A New Approach for Kinetic Modelling of El Lajjun Oil Shale Extracted Kerogen

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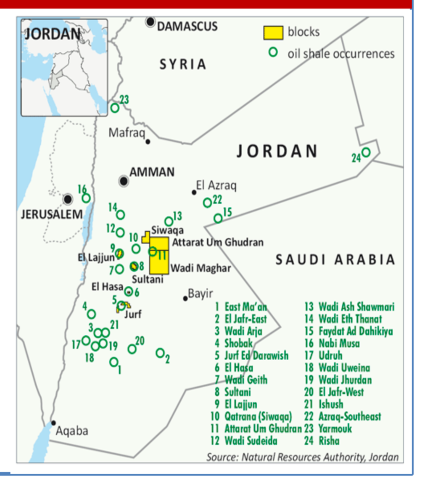
Oil Shale in Jordan

- Jordan is very rich in oil shale deposits.
- The main sites are located at El Lajjun, Sultani, and Jurf-Ed-Darawish located in west central Jordan; 20 to 75 km east of the Dead Sea.
- Jordan reserves of oil shale is around 50 billion tons.



Experimental Method

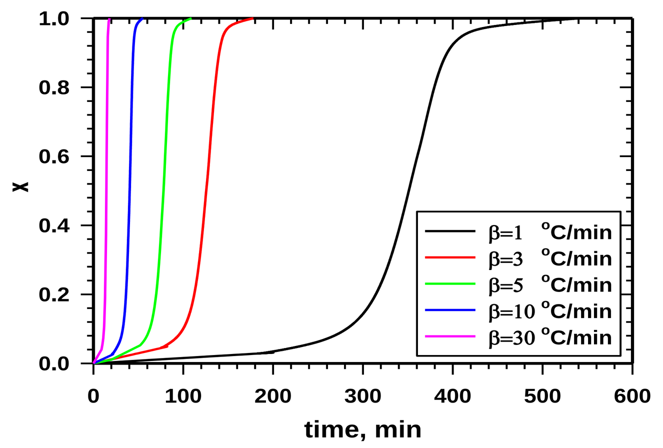
- Oil shale used in this study was obtained from El-Lajjun area in Jordan.
- Kerogen was isolated from raw oil shale by sequential HCl and HCl/HF digestion.
- Kerogen samples were pyrolyzed in a Thermogravimetric analyzer at different heating rates: β=1, 3, 5, 10, and, 30 °C/min up to a temperature of around 550 °C.

Experimental Findings

Mass composition of oil shale samples:

Moisture content	1.85%
Soluble organics before acid treatment	3.17%
Carbonate	46.46%
Silica and clay minerals	26.94%
Soluble organics after acid treatment	1.09%
Kerogen and insoluble minerals	20.49%

Experimental Findings

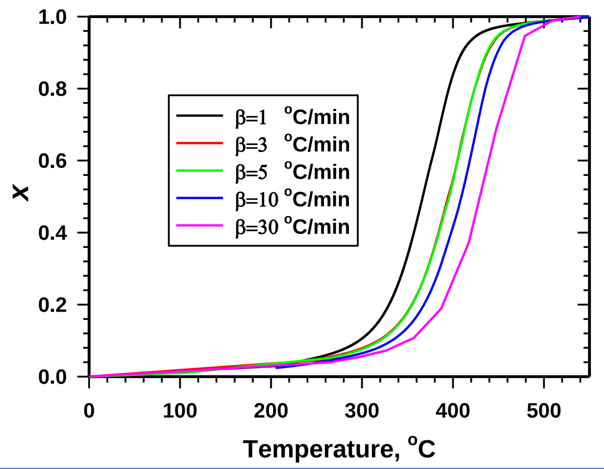


Kerogen Conversion Fraction ; *X*

$$x = \frac{W_0 - W_t}{W_0 - W_f}$$

X : Conversion fraction
W_0: Initial mass of the sample
W_t: Mass of the sample at t time
W_f: Final mass of the sample

Experimental Findings



Traditional Kinetic Approach

- Previous studies analyzed the non-isothermal kinetics of oil shale and its kerogen using the Arrhenius equation:

$$\frac{dx}{dt} = \beta \frac{dx}{dT} = Ae^{-E/RT} f(x)$$

where dX/dt is the rate of conversion for Thermogravimetric experiment at constant heating rate (β), E is the apparent activation energy, A is the pre-exponential factor and R is the gas constant.

Traditional Kinetic Approach

- The apparent activation energy and the pre-exponential factor are estimated using various mathematical strategies such as:

1. Friedman method.
2. Kissinger-Akahira-Sunose (KAS) method.
3. Flynn-Wall-Ozawa (FWO) method.
4. Coats and Redfern method.
5. etc…

Kinetic approach

- Pyrolysis of oil shale kerogen involves multiple reactions (no unique activation energy).
- Inaccurate kinetic findings of many previous works due to the unsafe assumption: fixing one E parameter in the mathematical formulations.
- The present study proposed a new approach to avoid such mathematical conflict.

New Kinetic approach

- The present work analyzed the non-isothermal kinetics of El Lajjun oil shale kerogen using Gaussian function of the form:

$$\frac{dx}{dt} = \beta \frac{dx}{dT} = ae^{-0.5\left(\frac{x-c}{b}\right)^2}$$

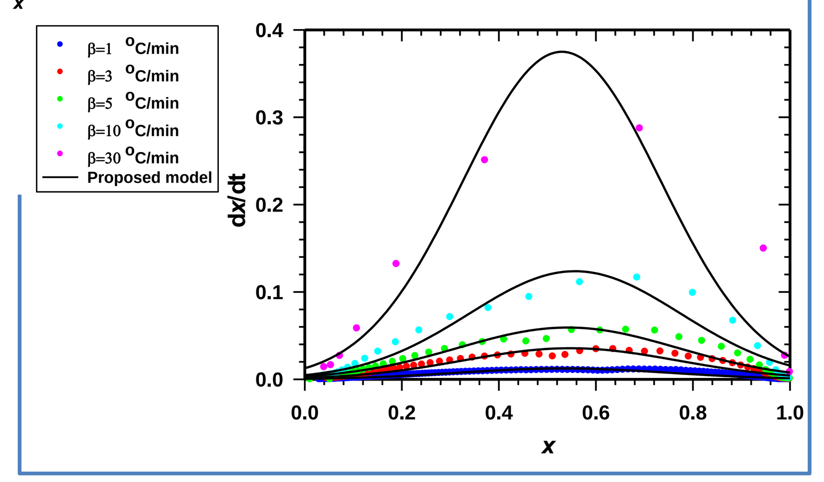
where a, b, and c are the kinetic model parameters.

New Kinetic approach

→ To find the proposed model parameters:

- The value of dx/dt has been calculated at each time point using fourth-order finite difference schemes.
- The resulting dx/dt values has been plotted against the corresponding *x* values.
- Least-square method has been used to estimate the three model parameters.

New Kinetic Model

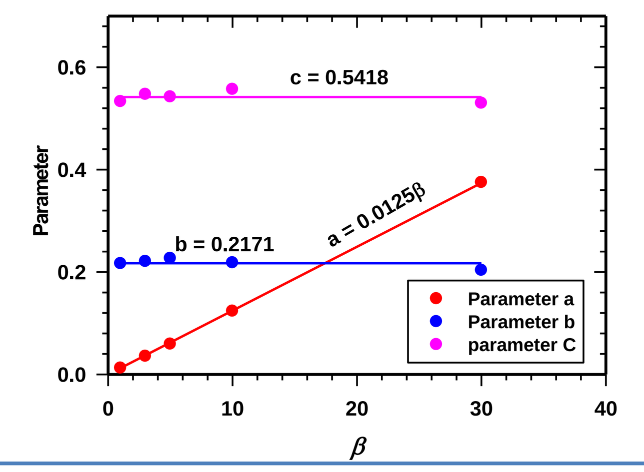


Findings of New Kinetic Model

The resulting kinetic parameters at different heating rates:

β; °C/min	a	b	c
1	0.0124	0.2165	0.533
3	0.0356	0.2207	0.5472
5	0.0593	0.2267	0.5422
10	0.1237	0.2182	0.5569
30	0.3750	0.2035	0.5298

Findings of New Kinetic Model



Conclusions

- Non-isothermal pyrolysis of El Lajjun oil shale kerogen can be modelled correctly as:

$$\frac{dx}{dt} = \beta \frac{dx}{dT} = 0.0125\beta e^{-0.5\left(\frac{x-0.5418}{0.2171}\right)^2}\ ;\ \left(\beta \le 30;\ T \le 550\ ^{o}\mathrm{C}\right)$$

- The present study shows that the pre-exponential parameter of the proposed Gaussian model increases linearly with increasing heating rate. The other two-exponential parameters are constant.
- It is recommended to try Gaussian law to model oil shale pyrolysis.