Elevation depth map of the Ludlow Rocks (data file: 10_top_ludlow.csv). The elevation depth of the Ludlow Rocks corresponds to the base of the model. Traces of regional fault zones are shown in red.*

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