Source Rock Kinetics: Goal and Perspectives*

Mathieu Ducros[1]

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Abstract

Despite international will and policies for reducing the dependency on fossil fuels, Petroleum is still considered as an essential resource to match the demand for petroleum in the coming decades. In order to match the long-term growing demand for petroleum, unconventional resources have taken a significant part of the petroleum offer (5-6 Mbd). The interest for these resources renewed the efforts of research on the mechanisms of petroleum generation, retention and expulsion. Since the source rock also acts as a reservoir in these systems, it also gave access to a large number of source rock samples compared to what was available when the interest was only on conventional petroleum systems, paving the way to interesting new studies.

Though some recent debates on the role of thermodynamics (Uguna et al., 2012) in the conversion of solid organic matter into fluid petroleum, the most accepted way to model this conversion remains the kinetic approach. This latter is mostly used, in combination with basin modeling or not, to predict the state of maturity of source rocks, the amount of generated petroleum and some other mechanisms related to expulsion and retention. Consequently, for exploration perspectives, the main objective when determining kinetics parameters is to get a predictive model of transformation of the organic matter in oil and gas under geological conditions (several millions of years at temperatures ranging between 80 to 200°C).

While first authors proposed kinetic models mostly basing their interpretations on field data (Lopatin et al., 1971; Tissot, 1969; Tissot and Pelet, 1971; Waples, 1980) kinetics parameters are currently mainly determined using artificial maturation procedures in laboratories. All these experimental maturation techniques are performed either using isothermal or non-isothermal temperatures with temperatures ranging between 200 and 700°C associated with heating times span varying from some minutes to few hundreds of hours (e.g., Behar et al., 2008; Lewan and Ruble, 2002). Thus, these laboratory conditions are far from the geological domain. A lot of efforts were put on compositional description of kinetics, and there was tremendous progress in analytical techniques and modeling capacities to better understand chemical processes and characterization of the generated petroleum composition (e.g., Behar et al., 2008; Fusetti et al., 2010). However, previous and recent studies emphasized some inconsistencies or shortcomings in the way kinetic parameters are currently determined (e.g., Prinzhofer, 1994, unpublished). They can lead to strongly erroneous prediction in the maturity of source rocks at regional scale. Indeed authors usually provided only a unique

possible solution to the kinetic parameters inversion problem; they dedicated little efforts to perform real validation of this unique proposed solution and did not assess their predictivity at laboratory or geological time scales. Even if the problem is not new (e.g., Ungerer and Pelet, 1987; Ungerer, 1989), it was kept at the bottom of the research priority list and remains unsolved. The recent attention to unconventional resources to supply global oil and gas needs has led to a rising interest both to better constrain the determination of kinetic parameters and assessing the uncertainties of their determination that appeared.

It seems now clear that in order to better constrain the determination of kinetic parameters for petroleum exploration, laboratory transformation data are not sufficient. Now, with new modeling techniques, such as basin modeling, we are able to better determine temperature history at basin scale, and then it is possible to estimate quite accurately the temperature history of any sample of rock. Based on the new data and samples derived from the production of unconventional resources, these reservoirs-source rocks can be used to better constrain kinetic parameters of organic matter conversion into petroleum by coupling basin modeling and laboratory experiments.

We applied this new approach, combining both usual laboratory immature source rock maturation results with observed characterization data coming from naturally mature samples also completed by laboratory maturations. For this natural series the temperature history was reconstructed based on basin modeling techniques. To get an uncertainty risk on the kinetic parameters, we provided not a unique set of kinetic parameters but the sets of parameters that fit equally well the constraining natural and artificial data. Finally the optimization procedure was revisited to keep the transformation description as simple as possible (no more complex than what is suggested by the data), using some inputs from the theory of information.

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Source Rock Kinetics: Goal and Perspectives

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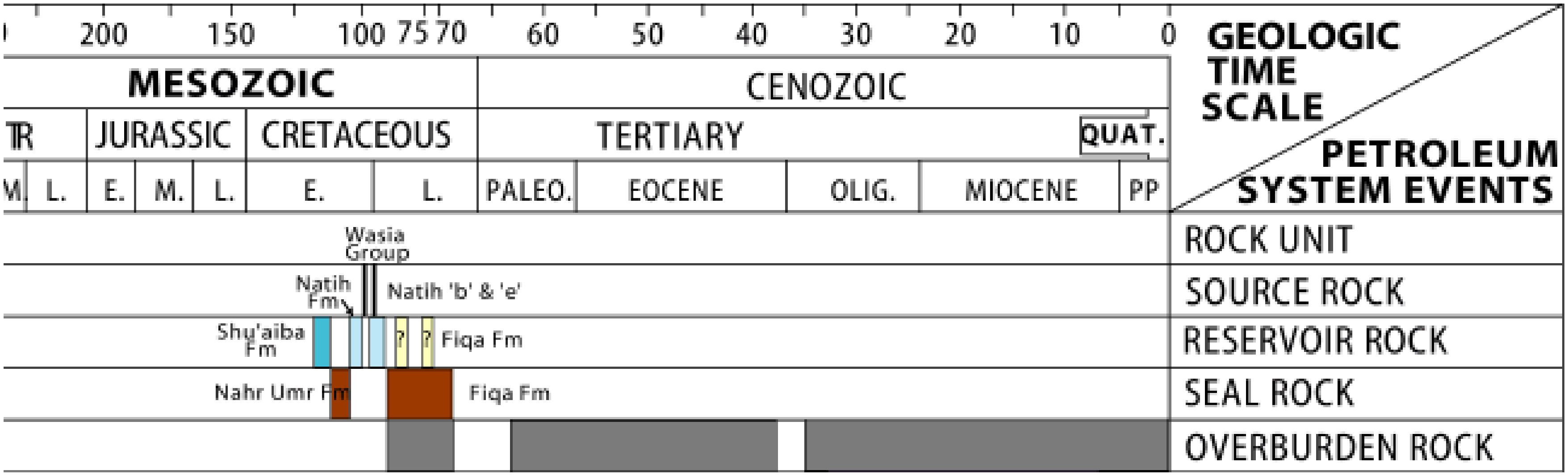
IFP Energies nouvelles

Introduction

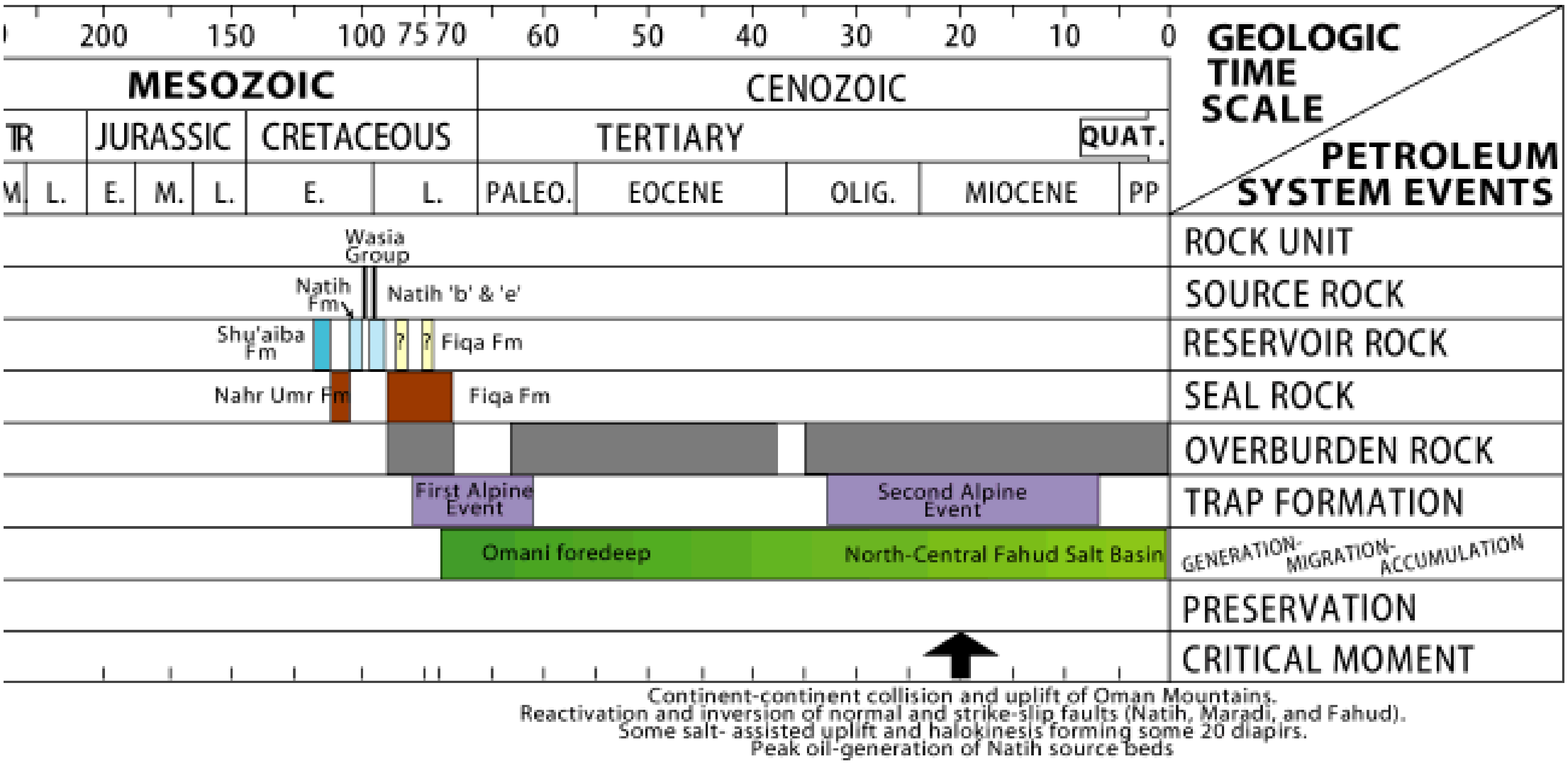
- Why do we need kinetics and how do we use them?
- Reminder on source rock maturation
- How do we determine kinetics and what are their current limitations?
- Current work and perspectives
  - Better constraints on kinetics
  - Better spatial prediction of source rock reactivity

Petroleum system



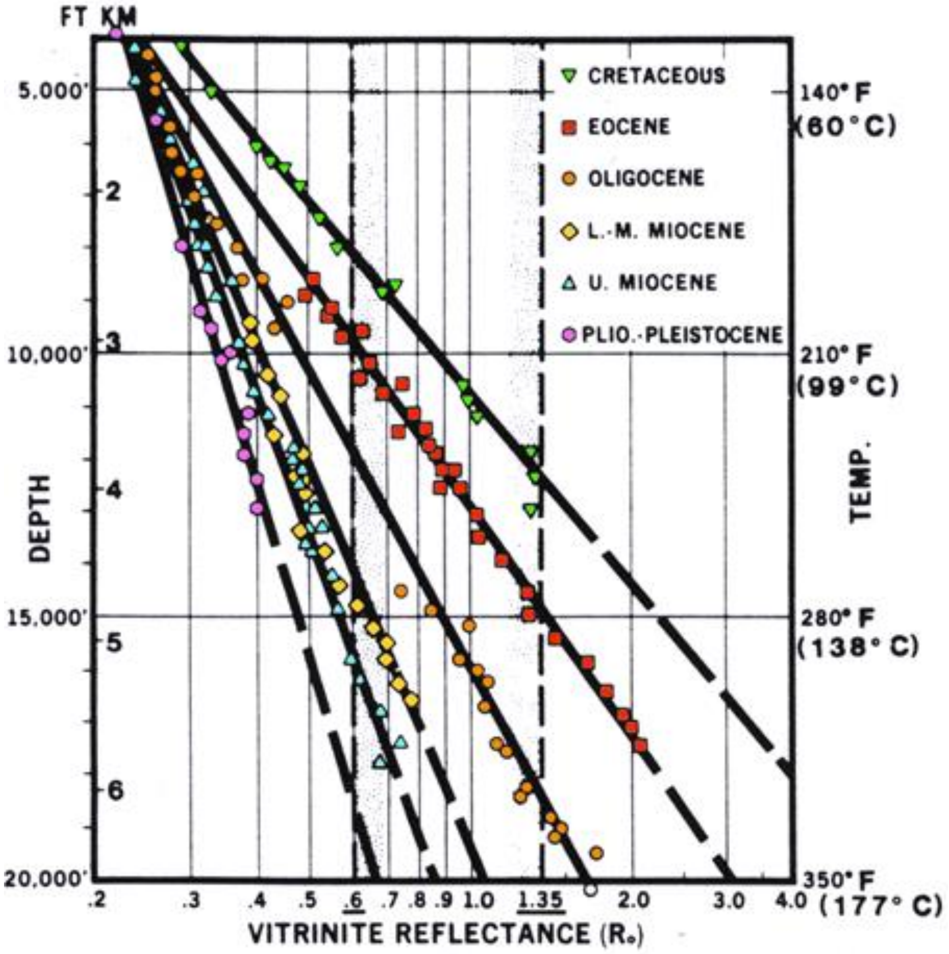
Natih Petroleum System (Pollastro, 1998)

Petroleum system



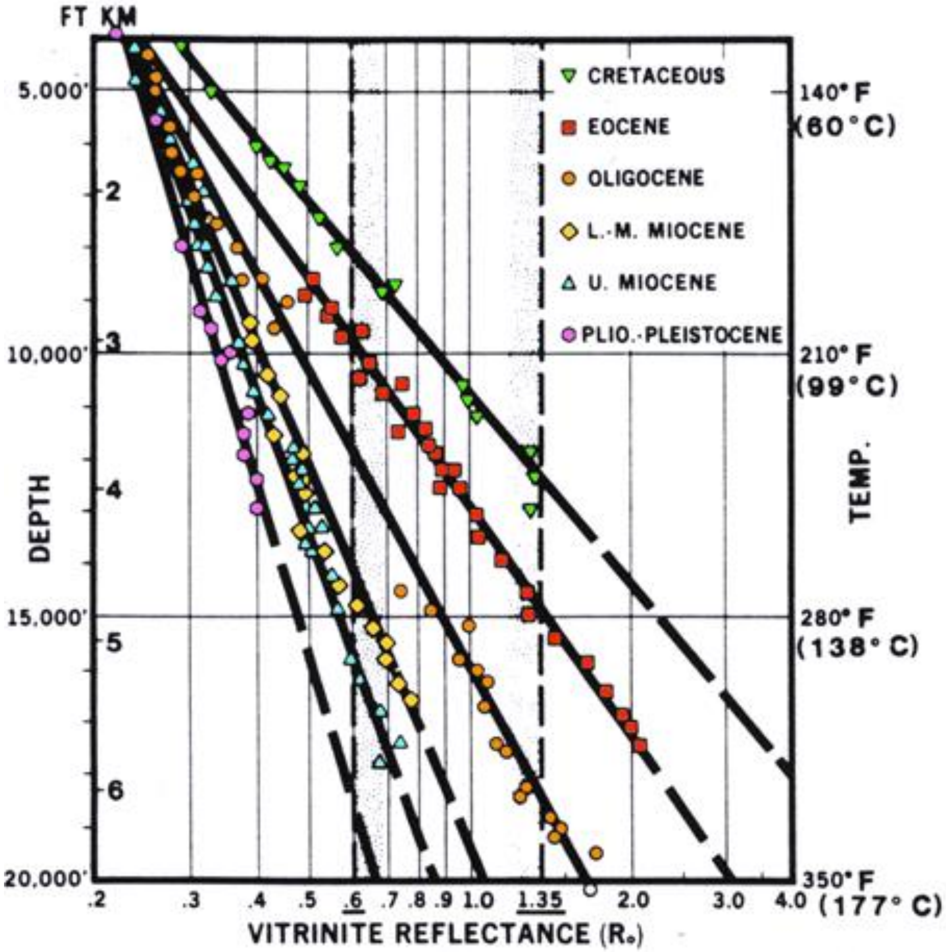
Natih Petroleum System (Pollastro, 1998)

Source rock maturation: reminder



Dow (1977)

Source rock maturation: reminder



Dow (1977)

Arrhenius' equation

$$\frac{dx}{dt} = -A.\exp^{(-E/RT)}\ x$$

x is the organic matter

t is the time

T is the temperature

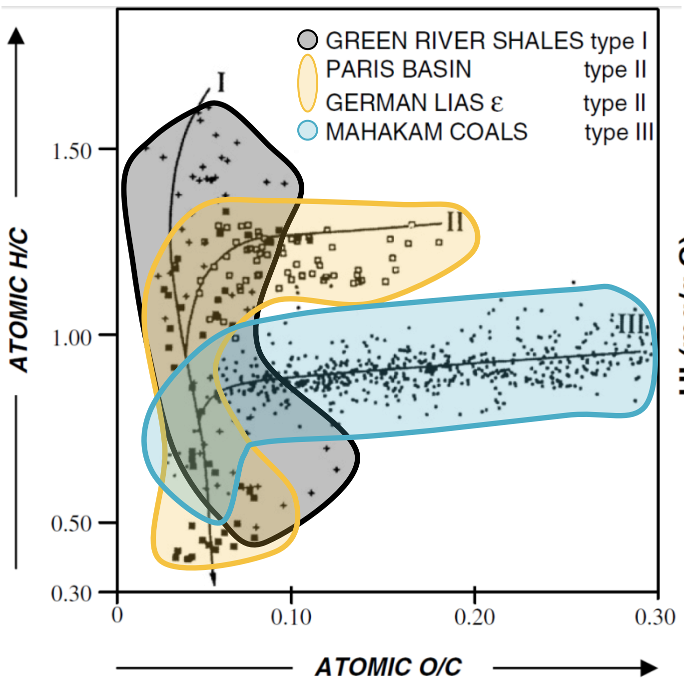
R is the constant of perfect gases

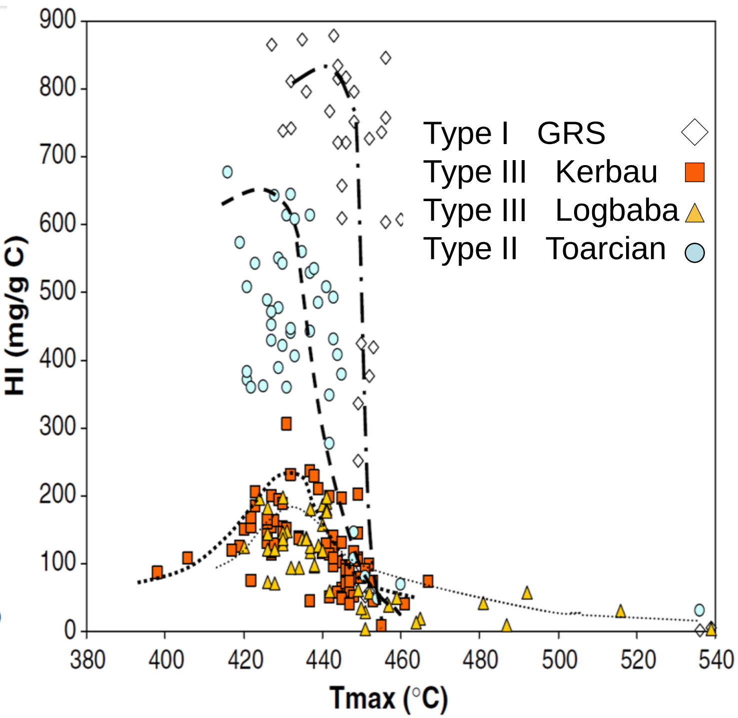
E is the activation energy

A is the frequency factor

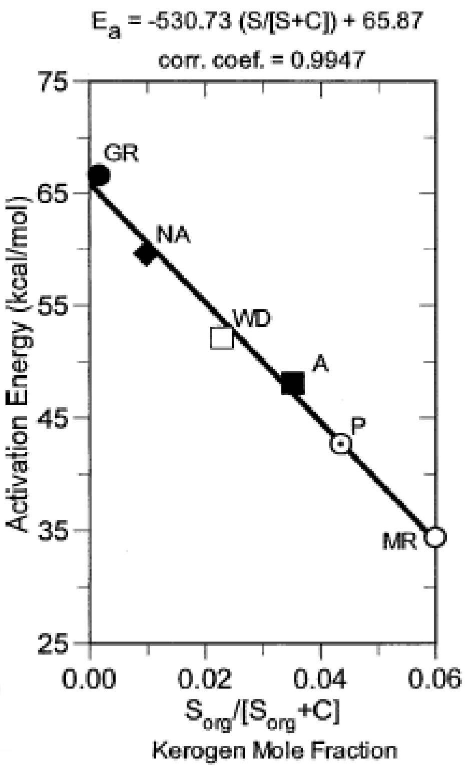
Source rock maturation: reminder

Atomic composition (organic matter type)



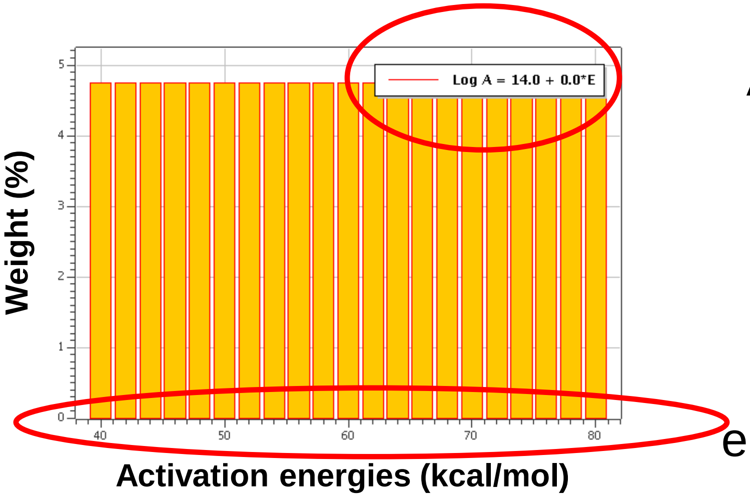


Modified from Vandenbroucke and Largeau (2007)



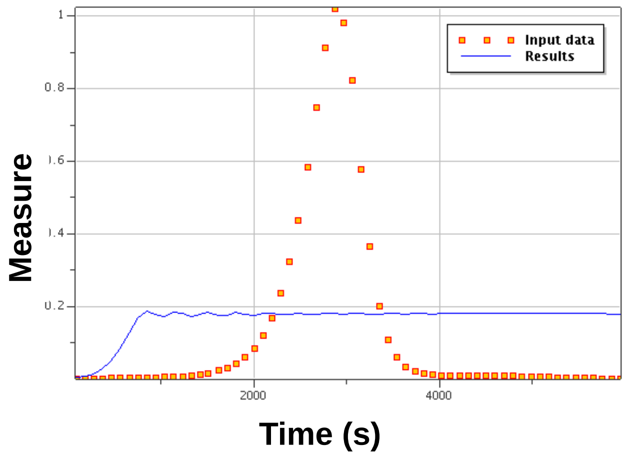
Lewan and Ruble (2002)

Kinetics:
Optimisation of kinetic parameters

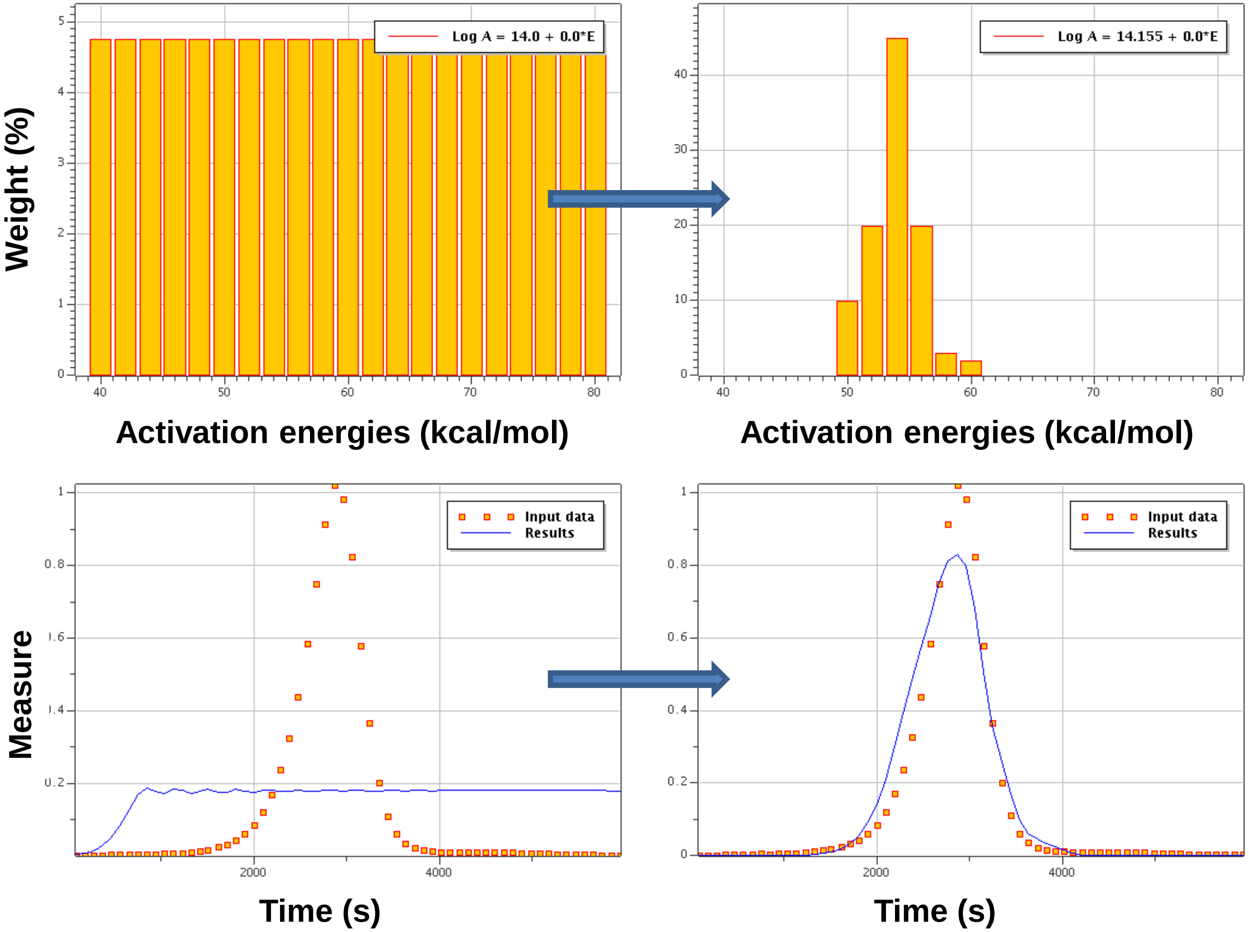


A = Frequency factor

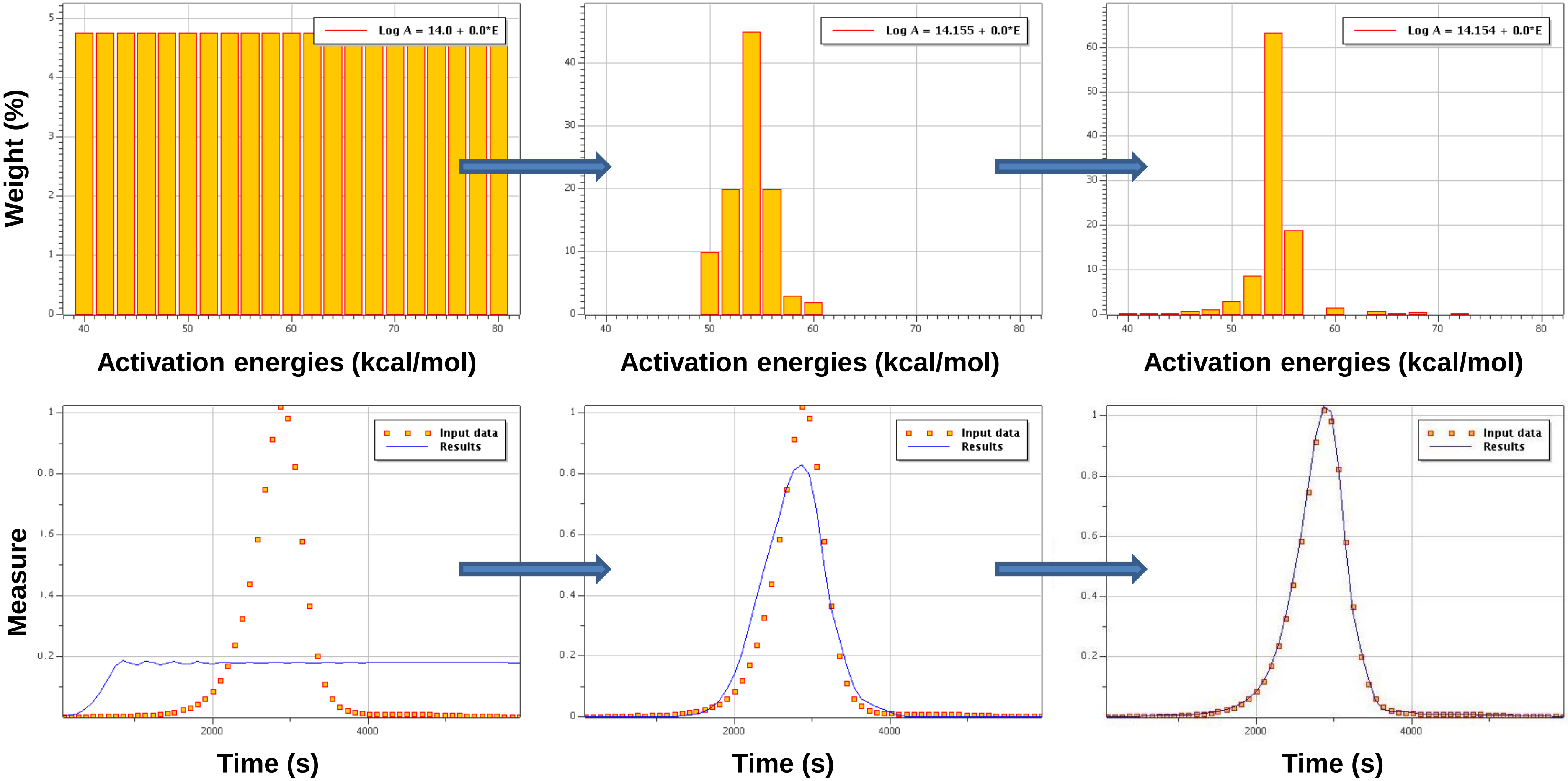
Distribution of activation energies (E) ranging between 40kcal/mol and 80kcal/mol



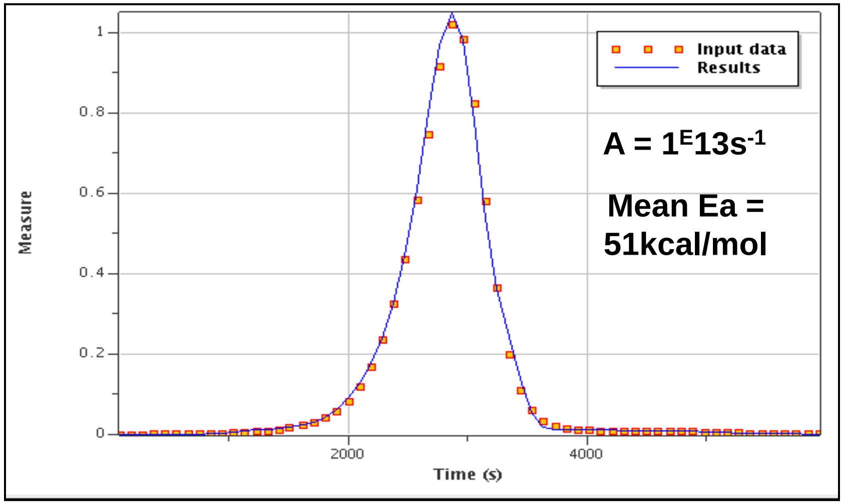
Kinetics:
Optimisation of kinetic parameters

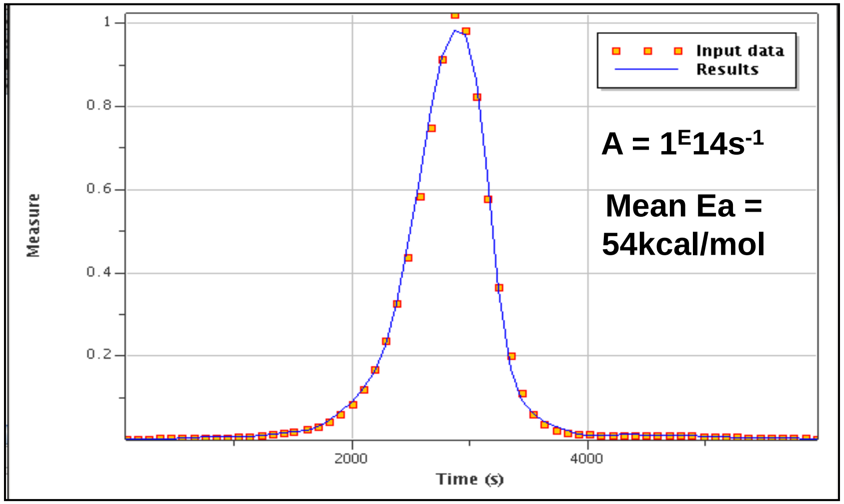


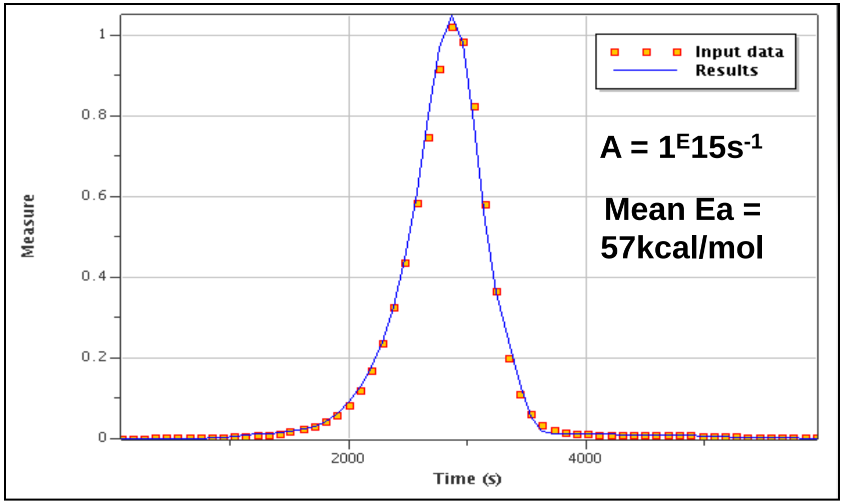
Kinetics:
Optimisation of kinetic parameters

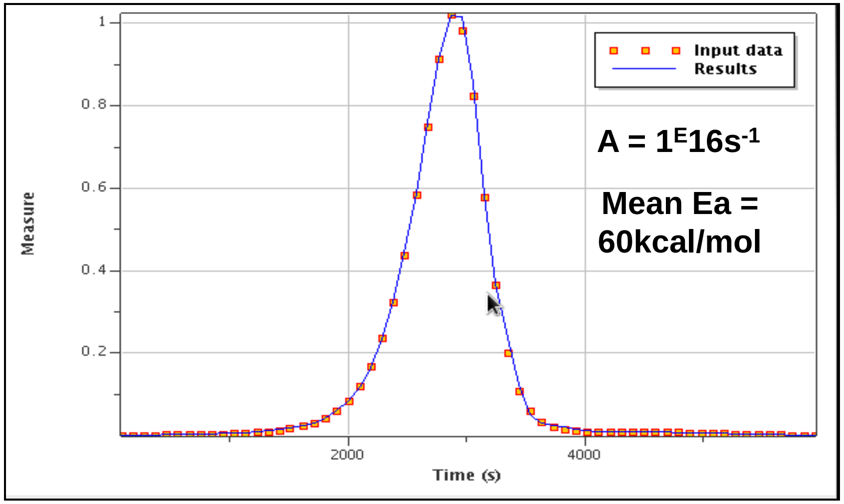


Kinetics:
Shortcomings and limitations



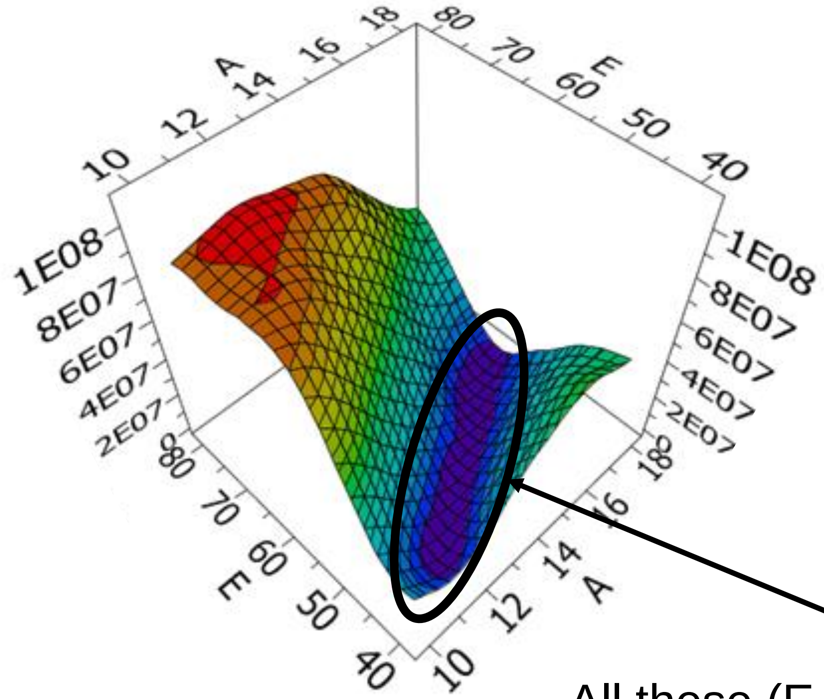






Kinetics:
Shortcomings and limitations

Graph illustrating the misfit of the kinetics on measured data as a function of the mean activation energy (E) and the frequency factor (A)

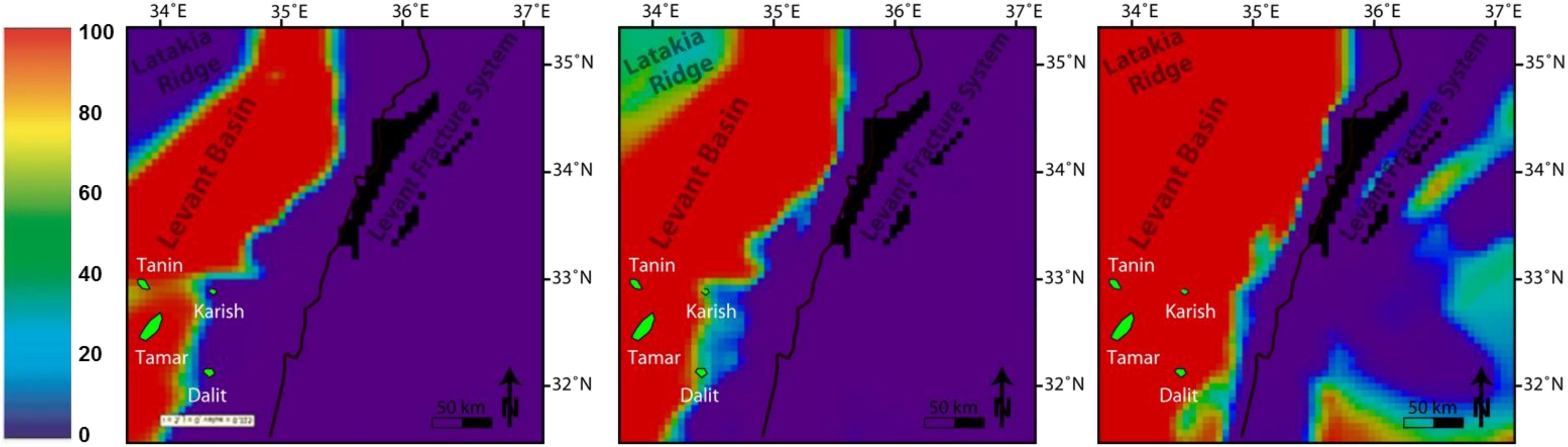


All these (E, A) couples are solution of the optimization problem

Kinetics:
Shortcomings and limitations

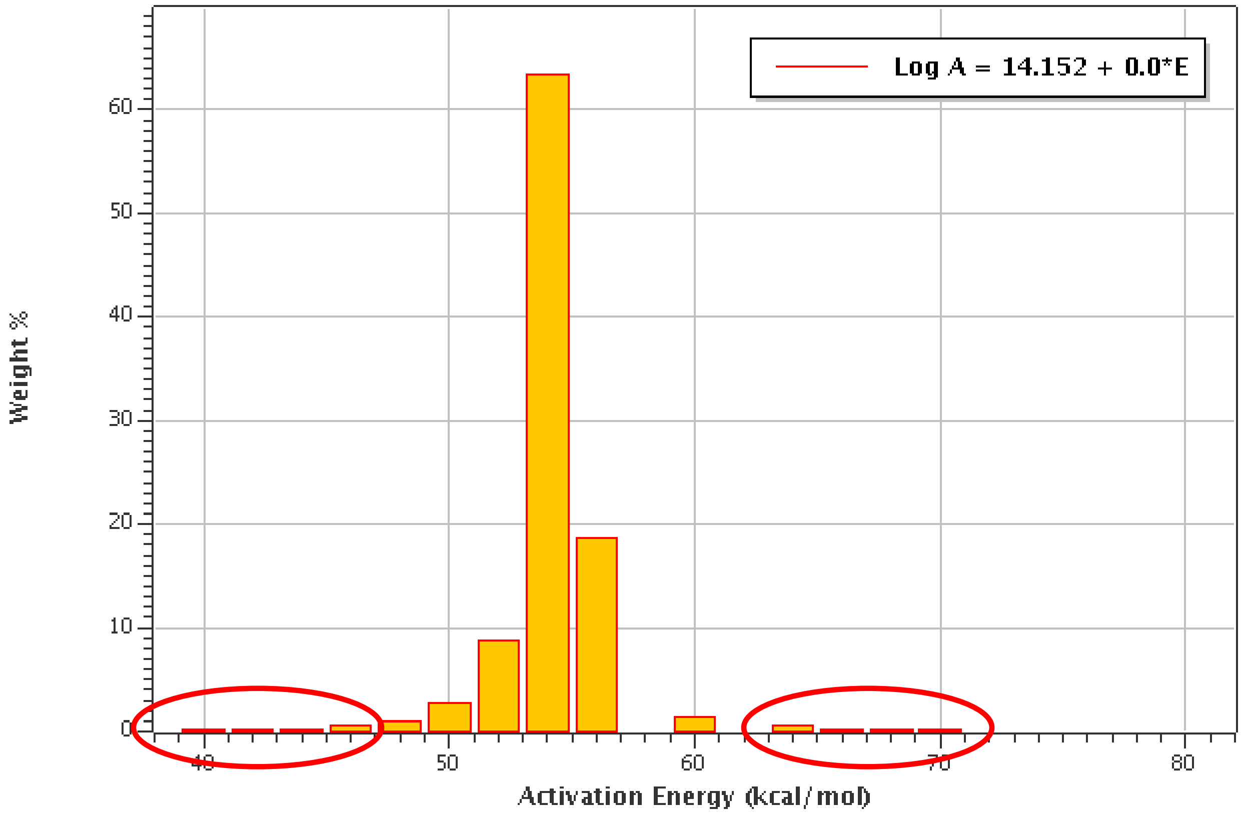
- Propagation of uncertainties on kinetics determination to maturity estimation at basin scale using TemisFlow:
  Application to the Cenomanian source rock of the Levantine Basin

Transformation ratio



P10 **P50** **P90**

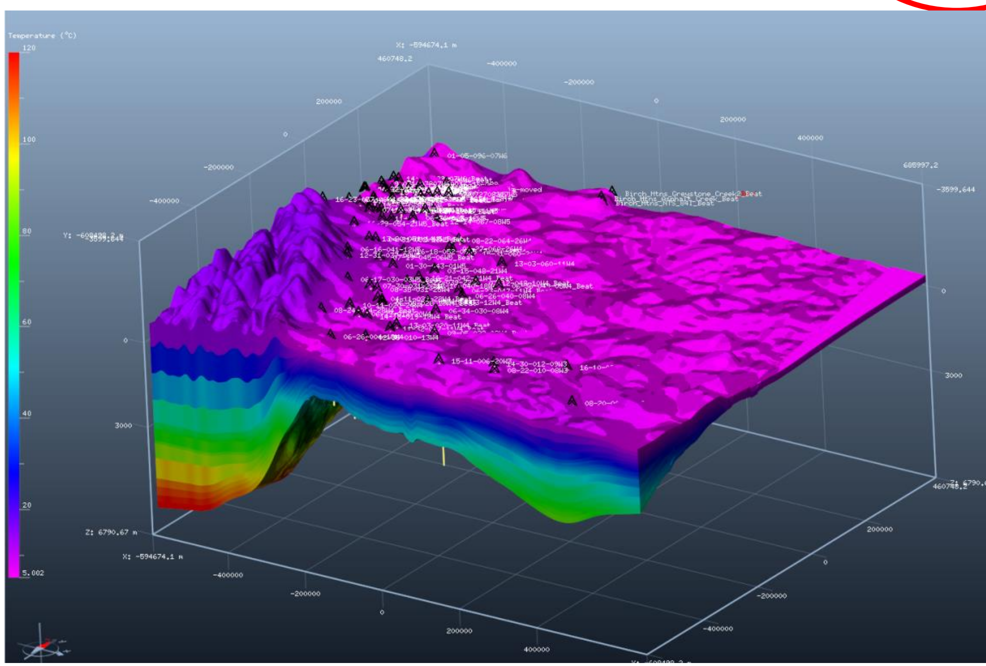
Kinetics:
Shortcomings and limitations



Noise or information?

Current work:
Back to the petroleum system

Puits	Prof foreurs (m)	Tmax (°C)	TOC (wt.%)	HI (mg/g)	**Reflectance de la vitrinite Ro%**
16-22-76-12W6	2187.4	467	3.60	56	**1.44 ± 0.08**
04-32-84-12W6	1581.4	435	2.74	506	**0.43 ± 0.04**
06-33-72-25W5	1595.5	429	3.04	486	**0.59 ± 0.06**
11-28-71-03W6	1861.6	436	2.34	530	**0.53 ± 0.03**
11-28-71-03W6	1845.2	437	2.33	513	**0.64 ± 0.08**
14-32-73-08W6	2066.6	443	1.17	190	**1.11 ± 0.11**

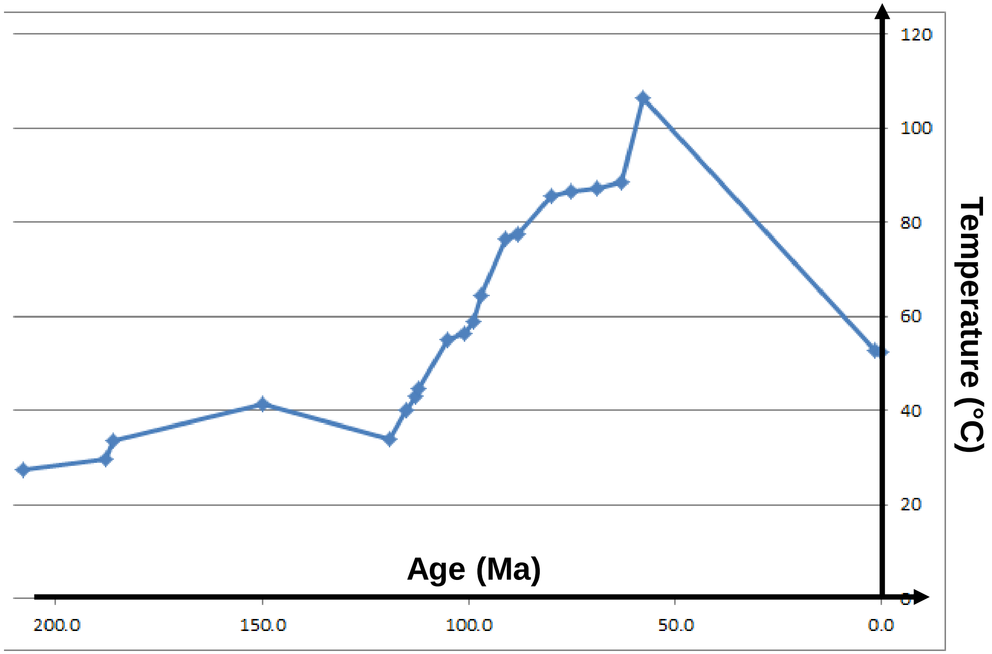


Romero-Sarmiento *et al.* (In progress)

Current work:
Back to the petroleum system

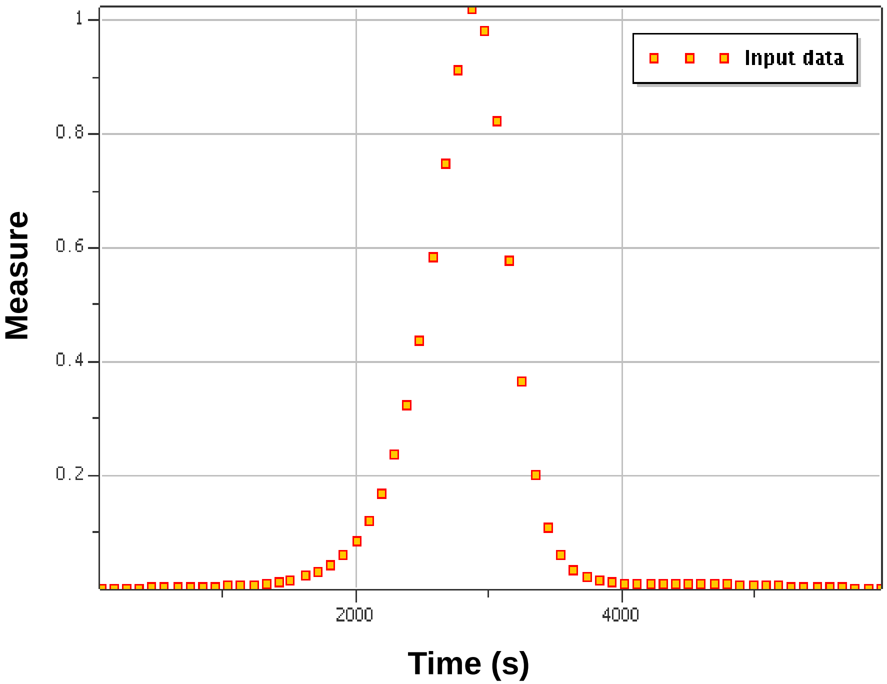
For each sample (mature or immature) we proceed to:

Reconstruction of paleo-temperatures



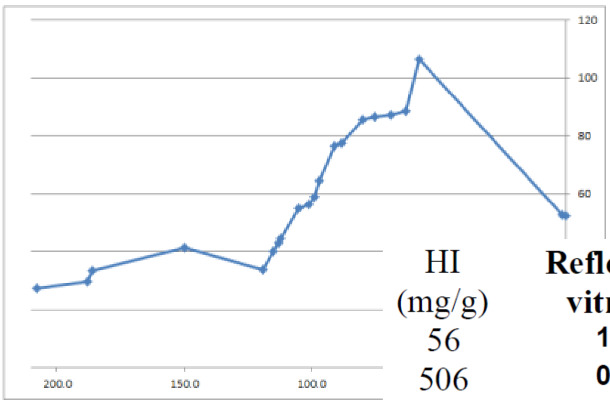
Romero-Sarmiento et al. (In progress)

Artificial maturation in lab



Current work:
New optimization procedure

Data: natural series and laboratory experiments



HI (mg/g)	Reflectance de la vitrinite Ro%
56	1.44 ± 0.08
506	0.43 ± 0.04
486	0.59 ± 0.06
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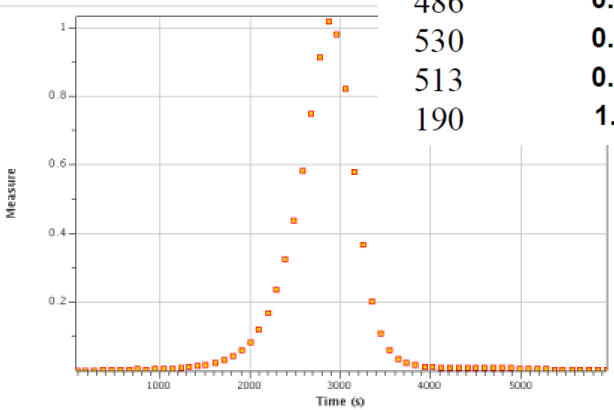
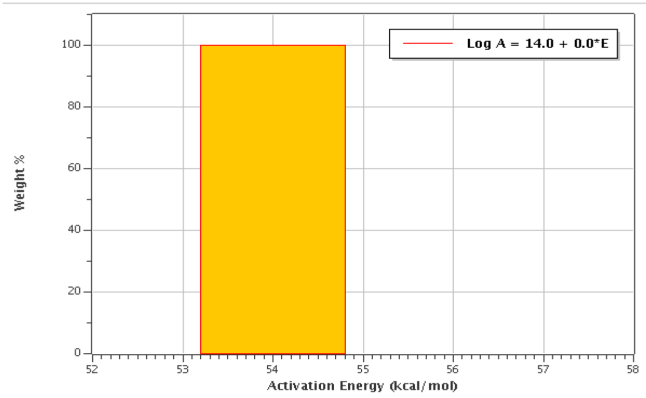
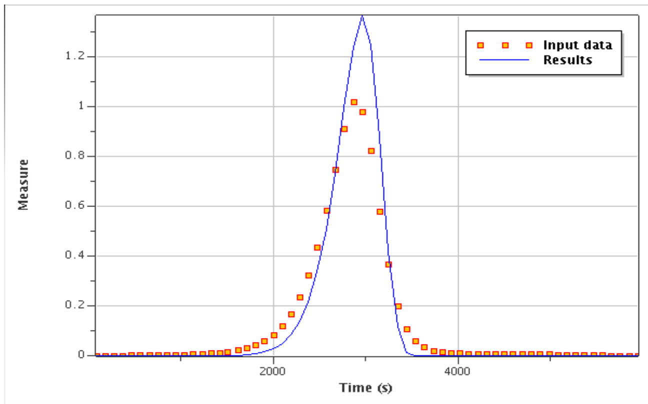
513	0.64 ± 0.08
190	1.11 ± 0.11







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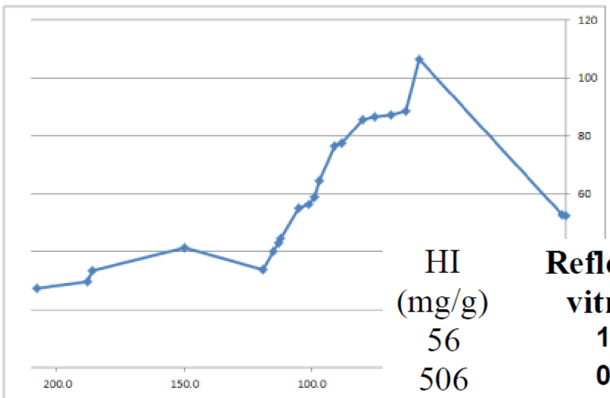

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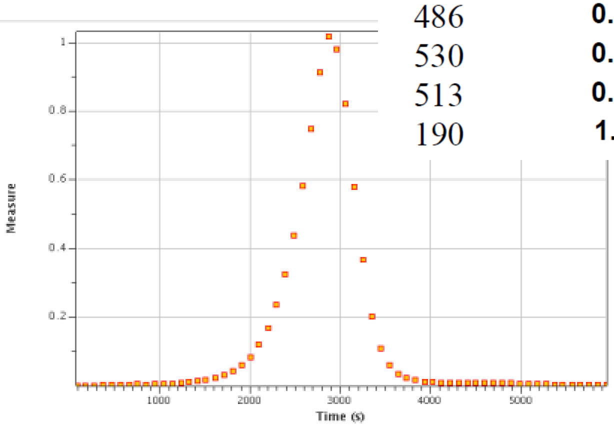

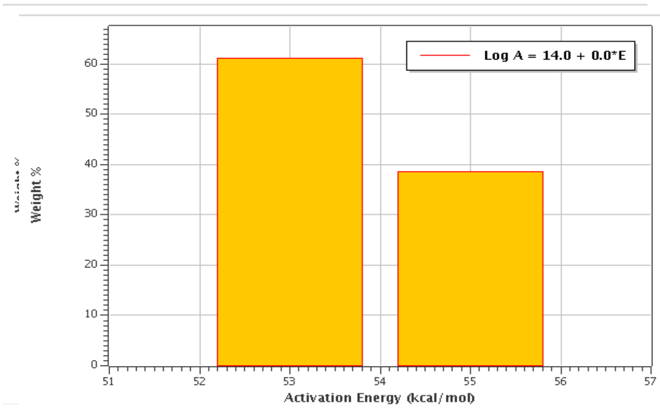

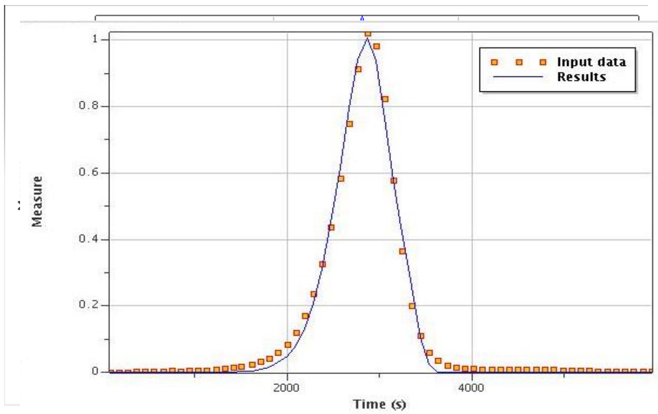

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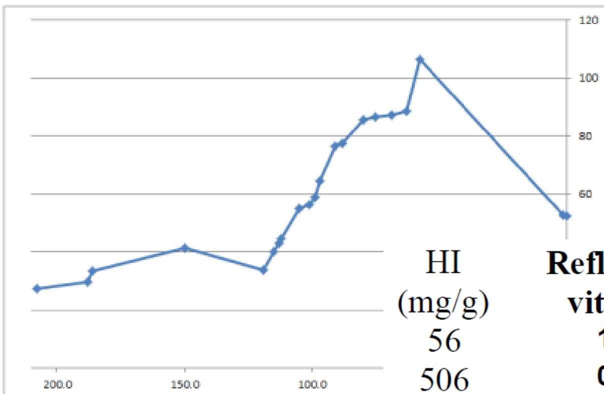

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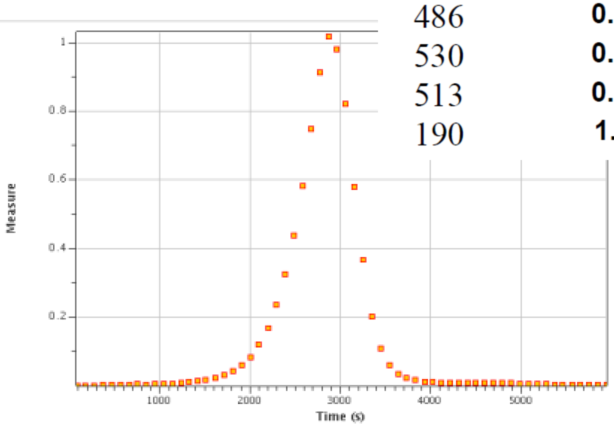

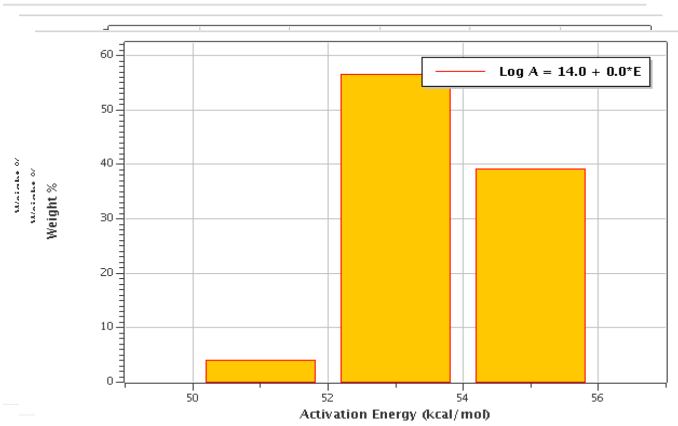

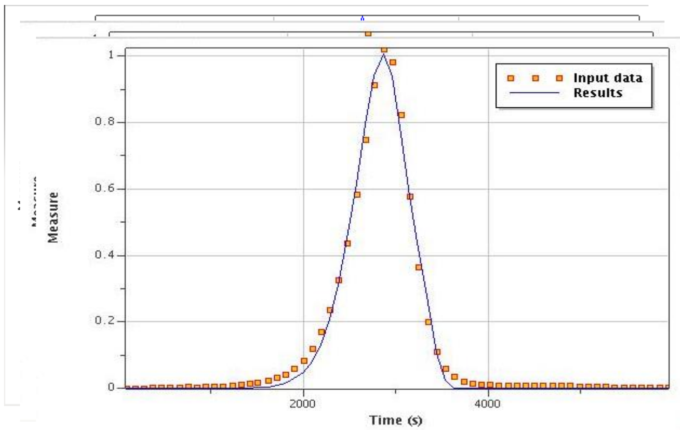

Current work:
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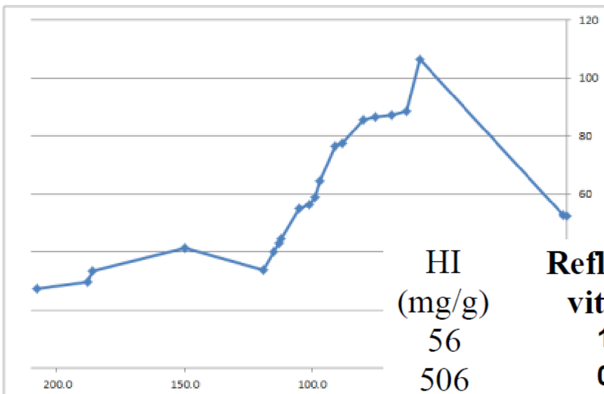
Data: natural series and laboratory experiments



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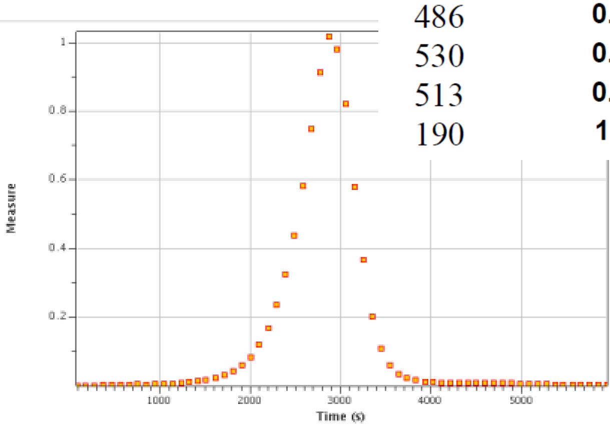
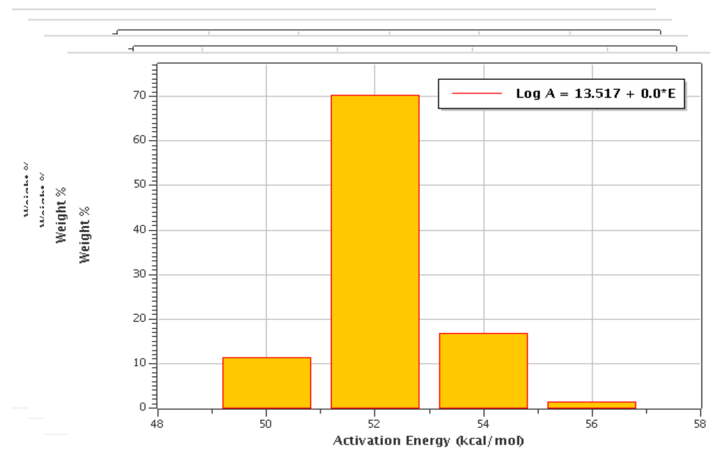
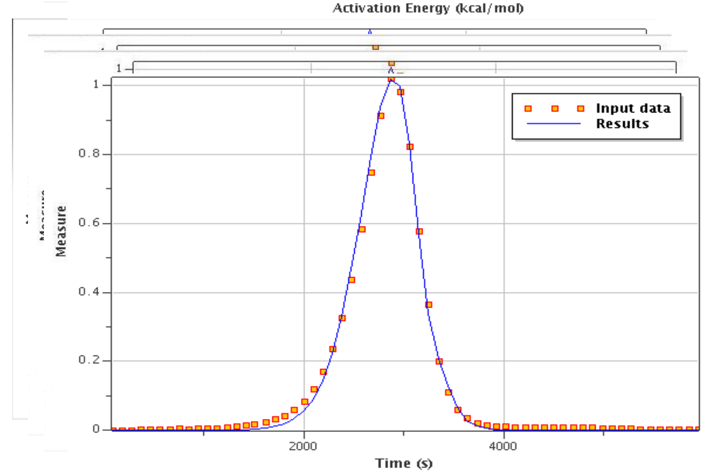
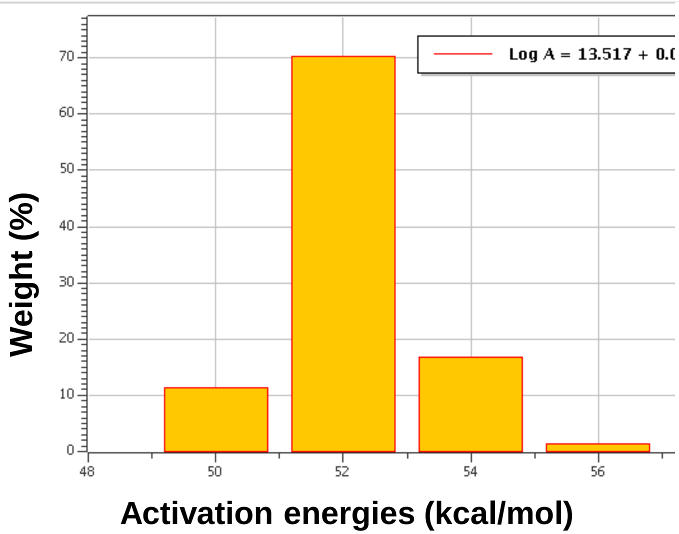




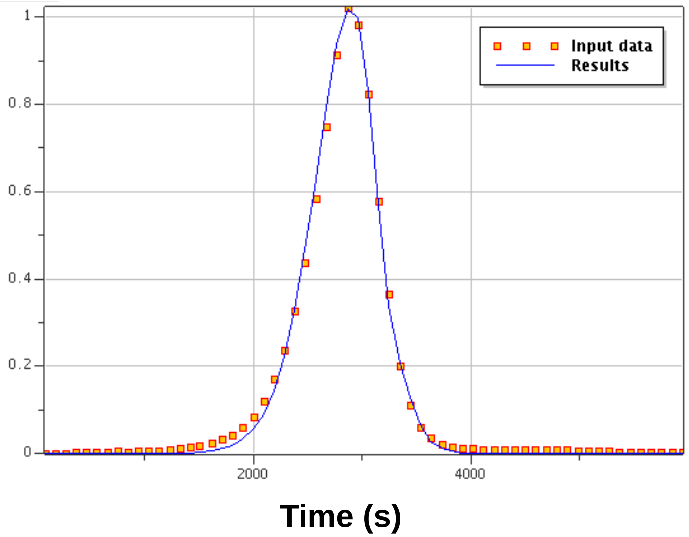


Current work:
New optimization procedure

Simpler kinetics



… still very well calibrated on laboratory data

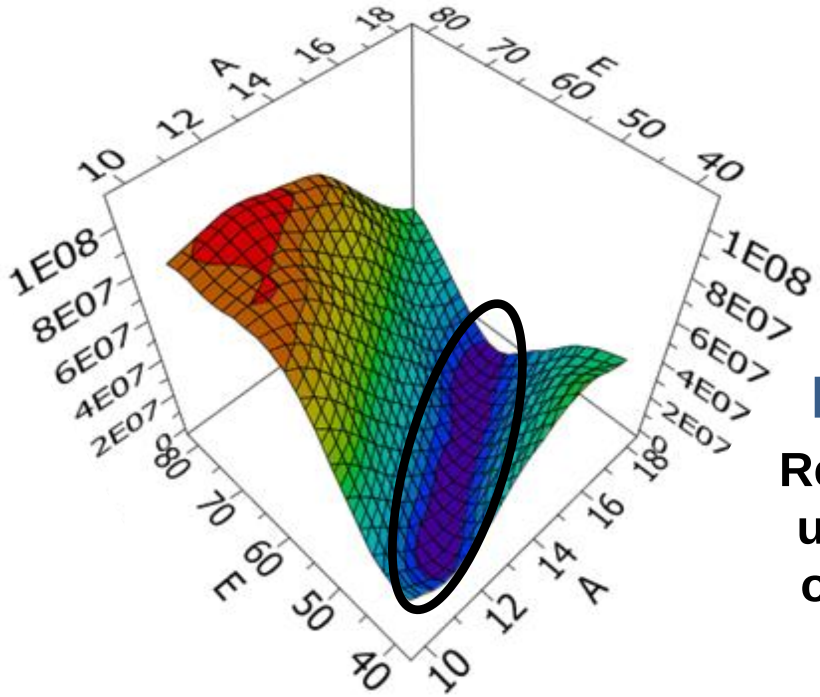


… and also on natural series

	Measured		Simulated	
Well	Tmax	HI	Tmax	HI
Well 1	467	56	470	40
Well 2	435	506	437	498
Well 3	429	486	430	510
Well 4	436	530	434	508
Well 5	437	513	436	505

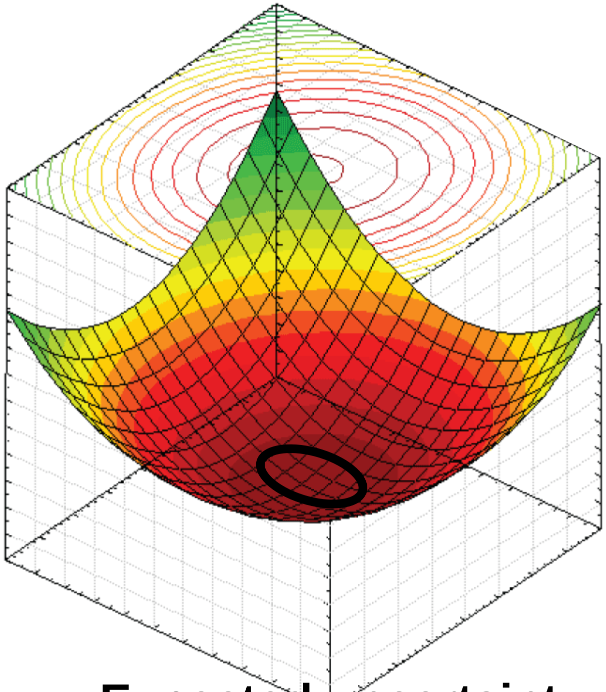
Current work:
New optimization procedure

Most important expected result from a basin analysis perspectives



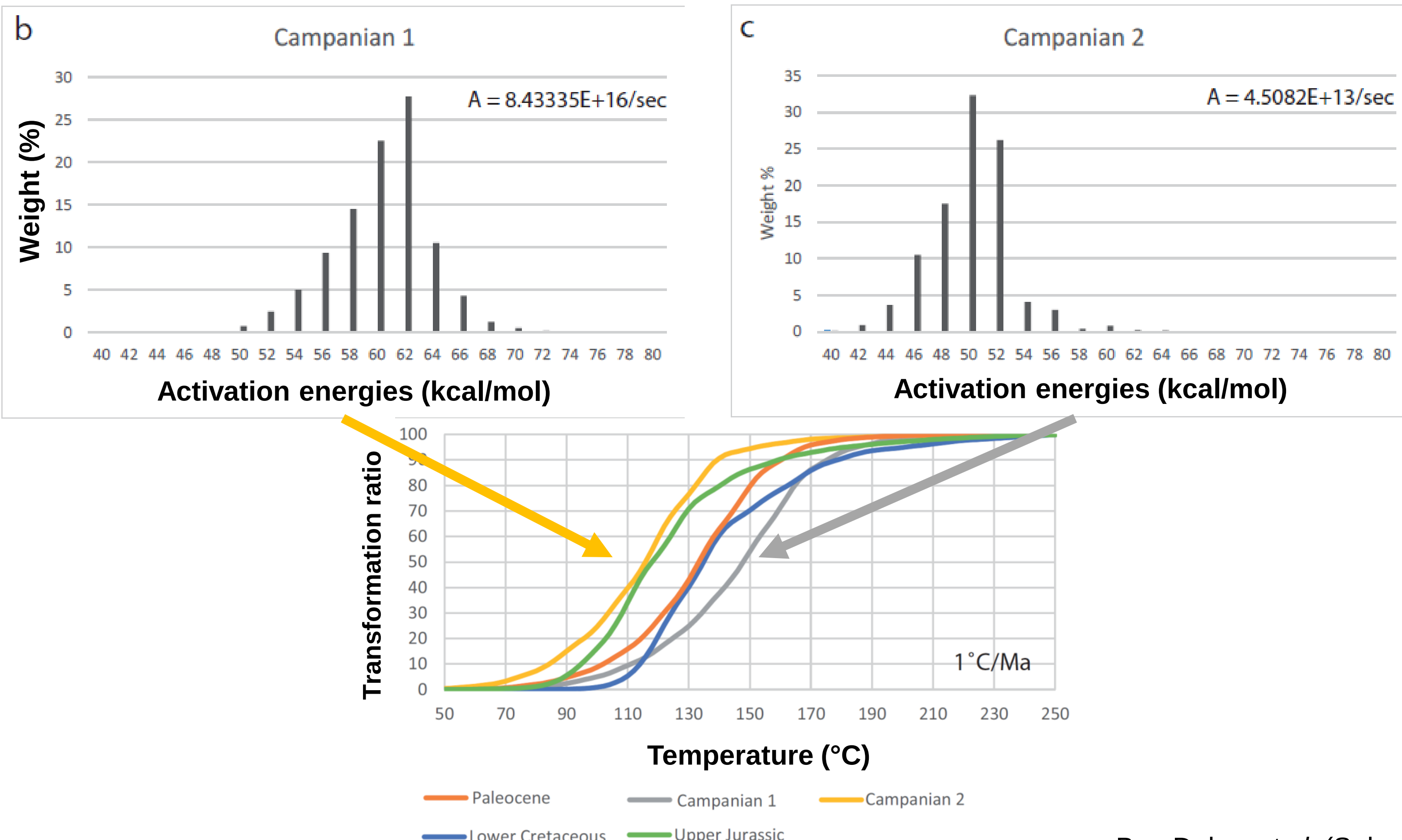
Current uncertainty on kinetics

Reduction of uncertainty on kinetics



Expected uncertainty

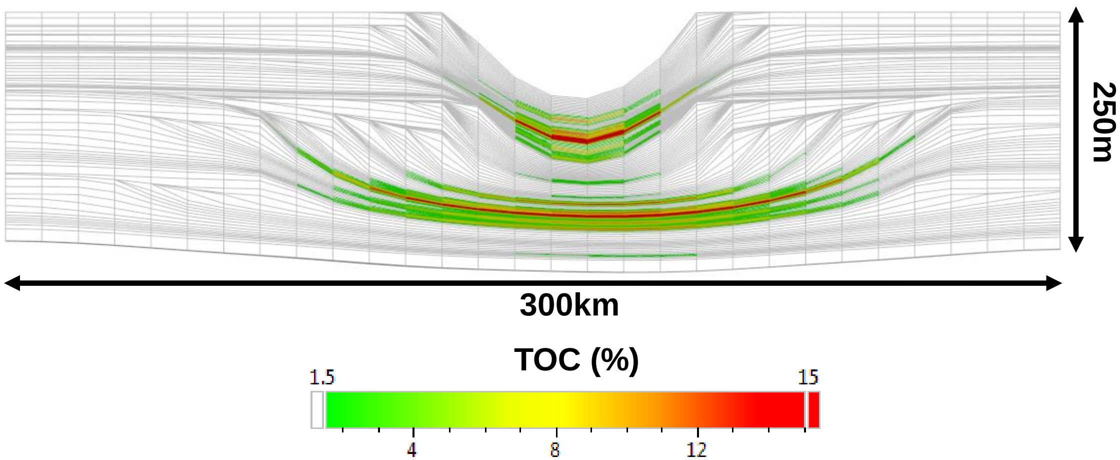
Kinetics: Perspectives

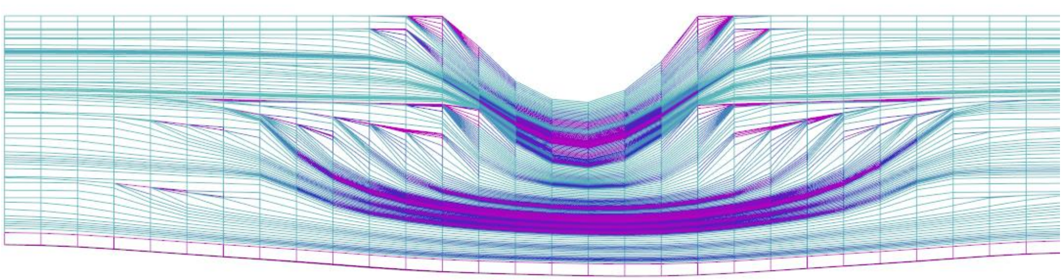


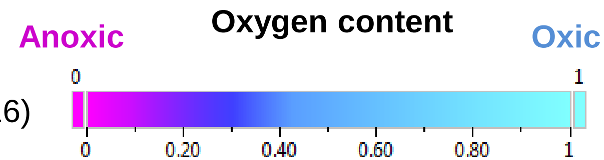
Bou Daher *et al.* (Submitted)

Perspectives

Modeling of the organic matter properties and distribution in the Natih Fm. using DionisosFlow

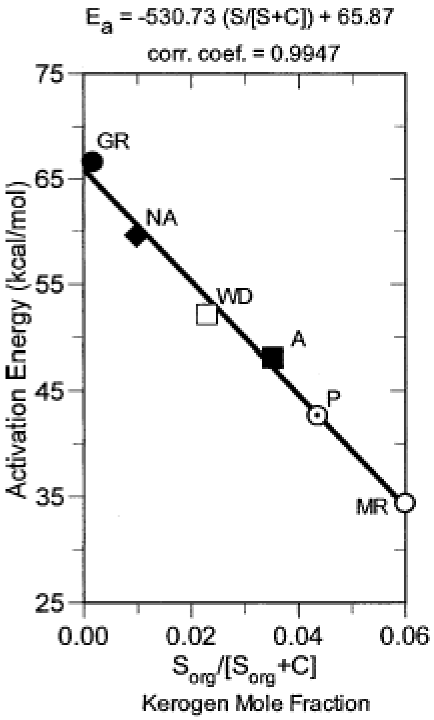






Chauveau *et al.* (2016)

Sulfur content



Lewan and Ruble (2002)

Conclusions

- Kinetics are important for petroleum system analysis
- Laboratory techniques are crucial to characterize source rock maturation BUT there are still limitations in kinetics predictivity
- Coupling laboratory data and natural series (with basin modeling paleohistory reconstruction) can lead to **more predictive kinetics (timing)**
- Stratigraphic models (e.g., DionisosFlow) could help to make the link between deposition environment and kinetics and lead to **more predictive generation timing at basin scale**

Thank you for your attention