MATURATION CHARACTERISTICS OF THE NEW ZEALAND COAL BAND: PART 2 – KEROGEN RESTRUCTURING AND IMPLICATIONS FOR MODELLING PETROLEUM FORMATION

Richard SYKES[1], Volker DIECKMANN[2,3], Brian HORSFIELD[2], Tiem T.A. VU[2] and Per Erling JOHANSEN[4]

1. GNS Science, PO Box 30368, Lower Hutt 5040, New Zealand
2. GeoForschungsZentrum Potsdam, Telegrafenberg, D-14473 Potsdam, Germany
3. Shell International Exploration and Production, Kessler Park 1, 2288 GS Rijswijk, Netherlands
4. Applied Petroleum Technology, Instituttveien 18, PO Box 123, 2027 Kjeller, Norway

The maturation characteristics of humic (i.e. vitrinite-rich) coals and coaly mudstones are fundamentally different to those of classic marine and lacustrine source rocks and, thus, for basin modelling purposes, require separate study. The unique maturation characteristics of coaly kerogen are well exemplified by the New Zealand Coal Band (Cretaceous–Cenozoic), which displays an unexpected, rank-related increase in HI of up to 150 mg HC/g TOC prior to the onset of oil expulsion (Sykes and Snowdon, 2002). This increase has been attributed primarily to kerogen restructuring (Killops et al., 2002; Sykes and Snowdon, 2002), which is thought to involve mainly aromatisation and polycondensation reactions reincorporating bitumen into the kerogen macromolecular structure and in the process, creating new, higher energy bonds (Schenk and Horsfield, 1998; Dieckmann et al., 2006). In this study, we have used Soxhlet extraction, TLC and open-system pyrolysis techniques to investigate evidence for progressive kerogen restructuring along the NZ Coal Band and to assess its implications for kinetics-based modelling of petroleum formation.

Thirteen well-characterised, rank series coals [Rank(S_r) 5.4–18.9, R_o 0.39–2.61%] of relatively uniform kerogen type from the NZ Coal Band were Soxhlet-extracted using an azeotropic solvent mixture for 72 hrs. The extracts are dominated by asphaltene and polar compounds. HI values of the extracted coals are up to c. 100 mg HC/g TOC less than those of the non-extracted counterparts (Fig. 1). Indeed, for coals of Rank(S_r) 12.6 (R_o 0.87%) or less, up to c. 30% of their S2 hydrocarbon yields is heavy bitumen-derived. Significantly, however, the extracted coals display the same rank-related increase in HI up to the onset of oil expulsion, confirming that the increase is indeed linked to the kerogen fraction.

For both the extracted and non-extracted sample sets, plots of the S2 hydrocarbon generation rate curves (normalised to mg HC/g initial C/°C) against Rock-Eval temperature reveal nesting of the curves for the three least mature samples [Rank(S_r) 5.4–6.6, R_o 0.39–0.45%), followed by progressive offset of curves to higher temperatures for successively more mature samples; i.e. each curve extends beyond the envelope of the preceding sample in the rank series. This distribution is consistent with the neo-formation of more refractory kerogen with progressive maturation – kerogen that is expected to generate late-stage, high-maturity gas (Dieckmann et al., 2006).

To further test this theory, hydrocarbon generation rate curves were obtained for the non-extracted coals at laboratory heating rates of 0.7, 2, 5 and 15 K/min and discrete activation energy and frequency factor distributions derived following the enhanced kinetics approach of Dieckmann (2005). Initial results are equivocal, probably because of the significant heavy bitumen component of many of the samples. However, irrespective of the kinetics results, the progressive offset of the S2 hydrocarbon generation rate curves beyond the immature envelopes indicates that hydrocarbon generation kinetics obtained from immature samples would likely result in erroneous predictions of petroleum formation histories at geological heating rates (Schenk and Horsfield, 1998).

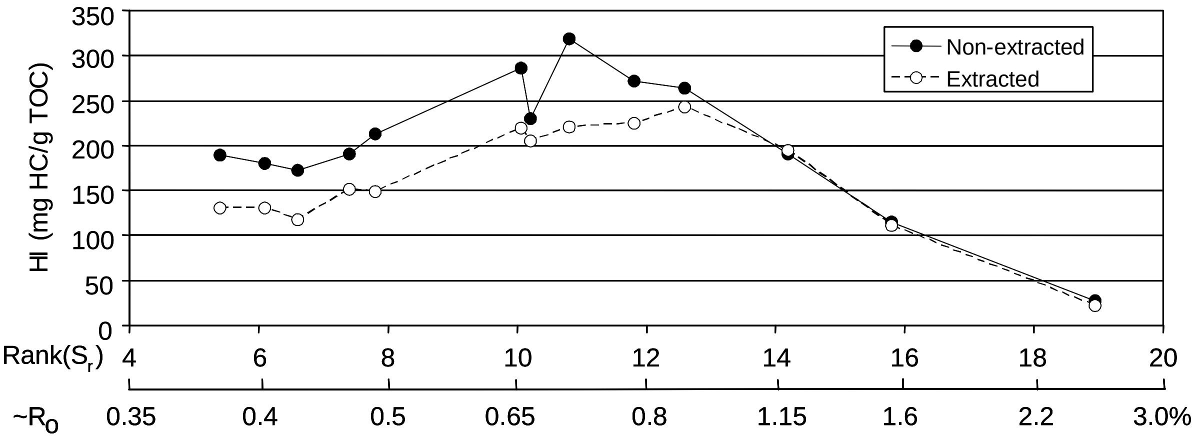

Figure 1. Plot of HI versus Rank(S_r) and equivalent R_o for selected coals from the NZ Coal Band, pre- and post-extraction.

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