Research paper

A data driven model for studying kerogen kinetics with application examples from Canadian sedimentary basins

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ABSTRACT

Source rock is an essential element in unconventional resource play evaluation, while kerogen kinetics is one of the most important components in source rock evaluation. Traditional approach for determining oil generation kinetics is done through laboratory pyrolysis analysis by mimicking the hydrocarbon generation processes with variable accelerated heating rates, thus the thermal energy required for hydrocarbon generation under geological conditions is inferred. Study suggests that for a given kerogen type, numerical kinetic models derived from a limited number of laboratory tests may result in unacceptable errors because of under-representation of variation in activation energy related to organic facies change and source rock heterogeneity. As economic margin of developing an unconventional resource play can be small, business success often depends on early identification of favourable area. A quick and robust method for resource play evaluation is critical. This study proposes a data driven statistical approach that utilizes existing Rock-Eval/TOC data by fitting the measured hydrogen index and Tmax to an exponential model. The model is designed so that all parameters have an explicit physical meaning and the ranges of parameter values are predictable. Once the empirical statistical model is established, hydrocarbon transformation ratio can be calculated to represent the hydrocarbon generation kinetics of the source rock. The main advantage of the proposed approach is the utilization of widely available Rock-Eval datasets so that 1) no additional specifically designed laboratory pyrolysis experiments are required; 2) the uncertainty due to facies variation or source rock heterogeneity (nature) and poor data quality (human) can be quantified through the statistical analysis of a large dataset; and 3) validation for temperature and geothermal rates, *in situ* pressure and other environmental conditions is not necessary as the input data for the model are all based on naturally matured samples. Rock-Eval datasets from four well-known Canadian source rock intervals, representing the most common kerogen types, are tested and used as examples to demonstrate the application of the proposed method. The examined source rocks with different kerogen types show distinct kinetic behaviours, and this is consistent with models derived from laboratory tests. Applications also indicate that the proposed method appears to be robust and convenient for modelling kerogen kinetics from Rock-Eval data directly.

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1. Introduction

Kerogen kinetics is important in resource evaluation for better understanding the thermal maturation of potential source rock and bulk composition of hydrocarbons (e.g., Dieckmann et al., 2004; Eseme, 2006; Lehne and Dieckmann, 2007; Kuhn, P. P., 2013), and are essential in petroleum system and basin modelling (Kuhn et al., 2012; Romero-Sarmiento et al., 2013). With gradual depletion of

conventional hydrocarbon resources and advancing in drilling and completion techniques, development of unconventional petroleum resources in low porosity and permeability tight reservoir has been playing an increasingly important role in adding energy supply to the market in North America and elsewhere. The traditional source rock in a conventional petroleum system becomes a self-sourced reservoir after being hydraulically fractured. As economic margin of developing such an unconventional resource play could be small, business success often depends on early identification of favourable area, and a quick and robust method for resource play evaluation is critical. While the quality, quantity and maturity of organic-rich shale/mudstone are the three key criteria in resource potential

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evaluation of the unconventional shale oil and gas plays (Jarvie, 2012a, b; Modica and Lapierre, 2012; Romero-Sarmiento et al., 2013), kinetic properties of the source rock are essential for characterizing the quality and thermal maturation of a source rock reservoir.

Hydrocarbon generation kinetics is usually determined in laboratory by exposing source rock samples of interest to high temperatures to accelerate the thermal conversion of kerogen to hydrocarbon. Kinetic parameters determined at these high temperatures are then extrapolated back to the geological conditions believed to exist at the time of hydrocarbon generation (Freund et al., 1993). As laboratory conditions such as temperature, pressure and fluid confinement may not be the same as the *in situ* subsurface setting, validation of the laboratory results against the environmental conditions over a wide range of temperatures and pressures has often resulted in controversial conclusions, especially as to whether or not pressure affects kerogen kinetics (Freund et al., 1993; Sajgo et al., 1985; Price and Wenger, 1991; Carr, 1999; Tian et al., 2008). On the other hand, although source rock kerogen can be arbitrarily classified as Type I, II or III based on their Rock-Eval hydrogen index (HI) values or their H/C ratios, such a classification is designed for appraisal of ultimate generation potential. Organic maters with similar generation potential may not show the same hydrocarbon generation kinetics because of differences in their molecular structure. There is a large variation in these hydrocarbon potential parameters among the source rocks containing the same type kerogen, and there are always overlapping transitional zones between kerogen types. As a result, no clear correlation can seem to be defined between classical kerogen types and measured kinetic parameters (Tegelaar and Noble, 1994). When applied to a source rock unit of different geological settings, such numerical hydrocarbon generation kinetic models as based on programmed laboratory pyrolysis experiments on limited number of source rock samples of pre-determined kerogen types can often introduce unacceptable errors (Peter et al., 2006).

Kerogen decomposition and hydrocarbon generation in a source rock progress with increasing burial and thermal exposure mainly due to the C−C bond cleavage under thermal stress. At shallower depths and lower geothermal conditions, weaker C−C bonds with lower activation energy in the long chain aliphatic structures are broken first, resulting in generally heavier hydrocarbon fluids in the early stage of oil window. With the advancing of the oil generation, stronger C−C bond with higher activation energy such as those in the short aliphatic chains and those connecting aromatic rings will be broken by the increased thermal stress at deeper burial, leading to lighter and more gaseous hydrocarbon fluids at late stage of oil window and in the gas window. This is reflected as upward shifting of activation energy over thermal maturation for a source rock. Jarvie (1991) demonstrated this by artificially maturing an immature Monterey sample. Nordeng (2014) noticed that average activation energy is positively correlated with Rock-Eval Tmax for the Ordovician Red River Formation source rocks in Williston Basin. This implies that for the same source rock, hydrocarbon generation rate can be indexed as a function of thermal maturation to represent the kerogen kinetics using Rock-Eval data directly.

Rock-Eval/TOC analysis and data interpretation provide a quick, fast and easy way in source rock evaluation (Peters, 1986; Bordenave et al., 1993). Major geochemical parameters obtained from Rock-Eval analysis include a) TOC (total organic carbon, in wt %) for the content for organic matter; b) S1 peak (mg HC/g Rock) for the amount of free hydrocarbons in the rock sample; c) S2 peak (mg HC/g Rock) for the amount of hydrocarbons that can be generated from a source rock upon further heating/burial; d) Tmax, a measure of the temperature at the maximum of S2 peak, for the thermal maturity of the sample; e) Hydrogen index HI (mg HC/g TOC) and

oxygen index OI (mg CO2/g TOC) for kerogen type classification. Typically, a Type I kerogen is assigned to immature source rocks with an HI > 700; Type II kerogen for immature source rocks with an HI between 400 and 700; and Type III kerogen if a source rock's HI < 400 (Bordenave et al., 1993). As the HI values of source rocks decrease with increasing thermal maturity due to hydrocarbon generation, the pathways of the variation of hydrogen index with Tmax have been used to measure the quality (type of kerogen) of source rock. With HI representing the hydrocarbon generating capacity of a source rock at certain maturity and Tmax being an indicator of how easy its kerogen can be further converted to hydrocarbons, the relationship between HI and Tmax also demonstrates the kinetic behaviour of the source rock, which is often expressed as hydrocarbon transformation ratio (Peters et al., 2005; Justwan and Dahl, 2005). When data cover the entire temperature range of hydrocarbon generation, the characteristics of oil generation kinetics can be derived from the data. Banerjee et al. (1998) provided a mathematical equation for fitting Rock-Eval hydrogen index and Tmax, but did not discuss its potential application to hydrocarbon generation kinetics characterization.

In this article, we propose a simple statistical approach to characterize oil generation kinetic property of organic matter using Rock-Eval/TOC data directly. Four real datasets from different Canadian sedimentary basins, representing the most common kerogen types, are tested and used as examples to demonstrate the application of the proposed method.

2. Methods

The proposed method utilizes the most commonly available geochemistry data from Rock-Eval/TOC analysis, and thus is a data driven method. This means that the kinetic property of the kerogen under investigation is quantitatively described by real data and no assumption is made regarding the geochemical property (e.g. maceral composition, type of organic matter) of kerogen under examination and the geological conditions of the source rock being investigated. However the statistical approach is based on the belief that the hydrocarbon generation (or transformation/conversion/decomposition) kinetics of kerogen in a given source rock can be characterized by its reaction path along thermal maturation, and this is best represented by natural samples from the same source rock unit with different thermal histories.

In our data driven model, the hydrocarbon generation profile is represented by the variation of hydrogen index HI as a function of thermal maturity index Tmax in the following form:

$$H_I = H_I^o \left[1 - \exp\left\{ -\left(\frac{T_{max}}{\beta}\right)^{\theta} \right\} \right] + c \tag{1}$$

where H_I^o is the initial hydrogen index, β and θ are unknown parameters specific to kerogen kinetics, and C is a constant indicating the magnitude of error in the measured hydrogen index at very high Tmax. By fitting the above relationship with a set of Rock-Eval data generated on a source rock unit covering the whole range of thermal maturation, an optimal H_I^o, β, θ and C can then be derived to characterize the hydrocarbon generation history, including the onset of oil generation, the width of oil window, and ultimate amount of hydrocarbon to be generated. This fitting practice is demonstrated in Fig. 1. From Eq. (1), it can be seen that HI = 0.63H_I^o when the Tmax equals β. This may suggest that the parameter β represents a Tmax value that corresponds to the beginning of massive hydrocarbon generation (>30%), and therefore is a reflection of the activation energy level required for initiating massive thermal decomposition of the kerogen. θ is a shape parameter and
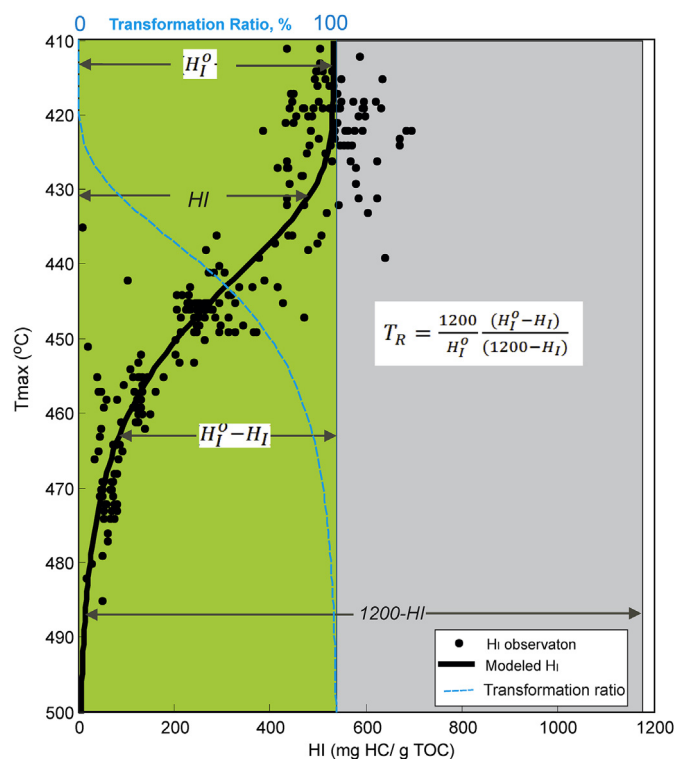
Fig. 1. A diagram showing the relationship between thermal history and hydrocarbon generation in terms of remaining hydrocarbon potential and transformation ratio of the source rock. Data points plotted are from Rock-Eval analysis on the Upper Devonian Duvernay Shale samples of Western Canada Sedimentary Basin. Tmax: thermal maturity indicator; Hydrogen index H_I: hydrocarbon generation potential; H_I^o original or initial hydrogen index; T_R: transformation ratio. Green and grey areas for generative organic carbon and inert carbon respectively.

is related to the width of hydrocarbon generation window or the distribution of activation energy of kerogen. It indicates the variability of maceral composition or chemical structure in the kerogen. If kerogen comprises various distinct organic macerals, the range of activation energy for thermal decomposition varies considerably, leading to a large range of Tmax for the hydrocarbon generation window. In contrast, a kerogen of unitary maceral composition will display a narrow distribution of activation energy for the thermal decomposition (Wang et al., 2011) and therefore shows a narrow range of Tmax (Bordenave et al., 1993). Therefore, the smaller the θ is, the more unitary structures the kerogen contains.

Hydrocarbon generation rate of a source rock is determined by its kerogen kinetics and is usually expressed as transformation ratio (T_R) that measures the degree of kerogen thermal decomposition or conversion. There are numerous ways to estimate the transformation ratio (Bordenave et al., 1993; Jarvie et al., 2007; Modica and Lapierre, 2012; Justwan and Dahl, 2005; Peters et al., 2005). In this paper, the transformation ratio is expressed as a function of hydrogen index. The derivation of the relationship is referred to Chen and Jiang (under review):

$$T_R = \frac{1200}{H_I^o} \frac{(H_I^o - H_I)}{(1200 - H_I)} \qquad (2)$$

where H_I is the present day hydrogen index obtained from Rock-Eval analysis, and H_I^o is the initial hydrogen index of the source rock before hydrocarbon generation and can be obtained through data fitting using Eq. (1). In Eq. (2), an assumption is made on an average of 83.3% carbon in the generated hydrocarbon (i.e., with a

hydrogen index of 1000*1/0.833 = 1200) for organic matter in the source rock samples.

By applying both Eq. (1) and (2) to a Rock-Eval dataset, a hydrocarbon transformation ratio vs maturity (i.e. T_R vs T_{max}) profile can then be obtained. Fig. 1 is an example of the data fitting and hydrocarbon transformation calculation from the Rock-Eval data on the Devonian Duvernay shale source rock unit in the Western Canada Sedimentary Basin. In addition to the modelled hydrogen index (HI) profile (solid black line), the modelled hydrocarbon transformation profile (dashed blue line) is also shown in Fig. 1.

3. Application examples

In this study, Rock-Eval datasets generated on four different Canadian source rock units containing three different kerogen types, I, II and III are used to illustrate the application of the proposed method for kinetic model construction and compare the kinetics of different types of kerogen.

3.1. Data sources and quality screening

The Rock-Eval data used in this study are from publically available data and the Geological Survey of Canada's in-house geochemistry database which consists of Rock-Eval analytical results produced by GSC's geochemistry laboratory during the last 40 years or so. The four datasets include the historical Rock-Eval analytical results on the Ordovician Yeomen kukersite samples from the Williston Basin, the Devonian Duvernay carbonaceous shale samples from the Western Canada Sedimentary Basin (WCSB), the Jurassic Nordegg shale samples from the WSCB, and shale/mudstone samples from terrestrial Tertiary Aklak Sequence of the Beaufort − Mackenzie Basin in Canadian Arctic region (Fig. 2).

Many factors could affect the quality of Rock-Eval data. Type of samples, such as cores, drill cuttings or outcrops, has a direct effect on the analytical results due to varying status of organic matter preservation. Contamination from drilling fluid additives can result in erroneous readings by Rock-Eval if not collected and prepared appropriately. The presence of a large amount of volatile hydrocarbon component in the sample can cause "depression" to the Tmax value (Snowdon, 1995). In addition, a normal loading of extremely organic-rich sample may result in incomplete combustion of organic matter in the Rock-Eval instrument furnace, leading to a reduced TOC measurement. All these factors may potentially introduce large variation and uncertainty to the analytical results. To eliminate the effect of poor quality data on the interpretation, the data have been scrutinized carefully in this study. Depending on the type of kerogen, different screening filters are applied to different datasets to ensure the data quality and minimize the uncertainty in model construction.

3.2. Devonian Duvernay shale

The Devonian Duvernay shale is one of the major contributors to conventional oil and gas accumulations in Devonian reef plays in the Devonian petroleum system of WCSB, and is also a proven liquid rich shale gas play in North America (Macedo, 2013). It has been extensively described by Stoakes and Creaney (1984, 1985), Creaney (1989, Creaney and Allan (1990), and Allan and Creaney (1991); Chow et al. (1995) and Stasiuk and Fowler (2002, 2004). The Duvernay shale is the basinal time-equivalent of Leduc reef growth during the Frasnian and comprises a sequence of dark brown to black, bituminous, slightly argillaceous carbonates interbedded with gray−green, calcareous shales. It was deposited under marine, deep-water, low-energy, basinal conditions surrounded by reefs and carbonate platforms. These sediments are
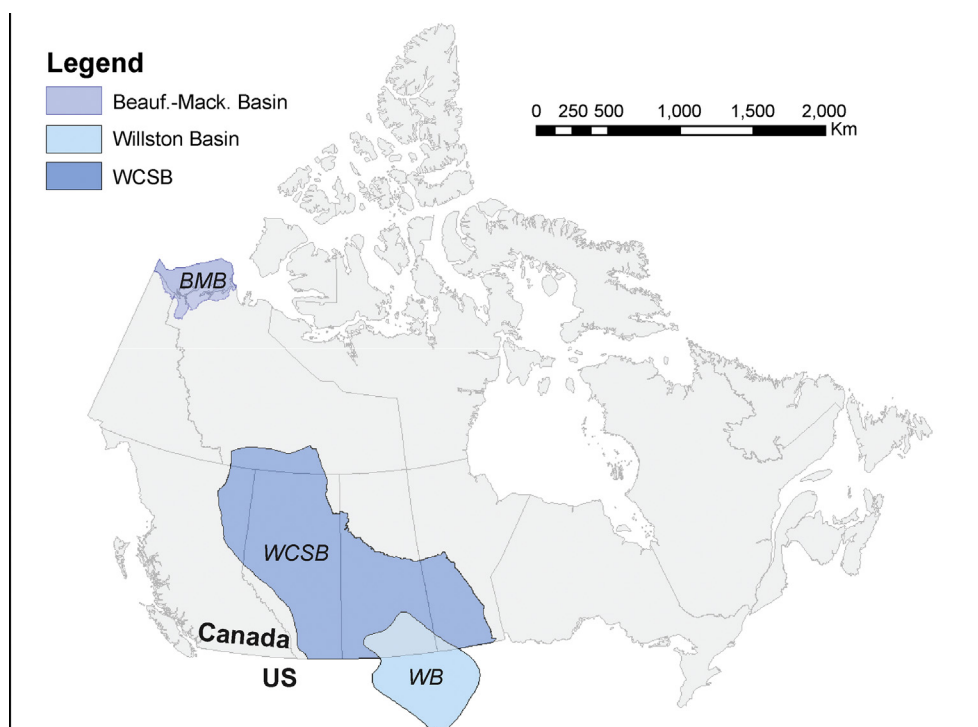
Fig. 2. Map showing Canadian sedimentary basins and locations of the example basins in this study.

characteristically organic-rich, with total organic carbon (TOC) values of up to 15% and maximum hydrogen index close to 700 mg HC/g TOC, and exhibit plane-parallel, millimetre-scale lamination (Creaney et al., 1994). Duvernay-sourced oils are low in sulphur (less than 0.5%) and have pristane/phytane ratios of 1.5–2.4, indicating source deposition in normal marine salinities in an oxygen-poor environment. Thermal maturation data show a large variation from immature to over-mature (Stasiuk and Fowler, 2002, 2004).

Data used in this study consist of Rock-Eval analytical results on core samples from 25 wells compiled by Alberta Geological Survey (Beaton et al., 2010) and additional GSC in-house Rock-Eval data on 60 wells, a total of 642 samples covering large part of the Duvernay shale basins in Alberta. To eliminate the potential effect of poor quality data on the analysis, the data were culled carefully by removing those with a TOC < 1.5%, and/or Tmax < 400 °C and/or S2 < 0.5. This resulted in a removal of 290 samples that were considered to be unreliable due to low TOC values or erroneous Tmax values.

Fig. 3a is a plot of hydrogen index against Tmax showing the kerogen kinetic characteristics of the Duvernay source rocks. A general trend of hydrocarbon generation potential with Rock-Eval Tmax temperature is clear from this diagram. The dataset was fitted by Eq. (1), producing an optimal quantitative trend of hydrogen index with increasing Tmax for the Duvernay dataset (solid black line in Fig. 3a). Also shown in Fig. 3a is the standard deviation interval as uncertainty measure of the model (dotted black line) associated with hydrocarbon generation potential forecast in Duvernay Formation. The residuals, defined as the difference between observed and modelled hydrogen index in Fig. 3b show a bell shaped histogram (approximately normally distributed). The distribution of the residuals is symmetric and centred around zero, indicating an unbiased model. Fig. 4a shows the residuals and the standard deviation as a function of Tmax of the model, showing that a) uncertainty changes with thermal maturity; and b) the residuals are statistically distributed around

zeros, an indication of an unbiased empirical model for the hydrocarbon generation potential. All estimated model parameters are given in Table 1. The parameter β = 440 may suggest the beginning of massive hydrocarbon generation for Duvernay shale. A transformation ratio profile can be then derived from Eq. (2) in combination with the established empirical numerical model in Eq. (1), showing the kerogen kinetic character of the Duvernay Shale for the purpose of quantitative source rock evaluation (Fig. 4b).

3.3. Jurassic Nordegg shale

The Nordegg Member of the Lower Jurassic Fernie Formation is a highly oil-prone marine source unit and consists of dark brown to black, variably phosphatic marlstone and calcareous mudstone, and shows very high gamma-ray response on geophysical logs. The Nordegg member rests uncomformably on Triassic and older formations and acts as both source and top seal for some conventional hydrocarbon accumulations, and is believed to be one of the major contributors to the liquid rich tight gas unconventional reservoirs in the Triassic Montney Formation in the WCSB. The "Nordegg" Member undergoes a facies change to a more proximal, brecciated and in part karsted chert- and sand-rich lithofacies. It contains up to 35% (wt) TOC with an average value of 7.98%. The hydrogen indices (HI) are commonly around 700 mg HC/g TOC for the immature samples and decreases with increasing Tmax once entering oil generation window (Fig. 5a).

The Rock-Eval data are from GSC in-house geochemistry database. Quality control screening criteria include Tmax > 400 °C, TOC > 1.0% and/or S2 > 0.5 mg HC/g TOC. The scrutinized data are plotted in Fig. 5a as HI vs Tmax together with the fitted empirical model, and the transformation ratio profile is displayed in Fig. 5b. The Nordegg shale source rocks show typical characteristics of type I to II kerogen, or a special type of sulphur-rich type II (II–S) kerogen. The determination of whether the Nordegg source rock is
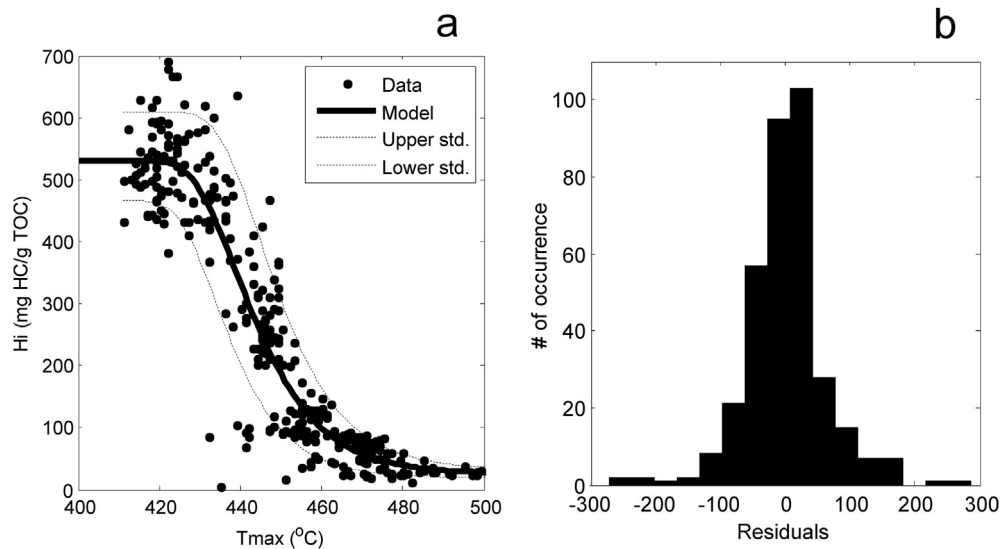
Fig. 3. (a) Rock-Eval data and fitted empirical model of hydrocarbon generation potential represented by hydrogen index HI vs thermal maturity Tmax for Duvernay shale together with the model uncertainty represented by an interval of standard deviation of the residuals (Upper std. and Lower std.); (b) The residuals (differences between the observation and prediction) shows uncertainty of the empirical model prediction in hydrogen index of the Devonian Duvernay Formation.
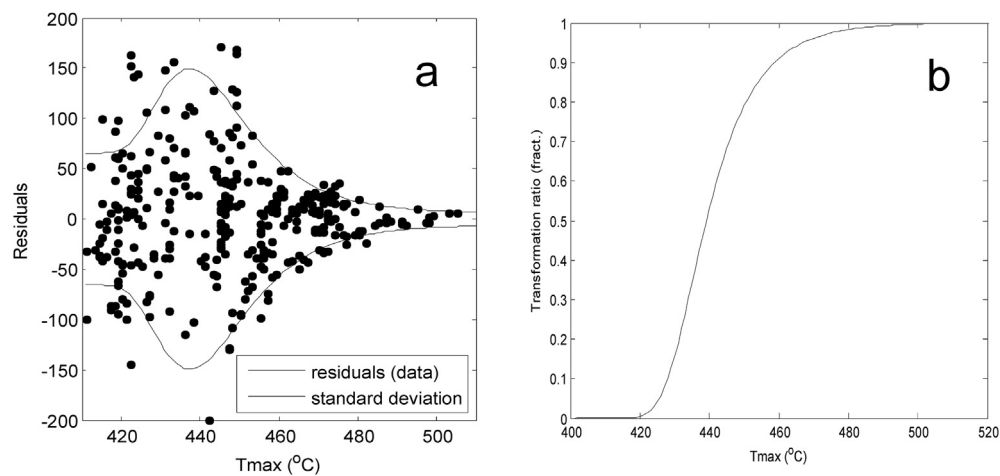

Fig. 4. A plot of residuals as a function of Tmax superimposed with uncertainty model of sample standard deviation (a); The standard deviation model is calculated from the residual data using a window length of 20 °C Tmax and incremental step of 1 °C Tmax. Hydrocarbon transformation ratio derived from the statistical model for Duvernay shale source rocks (b).

a Type II-S kerogen requires further geochemical analysis. The model parameters from the statistical fit are also listed in Table 1. It has a β value of 439, similar to the Duvernay, but a more negative θ value of −60 compared with that of −40 for the Duvernay shale.

3.4 Ordovician Red River formation

The source rock laminae, termed Kurkeriste in Red River formation of Yeomen Group in the Williston Basin has a TOC up to 35% and hydrogen indices (HI) in the range of 700−1000, but mostly > 900 mg HC/g TOC. The organic matter is typical Type I and composed dominantly of *Gloeocapsomorpha prisca* (Osadetz and Snowdon, 1995). The Ordovician petroleum system is largely a closed system in Canada with migration having taken place over relatively short lateral distances and vertically confined by extensive anhydrite seals. Discoveries were made in the Red River formation on both US and Canada sides of the Williston Basin.

Table 1
Summary of model parameters of the four source rocks for determining the hydrocarbon generation potential (hydrogen index) as a function of Tmax.

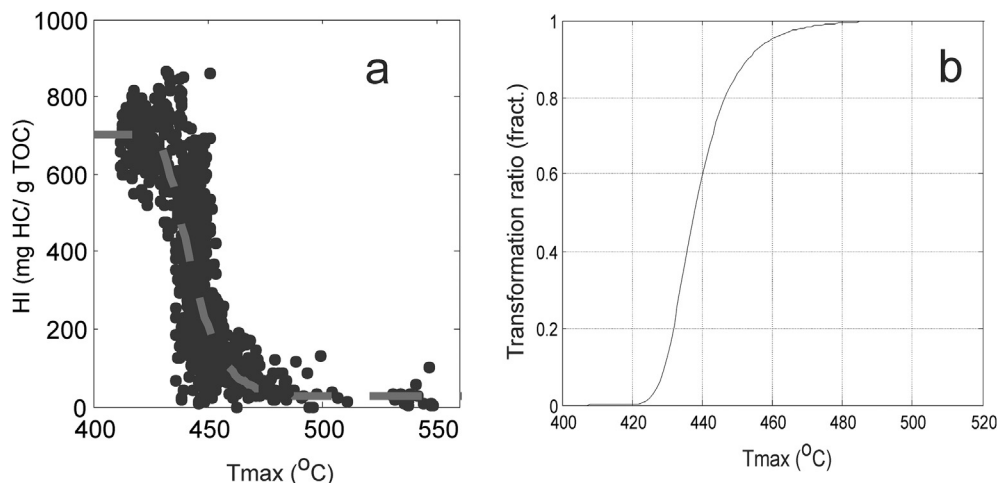| Formation	Basin	Age	β	θ	H_I^o	C	Kerogen type
Yeomen Fm	Williston	Ordovician	455	−120	900	20	I
Duvernay Fm	WCSB	Devonian	440	−40	506	25	II
Nordegg Fm	WCSB	Jurassic	439	−60	665	35	I + II or (IIs?)
Aklak Fm	Beaufort−Mackenzie	Tertiary	422	−42	180	15	III

Fig. 5. (a) Rock-Eval data and fitted empirical model of hydrocarbon generation potential represented by hydrogen index vs thermal maturity Tmax for Nordegg shale; and (b) Hydrocarbon transformation ratio derived from the empirical model for Nordegg source rocks.

The data used in this study are primarily from the Geological Survey of Canada Bulletin 487 (Osadetz and Snowdon, 1995) on Canadian Williston Basin with some data points from a recent public presentation by Nordeng (2014) on the North Dakota part of US Williston Basin. This is a relatively small dataset with samples covering maturity from immature to early mature. This example serves two purposes: a) demonstrating how to construct the kinetic model from limited Rock-Eval analytical results; and b) showing the kinetic characteristics of a source rock unit with predominant type I kerogen. The kinetic properties of the type I kerogen differ from type II and III because this type of kerogen comprises more unitary organic structures that need higher activation energy to start thermal decomposition in general. The Type I kerogen or source rock has a very narrow distribution of, but typically a higher average activation energy. This leads to a delayed onset of oil generation (i.e. Tmax of 445 °C) and a much narrower oil window (i.e., Tmax of 460 °C at the end of oil generation) compared with Type II and Type III kerogen/source rocks.

Data quality screening criteria include TOC > 1.0%, and S2 > 0.5 mgHC/gTOC and Tmax > 420 °C. Data points are plotted in Fig. 6a with the fitted model superimposed. The calculated transformation

ratio from the modelled hydrogen index is displayed in Fig. 6b showing general characteristics of type I source rock of the Red River formation. The model parameters for the empirical model of hydrogen index as a function of Tmax are listed in Table 1. A remarkable feature of the Red River source rock kerogen kinetics is its much higher Tmax for the onset of hydrocarbon generation as reflected by β value of 455, and its very narrow Tmax window (as represented by a θ vale of −120) for thermal decomposition of kerogen.

3.5. Tertiary Aklak formation

The late Paleocene-early Eocene Aklak Sequence of the Beaufort–Mackenzie Basin in the Canadian Arctic region (Fig. 2) was deposited in a shelf/pre-delta environment. The lithology of the Aklak Sequence consists of interbedded sandstone, siltstone and shale with some area containing abundant coal beds (Dixon et al., 1992). The TOC varies from <0.5% to up to 70% with a mean of 2.96% and median of 1.38%. The hydrogen indices (HI) are commonly below 300 mg HC/g TOC.
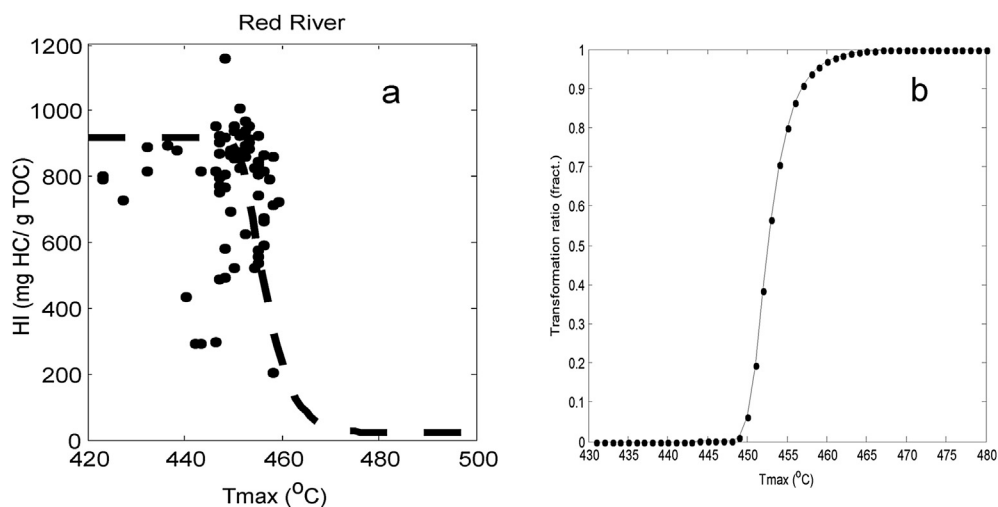

Fig. 6. (a) Rock-Eval data and fitted empirical model of hydrocarbon generation potential represented by hydrogen index vs thermal maturity Tmax for Ordovician Yeomen shale; and (b) Hydrocarbon transformation ratio derived from the empirical model for Yeomen source rocks.

The Rock-Eval data of the Aklak Sequence are from GSC in-house geochemistry database, with majority of the data generated during a recent GSC-industry research consortium project. Quality control screening criteria include Tmax > 380 °C, TOC > 0.5% and S2 > 0.5 mgHC/gTOC. The data used for the kinetic study are plotted in Fig. 7a with the fitted empirical model shown as dashed line. The Rock-Eval data from Aklak Sequence are scattered in a broad range of variation, suggesting a mixing of various organic matters with distinct thermal kinetics. The fitted empirical model represents the average kinetic behaviours of the source rock unit under thermal stresses. The transformation ratio profile derived from the empirical hydrogen index model is displayed in Fig. 7b, showing the average hydrocarbon generation trend of the type III source rock of late Paleocene-early Eocene Aklak Sequence in the Beaufort–Mackenzie Basin. The model parameters estimated are listed in Table 1 as well for comparison with other source rocks. The Aklak source rock has a β value of 425 and a θ value of −42, suggesting a very low onset temperature of oil generation and a broad oil window.

4. Discussion

Fig. 8 compares the modelled or generalized hydrocarbon generation potentials of the four different source rock units based on their Rock-Eval datasets in this study. The Ordovician Yeoman shale (kukersite) containing type I kerogen has the highest potential (i.e., >900 mgHC/gTOC), and the Tertiary Alklak source rock unit has the lowest hydrocarbon generation potential of less than 200, with the Devonian Duvernay and Jurassic Nordegg shales displaying a medium range. The compositional and/or structural features revealed by Rock-Eval data differ significantly for different source rocks, and this is also reflected in their kinetic behaviours as shown by the modelled hydrocarbon generation history (Fig. 9).

The data driven models are comparable with laboratory derived kinetic models for different types of kerogen that responds to thermal stresses differently as shown in Fig. 9. Type I kerogen represented by Yeomen kukersite in this study has an elevated onset temperature of hydrocarbon generation due to a uniform maceral composition or chemical structure that requires higher activation energy to start decomposition. The source rock samples from Yeomen Formation display a Tmax shift of about 15 °C upward as compared with a typical type II normal marine kerogen, such as the Duvernay or the Nordegg samples. Massive oil generation does not start until Tmax reaches 455 °C for Yeoman shale; while typical
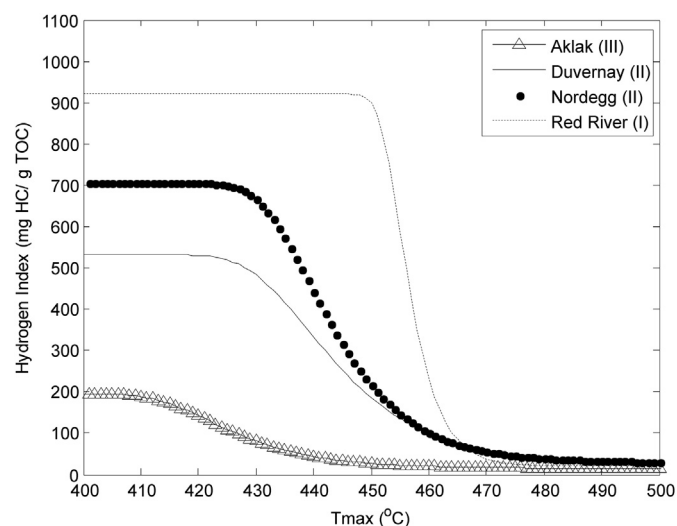

Fig. 8. Present-day hydrocarbon generation potential of different source rock/kerogen types as modelled from their Rock-Eval data. Type I shows highest hydrocarbon generation potential and potential decrease through type II to type III gradually.

marine type II kerogen start to generate significant oil at Tmax 440 °C. In addition, the type I kerogen shows a very narrow temperature window for hydrocarbon generation, with about 80% of thermal decomposition completed within 10 °C of Tmax temperature range. In contrast, typical normal marine type II kerogen shows a significantly broader temperature window for the completion of thermal decomposition (e.g., 80% of hydrocarbon transformation from Tmax of 430–460 °C).

Contrary to previous reports that Type III kerogens typically start to generate hydrocarbons at higher temperatures than Type I and II kerogens (Quigley et al., 1987; Tegelaar and Noble, 1994), the Tertiary Aklak source rock unit from the Beaufort–Mackenzie basin has a much lower β value compared with other three source rocks (i.e. 422 vs 439 and 440 for Nordegg and Duvernay shales, and 455 for Yeomen kukersite; Table 1) and display an onset hydrocarbon generation temperature at Tmax of 410 °C, even lower than that of the Type II Duvernay and Nordgegg shales. This is likely due to the presence of diterpenoid resinite in these deltaic sediments (Snowdon, 1980; Snowdon and Powell, 1982). As a unique maceral derived from higher plants, diterpenoid resinite has been observed being thermally labile and can convert to liquid hydrocarbons at
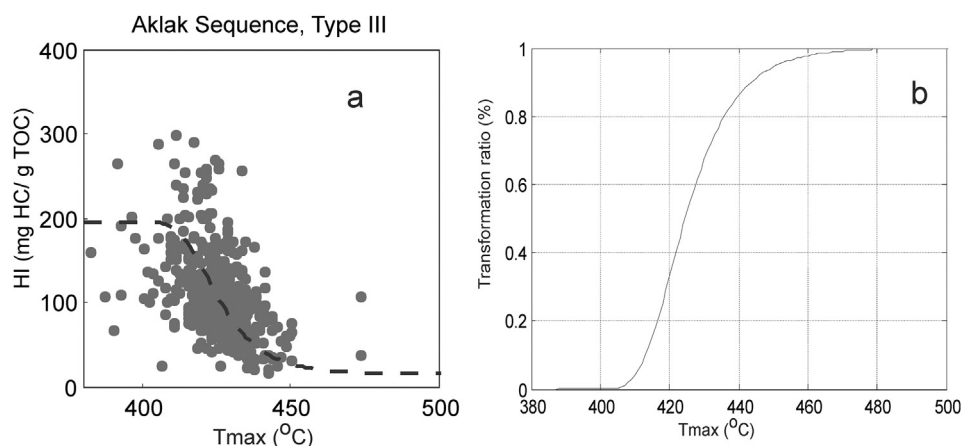

Fig. 7. (a) Rock-Eval data and fitted empirical model of hydrocarbon generation potential represented by hydrogen index vs thermal maturity Tmax for Tertiary Aklak shale; (b) (Hydrocarbon transformation ratio derived from the empirical model for Aklak source rock.
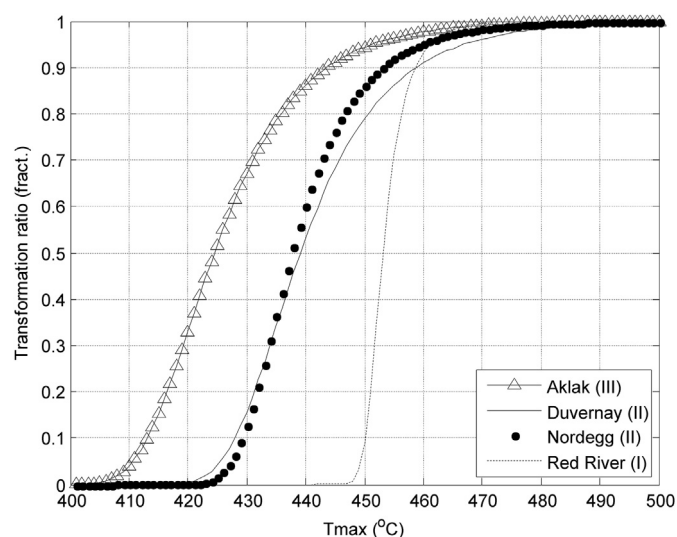
Fig. 9. Comparison of transformation ratio of different types of kerogen source rocks in this study as a function of thermal maturity Tmax. The required thermal energy for decomposing kerogen increases from type III through Type II to type I kerogen.

lower temperature than most types of organic matter (Snowdon, 1991; Tegelaar and Noble, 1994). The Tmax for 95% transformation is at about 450 °C, almost 20 °C lower than 470 °C for the Duvernay shale, suggesting that thermally labile components dominate in the Tertiary Aklak source rock, though other maceral components requiring higher thermal energy to generate hydrocarbons do exist as indicated by the wide range of variation along the fitted model (particularly on the right side) showing a mixing of different types of organic matters. This example demonstrates that hydrocarbon generation kinetic parameters developed for a specific source rock may not be applicable to other source rocks of the same type of kerogen but deposited in different facies and/or with different organic inputs. Therefore, Kerogen type is only an indicator of hydrocarbon generation potential, but not an equivalent of kerogen kinetics.

As a function of thermal maturity, Tmax is reflective of the kinetics of the cracking of organic matter (Bordenave et al., 1993). It is clear from Figs. 8 and 9 that thermal energy (temperature equivalent) required to start the decomposition increases from Tmax of 410 °C for resinite-dominated kerogen, to 430 °C for typical normal marine shale kerogen and 450 °C for kukersite-dominated kerogen (Fig. 9), showing a systematic upward shifting of activation energy from "type III" to "type I" kerogen in this study. This is consistent with the kinetics determined using laboratory pyrolysis of various source rock samples (Sundararaman et al., 1988; Jarvie, 1991; Petersen et al., 2010).

The advantage of the proposed data-driven approach is apparent from the above application examples. Firstly, Rock-Eval data are used directly to characterize kerogen kinetics and to model hydrocarbon generation from source rock (represented by transformation ratio) as a function of Rock-Eval Tmax. No specifically designed laboratory tests are required for estimating the kinetic parameters. Secondly, the data-driven model utilizes data measured on natural samples as input, thus no validation or calibration for environmental differences between nature and laboratory processes, such as subsurface *in situ* pressure, heating rate and pore fluids, is needed. Thirdly, the statistical model provides an unbiased and robust estimate of the model parameters and the variance from the model can be used to estimate the uncertainty associated with the data and model. Fourthly, this

proposed method can be used as a tool for the kinetic model construction when data coverage is limited. For example, the available data from the Ordovician Yeomen Formation cover only immature to early mature range, revealing first half of thermal decomposition trajectory in terms of remaining hydrocarbon potential. However, the model can construct the other half by extrapolating to the higher maturity area, providing a semi-hypothetical model useful for petroleum system modelling or quantitative calculation of generation potential. Fifthly, the numerical expression of the hydrocarbon generation potential as a function of maturity is simple, and all parameters in the model (Eq. (1)) have an explicit and predictable physical meaning. For example, the initial hydrogen index can be estimated by averaging the hydrogen index values of immature data when available. Parameter β represents a Tmax value that corresponds to the beginning of massive hydrocarbon generation, and therefore is a reflection of the activation energy level required for initiating significant thermal decomposition of the kerogen. The higher the β value, the more thermal energy level is required for the onset of hydrocarbon generation. θ, taking a negative value ranging from −120 to −20, is related to the width of hydrocarbon generation window or the distribution of activation energy of kerogen. It indicates the variability of maceral composition or chemical structure in the kerogen. A less negative θ value indicates the source rock kerogen comprises various distinct organic macerals, and the range of activation energy for thermal decomposition varies considerably, leading to a large range of Tmax for the hydrocarbon generation window or a broad oil window. In contrast, a kerogen of unitary maceral composition will have a more negative θ value, and thus display a narrow distribution of activation energy for the thermal decomposition and shows a narrow range of Tmax.

The methodology developed here is a cost-effective approach for quick and efficient evaluation of source rock units, and can be easily applied to unconventional resource assessment on shale formations for which large amounts of Rock-Eval results have been generated before during traditional organic geochemical evaluation. The concept has been employed to evaluate the organic porosity evolution and its effect on shale gas resource potential of the Duvernay shale of WCSB (Chen and Jiang, under review) and Utica shale of Quebec, Canada (Chen et al., 2014).

5. Conclusions

A data driven method has been proposed for studying hydrocarbon generation kinetics of source rocks. The approach utilizes existing Rock-Eval/TOC data by fitting the measured hydrogen index and Tmax to an exponential model and subsequently converting to hydrocarbon transformation ratio without involving specifically designed laboratory pyrolysis experiments. The proposed method has been tested and demonstrated using four Rock-Eval datasets with different kerogen kinetics from Canadian sedimentary basins. The results are consistent with the kinetic characteristics determined using laboratory pyrolysis of various source rock samples. The comparison of hydrocarbon generation kinetics of different kerogen types suggests that kerogen type may not be indicative of their kinetics. Depending on their maceral and chemical composition, the hydrocarbon generation kinetics of the same type of kerogens may differ significantly as exemplified by the Tertiary Aklak type III kerogen. In addition to its ease to implement and flexibility in data handling, the method is statistic in characteristics and allows for uncertainty from various sources to be quantified through the statistical analysis of a large dataset.

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