Oil, Bitumen, and Other Confusing Concepts: What do Lab Experiments Really Tell Us?

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ABSTRACT

Various types of experiments are used to derive chemical kinetic models for use in petroleum system modeling, but there are fundamental questions about the correspondence between nature and laboratory simulations that have never been answered. Qualitatively, we know that laboratory-based kinetic models extrapolate to natural generation timescales, but careful probing of data indicates that there are fuzzy definitional issues that make a quantitative comparison ambiguous.

The concept advocated here is that only by simultaneously matching closed system with open- or semi-open system experiments can one have confidence in any extrapolation. Furthermore, transport mechanism(s) in the open and semi-open system experiments, including how they may change with temperature and pressure, must be modeled explicitly.

Much has been made in the past about differences in kinetic parameters derived from open system and hydrous pyrolysis experiments. Neither can be claimed a priori to be extrapolatable to geological time scales, and an empirical demonstrate of their utility is complicated by the challenges of reconstruction of paleothermal histories. Misconceptions on both sides of that argument are explored here.

Most believe that open-system kinetics are a better predictor of natural maturation kinetics than published hydrous pyrolysis kinetics, but one must be careful about what comparison is actually being made. Open system kinetics are based on production of volatiles, which may or may not be primary products of kerogen decomposition and do not have the same molecular weight distribution. The most rigorous comparison is for kerogen disappearance, which has far less ambiguity in what is actually being compared.

Both compositional modeling and phase equilibrium calculations have been around for decades, but they have not been fully utilized to understand oil primary migration. Mechanistic models of kerogen transformation have been around for quite a while. Kerogen structural models are becoming sounder due to advances in spectroscopic characterization. Mechanistic modeling of sorption has also become possible. More powerful computers make a more fundamental approach feasible today. Time is ripe to put all these capabilities together to create more fundamentally based models of generation and primary migration that do not use archaic species that confuse the role of chemical kinetics and phase equilibria in the observed phenomena.