# PREDICTING PETROLEUM COMPOSITION USING BASIN MODELLING: COMPARISON OF DIFFERENT APPROACHES

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The advent of equation of state (EOS) based 3 phase multi-component modelling of fluid response to changing physical conditions during petroleum migration has significantly improved the predictive capacity of basin models with respect to fluid phase behaviour. The main constraints on this approach to date is a general lack of PVT-amenable compositional kinetic models of hydrocarbon generation and expulsion.

We have developed and tested a series of new methods for the determination of compositional kinetic models which correctly reproduce natural fluid compositions. The cornerstones of our approach are based on three specific observations made during the last 15-20 years of research:

a) analysis of source rocks by pyrolysis methods, especially closed-system, anhydrous pyrolysis (Horsfield *et al.*, 1989) correctly reproduce natural fluid gas to oil ratios (GOR) (di Primio & Skeie, 2004; Muscio *et al.*, 1991; Santamaria & Horsfield, 2004);

b) pyrolysis methods very closely mimic carbon chain length distributions of natural fluids (Horsfield, 1989)

c) no pyrolysis method is capable of correctly reproducing the natural composition of the petroleum gas phase (associate or free gas) (di Primio & Skeie, 2004; Mango, 1997; 2001; Mango *et al.*, 1994)

Comparison of source rock closed system pyrolysates and related natural fluids (data from live-fluid PVT reports) indicates that for comparable degrees of transformation pyrolysates very closely reproduce also the distribution of pseuocomponents of the liquid fraction (pseudocomponents are defined here as elution ranges representing steps along a resolved pyrolysate GC trace from one alkane to the next). Additionally, the average molecular weight of the liquid range (C6+) of closed system pyrolysates at increasing degrees of transformation mimics the evolution of C7+ molecular weight of natural fluid maturity series, whereby only fluids generated by the analysed source rock were compared.

This information indicates that it is possible to derive all necessary compositional information required for the definition of a compositional kinetic scheme from closed system pyrolysates, except for the gas composition.

In order to arrive at a better definition of natural gas compositions and develop a compositional kinetic model capable of predicting petroleum composition two techniques are available: the first (Tuning Method) uses a combination of bulk kinetics for the description of hydrocarbon generation and compositional information from a maturity series of related natural fluids (avoiding thus any analytical compositional artefacts). The method was described by di Primio and Skeie (2004), who defined such a compositional kinetic model using data from PVT reports from Snorre Field, North Sea. The results indicated that such a model can very closely reproduce natural fluid composition and phase behaviour in a basin model, allowing the reconstruction of compositional evolution and related physical properties of the reservoir fluids (GOR, saturation pressure).

The second technique is characterised by the correction of laboratory-derived gas compositions. Here again two different approaches are presented. The first uses an empirically determined set of correction factors for the gas composition as a function of bulk transformation ratio. This so called PhaseKinetic approach corrects gas compositions as discussed above, the corrected fluid compositions are then used to populate a bulk kinetic dataset with compositional information for different levels of conversion. This approach does not require the availability of natural data for its predictions. Comparison of predictions and actual natural fluid compositions using 2D and 3D basin modelling have also been succesfull.

The second gas compositional correction technique (Neural Net method) was developed in an industry collaboration. Here we noticed a very systematic behaviour of gas composition with respect to GOR, especially within samples series generated by source rocks belonging to the same organic facies. This allowed us to train a neural network to define natural fluid compositions based on closed system pyrolysis results obtained from source rocks. Integration of the corrected compositional data with kinetic data is performed using kinetics determined using the closed system pyrolysis approach. Compositional predictions in basin modelling based on this approach are accurate with respect to GOR, saturation pressure and even API gravity. If the relationship between source rock organic facies and gas composition is true, this method can allow us to predict generated petroleum compositions directly from experimental results very accurately.

Selecting which method to use in a given study depends on the exploration status of the study area. In frontier areas the PhaseKinetic approach should be used, where a series of samples representing different organic facies types have already been analysed and the

basin modeller can select which sample to use based on the supposed source rock depositional environment. Limitations here are that the models are constrained for primary cracking processes only. In moderately explored study areas, where source rock samples are available the Neural Net technique can be used. This approach allows the prediction of fluid compositions in the range of primary cracking and extends to include initial secondary cracking reactions, i.e. covers the oil window extending into the early gas window. In a mature study area, with abundant compositional information from PVT reports, the Tuning approach is easily implemented. Limitations are only given by the data range used in the definition of the compositional kinetic model (e.g. covering only a part of the oil window, the entire oil window or the oil and gas windows).

Our petroleum compositional description implemented in the kinetic models is sufficiently detailed to allow the assessment of effects of petroleum biodegradation on fluid phase behaviour. Initial results on this theme will also be presented.

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