Ceres2D: A Numerical Prototype for HC Potential Evaluation in Complex Area

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Résumé — Ceres2D : un prototype de modèle de bassin pour l’évaluation du potentiel pétrolier en zones complexes — Cet article décrit Ceres, prototype de modèle de bassin capable de prendre en compte la compaction des milieux poreux, les transferts de chaleur, la génération et la migration des hydrocarbures. De plus, Ceres a été conçu pour gérer des géométries qui évoluent au cours du temps à la suite des effets de la sédimentation, des érosions, de la tectonique salifère et des déplacements le long des failles.

Une étude avec Ceres comprend trois étapes principales. La première concerne la construction de la section à l’époque actuelle. Ceci est généralement effectué à partir des données sismiques, des données de puits et des données de terrain. La seconde étape est la restauration de la section. Cette phase consiste à déterminer, à partir de la section à l’époque actuelle et pour chaque couche définie sur cette section, les géométries intermédiaires en reculant dans le passé. Les simulations directes constituent la troisième et dernière étape du processus. Et, afin de pouvoir résoudre les équations généralement admises en modélisation de bassin, il nous a fallu développer des méthodes numériques originales basées sur des techniques de décomposition de domaines.

Le prototype a maintenant été utilisé pour l’étude de systèmes pétroliers. Dans un premier temps il a été testé pour des études de sensibilité concernant les perméabilités des failles en Bolivie et dans l’offshore du Congo. Dans le golfe du Mexique, il a permis d’étudier l’impact de la tectonique salifère sur la migration des hydrocarbures. Plus récemment, Ceres a été utilisé dans le cadre du consortium SubTrap dans des zones complexes comme les avant-pays canadiens et ceux du Venezuela. En ce qui concerne ces dernières études, l’implication des géologues structuralistes à toutes les étapes du processus s’est révélée véritablement bénéfique.

Abstract — Ceres2D: A Numerical Prototype for HC Potential Evaluation in Complex Area — This paper deals with the Ceres prototype which is a basin model able to account for porous medium compaction, heat transfer, and hydrocarbon generation and migration. Furthermore, Ceres was designed to handle changing geometry through time as results of sedimentation, erosion, salt or mud creeping and block displacement along fault.

The classical flow chart to perform a case study is composed of three main steps. The first step is the building of the present day section. This is generally done with data coming from the seismic interpretation, well data, field data and core data. The second step is the restoration of the section. Thus from the section at present day, the section is restored back in the past for each of the defined layer, and until the substratum is reached. The last step is the forward simulation. And, in order to solve the coupled
equations that are generally used in basin models, we had to develop original numerical methods based on domain decomposition techniques.

The Ceres prototype has now been used to study petroleum systems. It has been used to perform sensitivity studies on fault permeability in the Bolivian foothills and the Congo offshore. In the Gulf of Mexico, it allowed to study the impact of the salt tectonics on the hydrocarbon migration. More recently, the Ceres prototype has been tested, within the frame of the SubTrap consortium, in thrust areas such as the Canadian foothills and the Eastern Venezuelan foothills. For these last case studies, it has been beneficial that structural geologists were involved at all stages of the process.

INTRODUCTION

Basin modeling aims at reconstructing the time evolution of a sedimentary basin in order to make quantitative predictions of geological phenomena leading to pressure generation and hydrocarbons accumulations. It accounts for porous medium compaction, heat transfer, hydrocarbon formation and migration (e.g. Schneider et al., 2000b).

Today’s state-of-the-art sedimentary basin models are able to handle relatively simple geometries resulting from deposition, erosion and vertical compaction. Two main areas however are insufficiently or not at all treated:

- Basin geometry is often not precise enough. Most basins are cut by faults with significant offsets. In addition, basin geometry may be affected by the creeping of salt or mud which in turn may lead to the formation of diapirs.
- Fluid flow and convective heat transfer do not handle the permeability evolution of faults correctly. A fault can be pervious or acts as a seal, and it can change its behavior through time.

The aim of the Ceres project was to build a prototype that is able to simulate three-phase flow in a 2D section of a basin, whose geometry changes due to deposition, compaction, erosion of the sediments, salt or mud creeping, and blocks displacement along faults.

In the first part of the paper, Ceres modules are presented according to the classical work flow used to perform case studies. The second part of the paper is dedicated to a quick review of some cases performed with Ceres during the last years.

1. CERES PROTOTYPE

The software is composed of several modules. The main modules are a section editor, a restoration module and a forward simulation simulator. The other modules are a chronostratigraphy editor, a lithology editor, a kerogen editor, fluid editors, a mesh editor, a run editor and visualization modules. All these modules are managed by a study browser.

1.1 Edition of the Initial Section

The initial section is composed of a chronostratigraphic column and a 2D cross section. In the study browser, this first composite object is represented by the root of a tree. The number of horizons, the corresponding number layers, the ages of the horizons, and the values of the eustatism level are edited with the chronostratigraphic editor.

The section can be edited directly from scratch or its geometry can be imported from other softwares. It is recommended, at this stage to use a structural software (e.g. Locace) that is able to balance the section. The edition of the section is split into three steps. First, the geometry of the section is defined (Fig. 1a). Second, the geological attributes are affected. These attributes may be horizon, fault, section boundary, facies change limit. At this stage a decollement level is defined by superimposing an horizon with a fault. At the end of this second step, the section is filled with the lithologies (Fig. 1b). The third step of the edition of the section, is the numerical step. At this stage, the blocks, which represent the smallest kinematics units, are defined (Fig. 1c). Then, each of the blocks is gridded (Fig. 1d). One specificity of the gridding is that each block holds its own grid with no constraint coming from the other blocks. The faults are not gridded in the initial section because their grids are created dynamically during the forward simulation.

The initial section (Fig. 2), once edited, holds the upper mantle, the ductile lower crust, the brittle upper crust and the considered sedimentary part. The faults can exist in the sediments and in the brittle upper crust; they may be rooted at the interface of the brittle upper crust with the ductile lower crust or at predefined decollement levels.

1.2 Restoration of the Section

Once the edition of the initial section is terminated, a backward process, which includes a kinematics restoration, backstripping, and thickness modification, allows determining the input data for the forward calculator. During the backward process, all the periods defined in the chronostratigraphic column should be restored. For this step, it is recommended, especially for complex area, to use a structural forward model (e.g. Thrustpack) in order to constrain the geometry through time and to provide a reliable estimation of the eroded parts. At the study browser level, a restoration scenario from the initial section to the final section, only composed of the basement, is represented by a
The main steps of the section editor are: (a) edition of the geometry; (b) edition of the geology; (c) creation of the kinematic blocs; (d) building of the grid for each bloc.

Resulting section at the end of the edition.
branch of the tree. Each leaf of the branch is the section at the corresponding age. For each restoration, the backward process is composed of different steps.

The first step is the edition of the eroded parts if erosion has occurred during the considered period (Fig. 3b). This edition may be helped by importing templates. The second step is an automatic popping of the section. It allows taking off what has been sedimented during the considered period. Once the erosion and the sedimentation accounted for, the resulting section is decompacted using porosity depth relationships.

The backstripped section is then restored from a kinematics point of view (Fig. 3c). At this stage, the displacements along faults are accounted using translations and vertical shear. As for the edition of the eroded parts, this operation may be constrained with the use of templates.

Once the section is restored, the last step of the backward process is the thickness modifications (Fig. 3d). This step allows accounting for salt or mud tectonics. Correction of the edition of the erosion may be done at this stage. Nevertheless, the main use of this editor, is to account for thickness modifications due to salt tectonics or mud creeping.

These steps should be performed for each layer initially defined in the section at present day. The result is a scenario of restoration (Fig. 4) that should be validated against the previous structural study.

1.3 Forward Simulations

In these complex geometries, faults cut the basin into blocks that naturally define computational sub-domains. In the
blocks, the model accounts for the porous medium compaction, erosion, heat transfer, hydrocarbon formation (see Appendix 2) and migration (Fig. 5). The equations are mass conservation of solid and fluids (water, oil, gas) coupled with the Darcy’s law and a compaction law (see Appendix 1). The faults have a constant thickness and their permeability may evolve with time. The prototype allows using three permeability models for the faults: faults may be impervious, pervious or may have a permeability that is a function of the neighboring lithologies and of the strain rate.

In order to solve the three-phase flow in a basin cut by faults along which block displacements can occur, Domain Decomposition Methods (DDM) are used (Willien et al., 1998a, 1998b). The classical techniques used in the first version have been improved by using optimized interface conditions (Faille et al., 2002). In these methods, the faults are considered as subdomains with their own geological properties. However, because of the very small width of the faults in comparison with the size of the basin we are studying another approach where the faults are characterized as interfaces between blocks (Faille et al., accepted). In all the cases, the equations are discretized using a cell-centered finite volume scheme in space. Finite volume methods are known to be robust and cheap methods for the discretization of conservation laws in heterogeneous media and have the important property to be conservative.

Different time discretizations coupled with several DDM algorithms have been tested. In a first stage, a classical IMPES scheme (Implicitly advances the Pressure and Explicitly updates the Saturation in time) was used. But, it is well known that this scheme needs time step limitations for stability reasons. In order to use larger time steps, we have tested (Flauraud et al., 2000) a sequential scheme, called IMPIMS (Implicitly advances the Pressure and Implicitly advances the Saturation in time). It consists in solving two nonlinear systems, one for the pressure (as in the IMPES scheme) and one for the saturation.

2 CASE STUDIES

This prototype has now been used to study petroleum systems all around the world. In the Bolivian foothills, where faults are supposed to be the most important carrier beds for hydrocarbon migration it has been used to perform a sensitivity study on fault permeability (Schneider et al., 1999). In the Congo offshore, it has also been used to study the impact of faulting on maturity of the organic matter and hydrocarbon migration (Schneider et al., 1999). In the Gulf of Mexico, it has been tested for studying the impact of the timing of salt withdrawal on hydrocarbon migration (Schneider et al., 2000a).

More recently, Ceres has been tested within the frame of the IFP Subtrap consortium in thrust area such as the Canadian foothills and the Eastern Venezuelan foothills. The prototype has been used to quantify the fluid flow and to reconstruct the pore fluid history of the subthrust reservoirs. The use of Ceres implies a backward restoration. Although the backward restoration is fully appropriate for modeling an extensional basin well balanced (e.g. with Locace), it may turn difficult to constrain successive intermediate evolutionary stages, as far as the topography (prediction of erosion) and thrust geometry are concerned. In consequence, we have decided to use also the Thrustpack forward kinematic software to elaborate a better structural scenario. These successive intermediate geometries constructed with Thrustpack were then used as templates for the Ceres modeling.

2.1 Venezuelan Transect

As defined previously, the first work to perform at the beginning of a Ceres study is the definition of the initial
section (Fig. 6). This was done with data coming from the seismic interpretation, well data, field data, core data. Then, the available data and the Thrustpack scenario have been used to build the Ceres dataset.

From the data available, it is clear that the El Furrial structure is closed today as it is overpressured while the equivalent layers of the southern part have nearly hydrostatic pressures. The initial geometry (Fig. 7a) did not allow closing the El Furrial structure. Thus a second lithology distribution (Fig. 7b) has been defined by the introduction of a shaly layer at the top of the Oligocene. With this new geometry, the El Furrial structure that was not properly sealed in its northern part and in its southern part is now closed today at both sides.

The El Furrial trend from the Eastern Venezuelan transect displays two distinct episodes of quartz cementation. The first generation of quartz overgrowths, which account for more than 90% of the cements, is developed during the active dewatering processes in the Oligocene strata of the underthrust foreland. This is evidenced by the $\delta^{18}O$ signature and by the Ceres fluid flow simulations (Schneider et al., 2001). In contrast, the second generation of quartz overgrowths displays quite distinct $\delta^{18}O$ values. These cements are originated when the deeper aquifer of the Lower Cretaceous Barranquin formation from the Pirital hanginwall started to expell its fluids towards the Oligocene reservoir of the adjacent El Furrial footwall unit. This is well evidenced by the Ceres fluid flow simulations (Schneider et al., 2001).

### 2.2 Canadian Transect

As for the Venezuelan transect the first work to perform at the beginning of a Ceres study is the definition of the initial section (Fig. 8). Then, one scenario for the geometry evolution has been defined (Fig. 9). It is characterized by five major episodes in the geodynamic evolution:

- pre-flexural deposition during the Paleozoic and lower Mesozoic on a Precambrian substratum;
- deposition of synflexural formation from $-100$ Ma to $-76$ Ma;
- a main thrusting phase between $-76$ Ma and $-55$ Ma;
- a strong erosion from $-55$ Ma to $-20$ Ma;
- since $-20$ Ma the area is uplifted.
Figure 6
Geometry and lithology distribution of the Venezuelan section at present day. The white dot indicates the El Furrial structure.

Figure 7
Initial lithology distribution (a) and new lithology distribution (b) where impervious sediments are involved in the El Furrial thrust. The white dot indicates the El Furrial structure.
Figure 8
Geometry and lithology distribution of the Canadian section at present day.

Figure 9
Geometrical evolution of the Canadian section from –76 Ma to present day.
Unlike in Venezuela, where modern fluid flow is still controlled by the compressive evolution of the foothills, the Ceres fluid flow simulations shown that a dramatic change occurred since the end of the Laramian Orogeny. Indeed, more than 4 km of Mesozoic and Cenozoic series have been eroded and the hinterland and the foreland were progressively uplifted. Thus, the present day fluid flow is mainly controlled by the topography and the geometry of the aquifer (Fig. 10).

CONCLUSION

Ceres is a new tool that enable to perform basin modeling in complex area where faults or salt tectonics may constrain the petroleum system. This prototype has been tested successfully worldwide. It may now be used to understand much more petroleum systems as the ones generally addressed with classical basin models.

The Ceres software, when coupled with a forward kinematics tool, such as Thrustpack, can be used for the simulation of the very complex structures of the foothills. It can provide reliable values for the velocity of the paleo-fluid circulations and for the paleo-fluid pressure.

It should be noticed that for these studies, it was of real importance to work closely with the structural geologists in order to define the initial section and the scenario for the kinematics restoration (Schneider et al., 2002).

REFERENCES


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APPENDIX

1 PHYSICAL CONCEPTS
AND MATHEMATICAL FORMULATIONS

The energy equation (or heat equation) is:

\[ \rho \phi \frac{\partial T}{\partial t} + \nabla \cdot (\phi \rho \mathbf{V} T) = \nabla \cdot (k \nabla T) + \frac{S}{T} \pm \left( \frac{1}{T} \right) \]  

where \( \rho \) is the density, \( \phi \) is the saturation, \( T \) is the temperature, \( k \) is the thermal conductivity, and \( S \) is the source term.

Mass Balance Equations

For each phase \( \alpha \in \{ s, w, o, g \} \) (\( s \) = solid, \( w \) = water, \( o \) = oil, \( g \) = gas), the mass balance equation is:

\[ \nabla \cdot (\phi \rho \mathbf{V}) = 0 \]  

where \( \phi \) is the volumetric fraction of the phase, \( \rho \) is the density, \( \mathbf{V} \) is the velocity, and \( \nabla \cdot \) denotes the divergence operator.

Fluid and Porous Medium Rheologies

The fluid is supposed to obey to the generalised Darcy’s laws. Its mathematical formulation is for each of the phase (\( \alpha \in \{ w, o, g \} \)):

\[ \mathbf{U}_\alpha = \phi_\alpha \mathbf{V}_\alpha \pm \mathbf{g} = \pm k \eta_\alpha \nabla (P_\alpha) \pm \rho_\alpha \mathbf{g} \]  

where \( \mathbf{U}_\alpha \) is the Darcy velocity of the phase \( \alpha \) in the porous medium, \( k \) is the intrinsic permeability tensor, \( \eta_\alpha \) is the mobility of the phase \( \alpha \) in the porous medium with respect to the other phases, and \( P_\alpha \) is the pore pressure of the phase \( \alpha \).

The intrinsic permeability tensor is written as the product of an anisotropy tensor by the intrinsic permeability:

\[ k = a k(\phi) \quad \text{with} \quad a = \begin{bmatrix} a_{xx} & a_{xy} \\ a_{yx} & a_{yy} \end{bmatrix} \]  

where \( S \) is the specific surface area of the porous medium. \( m \) is an exponent, which generally equals to 3. The velocity of the phase \( \alpha \) is given by:

\[ \mathbf{U}_\alpha = \frac{k(\phi)}{\mu_\alpha} \]  

where \( \mu_\alpha(T) \) is the fluid viscosity given by the Andrade formula:

\[ \mu_\alpha(T) = \mu_\alpha^0 \exp \left( b_\alpha \left( \frac{1}{T} \pm \frac{1}{T^*} \right) \right) \]  

where \( T \) is the temperature in Kelvin. The triphasic relative permeabilities are computed from the three two-phase couples of relative permeabilities by using the following formula:

\[ \begin{align*}
(S_o + S_g) k_{ro} &= S_o k_{aro}(S_w) + S_g k_{rwo}(S_w) \\
(S_w + S_g) k_{rw} &= S_w k_{arw}(S_o) + S_g k_{rwo}(S_o) \\
(S_o + S_w) k_{re} &= S_o k_{re}(S_g) + S_w k_{rwe}(S_g)
\end{align*} \]  

Each of the relative permeabilities is given by:

\[ S_\alpha \leq S_{i\alpha\beta} \quad k_{\alpha\beta} = 0 \quad \text{for} \quad S_{i\alpha\beta} < S_\alpha \leq 1 \quad k_{\alpha\beta} = \frac{S_\alpha \pm S_{i\alpha\beta}}{1 \pm S_{i\alpha\beta}} \]  

This original formalism has been developed for this model in order to be able to account for the possible symmetrical behaviour of each phase and to ensure numerical stability.

Compaction at basin scale and at geological time scale is supposed to be vertical. This choice is the result of a
compromise between accuracy and costs in term of cpu time (Lamoureux-Var V., 1997). The behaviour law is then given by a volumetric rheology (Schneider 1993; Schneider et al., 1994, 1996):

\[
\frac{d \sigma}{dt} = \pm \beta(\sigma) \frac{d \sigma}{dt} \pm \alpha(\sigma) \sigma
\]

\[
\beta(\sigma) = \frac{\phi_\alpha}{E_a} \exp \left( \pm \frac{\sigma}{E_a} \right) + \phi_\beta \exp \left( \pm \frac{\sigma}{E_\beta} \right) \sigma \geq \sigma_m
\]

\[
\alpha(\sigma) = \frac{1}{E_c} \sigma < \sigma_m
\]

\[
\alpha(\phi) = (1 \pm \phi) \frac{1}{\mu_b (T)} \sigma > 0 \text{ and } \phi > \phi_{\text{min}}
\]

\[
\alpha(\phi) = 0 \sigma = 0 \text{ or } \phi \leq \phi_{\text{min}}
\]

\[
\phi(t = 0) = \phi_r + \phi_\alpha + \phi_\beta
\]

(A1-13)

where \(\sigma\) is the mean effective stress defined as follows:

\[
\sigma = \left( \frac{1 + 2 K_o}{3} \right) (P_b + b P_f)
\]

(A1-14)

\[
P_j = \frac{1}{\phi} (\phi_\alpha P_\alpha + \phi_\beta P_\beta + \phi_\gamma P_\gamma) = S_w P_w + S_o P_o + S_g P_g
\]

where \(K_o\) is the ratio between the horizontal stress and the vertical stress, \(b\) is the effective stress coefficient (Schneider et al., 1993) and \(P_j\) is the mean pore pressure. The pore pressure of each of the phases are related to each other by the capillary pressures.

\[
\begin{align*}
P_o &= P_w + P_{\text{cow}} \\
P_g &= P_w + P_{\text{gw}} \\
P_g &= P_o + P_{\text{go}}
\end{align*}
\]

(A1-15)

If we make the assumption that the water phase is always present, this means that the porous medium is water wet, only the two first relations are necessary because we can write:

\[
P_{\text{go}} = P_{\text{gw}} \pm P_{\text{cow}}.
\]

(A1-16)

By introducing the mean pore pressure, we obtain:

\[
\begin{align*}
P_w &= P_j + P_{\text{w}} \\
P_o &= P_j + P_{\text{w}} \quad \text{with} \quad P_{\text{w}} = P_{\text{cow}} = \pm S_w P_{\text{cow}} \pm S_g P_{\text{gw}} \\
P_g &= P_j + P_{\text{w}} \\
P_{\text{go}} &= P_j + P_{\text{gw}} \quad \text{with} \quad P_{\text{gw}} = \pm S_w P_{\text{gw}} \pm S_g P_{\text{go}}
\end{align*}
\]

(A1-17)

Under the assumption that water is always present, we can write:

\[
\begin{align*}
P_{\text{w}} &= \pm S_w P_{\text{cow}} \\
P_{\text{w}} &= \pm S_g P_{\text{gw}} \\
P_{\text{w}} &= \pm (1 \pm S_w) P_{\text{cow}} \pm S_g P_{\text{gw}}
\end{align*}
\]

(A1-18)

As for the relative permeabilities, the three-phase capillary pressures are derived from the two-phase capillary pressures. With the assumption that water is always present, only the oil-water and the gas-water capillary pressure curves are necessary. They are given by the following formula:

\[
\begin{align*}
\frac{d S_{\text{w}}}{dt} &\leq S_{\text{uw}} P_{\text{uw}} \quad P_{\text{uw}} = P_{\text{uw}} \, P_{\text{uw}} \\
S_{\text{uw}} &< \frac{d S_{\text{w}}}{dt} + (P_{\text{uw}} + P_{\text{uw}} P_{\text{uw}}) (\frac{S_{\text{uw}} + S_{\text{uw}}}{1 + S_{\text{uw}} + S_{\text{uw}}})^{\gamma_{\alpha}} \\
S_{\text{uw}} &\geq 1 + S_{\text{uw}} P_{\text{uw}} \\
P_{\text{uw}} &= P_{\text{uw}} P_{\text{uw}} \quad (A1-19)
\end{align*}
\]

with: \(\frac{d S_{\text{w}}}{dt} = \frac{S_{\text{w}}}{S_{\text{w}} + S_{\text{w}}} \) and \(0 < \gamma_{\alpha} \leq 1\).

State Equations

The density of each phase is supposed to be constant and is then given by: \(\rho_{\alpha} = \rho_{\alpha}^0\).

Closure of the Problem

The problem consists in the resolution of a system composed of 13 equations with the 13 unknowns \(\phi_{\alpha}, V_{\alpha}, P_{\alpha} , T\). Once the boundary conditions are given, the system is well posed.

Boundary Conditions

At the upper boundary, the pressures are imposed by the atmospheric pressure and by the bathymetry. The temperatures are imposed as a function of the altitude or function of the water depth.

At the lower boundary, there is no fluid flux and the displacements are imposed. The heat fluxes or the temperatures are imposed.

At the lateral boundaries, there is no heat flux and the displacements are only vertical. The fluid flux or the pressure may be imposed as a function of space and time.

2 HYDROCARBONS GENERATION

The hydrocarbon generation is performed with a conservative physical model which considers three components (oil, gas, and coke). In this model, the oil component is entirely in the hydrocarbon liquid phase, the gas component is entirely in the hydrocarbon vapour phase, and the water component is entirely in the water phase.

Description of the Porous Medium

The porous medium is composed of immobile components (solid, kerogen, and coke) and mobile components (oil, gas, water).
The porous medium is characterised by its initial composition (see Table 1). We make the assumption that the initial existing components are the solid, the water and the kerogen. The initial porosity is given by the behaviour law (see Appendix 1). The initial mass of kerogen is introduced by the TOC (Total Organic Content) which is given in grammes of organic carbon per grammes of dry rock. We admit that the TOC is given by the following formula:

$$\text{TOC} = \frac{c M_k^c}{M_k^c + M_s^c} \quad (A2-1)$$

where \(c\) is the mass carbon ratio of the kerogen that is a characteristic datum of the kerogen.

**TABLE 1**

<table>
<thead>
<tr>
<th>Component</th>
<th>Density</th>
<th>Volumetric fraction</th>
<th>Volume</th>
<th>Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Immobile</td>
<td>Solid</td>
<td>(\phi_s)</td>
<td>(V_{l,s})</td>
<td>(M_{l,s})</td>
</tr>
<tr>
<td></td>
<td>Kerogen</td>
<td>(\phi_k)</td>
<td>(V_{l,k})</td>
<td>(M_{l,k})</td>
</tr>
<tr>
<td></td>
<td>Coke</td>
<td>(\phi_c)</td>
<td>(V_{l,c})</td>
<td>(M_{l,c})</td>
</tr>
<tr>
<td>Mobile</td>
<td>Oil</td>
<td>(\phi_o)</td>
<td>(V_{l,o})</td>
<td>(M_{l,o})</td>
</tr>
<tr>
<td></td>
<td>Gas</td>
<td>(\phi_g)</td>
<td>(V_{l,g})</td>
<td>(M_{l,g})</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>(\phi_w)</td>
<td>(V_{l,w})</td>
<td>(M_{l,w})</td>
</tr>
</tbody>
</table>

### Primary Cracking

During the primary cracking, the kerogen is transformed with \(n\) parallel reactions, into oil, gas and coke.

$$\begin{align*}
x_i & \rightarrow \alpha_{i}^o \text{ oil } + \alpha_{i}^g \text{ gas } + \alpha_{i}^c \text{ coke} \\
x_j & \rightarrow \vdots + \vdots + \vdots \\
x_n & \rightarrow \alpha_{n}^o \text{ oil } + \alpha_{n}^g \text{ gas } + \alpha_{n}^c \text{ coke}
\end{align*} \quad (A2-2)$$

\(x_i\) is the normalised partial potential of reaction \(i\). It is a datum of the kerogen which obeys to the following relation:

$$\sum_{i=1}^{n} x_i^0 = 1. \quad \alpha_{i}^o (\text{respectively } \alpha_{i}^g \text{ and } \alpha_{i}^c) \text{ is the oil (respectively the gas and coke) quantity produced by reaction } i. \text{ We have: } \alpha_{i}^o + \alpha_{i}^g + \alpha_{i}^c = 1.$$

Each of these elementary reactions are supposed to be controlled by a first order kinetic given by the following equation:

$$\frac{dx_i}{dt} = \pm k_i x_i \quad \text{with} \quad k_i = A_i e^{\frac{E_i}{RT}} \quad (A2-3)$$

\(A\) is the frequency factor. \(E\) is the activation energy. \(R\) is the perfect gas constant. \(T\) is the temperature in Kelvin.

### Secondary Cracking

The oil produced by the primary cracking is then transformed, during the secondary cracking, into gas and coke.

This reaction is supposed to be controlled by a first order kinetic given by the following equation:

$$\begin{align*}
\text{Oil} & \rightarrow \beta_o^c \text{ Gas } + \beta_o^g \text{ Coke } \\
k_o = A_o e^{-\frac{E_o}{RT}} 
\end{align*} \quad (A2-4)$$

\(\beta_o^c\) and \(\beta_o^g\) are the stoechiometric coefficients of the reaction which respect the following condition: \(\beta_o^c + \beta_o^g = 1\).

### Transformation Ratio

The equations which described the primary cracking are discretized with an implicit scheme for the partial potential and with explicit temperatures. Thus, we have:

$$\begin{align*}
\frac{dx_i}{dt} & = -k_i x_i \Rightarrow x_i^{m+1} = x_i^m + \frac{x_i^m}{1 + k_i^{m+1} \Delta t} \\
\Delta t & \text{ is the time step. The } m \text{ exponent indicates values taken at } t, \text{ while the } m+1 \text{ exponent indicates values taken at } t + \Delta t.
\end{align*} \quad (A2-5)$$

The transformation ratio (TR) of the organic matter is then given by:

$$\text{TR} = 1 - \sum_{i=1}^{n} x_i^{m+1} \quad (A2-6)$$