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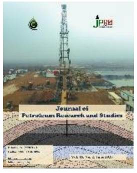

Determination of Relative Kinetic Parameters of Middle to Upper Jurassic Petroleum Source Rock Formations of Different Maturity Levels by Means of Elemental Analysis

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Abstract

The kinetic parameters of Middle to Upper Jurassic formations rich in organic matter in northern Iraq are examined, with a particular emphasis on sulfur-rich kerogen. The study simulates natural oil generation and ejection utilizing hydrous pyrolysis to evaluate the consequences of sulfur content on activation energy, frequency factors, and thermal maturity. A comparison between both pyrolysis methods (open vs. closed) reveals the effects of system parameters on the quality and content of the petroleum produced. The effects of sulfur levels as indicated by atomic Sorg/C ratios exceed 0.04 and should not rear exceed 0.4%. The findings show that these sulfur intensities are exist in the Type II-S kerogens in the Middle to Upper Jurassic formations; these levels are associated with lower maturation temperatures and early oil generation. The results offer substantial information for assessing the Jurassic petroleum system in carbonate facies that are high in sulfur.

Keywords: Kerogen, Source rock, Hydrous pyrolysis (HP), Open system pyrolysis, Closed system pyrolysis, Jurassic, Sulfur content, Petroleum generation.

تحديد المعلمات الطاقة الحركية النسبية لتكوينات الصخور المصدرية للهايدروكاربون من العصر الجوراسي الأوسط إلى العصر الجوراسي العلوي بمستويات نضج مختلفة عن طريق التحليل العنصري

الخلاصة:

تم دراسة المعلمات الطاقة الحركية لتكوينات الجوراسي الأوسط والأعلى الغنية بالمواد العضوية في شمال العراق، مع التركيز بشكل خاص على الكيروجين الغني بالكبريت. تتحدث الدراسة توليد النفط الطبيعي وقذفه باستخدام التحلل الحراري المائي لتقييم عواقب محتوى الكبريت على طاقة التنشيط وعوامل التردد والنضج الحراري. تكشف المقارنة بين طريقتي التحلل الحراري (المفتوحة والمغلقة) عن تأثيرات معلمات

النظام على جودة ومحتوى النفط المنتج. تتجاوز تأثيرات مستويات الكبريت كما هو موضح بنسب Sorg/C الذرية 0.04 ولا ينبغي أن تتجاوز 0.4٪. تظهر النتائج أن هذه الكثافة الكبريتية موجودة في الكيروجينات من النوع II-S في تكوينات الجوراسي الأوسط والأعلى؛ ترتبط هذه المستويات بدرجات حرارة النضج المنخفضة والتكوين المبكر للنفط. تقدم النتائج معلومات جوهرية لتقييم نظام النفطي الجوراسي في السحنات الكربونية التي تحتوي على نسبة عالية من الكبريت.

1. Introduction

Chemical kinetics, also known as reaction kinetics, is the main parameter for determining the nature and rate of any chemical reaction. It is diverse from chemical thermodynamics, which concerned with the trend in which a reaction arises [1]. Chemical kinetics includes investigations of experimental settings effect on the rate of a chemical reaction and provide evidence on the reaction’s mechanism and evolution, besides the offering of mathematical simulations that also can define the appearances of a chemical reaction [2].

Kinetic parameters are critical for knowing the timing and amount of producing hydrocarbon within a petroleum system. Various laboratory techniques, particularly hydrous pyrolysis (HP) and Rock-Eval (RE) pyrolysis, are utilized to establish these parameters. Studies indicate significant differences in results for diverse kinds of kerogen [3], particularly in source rocks containing low amount of sulfur and high-sulfur kerogen [4;5].

Significant differences could be detected when comparing varying pyrolysis methods and experimental settings (open *vs.* closed systems, hydrous *vs.* anhydrous, pressure, and heating procedures). Notably, open system pyrolysis appears to generate products dominated by polar compounds, while closed system pyrolysis yields more natural-looking petroleum [3;6;7;8]. The concern of expecting quantity, quality, and constituents of petroleum utilizing anhydrous pyrolysis results have been investigated [9;10;11]. Nevertheless, no effort has combined the external and internal characteristics of produced petroleum anticipated by simulated progress through HP and associated them to ordinary oil from comparable source rocks.

The kinetic EASY vitrinite reflectance (%Ro) model was applied to simulate thermal maturity during the reconstruction of the burial history of the Jabel Qand Oilfield, yielding results that differed from those reported in subsequent studies [12]. Owing to the lack of available kinetic parameters and elemental analysis data, later investigations adopted the Type-II-S kerogen kinetics of the Phosphoria Formation as an alternative approach. These kinetics exhibit constraints that are generally comparable to those of Jurassic source rock formations [13;14].

It is undoubtedly that Ro% is a decent for maturity impact indication as demonstrated by Sweeney and Burnham [15], but it’s not a decent indicator of *transformation ratio* (TR) from Type-II-S kerogen, which surprises and terminates at lower vitrinite reflectance values [16]. This is why it is important to have HI or kerogen atomic H/C ratios to check whether the kinetic parameters are in line with the data that indicated oil generation.

The significant concern is the kinetics and interpretation that used for oil cracking to gas (i.e., secondary gas) [17]. Certainly, oil cracks to gas at VR more than 1.5%Ro. They showed that oil cracking is more than 80% complete at VR 0.81 to 0.99 %Ro. This is not reinforced by other studies. If the gas they observed is dry and not associated with oil, it is most likely from a deeper source in the basin where trapped oil remains in coherent traps. Hydrous-pyrolysis kinetic parameters for Sargelu Formation were used to determine timing of hydrocarbon generation in Iraqi Kurdistan [18]. He used activation energy (Ea) of 41.52 kcal per mole in his study on petroleum generation modeling in northern Iraq.

The study's aim is to utilize hydrous analysis to mimic ordinary petroleum generation and ejection processes in order to identify the Ea and frequency factor (A_o) for petroleum generation from sulfur-rich Middle to Upper Jurassic source rocks. Iraqi Jurassic formations are not directly involved in this investigation.

This study uses data from similar formations in the United States and Iran to evaluate the effects of sulfur content on hydrocarbon output and thermal maturity. In order to comprehend how various experimental settings, affect the timing and content of produced petroleum, it also compares results from isolate and non-isolate analysis to investigate how diverse settings influence the timing of the generated petroleum. This information may then be applied to similar kerogen types around the world.

1.1 Hydrous pyrolysis (HP) *vs.* anhydrous pyrolysis

Anhydrous analysis settings lead to overlay reactions causing to produce of bitumen and liquid petroleum dominated by polar composites [19], denoted by the Rock-Eval's S_2 peak [20]. On the other hand, simulated maturing in hydrous pyrolysis (closed setting) produces a petroleum reasonably-seeming natural [21]. This resemblance likely accredited to the decomposition of polar composites (resins and asphaltenes) into paraffin and aromatic composites [4]. HP experimentations have been utilized to examine the configuration and feature of hydrocarbon produced from a Barazilian source rock during progressing thermal maturation. Outcomes display that organic matter primarily cracks to a polar compound, which break partially to liquid petroleum [22].

Contrasting anhydrous isolated analysis techniques, hydrous analysis produces a hydrocarbon that is structurally analogous to naturally generated hydrocarbons [8]. Expelled hydrocarbons from HP are enhanced in paraffin primarily resulted from the breakdown of bitumen due to increasing maturity (i.e., resins and asphaltenes) [16;23;24].

The attendance of water during hydrocarbon generation is necessary in laboratory and nature as a hydrogen provider in developing generated petroleum [25;26]. Consequently, bonding pair in the bitumen crack, generating liquid petroleum. This proposes that the driving apparatus replicated by hydrous analysis aligns with the perception that oil ejection is a result of its expulsion within a rock [27].

Lacking water in pyrolysis, leads hydrocarbon-enriched oil to be not discriminated from bitumen especially polar compounds, besides no remaining quantity surge arises to force the hydrocarbon from the bitumen-saturated rock, which built on investigational assessments [8;28]. Furthermore, this type of pyrolysis has proven valuable understanding of kinetics of hydrocarbon generation [20;29;30;31;32]. So, hydrous pyrolysis is the best applicable analysis system to mimic oil expulsion and generation, which is why it’s utilized herein to assess alterations in hydrocarbon configuration and feature with growing maturity.

2. Methods

The samples from Middle-Upper Jurassic formations were gathered from surface sections after removing weathered parts in northern Iraq and south western Iran (Table 1). The representative rock samples were analyzed earlier by English et al. [33] and Shekarifard et al. [34]. These elemental analysis results were used to determine the Ea and A_o of Jurassic source rocks in northern Iraq. The determination is based on comparing of organic sulfur amount presence in Jurassic formations in Iraq and Iran with organic sulfur content and Ea and A_o of diverse source rocks in United States and Iran that were published by Lewan and Ruble [3], Higley and Lewan [35], and Pak et al. [36].

Table (1): Elemental components (wt. %)* of Jurassic organic matter from the northern Iraq (the data from [33^1;34^2]).

Location	Formation	C	H	O	N	Fe	S	Ash	Sorg	Atomic S_{org}/C
^{1}Amedi	Chia Gara -a	64.37	5.75	4.76	0.96	2.20	13.13	8.83	10.60	0.062
	Chia Gara -b	63.78	5.72	4.56	0.94	2.07	12.82	10.11	10.44	0.061
^{1}Barsarin	Naokelekan-a	75.07	4.00	3.53	1.17	0.88	11.79	3.56	10.78	0.054
	Naokelekan-b	75.29	4.03	3.42	1.19	0.85	11.71	3.51	10.73	0.053
1Gara	Naokelekan-c	70.41	7.00	2.46	0.89	2.91	14.60	1.73	11.26	0.060
	Naokelekan-d	69.44	7.01	-	0.88	3.16	13.18	6.33	9.55	0.052
	Naokelekan-e	68.45	6.63	9.20	0.94	0.16	8.85	5.77	8.67	0.047

	Naokelekan-f	68.11	6.50	9.37	0.94	0.16	8.15	6.77	7.97	0.044
[1]Amedi	Sargelu-a	66.47	5.84	12.81	1.31	0.11	8.73	4.73	8.60	0.048
	Sargelu-b	66.40	5.77	12.84	1.30	0.12	8.45	5.12	8.31	0.047
[2]Qalikuh	Sargelu-c	53.00	5.10	2.80	1.00	2.00	9.40	26.70	7.10	0.050
	Sargelu-d	55.20	5.50	2.80	0.90	2.30	9.90	23.40	7.26	0.049
	Sargelu-e	69.50	6.50	2.20	1.00	0.50	10.60	9.70	10.03	0.054
	Sargelu-f	64.00	6.00	4.30	0.90	0.40	9.80	14.60	9.34	0.055

values are corrected to atomic ratios from the mass ratios [33] [34].

3. Results and Discussion

The relationship between sulfur content and the type of source rocks has been extensively discussed in previous studies. Hunt [37] emphasized that carbonates often contain higher sulfur levels due to reduced iron availability in detrital sediments. This designates the role of mineralogical composition in determining sulfur content. Gransch and Posthuma [38] highlighted that oils originated from carbonate dominated source rocks typically exhibit sophisticated sulfur content compared to those from siliciclastic sources. This distinction is crucial for understanding the geochemical signatures of different petroleum systems and their implications for exploration and production. Higher-quality oils are derived from source rocks with lower sulfur content, emphasizing the importance of source rock evaluation in predicting petroleum quality [39].

Type II-S kerogen needs less heat and time than regular kerogen type II to generate petroleum due to the presence of sulfur in kerogen that influences the thermal maturation process [40;41]. Collected data indicating varying T_{max} values for petroleum generation in high-sulfur organic matter, suggesting that oil generation occurs at lower thermal maturities in these systems [42]. Table (1) shows elemental components of some Jurassic formations in northern Iraq and south western Iran. The organic matter of Jurassic formations in Iraq and Iran are analogous to sulfur-rich organic matters in United States (Table 2), and atomic S_{org}/C proportions properly in surplus of 0.04 categorizes them as kerogen type II-S [16;43]. The elemental analysis includes sulfur, carbon, iron, hydrogen, nitrogen, and oxygen. The amount of organic sulfur (S_{org}) determined on the postulation that entirely iron is existing as neat pyrite (FeS_2)—i.e., $\%S_{org} = \%S_{total} - (1.1482 \text{ x } Fe)$.

Table (2): Kinetic factors obtained through hydrous pyrolysis l experimentations.

Formation	**Atomic S_{org}/C**	**Activation energy, Ea (kcal/mol)**	**Source**
New Albany	0.010	59.63	[4]
Duvemay	0.012	58.30	[35]
Kazhdumi	0.014	57.00	[36]
Exshaw	0.022	53.70	[35]
Sarvak	0.023	53.40	[36]
Doig	0.025	52.30	[35]
Woodford	0.023	52.16	[4]
Ostracod	0.029	50.40	[35]
Alum	0.036	48.10	[4]
Phosphoria	0.045	42.71	[4]
Poker Chip A	0.057	37.50	[35]
Gordondale	0.057	37.50	[35]
Monterey	0.064	34.32	[4]

The organic sulfur content of Jurassic source rocks is presented in Table (1). From relationship between Ea and organic sulfur content (Figure 1), the Ea of Middle to Upper Jurassic formations can be resolute (Table 3). The mean Ea of Chia Gera, Naokeleken, and Sargalu formations are 34.97, 39.44, and 40.36 kcal/mol, respectively.

From the Table (3) appears that Ea of Jurassic source rocks are ranging between 34.65 kcal/mol for Chia Gara Formation in Amedi locality and 43.42 kcal/mol for Naokelekan Formation in Gara Mountain. These low Ea are common for kerogen Type II-S which expels liquid hydrocarbon in lower than regular thermal maturity temperatures that are documented for regular Type II kerogen. The Ea and A_o of five different formations in United States which contain Type II-S kerogen are shown in Table (4) and from a linear relationship between them (Figure 2), the A_o of Jurassic petroleum source rock formations in northern Iraq can be determined (Table 5).

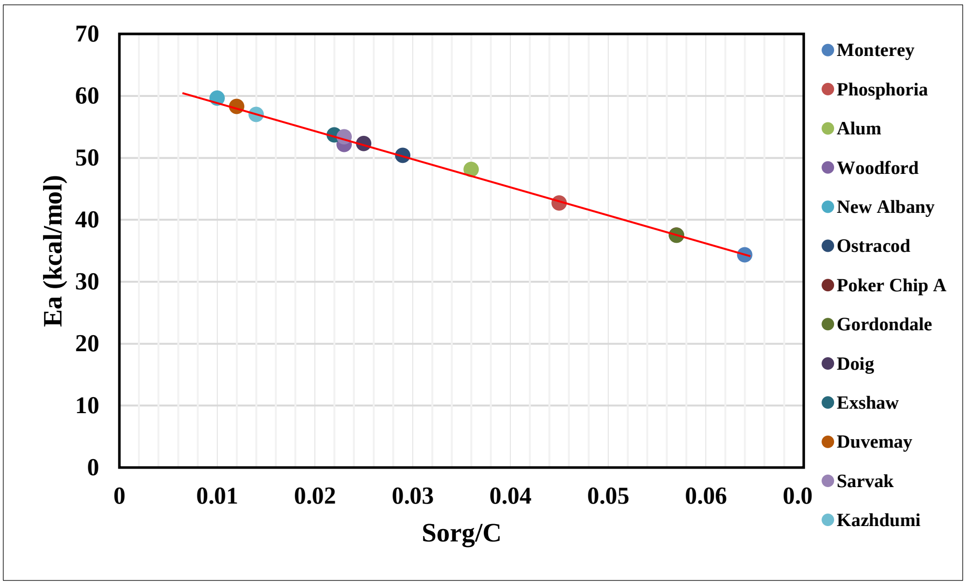

Fig. (1): Atomic weight of organic sulfur to carbon ratio (S_{org}/C) *vs.* activation energy (Ea) of different formations in United States and Iran [3;35;36].

In the nature and laboratory, thermal impact has been revealed by electron spin resonance (ESR) spectroscopy to aid growing unpaired electrons that surge in number [44]. The hydrogen atom from a methyl assemblage of saturated (aliphatic) originates thermal crashing of carbon-carbon bonds [45;46]. Accordingly, thermal breakdown is likely to accelerate in fraction to the quantity of carbon–sulfur and sulfur–sulfur linkage in the immature type-II kerogen. The break of the carbon–sulfur and sulfur–sulfur links is not liable for generating various components of petroleum, but relatively offers the originating unpaired electrons that permit the breaking of carbon–carbon linkages to arise at an earlier time and lower stage of maturation [47].

Table (3): kinetic factors obtained for expelled-hydrocarbon generation by comparison with activation energy (Ea) of petroleum source rocks in United States and Iran.

Formation	Sample location		Atomic S_{org}/C	Ea (kcal/mol)
Chia Gara	Amedi	b	0.061	35.48
		a	0.062	34.95
Naokelekan	Gara	e	0.047	42.06
		f	0.044	43.42
		c	0.060	35.93
		d	0.052	39.46
	Barsarin	a	0.054	38.80
		b	0.053	39.10
Sargelu	Amedi	b	0.047	42.06
		a	0.048	41.52
	Qalikuh	f	0.055	38.16
		d	0.049	41.11
		c	0.050	40.70
		e	0.054	38.60

Table (4): Formation names, activation energies (Ea), and frequency factors (A_o) for five formations in United States [3].

Formation name	**Ea (kcal per mol)**	**A_o (h^{-1})**
Monterey	34.32	$7.59x10^{10}$
Phosphoria	42.71	$4.92x10^{13}$
Alum	48.10	$1.77x10^{15}$
Woodford	52.16	$6.51x10^{16}$
New Albany	59.63	$1.36x10^{19}$

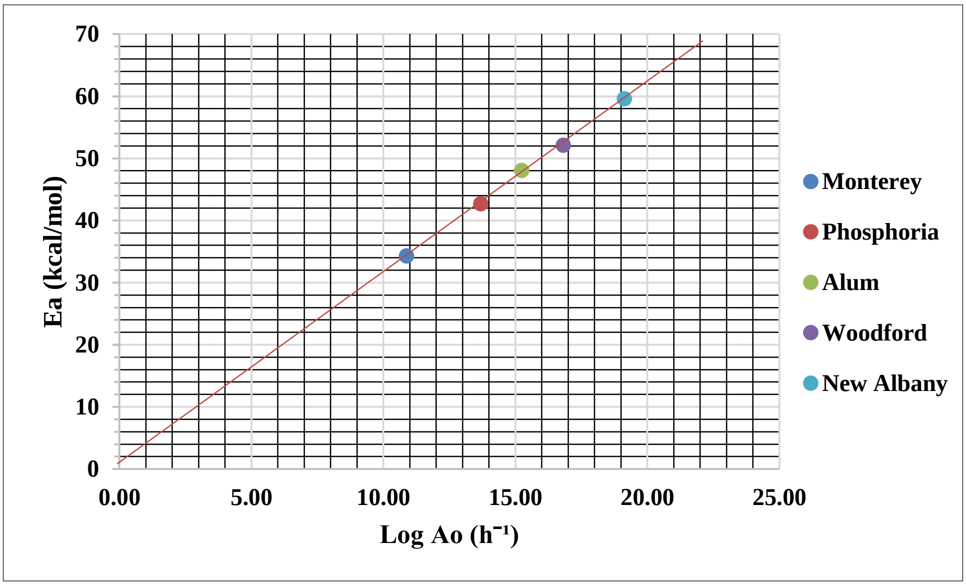

Fig. (2): The plot shows the linear relationship of activation energy (Ea) with frequency factors (A_o) of different formations in United States [3]. The linear regression is very good as expressed by Log A_o = 0.3264Ea -0.312 with a correlation coefficient, $R^2 = 0.9991$.

Table (5): The kinetic parameters of Jurassic formations in northern Iraq.

Formation name	Ea (kcal/mol)	A_o (h^{-1})
Chia Gara-a	34.95	$7.63x10^{10}$
Chia Gara-b	35.48	$8.11x10^{10}$
Naokelekan-c	35.93	$8.91x10^{10}$
Sargelu-f	38.16	$6.71x10^{11}$
Sargelu-e	38.60	$6.92x10^{11}$
Naokelekan-a	38.80	$6.14x10^{11}$
Naokelekan-b	39.10	$7.35x10^{11}$
Naokelekan-d	39.46	$1.64x10^{12}$
Sargelu-c	40.70	$2.24x10^{12}$
Sargelu-d	41.11	$1.02x10^{13}$
Sargelu-a	41.52	$1.21x10^{13}$
Sargelu-b	42.06	$1.67x10^{13}$
Naokelekan-e	42.06	$1.67x10^{13}$
Naokelekan-f	43.42	$5.93x10^{13}$

4. Conclusions

This study provides significant information about the impacts of Type II-S kerogen on thermal maturity and petroleum output. The kerogen from the Middle to Upper Jurassic succession were classified as Type II-S because their ratio of atomic weight of organic sulfur to carbon content levels were higher than 0.04%. The average Ea for the Chia Gera, Naokeleken, Sargalu formations are 34.97, 39.44, and 40.36 kcal/mol, respectively. These values corresponded to average A_o of $7.61\text{x}10^{10}$, $1.32\text{x}10^{13}$, and $1.44\text{x}10^{13}$ h^{-1}, in that order. In contrast to conventional Type II kerogen, these results highlight the unique function of sulfur in promoting earlier and lower-temperature oil formation in Jurassic carbonate source rocks. Additionally, a comparison of pyrolysis in isolated and non-isolated systems showed that the former favor the creation of polar compounds, which affects the overall composition of hydrocarbons, while the latter produce petroleum that is more natural-like. This work improves our knowledge of the kinetics of petroleum systems in sulfur-rich deposits.

Author Contributions Statement: Rzger A. Abdula contributed to the Conception; Methodology; Experiments; Data Analysis and Interpretation; Writing – Original Draft; Writing – Review & Editing. Parween R. Abid contributed to the Data Interpretation; Writing – Original Draft; Writing – Review & Editing. All authors have read and approved the final version of the manuscript.

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