# SOME RECENT ADVANCES AND CHALLENGES IN PETROLEUM SYSTEMS MODELING

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Petroleum systems modeling has become an essential tool for exploration in the last few years. Geologic processes like heat transfer, source-rock maturation, petroleum generation, expulsion, migration and accumulation, as well as the prediction of oil and gas compositions, are dynamically modeled and quantitatively assessed during basin history in increasingly complex and detailed three-dimensional models. Several scientific, software and computational advances have allowed petroleum geologists to thoroughly investigate the efficiency of each process, contemplating a large number of alternative scenarios and thus providing a probabilistic assessment of risk for decision-making.

Even though progress has been fast in software development and computational capabilities, there is a number of topics that still deserve scientific research in order to improve the reliability of predictions given by petroleum systems modeling. Therefore, the main goal of this work is to provide an overview of some recent advances in basin modeling, and to highlight some of the challenges that must be overcome in the future to make this technique even more robust in terms of predictive capabilities. Below we address the following developments and challenges: a) Crustal stretching in rifted continental margins; b) Misconceptions on heat flow histories; c) Applications of compositional kinetic modeling; d) Sensitivity studies in migration modeling; e) Increased use of biomarker and isotopic maturity data; and f) Modeling of petroleum biodegradation.

a) Crustal stretching in rifted continental margins: basins in continental margins have traditionally been assumed to form by pronounced extension and thinning of the lithosphere. The partition of the sedimentary basins in rift, evaporite and open-marine megasequences was convenient because the vertical motions associated with these megasequences could be roughly unified by simple rifting models. The observed initial subsidence in passive margins is usually rift-related and the thinning of the crust associated with it could theoretically explain elevated heat flow anomalies in the past and the subsequent long-term, exponential-like, subsidence. It might not be clear to many petroleum geologists that, in order to produce post-rift subsidence, there must be considerable syn-rift subsidence. Royden and Keen (1980) reported extra subsidence during the thermal phase in the Atlantic margin of Canada. They proposed a two-layer stretching model in which mantle and lower crust can deform more than the upper crust in order to explain the extra-subsidence. Driscoll and Karner (1998) reported that subsidence in the Exmouth Plateau (off Northwest Australia) did not involve upper crustal extension. This is a major problem with the current knowledge of extensional margins and is known as the "Upper Plate" or "Extra Subsidence" paradox. This problem is also reported for Brazilian and African margins and represents a serious challenge to predict heat flow histories.

b) Misconceptions on heat flow histories: the issue addressed above concerns rift-related heat flow, which is a smooth first order effect in the lithosphere. By definition, heat flow is a depth-dependent variable, but geologists used it as a boundary condition either at the bottom of the sedimentary column or at the bottom of crust without the proper care of this aspect. If the whole lithospere is part of the framework simulated, the resultant heat flow history at the bottom of the sedimentary column becomes noisy in time and can confuse most petroleum geologists. This is because the lithospheric heat flow interacts with cold sedimentary rocks and other thermal effects (radiogenic heat sources, conductivity variations and overpressure generation), which reduce and create variable effects in time, depending on the sedimentary evolution of the basin.

The misuse of heat flow has some unwanted consequences. Even with simple heat flow histories, observed and estimated vitrinite and temperature data can be matched but hydrocarbon expulsion from source rocks might be incorrect by several million of years. Very often fitting calibration data is not possible at all. In this case, there are software (e.g. PetroFits) that might help to minimize the differences between observed and estimated thermal data. However, this kind of software tends to work with low-order mathematical functions, which will not restore the high-frequency content of the "true" heat flow history. We elaborate on this issue and how the incorrect handling of heat flow histories can lead to incorrect estimates of the timing and degree of maturation of source rocks, mainly of those located in frontier areas.

c) Applications of compositional kinetic modeling: despite intensive research undertaken in the last thirty years, modeling of petroleum generation is not a totally consensual matter. Several questions have been arisen about the processes of acquisition of kinetic data for primary cracking. Those questions revolve around the nature of the sample used for laboratory artificial maturation experiments (whole rock *versus* isolated kerogen), the type of experiment (open *versus* closed system pyrolysis) and the presence or absence of water (hydrous *versus* anhydrous pyrolysis; e.g. Lewan & Ruble, 2002). Whereas in nature petroleum generation from kerogen in source rocks takes place in the presence of minerals and water, their role in artificial maturation under laboratory conditions is somewhat controversial. Besides the debate about any catalytic effect caused by minerals in artificial maturation, retention effects must be assessed adequately since the retained petroleum will undergo secondary cracking with further maturation. Another issue underlying the choice of the method of kinetic data acquisition is a good understanding of the type of cracking reactions that occur under the time, temperature and pressure conditions of each equipment.

Compositional kinetic models are becoming increasingly complex and powerful since their first appearance in the mid-seventies. Once again, several issues are associated with the method of data acquisition. First of all, the amount, production rates and composition of the generated products is strongly dependent on the pyrolysis method due to the variable extent of secondary cracking. The quality of the compositional prediction given by open or closed-system derived kinetics will depend largely on the availability and quality of class-specific secondary cracking kinetics. It is clear that the amount of petroleum generated in open-system experiments is larger than that from closed system. Furthermore, oil from open pyrolysis is considerably heavier than reservoired oils.

Kinetic data from different analytical techniques have been available for the modeling of petroleum generation in numerical simulators. Nevertheless, a detailed comparison and analysis of the kinetics results (amount and composition of reactants and products, rates) obtained from the various laboratory techniques is necessary for a proper evaluation of their impact in the assessment of petroleum generation. The types of primary cracking reactions that take place in each laboratory apparatus must be better understood before extrapolating their kinetics to geologic conditions. In addition, calibration of kinetic models with natural source-rock and petroleum compositions data is absolutely essential for an adequate choice of the type of compositional kinetics used as input in basin simulators.

d) Sensitivity studies in migration modeling: the comprehension of secondary migration in basin scale has not increased over the years, although the market offers programs to simulate migration of progressively larger models and in shorter computation time. Due to the complexity of hydrocarbon migration, geologists tend to approach the problem in a statistical way directly using risk assessment tools (e.g., Petrorisk) without understanding the system. Considering the large number of faults, rock types and related variables that might exist from source to trap, the use of few parameters in a risk tool only gives an artificial feeling of comprehensive and independent assessment.

e) Increased use of biomarker and isotopic maturity data: the location, volumes and compositions of real petroleum accumulations have been used for the calibration of migration models. It must be pointed out, however, that a vast array of source and maturity indicators from biomarkers in the oil can be used for calibration in basin models (e.g. Peters et al., 2005). This approach has not been intensively used in petroleum systems modeling. For instance, biomarker and isotopic parameters can provide quantitative assessments of the source-rock maturity at the moment of petroleum expulsion, as well as an evaluation of any further secondary cracking oil might have undergone after reservoir filling.

f) Modeling of petroleum biodegradation: a major challenge still persists when it comes to prediction of post-accumulation alteration processes, i.e. biodegradation modeling. Several approaches are currently being tried by different research groups. The experimental approach consists in the simulation of bacterial degradation of petroleum under laboratory conditions. Since anaerobic biodegradation seems to prevail in geologic conditions, the experimental approach becomes relatively complicated and takes a long time to perform. In addition, biodegradation rates and compositional alterations derived from laboratory experiments might not be straightforwadly applicable to natural conditions. The study of metabolites and metabolic pathways is an alternative way of getting insights into the mechanisms of biodegradation in nature. However, a more practical way of simulating biodegradation rates and compositional changes involves the modeling of reservoir filling history. This task demands a relatively detailed reservoir model within a basin-scale simulation in order to take into account the overall petroleum generation, migration and accumulation processes. The coupling of the reservoir filling history with compositional gradients in the oil column given by geochemical data will certainly provide a means of estimating biodegradation rates which might be compared in different geologic settings.

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