



Full Length Article

Inversion of source rock hydrocarbon generation kinetics from Rock-Eval data



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HIGHLIGHTS

- Numerical inversion for estimating petroleum generation kinetic parameters from Rock-Eval data.
- A complementary tool to characterize the thermal decomposition of source rock.
- Improved spatial resolution of source rock generation kinetics.
- Useful for less well-known petroleum systems where no information on generation kinetics is available.

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ABSTRACT

Basin and petroleum system modeling requires source rock kinetics as input for the reconstruction of hydrocarbon generation history. For less well-studied petroleum systems, there may be little information on petroleum generation kinetic parameters publically available; thus, an analog of representative source rock kinetics must be chosen from available kinetics databases. Recent studies suggest that source rock kinetics may vary considerably even when they contain the same type of kerogen. Thus, kinetic parameters from analog basins/source rocks may lead to erroneous results in petroleum generation history reconstruction. Rock-Eval data contain information about source rock kinetics, and can be used to improve the kinetic model in petroleum system modeling. However, the kinetic information in Rock-Eval data is not in the form of activation energies and frequency factors required to solve the temperature dependency of reaction rate in the Arrhenius equation. This article proposes a kinetic inversion method so that the analogous kinetic model chosen by the user can be improved based on Rock-Eval data of the targeted source rock. We demonstrate the method using a synthetic dataset in a case study for method validation and its application to real source rock evaluation for examples from the Devonian Duvernay Shale in the Western Canada Sedimentary Basin (WCSB).

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1. Introduction

To better understand resource potential in both conventional and unconventional petroleum systems, basin and petroleum system modeling is often applied to reconstruct petroleum generation histories so that the timing of generation and the quantity and fluid types of the petroleum products can be inferred. Theoretical chemical reaction models using kinetic parameters in the form of activation energy distributions coupled with a frequency factor have been applied to reconstruct petroleum generation history in basin and petroleum system modeling [1,2].

The most common approach to determine hydrocarbon generation kinetics utilizes laboratory pyrolysis of source rock or kerogen samples at variable heating rates to provide insight into the processes of kerogen thermal decomposition. Thus, the thermal energy required for hydrocarbon generation under geological conditions can be inferred [3–6]. Based on laboratory pyrolysis experiments, Braun and Burnham [7] and Burnham et al. [8–11] discussed different techniques to estimate kinetic parameters. Their studies suggest that a single activation energy is sometimes insufficient to characterize complex chemical reactions during hydrocarbon generation, and a distribution in activation energies, or most rigorously, a distribution in both activation energies and frequency factors can offer better kinetic models. To make the mathematical model manageable but reasonably representative of the processes, kerogen thermal decomposition in source rock

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is approximated by a series of n^{th} -order, independent and parallel chemical reactions. To facilitate the implementation of the parallel n^{th} -order chemical reactions mathematically, a distribution of activation energies was proposed to quantify the thermal transformation of various kerogen components having different molecular structures [7].

However, the traditional approach to estimate the distribution of activation energies and the frequency factor has at least three deficiencies: (a) it requires special laboratory procedures, expertise and equipment, and the source rocks that have been analyzed for kerogen kinetics are limited to well-known source rock beds (e.g., [12–17]); (b) full exposure of the transformation behaviors of kerogen requires immature samples, which constrains the availability and spatial representation of source rock samples; and (c) large uncertainties may exist in the inferred reaction rates under geological conditions due to differences between laboratory settings and natural environments, such as variable heating rates, formation pressure, geochemistry of formation water and mineral contents [18,19].

Alternatively, kerogen kinetics can be expressed as the present-day hydrocarbon transformation status with thermal maturation in a series of data points on a Tmax vs HI cross-plot. Chen and Jiang [20] demonstrated that the relationship between Tmax and HI can be approximated statistically using an empirical model that was subsequently converted to hydrocarbon transformation ratio (TR) as a function of thermal maturity indexed by Tmax or vitrinite reflectance. The TR can then be used in petroleum resource potential evaluation where reconstruction of petroleum generation histories in geological time is not essential [21,22]. There are two advantages of applying such an empirical relationship in source rock evaluation: (a) geological calibration of laboratory generated data is not required since the hydrocarbon generation model is built on analytical data generated directly from geological samples; (b) the Rock-Eval data may cover the entire study area, and thus are more representative of the targeted source rock unit in a basin than parameters inferred from a few pyrolysis experiments carried out on a limited number of immature samples collected from restricted geographic locations.

In many cases, basin and petroleum system modeling is an essential part of petroleum resource potential assessment in less explored sedimentary basins or new conceptual plays in well explored basins, where there are no publically available kinetics parameters. The use of analog source rock kinetics based on similarity of kerogen types and organofacies may jeopardize the reliability of reconstructed petroleum generation history because source rock generation kinetics can vary considerably for the same type of kerogen [13,14,17,20,23]. Rock-Eval analytical data exist for many basins and contain information about hydrocarbon generation kinetics. We may use the information in archived Rock-Eval data to constrain the kinetic model derived from analogues.

By assigning an activation energy distribution and frequency factor based on a single immature sample, the traditional approach may not be representative and ignore organofacies changes. The objective of this study is to discuss a complementary method for studying hydrocarbon generation kinetics in basins, where no immature samples are available, using widely available and spatially representative Rock-Eval data. We propose kinetics inversion of Rock-Eval data to infer the distribution of activation energies directly from Tmax-HI data pairs employing an optimization algorithm. We validate the method using a synthetic dataset and then demonstrate its application through a real case study from the Devonian Duvernay Shale in the Western Canada Sedimentary Basin.

2. Methodology

2.1. Theoretical background

Burnham and Braun [25] reviewed a variety of kinetic methods that have been developed for analyzing complex chemical reactions and outlined the important characteristics of the various models with guidance in model selections. Like most other chemical reactions, the rate of hydrocarbon generation from kerogen in source rocks is temperature-dependent, and the rate constant, $k(T)$, can be approximated by the Arrhenius equation though other alternative equations for the rate constant are also available [3]:

$$k(T) = A \cdot \exp\left(-\frac{E_{act}}{RT}\right) \quad (1)$$

where A is the pre-exponential or frequency factor, E_{act} the activation energy, R the gas constant, and T the absolute temperature.

The rate of chemical reactions can be expressed as follows:

$$\frac{dx}{dt} = k(T)f(x) = A \cdot \exp\left(-\frac{E_{act}}{RT}\right) \cdot f(x) \quad (2)$$

Hydrocarbon generation from source rocks in the subsurface has been approximated in the laboratory through pyrolysis of rock samples at ramped temperatures. Assuming a constant heating rate ($\xi = \frac{dT}{dt}$) the rate of kerogen transformation can then be related to the temperature in the following form:

$$\frac{dx}{dT} = \frac{1}{\xi} k(T)f(x) = \frac{A}{\xi} \cdot \exp\left(-\frac{E_{act}}{RT}\right) \cdot f(x) \quad (3)$$

where $f(x)$ is a mathematic function of x , representing the amount of kerogen. Normally, we assume a pseudo first-order reaction for $f(x)$ for hydrocarbon generation kinetics in basin and petroleum system modeling. Eq. (3) cannot be integrated in a closed form and a common approximation for the kinetic integral, with an assumption of an Arrhenius dependence to $k(T)$, is used [3,24–27],

$$\int_0^t k(T)dt \approx \frac{A \cdot R \cdot T^2}{\xi \cdot E_{act}} \left(1 - \frac{2RT}{E_{act}} + 6\left(\frac{RT}{E_{act}}\right)^2\right) \exp\left(-\frac{E_{act}}{RT}\right) \quad (4)$$

By applying a first-order reaction in Eq. (4), we have:

$$x = 1 - \exp\left(\frac{-ART^2}{\xi \cdot E_{act}} \left(1 - \frac{2RT}{E_{act}} + 6\left(\frac{RT}{E_{act}}\right)^2\right) \exp\left(-\frac{E_{act}}{RT}\right)\right) \quad (5)$$

We compared the results from the approximation using Eq. (4) with those from numerical integration by Eq. (3). The differences are in the order of 1/1000 for activation energy ranging from 40 to 70 kcal/mol commonly found for various kerogens in source rocks, which are far less than the uncertainty range of remaining generation potential indicated by the variance of GSC laboratory standard sample 9107 [28].

Pyrolysis reaction results may not always be adequately approximated by using a simple value of activation energy. To overcome this difficulty, a finite set of independent parallel first-order reactions [25,29] characterized by a spectrum of activation energies was introduced to the equations. The cumulative amount of hydrocarbons generated at temperature T is the sum of the contributions from each individual kerogen component of distinct activation energy:

$$x = x_0 \int_0^\infty \exp\left[-\frac{A}{\xi} \cdot \int_0^T \exp\left(-\frac{E_{act}}{RT}\right) dT\right] D(E)dE, \quad (6)$$

where $D(E)$ is a density function representing the relative abundances of various kerogen components with specific ranges of acti-

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