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Review article

Guidelines for kinetic input to petroleum system models from open-system pyrolysis

K.E. Peters[a,*], A.K. Burnham[b,c], C.C. Walters[d], O. Schenk[e]

[a] Schlumberger, 18 Manzanita Place, Mill Valley, CA 94941, USA
[b] Department of Geological Sciences, Stanford University, 450 Serra Mall, Stanford, CA 94305, USA
[c] Department of Energy Resources Engineering, Stanford University, Green Earth Sciences Building, 367 Panama Street, Stanford, CA 94305, USA
[d] ExxonMobil Research and Engineering Company, 1545 Route 22 East, Annandale, Clinton, NJ 08801-0998, USA
[e] Schlumberger Center of Excellence for Petroleum Systems Modeling, Ritterstraße 23, D-52072 Aachen, Germany

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ABSTRACT

Reliable basin and petroleum system models (BPSM) require accurate kinetic parameters for the conversion of source-rock kerogen to petroleum. The purpose of this paper is to dispel widespread uncertainty about kinetic input to BPSM by providing guidelines based on interpretation of previously published data for 81 worldwide source rocks containing various kerogen types.

• Kinetic response is unrelated to kerogen type as defined by Rock-Eval pyrolysis hydrogen index. Default kinetics in BPSM software may differ from that for the same kerogen type in different study areas. Use default kinetics with caution when appropriate measured kinetics are unavailable.

• Measure kinetic parameters using thermally immature equivalents of the source rock, which may require multiple samples because kerogen kinetics can vary laterally and vertically in each source rock.

• Descriptions of depositional environment are insufficient to define kerogen type or kinetic response in different basins.

• Optimize multiple-run programmed pyrolysis results for both the activation energy (E_a) and frequency factor (A). Assuming a universal value of A rather than optimizing both E_a and A can yield temperature errors of 20 °C or more when extrapolated to geologic time.

• Alternative kinetic models to calculate vitrinite reflectance (R_o) may be more accurate than Easy%R_o for BPSM calibration. In the Aurora-1 and Inigok-1 wells in Alaska, Basin%R_o and Easy%R_oDL, more accurately replicates the dogleg in vitrinite reflectance versus depth commonly observed in wells at depths corresponding to ~0.7–1.0% R_o.

1. Introduction

Computerized BPSM provides useful exploration information for conventional and unconventional resources when accurate kinetic parameters for the thermal decomposition of source-rock kerogen to oil and gas are available (Hantschel and Kauerauf, 2009). Kerogen consists of the insoluble particulate organic matter of various origins in sedimentary rocks. The purpose of this paper is to increase awareness among modelers and geochemists regarding some myths and realities of kinetic input and calibration. The kinetic guidelines provided in this paper are critical for preparation of more accurate and reliable models.

1.1. Fundamentals of petroleum generation kinetics

The transformation of kerogen to oil and gas during burial of petroleum source rocks proceeds through a series of quasi-irreversible reactions controlled by first-order chemical kinetics. The assumption of independent first-order reactions may be oversimplified (Stainforth, 2009), but kinetic models based on this assumption yield predictions that appear to be supported by observations of source rock maturation in nature. Mathematical modeling of this complex process requires simplified kinetic concepts in which fractions of product yields replace precise molecular compositions (Tissot and Espitalié, 1975). Extrapolation of kinetic measurements from short-term pyrolysis experiments to geologic time requires that the same or similar reactions occur under both conditions (e.g., Braun and Burnham, 1990; Ungerer, 1993;

* Corresponding author.
E-mail addresses: kpeters2@slb.com (K.E. Peters), aburnham@stanford.edu (A.K. Burnham), clifford.c.walters@exxonmobil.com (C.C. Walters), OSchenk@slb.com (O. Schenk).

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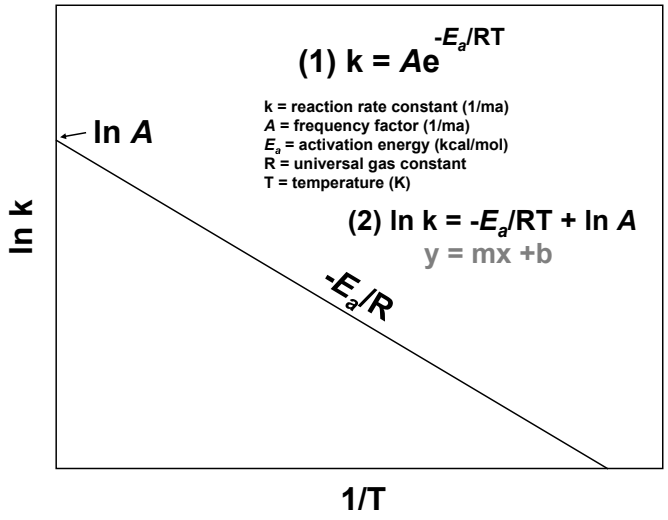

Fig. 1. The rate of a simple chemical reaction increases exponentially with increasing temperature as described by the Arrhenius equation (1). The logarithmic form of the Arrhenius plot (2) helps to explain ln A and $-E_a/RT$. Higher T and lower E_a favor fast rates for chemical reactions. Because kerogen is heterogeneous, the usual simplification in BPSM software comprises a distribution of E_a values (discrete activation energy distribution) at 1-kcal/mol intervals with a common A that applies to all components in the thermal transformation of kerogen to petroleum (Fig. 2).

Schenk et al., 1997). Documented validations of the predictive value of laboratory-based kinetic models include: (1) studies of the generative potential of kerogen at different levels of maturity induced by hydrous pyrolysis (e.g., Burnham et al., 1995; Barth et al., 1996) and (2) studies along transects of increasing maturity in the same source rock (e.g., Ungerer, 1990; Schenk and Horsfield, 1998).

1.2. Kerogen types

This paper identifies several common misconceptions about bulk petroleum generation (oil and hydrocarbon gas) and kinetic input to BPSM (E_a and A; Fig. 1). The first misconception concerns kerogen type. Kerogen is heterogeneous and represents a mixture of components with unique Arrhenius parameters for reactions that proceed in parallel. Kerogen Types I, II, II/III, III, and IV (very oil-prone, oil-prone, oil and gas-prone, gas-prone, and inert) have Rock-Eval pyrolysis hydrogen index (HI) values of > 600, 300–600, 200–300, 50–200 and < 50 mg hydrocarbons (HC)/g total organic carbon (TOC), respectively (Peters and Cassa, 1994). Examples of sulfur-rich kerogens include Types IS and IIS (Orr, 1986; Peters et al., 1996).

Although some papers suggest that kinetic response can be predicted from kerogen type as defined by Rock-Eval pyrolysis hydrogen index (HI, mg hydrocarbons/g TOC; e.g., Pepper and Corvi, 1995), we show that there is no systematic link between kerogen type and kinetic response (Peters et al., 2006). Large ranges of kinetic response can characterize each kerogen type. For example, Type II kerogen from one basin may not respond to maturation in the same way as Type II kerogen from another basin because the chemical bonds and their thermal reactivity may differ (Tegelaar and Noble, 1994). Furthermore, simple descriptions of the source rock depositional environment cannot reliably predict kinetic behavior. For example, lacustrine source rock may contain virtually any kerogen type (e.g., I, IS, II, IIS, II/III, III, IV; e.g., Wanli et al., 1985; Horsfield et al., 1994). Default kinetics for kerogen in BPSM software obtained using source rocks from other basins can introduce unacceptable errors into numerical simulations of petroleum generation in a studied basin. Kinetic parameters measured on thermally immature equivalents of the source rock may be more accurate than default kinetics based on another source rock, but may be inadequate to account for organofacies variations, which result in lateral and vertical differences in kinetic response. Organofacies are portions of a rock unit that contain a distinct assemblage of organic matter without regard to the mineralogy (Jones, 1987).

Multi-component kinetics based on the PhaseKinetics method (di Primio and Horsfield, 2006) can be used to predict detailed fluid compositions and properties (e.g., Baur et al., 2012), but is not discussed further here. When assigning bulk kinetic parameters to source rock using BPSM software, modelers must (1) select default kerogen decomposition kinetics from a list of stored measurements from various publications, or (2) use their own measured kinetics. Kinetic measurements generally require laboratory experiments on thermally immature stratigraphic equivalents of more deeply buried, thermally mature source rock. These samples must have undergone diagenesis and lithification, but they must remain thermally immature (i.e., no significant catagenesis). Stored default kinetic values are from standard source rock or kerogen samples that may or may not behave like those from a given study area, whereas measured kinetics use one or more samples collected from the study area. Both approaches involve uncertainty. For example, the organofacies of the source rock that generated and expelled petroleum in the thermally mature part of the study area may differ from a thermally immature stratigraphic equivalent selected for kinetic analysis.

1.3. Open-system vs. other pyrolysis kinetics

First-order kinetics based on hydrous pyrolysis (e.g., Lewan and Ruble, 2002) yields only one activation energy and frequency factor that cannot adequately represent the thermal decomposition of

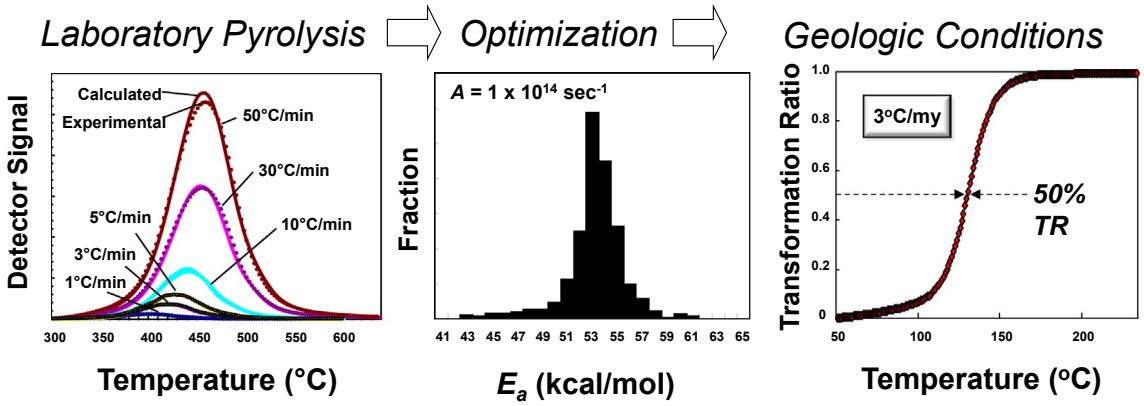

Fig. 2. Discrete activation energy (DAE) modeling requires optimization of both E_a and A to determine the rate of kerogen decomposition at any laboratory temperature. The "compensation law" shows that many combinations of E_a and A satisfy the Arrhenius equation for the laboratory rate constant, but extrapolation of inaccurate E_a and A to geologic time gives incorrect temperature predictions.

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