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Development of compositional kinetic models for hydrocarbon generation and phase behaviour modelling

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Petroleum composition directly controls the physical response of the fluid to changing pressure and temperature conditions (PVT behaviour) during migration. Modern basin modelling software now include the possibility to model petroleum composition and PVT behaviour during hydrocarbon generation and migration. While various compositional kinetic models of petroleum generation have been published in the last few years, none of the studies presented have attempted to match the composition and phase state of known petroleum accumulations.

Using compositional data from closed-system non-isothermal pyrolysis experiments we have developed compositional kinetic models of hydrocarbon generation for a variety of petroleum-type based source rock organofacies which use 14 components to describe the generated fluid and take compound generation and cracking reactions into account. The data format selected is compatible with the compositional resolution used in reservoir engineering, allowing thus a direct comparison of predicted compositions and phase behaviour to PVT data of natural fluids. Compositional predictions of the model are tuned to natural fluid compositions and the calibrated models implemented in 2 and 3D basin modelling studies.

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Petroleum generation kinetics based on oil asphaltene pyrolysis

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Establishing the reaction kinetics of petroleum generation by various pyrolysis techniques using different immature source rock types/kerogen has long been employed to constrain basin models and predict the timing of generation/migration. It may be possible to measure generation kinetics of a particular petroleum system more specifically using the modified reactant (asphaltene) retained and transported with the product (petroleum). Previous work [1] suggests that asphaltene pyrolysis was useful in determining the temperature of petroleum formation. In the present study, 14 asphaltene samples from crude oils were obtained by hexane precipitation. Seven of the samples were from oils generated from carbonate sources of varying ages and environments and the other seven samples are from marine shale source rocks with little or no terrigenous influence. Additionally, asphaltenes were obtained from source rock kerogen, source rock bitumen, and corresponding oils representing five other well characterized petroleum systems: 1) Middle Cretaceous Shilaif carbonate/marl source; 2) Upper Jurassic Tuwaiq Mountain carbonate source; 3) Upper Jurassic Bazhenov shale source; 4) Frasnian RAD shale of the Ghadamas Basin; and 5) Upper Jurassic Kimmeridge Formation. Multiple oils of different thermal maturity, as determined by terpane and sterane biomarkers, were used from each petroleum system. Asphaltene samples were pyrolyzed using a SR Analyzer at different rates (1, 3, 10, 30, 50 °C/min), and a discrete model was employed to calculate activation energy (Ea) distributions. Onset (10% reaction) and peak generation temperatures were calculated based on a 3.3 °C/my model. Of the 14 initial oil sample asphaltenes, the results were not atypical of immature kerogen pyrolysis: some samples had broad Ea distributions about 53 to 54 kcal/mole maximums while a few had essentially a single Ea at 54 kcal/mole. Onset temperatures varied from 124 to 139 °C and peak generation temperatures ranged from 144 to 153 °C. Weighted average Ea correlated well positively to onset temperatures. A less well defined positive correlation was observed between peak generation temperature and apparent oil thermal maturity as defined by triaromatic steranes. The estimated sulfur concentration in oil asphaltenes (higher in carbonate-sourced oils compared to oils from shales) generally correlated to a measure of the broadness of the Ea distribution, with asphaltenes from carbonates having a separate trend than shale asphaltenes.

Reference

[1] di Primo et al. (2000) *Nature* **106,** 175-176.