Assessment of Thermal Reactivity for Source Rock Chracterization and Optimization of Kinetics in Basin Modeling

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Abstract

The conversion of kerogen to petroleum in source rock is regarded as a series of irreversible reactions controlled by first-order chemical kinetics, which can be described by Arrhenius Equation ($k = A\ e^{-Ea/RT}$). The equation determines the rate of the transformation of kerogen to hydrocarbon (***k***) under thermal stress during burial history of the source rock, and demonstrates the effect of temperature (***T***) and time (***t***) on petroleum generation. The kinetic parameters, activation energy (***Ea***) and frequency factor (***A***), are critical inputs for a source rock in basin modeling to quantify generation, retention and expulsion of petroleum and to determine the timing of these processes.

The study focuses on the bulk kinetics that describes the transformation of kerogen to hydrocarbon. Because kerogen is heterogeneous, the usual format of the kinetic parameters comprises a discrete distribution of ***Ea*** values at one kcal/mol interval with a common ***A***. It is recommended to apply all derived kinetics with a geological heating rate (thermal history) to test their validity and thermal reactivity before implementing measured kinetics in a basin model. **Thermal reactivity** here is defined as the chemical reactivity of source rock under thermal stress. Lower reactivity means that it is more difficult to crack kerogen into hydrocarbons under certain thermal stress, suggesting that higher temperatures and/or a longer time is needed to complete certain ratio of kerogen transformation in geological situation.

The study developed a new method to convert the complex format of kinetic parameters to a couple of weighted average ***Ea*** and ***A.*** A cross-plot is used to compare the simplified kinetic parameters between different source rocks. The method allows to evaluate the thermal reactivity based on both measured and published bulk kinetic parameters, for both kerogen and oil cracking, without using basin modeling software. The reactivity defined by kinetics therefore can be used as an independent variable, beyond quantity, quality and thermal maturity of organic matter, for source rock characterization. The reactivity rank, as a quick indicator of the kinetic behavior, may help selection and assignment of kinetic parameters in basin modeling.