GEOCHEMICAL CALCULATION SOFTWARE

GEOWORKS

Modeling/Quick-Multi Kinetics modules

In this note we will take for example an immature sample (Tmax<420°C) from a surface sampling in the Toarcian layer of the eastern edge of the Paris basin near the village of Fécocourt.

For our modeling we will therefore use a burial rate and temperature model characteristic of the Paris basin based on experimental and extrapolated well data. The points representing the Paris basin in the "Quick Modeling" are based on geological studies of a sedimentary layer belonging to the Lias (lower Jurassic): the Toarcien (deposited about 180Ma ago). These data were acquired using drilling study and extrapolations and represent the evolution of the maturity of the Toarcian stratigraphic layer in the Paris basin where it underwent its deepest burial. These data are also valid for the other layers of the same basin provided that the time and physical differences between these layers are taken into account.

The examples included in Geoworks (Paris Basin and Vicking Graben) are well known series in France and must serve as examples for users and/or as a control for the kinetic distributions of type II and III that they can obtain. For more accuracy, it is up to users to create their own models based on the burial laws of the sedimentary basin considered in their study put it in relation with the kinetic distributions of source rocks.
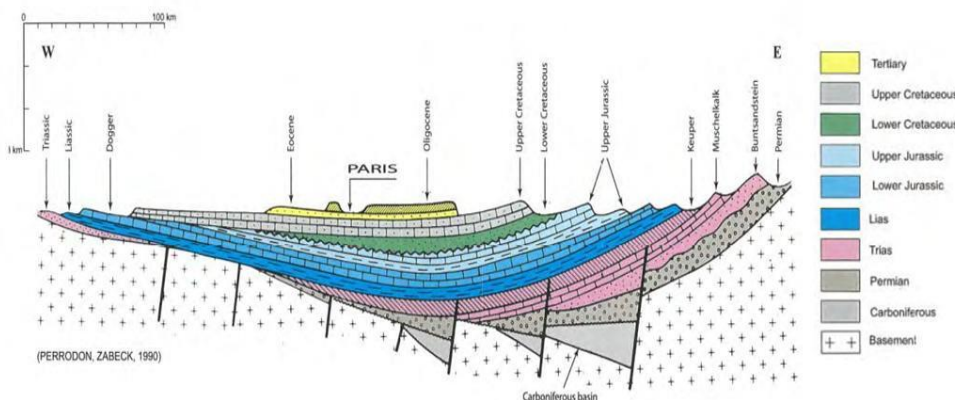
Simplified geological section (AB) oriented WNW / ESE of the Paris Basin
(Perrodon A., 1990)

Step 1: prerequisites

The studied sample should not be too mature. If it is too mature cracking doesn't occur and there is no kinetics study possible.

It is necessary to know burial history data of the basin (or similar) from which the sample comes.

The S1 peak and the potential drilling mud pollution must have been extracted from the sample either manually before Rock-Eval analysis or using GEOWORKS CleanSim module.

The the oil cracking reaction must be complete.

Step 2: Kinetics

Start by going to "Compute" then "Kinetic options" in order to obtain the best kinetic fit for your sample as well as the associated data (<u>pre-exponential factor</u> (A), activation energies (Ea), etc.)

Concerning the "Parallel reactions tab", unless you know the <u>pre-exponential factor</u> required for the sample you are working on, it is recommanded to use the tool « optimize A in range » between 1e+13 and 1e+15 (according to the littérature). Depending on your analysis, it is also often more accurate to use 1kcal/mol as « ΔE ».

In the « Compute option » tab choose wathever fits best your HC curve. However, S1 peak should not be taken into account for kinetics as it is not kinetics so the curve fitting you choose should not include the isotherm section of the analysis. Finally, if you used a RE6 for your analysis choose « Interpolated temperature » for « Reaction velocities », if you used a RE7 chose « Pyrolysis temperature data ».
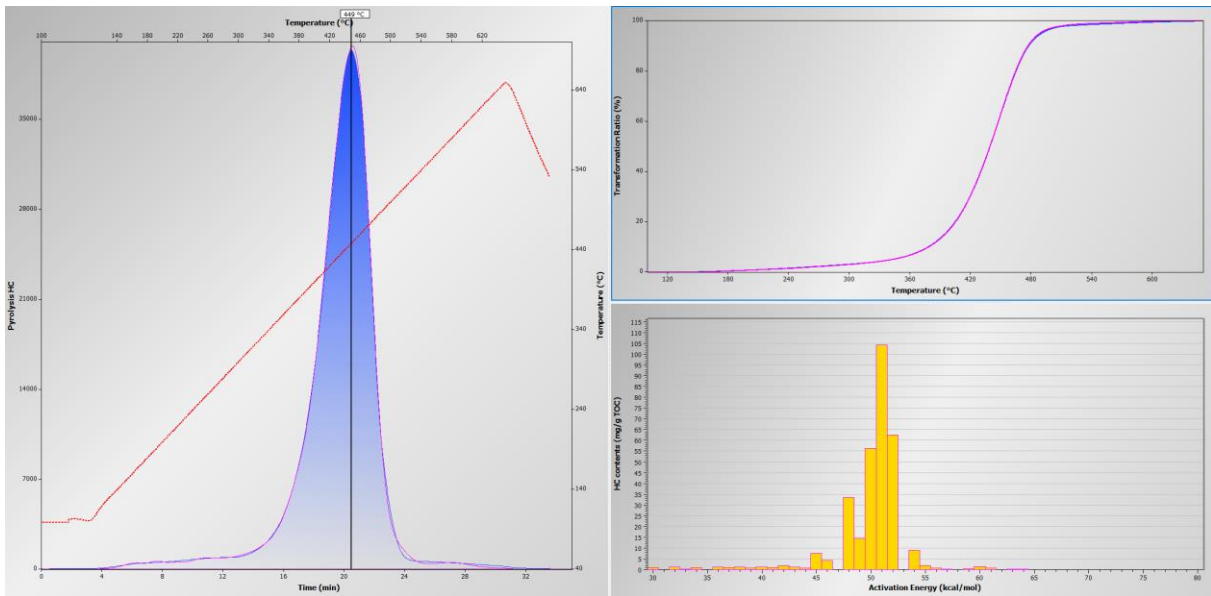
Here is the result obtained in the case of the example considered when following those simple steps:

A = 3.460639e + 13
Main Ea = 51 kcal / mol
Residual error = 1.181507e-06
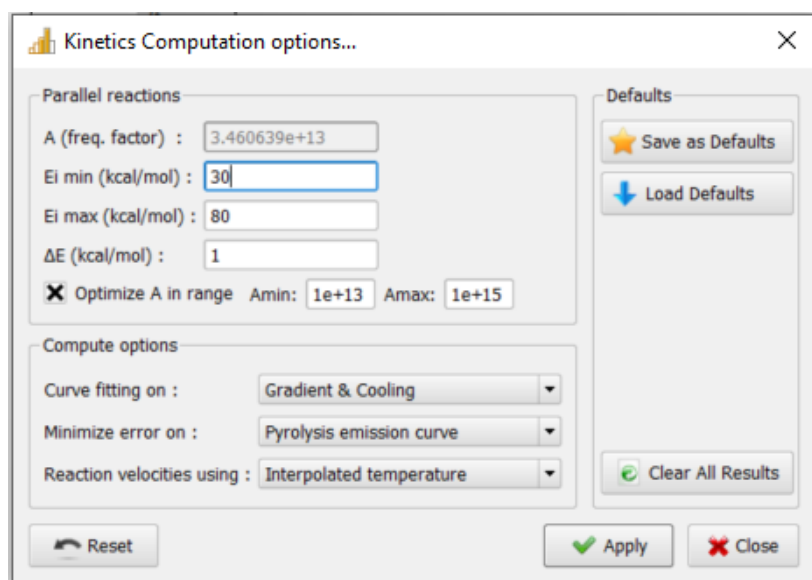
This can also be done using the multi-heating kinetics module if more accuracy is needed.

Step 3: Modelling

Open the modelling module and in the display tab uncheck "Initial burial only".
In the compute tab, "modelling options" add your basin burial and temperature model and experimental data.

The Depth (m) VS Oil + Gas (mg/g TOC) graph should show two curves:
-   Your sample curve (green in this example)
-   Your model curve (yellow in this example)

If the kinetics study/fit is right the last point of your sample curve should be on the model curve which is often not the case as there is many kinetics fits for the same HC curve.

Last point of the sample out of the model curve
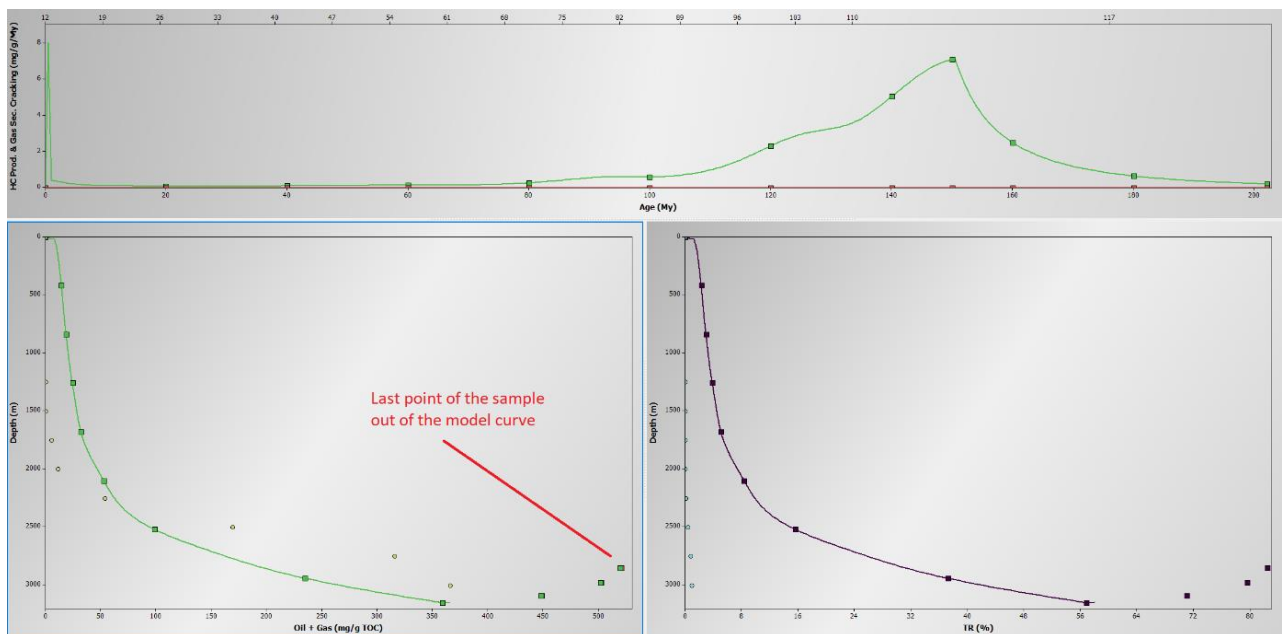
It is now appropriate to play with the A in the Kinetics options until the last point of our sample appears on the curve of the model (be careful to click on "Valid current kinetics parameters and results" every time you change the kinetics options. If this is not done the modeling curve will not be affected by the changes you made).
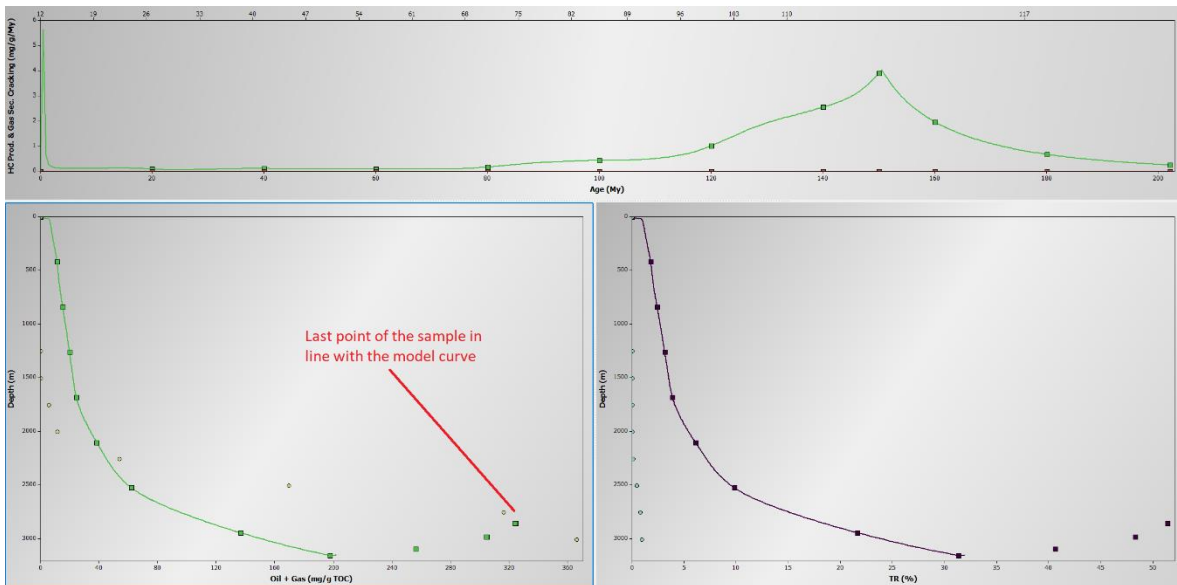
Once you have found an A which allows the last point of the sample to be located on the model curve, it is possible to use the "optimize A in range" tool by defining a more restricted range based on what you already know to refine your result (in this example we found an A of 3.5e + 14, then "optimize in range" between 3e + 14 and 3.6e + 14 to finally obtain an A of 3.527286e + 14). It goes without saying you must always check that the fit of the HC curve remains correct.

Here is the new result obtained in the case of the example considered when following those simple steps:

A = 3.527286e+14
Main Ea = 54 kcal / mol
Residual error = 8.182819e-07

To facilitate this last step you can reduce all the windows of the software except kinetics and modeling, right click on the software background and then select "Tile horizontaly" to have everything on the same screen and see changes made live on the curves. In the modeling module, it should be understood that only the last point represents the studied sample, the previous points only represent stages of maturation through which it went.

Nanterre, May 9th 2019

Signed:

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