

## **COMPOSITIONAL KINETICS FOR HYDROCARBON GENERATION AND DESTRUCTION IN SOURCE ROCKS AND PREDICTION OF IMPORTANT FLUID PROPERTIES**

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Kinetic parameters for hydrocarbon generation and destruction are, amongst others, key input parameters in basin modelling computations. Increasing need of the last two decades to integrate Petroleum System Analysis and Reservoir engineering highlighted the need to have compositional kinetic data that allows - in combination with PVT-simulation and Shell's earlier reported fully coupled generation and expulsion module – accurate prediction beyond only hydrocarbon (HC) masses. Estimation of parameters such as oil gravity, gas to oil ratio (GOR/CGR), and/or aromaticity is a key in a pre-drill phase of exploration. Moreover, the composition has to be directly compatible with the HC mass fractions used by reservoir engineers within their models. Present basin modelling software packages, however, use kinetic data and utilise kinetic models that are often too simplistic to attain the quality-levels necessary for the correct prediction of these parameters. In contrast to Shell, they use a decoupled approach to model generation and subsequently expulsion. These packages predict very inaccurate gas compositions (too wet in comparison to actual natural gas composition), or oil compositions of too aromatic a character. Such assumptions can jeopardise a serious effort at predicting phase compositions along migration pathways and within reservoirs.

To address the lack of predictive ability a comprehensive and complex analytical scheme has been developed to first characterize the organic matter, including series of closed (gold tube) pyrolysis experiments. Different source rocks types from well-known major hydrocarbon systems such as the North Sea, Green River or LaLuna have been studied. The analytical scheme included careful sample preparation, fractionation and detailed characterization of various fractions, including careful C, H, N, and O quantification. Data obtained allowed for generation of compositional kinetic values for the saturate, aromatic, resin and asphaltene (SARA) fractions in the C15+ domain, the saturate and aromatic C6-14 fractions, and hydrocarbon as well as non-hydrocarbon gases.

We will demonstrate that kinetic values obtained for various fractions enable fluid property predictions (through data fitting and modelling) that match the actual field/well fluid properties and compositions in the reservoirs of the natural petroleum systems. In order to achieve a high predictive standard a newly developed PVT module, based on well established EOSs and calibrated against standard tools such as PVT-Sim, was linked to Shell's generation and expulsion engine, within Shell's inhouse 3-D basin modelling software. Without such a linkage, a petroleum generation model is incomplete.

The results generated by the models are directly comparable to standard geochemical criteria such as SARA composition, aromaticity, gas wetness and GOR/CGR. The accuracy of our modelling capabilities will be demonstrated at a regional and prospect scale. These improvements provide a new perspective on the use of large regional calibrations which were always a laborious necessity in the previous more simplistic models.