**A thermal maturity map based on vitrinite reflectance of British coals**

Bullock, L. 1, 2\*, Parnell, J. 2, Muirhead, D. 2, Armstrong, J. 2, Schito, A. 3, Corrado, S. 3

1 *Ocean and Earth Science, University of Southampton, National Oceanography Centre, Southampton, SO14 3ZH, UK.*

2 *School of Geosciences, University of Aberdeen, Aberdeen AB24 3UE, UK.*

3 *Dipartimento di Scienze, Sezione di Scienze Geologiche, Università degli Studi Roma Tre, Largo San Leonardo Murialdo 1, 00146, Roma, Italy.*

*\*Correspondence (L.A.Bullock@soton.ac.uk)*

**Abstract:** A compilation of new and previously published vitrinite reflectance (Ro) data from Carboniferous coals constitutes the most comprehensive map of reflectance across Great Britain. Values of Ro range from 0.38 to 3.29 %, recording an ambient thermal maturity in the early oil window (standard reference point for reflectance studies), modified by elevated heat flow in northern England and along the Variscan orogenic front. The map provides a context for other geological data sets.

We present a map of vitrinite reflectance data for Great Britain (Figs. 1 and 4). The map is the most comprehensive that is publicly available. Maturity data previously compiled by the National Coal Board was obtained from the content of volatile matter (Creedy 1986, 1988). A recent limited compilation of data from some sedimentary basins in Britain (Linley 2014) is accessible only by subscription. The map presented herein incorporates data from several minor coalfields not included in earlier compilations. The data plotted are exclusively from coals of Great Britain of Carboniferous age (Fig. 2). They are collated from published sources and newly measured samples. The published sources include information hitherto not reported in geological literature.

**Use of vitrinite reflectance data**

Vitrinite reflectance is a measure of the cumulative thermal maturity of coalified plant remains. The use of vitrinite reflectance data is diverse. Ten examples are:

1. Estimation of remaining potential to yield hydrocarbons, including conventional oil and gas, and shale gas (e.g. Hackley & Cardott 2016).
2. Determination of palaeogeothermal gradients, by measuring changes in vitrinite reflectance with depth (e.g. Marshall et al. 1994).
3. Assessing broad regional variations in maturity due to metamorphism and/or tectonic history (e.g. Creaney 1980).
4. Assessing local variations in maturity due to igneous intrusions (e.g. Bishop & Abbott 1995).
5. Measurement of displacement across major faults through contrast in maturity across the fault (e.g. Cavailhes et al. 2018).
6. Assessing provenance of clasts containing coaly matter, in sedimentary successions (e.g. Vandenberghe 1976).
7. Identification of potential sites for exploitation of geothermal energy (e.g. Manning et al. 2007).
8. Identification of palaeogeothermal anomalies to guide mineral exploration (e.g. Maynard et al. 2001).
9. Combination with apatite fission track data to deduce the thermal histories of basins (e.g. Bray et al. 1992).
10. Assessing provenance of coal fragments encountered in archaeological sites (e.g. Smith 1996).

The wide-ranging applicability of vitrinite reflectance data makes a database of compositions valuable.

**Methodology**

There are 14 new analyses in this study, from: Inninmore Bay, East Trodigal, High Tirfergus, Uddingston, Arran, Ascog (Bute), Kello Water, Jenkin Beck, Tan Hill, Rowanburn, Wrexham, Hanwood, Pembroke and Midsomer Norton. Samples for new vitrinite reflectance analyses were crushed and then mounted in epoxy resin and polished, according to the method of Bustin et al. (1990). Samples were analysed in reflected, non-polarized, monochromatic light (λ=546 nm) under oil immersion (ν=1.518) using a Zeiss Axioskop MPM400 microscope equipped with MPS 200 system by J&M Analytik AG. The standard materials used to calibrate the microscope depends on the coal rank and are: Spinel with relative reflectance of 0.426% (Rr), Sapphire with Rr of 0.585%, YAG (Yttrium-Aluminium-Garnet) with Rr of 0.905%, GGG (Gadolinium- Gallium-Garnet) with Rr of 1.72 and Cubic Zirconia with Rr of 3.09. About 50 measurements for each sample were made in order to statistically constrain heterogeneities in the analysed kerogen.

**Data**

The vitrinite reflectance (Ro) values range from 0.38 to 3.29 % (Figs. 3-4; Table 1 and Appendix I). The distribution of values (Fig. 3) shows that a majority of samples have Ro values in the range up to 0.80 %. A smaller group are in the range 0.80 to 1.0 %, and a third group in the range from 1.0 % upwards has a distinct geographic distribution (Fig. 4). Depths given for samples in Table 1 are estimated based on information (where available) on coal seam depth, depth of extraction or depth of the colliery from where the samples were taken. In general, samples from boreholes are stratigraphically well constrained, whilst spoil and ex-situ samples are less accurate. Borehole sampling also provides a better opportunity to sample at greater depths than what may be achievable for samples collected through conventional shaft sinking excavation. Depths presented are also subject to available data in references or obtainable colliery/site information. The depths presented do not account for any uplift, burial or erosion, and therefore may not fully represent the maximum burial experienced by the samples whilst in-situ. No correlation is observed between estimated sample depth and Ro%.

**Discussion**

Reflectance data presented here are constrained to the highest possible accuracy, in terms of considering Ro% standard deviation of each samples for newly acquired data (see Appendix I), and assessing the adequacy of methods used in published data. However, it is important to note that when interpreting the values presented, there are inherent expected variations of reflectance with vertical depth in a Coal Measures sequence and in the source data referenced. Data presented and assumptions made here represent conservative interpretations, which can be more rigorously tested with additional data (e.g. more samples for areas where 1 or few samples have been analysed) and studies on a given sample, region or stratigraphic section. The values below 1.0 % are typical of sedimentary basins in western Europe, where Carboniferous sediments are in the window of oil generation. The oil generation window extends from 0.5 % to 1.3 %, equivalent to coals that are classified as bituminous (Tissot & Welte 1984; Petersen 2006), typically formed at 2-6 km depth and 50-150 °C (Bjørlykke 2015; Mani et al. 2017).

The values above 1.0 % are from regions which have experienced anomalous localized heating. The samples from South Wales, the Bristol region and Kent form a linear belt in the vicinity of the Variscan (Hercynian) orogenic front. During orogenesis, hot fluids were expelled northwards, causing mineralization in South Wales, and contributing to the maturation of coal (Gayer et al. 1997, Alderton et al. 2004). The Variscan thrust system propagated northwards into the coalfield even as Pennsylvanian sedimentation was continuing (Gayer et al. 1998). The pattern of elevated reflectance in coals adjacent to the orogenic front extends west across Ireland (Clayton et al. 1989) and east in continental Europe (Koch 1997). In the north of England, coals on the Alston Block were subject to anomalous heat flow from the Devonian Weardale Granite (Creaney 1980, Manning et al. 2007). There is a marked change in reflectance over just a few kilometres from high values in the Pennines to low values in the Ingleton Coalfield, across the Craven Faults. The coal on Arran was metamorphosed by the intrusion of Palaeogene granite (Fyfe et al. 1993). Contact metamorphism associated with laterally extensive Tertiary basaltic dykes may have also affected coals across Ayrshire (southern Scotland), Cleveland (north Yorkshire), Anglesey (North Wales) and central England.

The data imply that the potential for definitive discrimination of source regions in provenance studies is limited. Coals from along the Variscan orogenic front can be identified, and a regional distinction can be made between northern England and regions to the north and south. Consequently, where reflectance has been used for provenance in archaeological studies (Smith 1996, 2005, Erskine et al. 2008), the results are confirmatory rather than definitive.

Contact metamorphism can play a pivotal role in organic matter thermal maturity (Bishop and Abbot 1993, 1995). Some coals may have experienced short-term additional heating. For example samples from Bute and Fife exhibit veining by calcite due to hydrothermal activity. However, reflectance is a kinetically-controlled parameter, so is influenced by long-term heat flow rather than short-term events, as observed elsewhere (Parnell et al. 2005).

**Conclusions**

The reported database is the first comprehensive collation of vitrinite reflectance for British coals. In addition to providing a frame of reference for thermal maturity in sedimentary sections of Carboniferous age, the database of vitrinite reflectance has applications for diverse purposes that involve national surveys. For example, the data can be used in assessments of coal bed methane (DECC 2013), shale gas potential (Smith et al. 2011), geothermal energy (Gluyas et al. 2018) and the interpretation of trace element data in coals (Bullock et al. 2018).

**Acknowledgements**

The authors wish to thank Professor Barry A. Thomas for supplying Wrexham coal samples and David Richardson for sharing samples and data for coals from New Cumnock. The authors are grateful for the constructive comments from Dr David P. Creedy and Dr Onoriode Esegbue, as well as the careful editorial handling of Dr Veerle Vandeginste. This work was partially funded by NERC grant NE/M010953/1.

**References**

Alderton, D.H.M., Oxtoby, N., Brice, H., Grassineau, N. & Bevin, R.E. 2004. The link between fluids and rank variation in the South Wales Coalfield: evidence from fluid inclusions and stable isotopes. Geofluids, 4, 221-236.

Andrews, I.J., 2013 The Carboniferous Bowland Shale gas study: geology and resource estimation. London, UK, British Geological Survey for Department of Energy and Climate Change, 64pp. Data including: Appendix A: Estimation of the total in-place gas resource in the Bowland-Hodder shales, central Britain. http://nora.nerc.ac.uk/id/eprint/503839/.

Armstroff, A., 2004. Geochemical Significance of Biomarkers in Paleozoic Coals. Doctoral Thesis (Ph.D), Technischen Universität Berlin.

Asuen, G.O., Onyeobi, T.U.S., 2013. Evaluation of the optical properties of some coal types. Journal of Geography and Geology, 5, 3, 176-185.

BCURA (The British Coal Utilisation Research Association), 2002. The BCURA Coal Sample Bank: A Users Handbook. http://www.bcura.org/coalbank.html.

Bishop, A.N. & Abbott, G.D. 1993. The interrelationship of biological marker maturity parameters and molecular yields during contact metamorphism. Geochimica et Cosmochimica Acta, 57, 15, 3661-3668.

Bishop, A.N. & Abbott, G.D. 1995. Vitrinite reflectance and molecular geochemistry of Jurassic sediments: the influence of heating by Tertiary dykes (northwest Scotland). Organic Geochemistry, 22, 165-177.

Bjørlykke, K. 2015. Introduction to Petroleum Geology. In: Bjørlykke, K. (Ed.), Petroleum Geoscience. Springer, Berlin, Heidelberg.

Bray, R.J., Green, P.F. & Duddy, I.R. 1992. Thermal history reconstruction using apatite fission track analysis and vitrinite reflectance: a case study from the UK East Midlands and Southern North Sea. In: Hardman, R.F.P. (Ed.), Exploration Britain: Geological Insights for the Next Decade. Geological Society Special Publication, No. 67, pp. 3-25.

British Geological Survey 1999. Coal Resources Map of Britain. Natural Environment Research Council and The Coal Authority.

Bullock, L.A., Parnell, J., Feldmann, J., Armstrong, J.G., Henn, A.S., Mesko, M.F., Mello, P.A. & Flores, E.M.M. 2018. Selenium and tellurium concentrations of Carboniferous British coals. Geological Journal, doi: 10.1002/gj3238.

Burnett, R.D. 1987. Regional maturation patterns for Late Visean (Carboniferous, Dinantian) rocks of northern England based on mapping of conodont colour. Irish Journal of Earth Sciences, 8, 165-185.

Bustin, R.M., Barnes, M.A. & Barnes, W.C. 1990. Determining levels of organic diagenesis in sediments and fossil fuels. In: McIlreath, I.A. & Morrow, D.W. (Eds.), Diagenesis. Geological Association of Canada, pp. 205–226.

Cavailhes, T., Rotevatn, A., Monstad, S., Khala, A.B., Funk, E., Canner, K., Looser, M., Chalabi, A., Gay, A., Travé, A., Ferhi, F., Skanji, A., Chebbi, R.M. & Bang, N. 2018. Basin tectonic history and paleo-physiography of the pelagian platform, northern Tunisia, using vitrinite reflectance data. Basin Research, 30, 926-941.

Clayton, G., Haughey, N., Sevastopulo, G.D. & Burnett, R. 1989. Thermal maturation levels in the Devonian and Carboniferous rocks in Ireland. Geological Survey of Ireland, Dublin.

Cloke, M., Lester, E. & Gibb, W. 1997. Characterization of coal with respect to carbon burnout in p.f.-fired boilers. Fuel, 76, 1257-1267.

Creaney, S. 1980. Petrographic texture and vitrinite reflectance variation on the Alston Block, NE England. Proceedings of the Yorkshire Geological Society*,* 42, 553-580.

Creaney, S. 1982. Vitrinite reflectance determinations from the Beckermonds Scar and Raydale boreholes, Yorkshire. Proceedings of the Yorkshire Geological Society, 44, 99-102.

Creedy, D.P. 1986. Methods for the evaluation of seam gas content from measurements on coal samples. Mining Science and Technology, 3, 141-160.

Creedy, D.P. 1988. Geological controls on the formation and distribution of gas in British Coal Measure Strata. International Journal of Coal Geology, 10, 1-31.

DECC (Department of Energy and Climate Change) 2013. The Unconventional Hydrocarbon Resources of Britain's Onshore Basins - Coalbed Methane (CBM). HM Government, Department of Energy and Climate Change, London. 45 pp.

Duncan, W.I., Green, P.F. & Duddy, I.R. 1998. Source rock burial history and seal effectiveness: Key facets to understanding hydrocarbon exploration potential in the East and Central Irish Sea basins. AAPG Bulletin, 82, 1401-1415.

Durucan, S., Ahsan, M. & Shi, J-Q. 2009. Matrix shrinkage and swelling characteristics of European coals. Energy Procedia, 1, 3055-3062.

Erskine, N., Smith, A.H.V. & Crosdale, P.J. 2008. Provenance of coals recovered from the wreck of HMAV *Bounty*. The International Journal of Nautical Archaeology, 37, 171-176.

Fyfe, J.A., Long, D. & Evans, D. 1993. United Kingdom Offshore Regional Report: The Geology of the Malin-Hebrides Sea Area. London, HMSO.

Gayer, R. & Fowler, R. 1997. Variations in coal rank parameters with depth correlated with Variscan compressional deformation in the South Wales Coalfield. In: Qi, Y. (Ed.), Proceedings of the 30th International Geological Congress, No. 18, B, pp. 77-98.

Gayer, R., Fowler, R. & Davies, G. 1997. Coal rank variations with depth related to major thrust detachments in the South Wales coalfield: implications for fluid flow and mineralization. Geological Society of London, Special Publications, 125, 161-178.

Gayer, R.A., Garven, G. & Rickard, D.T. 1998. Fluid migration and coal-rank development in foreland basins. Geology, 26, 679-682.

Gluyas, J., Adams, C.A., Busby, J.P. & Craig, J. 2018. Keeping warm: A review of deep geothermal potential of the UK. Proceedings of the Institution of Mechanical Engineers Part A Journal of Power and Energy, 232, doi: 10.1177/0957650917749693.

Hackley, P.C. & Cardott, B.J. 2016. Application of organic petrography in North American shale petroleum systems: A review. International Journal of Coal Geology, 163, 8-51.

Koch, J. 1997. Upper limits for vitrinite and bituminite reflectance as coalification parameters. International Journal of Coal Geology, 33, 169-173.

Linley, K.A. 2014. User Guide for the Vitrinite Reflectance dataset. British Geological Survey Open Report, OR/14/055.

Mani, D., Kalpana, M.S., Patil, D.J. & Dayal, A.M. 2017. Organic matter in gas shales: Origin, evolution and characterization; In: Daval, A.M. & Mani, D. (Eds.), Shale gas: Exploration and environmental and economic impacts. Elsevier, pp. 25–52.

Manning, D.A.C., Younger, P.L., Smith, F.W., Jones, J.M., Dufton, D.J. & Diskin, S. 2007. A deep geothermal exploration well at Eastgate, Weardale, UK: a novel exploration concept for low-enthalpy resources. Journal of the Geological Society, London, 164, 371-382.

Marshall, J.E.A., Haughton, P.D.W. & Hillier, S.J. 1994. Vitrinite reflectivity and the structure and burial history of the Old Red Sandstone of the Midland Valley of Scotland. Journal of the Geological Society, 151, 425-438.

Maynard, J.B., Elswick, E.R. & Hower, J.C. 2001. Reflectance of dispersed vitrinite in shales hosting Pb-Zn-Cu deposits in Western Cuba: Comparison with clay crystallinity. International Journal of Coal Geology, 47, 161-170.

New Age Exploration Ltd., 2014. Lochinvar Coking Coal Project. ASX Release: 29 August 2014, http://nae.net.au/wp-content/uploads/2014/08/Lochinvar-Resource-Upgrade.pdf.

Northern Mine Research Society, 2015. Coal Mining in the British Isles (Interactive map). https://www.nmrs.org.uk/mines-map/coal-mining-in-the-british-isles/.

Parnell, J. 1992. Burial histories and hydrocarbon source rocks on the North West seaboard. In: Parnell, J. (Ed.), Basins on the Atlantic Seaboard: Petroleum Geology, Sedimentation and Basin Evolution. Geological Society Special Publication, No. 62, pp. 3-16.

Parnell, J., Green, P.F., Watt, G. and Middleton, D. 2005. Thermal history and oil charge on the UK Atlantic margin. Petroleum Geoscience, 11, 99-112.

Pearson, M.J. & Russell, M.A. 2000. Subsidence and erosion in the Pennine Carboniferous Basin, England: lithological and thermal constraints on maturity modelling. Journal of the Geological Society, 157, 471-482.

Petersen, H.I. 2006. The petroleum generation potential and effective oil window of humic coals related to coal composition and age. International Journal of Coal Geology, 67 (4), 221-248.

Raymond, A.C. & Murchison, D.G. 1991. Influence of exinitic macerals on the reflectance of vitrinite in Carboniferous sediments of the Midland Valley of Scotland. Fuel, 70, 155-161.

Shelley, A.E. 1967. Analyses of two coals from the Great Scar Limestone near Ingleton, Yorkshire. Proceedings of the Yorkshire Geological Society 36, 51-56.

Smith, A.H.V. 1996. Provenance of coals from Roman sites in U.K. counties bordering River Severn and its Estuary and including Wiltshire. Journal of Archaeological Science, 23, 373-389.

Smith, A.H.V. 2005. Coal microscopy in the service of archaeology. International Journal of Coal Geology, 62, 49-59.

Smith, N., Turner, P. & Williams, G. 2011. UK data and analysis for shale gas prospectivity. Geological Society, London, Petroleum Geology Conference Series, 7, 1087-1098.

Tissot, B.P. & Welte, D.H. 1984. Petroleum Formation and Occurrence. Springer-Verlag, Berlin.

Vandenberghe, N. 1976. Phytoclasts as provenance indicators in the Belgian septaria clay of Boom (Rupelian age). Sedimentology, 23, 141-145.

Vincent, C.J. & Rowley, W.J. 2004. Thermal Modelling in the Midland Valley of Scotland using BasinMod™ and HotPot. British Geological Survey Internal Report, IR/04/144. 48pp.

Waters, C. N., Browne, M. A. E., Dean, M. T., and Powell, J. H. 2007. Lithostratigraphical framework for Carboniferous successions of Great Britain (Onshore). British Geological Survey Research Report, RR/07/01. 60pp.

**Figure captions**

**Fig. 1.** Map of Great Britain, showing exposed British coalfields (grey), sample localities (black dots) and identification numbers (see insets) used in Table 1 (base map after British Geological Survey 1999).

**Fig. 2.** Stratigraphy of coal-bearing Carboniferous section, UK (Waters et al. 2007), including units identified in Table 1.

**Fig. 3.** Distribution of reflectance values for total data set.

**Fig. 4.** Vitrinite reflectance (Ro %) map of Great Britain with Ro values delimited by spot size. Numbers in map correspond to amount of samples analysed per locality (where information is available). Exposed British coalfields (grey) also shown.

**Table captions**

**Table 1.** *Vitrinite reflectance data for localities and coalfields across Great Britain.*