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Integration of biodegradation and migration of hydrocarbons in a petroleum system model: Application to the Potiguar Basin (Brazil)

Mathieu Ducros*, Bernard Carpentier, Sylvie Wolf, Marie-Christine Cacas.

IFP Énergies nouvelles, Direction Géologie-Géochimie-Géophysique, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex - France.

* Corresponding author.

E-mail address: mathieu.ducros@ifpen.fr (M. Ducros)

ABSTRACT

Prediction of oil quality is a major issue as exploration extends towards costlier areas such as high water depth basins. Biodegradation, responsible for the major part of heavy oil reservoirs in the world (Roadifer, 1987), is the most important oil alteration process. Several studies have already been performed to determine qualitative biodegradation scales (Moldowan *et al.*, 1992; Peters *et al.*, 2005) or quantitative levels of biodegradation through basin and petroleum system modeling (Larter *et al.*, 2003; Walters *et al.*, 2009).

Until now, the different proposed approaches to simulate biodegradation processes and quantify their impact on the quality of trapped hydrocarbons remain post-processing solutions. This is not fully satisfactory due to the complexity of the history of a petroleum system and of the processes involved (generation, migration, alteration, preservation...). For instance, mixing of biodegraded and fresh oil, as well as effects of

viscosity changes on migration, are poorly taken into account. Moreover, the description and the evolution through time of the oil-water contact, which is known to play a key role in the biodegradation (e.g. Larter *et al.*, 2003), are usually oversimplified.

In our work we integrated the biodegradation processes within a basin and petroleum system forward simulator. Based on a Darcy's migration calculator, we simulated the evolution through time of hydrocarbon properties. An innovative way to determine the intensity of microbial activity and the evolution of the oil-water contact, where biodegradation is confined, has been developed. This new approach has been applied on the Potiguar basin and it appeared that besides the residence time in the biodegradation temperature window, rate of reservoir infill and migration paths are key controlling factors of the biodegradation. Our results fit satisfactorily the observed data and highlight the improvements brought by a fully coupled approach to the determination of oil quantity, quality and migration timing.

1. Introduction

Biodegradation is a complex series of bio-chemical processes of decomposition of organic matter by micro-organisms in the subsurface. These processes, which generally involve a pool of micro-organisms working in association (e.g. Dolfing *et al.*, 2008), result mainly in the generation of methane and carbon dioxide from hydrocarbons (e.g. Zengler *et al.*, 1999). If biodegradation risk is not accounted for, it can lead to lower revenues than expected due to high hydrocarbon density and viscosity, increase of corrosion risks, increase of refining costs, etc...

Among others, organic matter richness and maturity, hydrocarbon expulsion, migration and preservation are of uppermost importance when assessing oil quantity and quality. Biodegraded oils are considered to represent the main part (bituminous and heavy oils) of the world petroleum reserves (Roadifer, 1987) and should be very common in future deep water discoveries like in the Atlantic African margin (Head *et al.*, 2003). In that context of very high drilling costs, prediction of oil quality becomes a critical issue since it is a major control of cost-effectiveness.

Recent advances in the understanding of the biodegradation processes open the way to the quantitative modeling of their effects. Several researches have already been performed to provide tools for characterizing oil biodegradation by determining qualitative biodegradation scales (Connan, 1984; Johns, 1986; Moldowan *et al.*, 1992; Yu *et al.*, 2002; Peters *et al.*, 2005) or quantitative levels of biodegradation in reservoirs (Larter *et al.*, 2003; Blumenstein *et al.*, 2008; Dzou *et al.*, 2009; Walters *et al.*, 2009; Haeseler *et al.*, 2010). Most of these models consider biodegradation processes occurring in the reservoir apart from the basin history and without information on hydrocarbon migration.

As noticed by Blumenstein *et al.* (2008), it is natural to tie biodegradation processes, migration processes and petroleum system evolution. Most of the latter works tended to make the link between hydrocarbon migration and biodegradation. Before the first attempts to link biodegradation processes and petroleum system modeling, some authors had already worked at the geological scale to provide qualitative tools for the description and the prediction of the biodegradation risk in reservoirs. Wenger *et al.* (2001) and Peters *et al.* (2005) proposed for instance a biodegradation qualitative scale based mostly on empirical field observations where biodegradation processes are considered as stepwise processes. Then Yu *et al.* (2002) proposed a numerical solution, providing results as a qualitative risk, called BDI (Biodegradation Index). This numerical model was designed to qualitatively predict the biodegradation degree of hydrocarbons as a function of temperature history and of residence time of oil in the reservoir. It had to be used carefully as it did not take into account the dynamic of petroleum charge. Moreover BDI formulation assumed a simple thermal history (no uplift and no erosion) because potential paleopasteurization were not taken into account in the case of complex geological history. Wilhelms *et al.* (2004) improved this approach by adding a term which accounted for reservoir filling history. It was still not fully coupled to the petroleum system modeling and did not take into account some important phenomena such as oil mixing and reservoir spilling.

A much more documented and quantitative approach was developed by Larter *et al.* (2003, 2006). Their solution added the notion of degradation flux (expressed in $\text{kg m}^{-2} \text{y}^{-1}$) derived from laboratory experiments (Larter *et al.*, 2006). Their work resulted in a first method to quantitatively assess biodegradation risk. Blumenstein *et al.* (2008), who pointed out the limitations of the previous solutions described here above, aimed at

improving the modeling of biodegradation processes in their Biodexx approach by strengthening the link with petroleum system history. Thus, they focused their work on the effects of reservoir geometry, filling rates and oil composition in the reservoir. However, all these solutions are still based on post-processing calculations what cannot be fully satisfactory to properly quantify biodegradation effects. Indeed it is absolutely essential to fully combine migration and biodegradation mechanisms in order to properly take into account the effects (i) of mixing of biodegraded and fresh oil (which changes petroleum properties), (ii) of biodegradation processes during reservoir filling (which can delay spilling and thus reduce distance of petroleum migration) and (iii) of the control of biodegradation on oil viscosity and density regarding to migration. Besides a poor link between biodegradation model and petroleum system simulation in the previous approaches, the description of biodegradation location was either vague or arbitrary and did not take reservoir porosity and permeability into account. As a consequence, there was no difference that could be accounted for in the description of the biodegradation between reservoirs of unequal quality (in terms of permeability and porosity) reducing at the same time the prediction capability of the models. It appears also important to mention that theses approaches are generally based on schematic representations of reservoir architecture (Larter *et al.*, 2003) and its evolution through time was barely taken into account, as well as input parameters such as temperature which has to be adjusted manually (Blumenstein *et al.*, 2008).

The present work aims at developing a new approach for determining hydrocarbon losses and oil quality evolutions, using a methodology based on biodegradation rates and on previous case studies (Carpentier *et al.*, 2005; Behar *et al.*, 2006; de Barros Penteado *et al.*, 2007). It is integrated in a petroleum system modeling (PSM) simulator,

thus allowing for biodegradation processes model to be fully coupled with migration simulation. The proposed approach was tested on a 2D numerical model of the Potiguar Basin (Brazil) which is well known thanks to several studies conducted in the past (Trindade *et al.*, 1992; Blanchet *et al.*, 2005; de Barros Penteado *et al.*, 2007).

2. Methodology: description of the conceptual model

PSM aims at assessing and de-risking prospect evaluation in petroleum exploration. It uses information on the reconstruction of the basin history to describe, in a deterministic manner, the main mechanisms impacting reservoirs potential. Therefore, as a basic, PSM calculates burial history, thermal history and pressure fields which control source rock maturity, expulsion, migration and hydrocarbon trapping . It seems natural to introduce biodegradation concepts within PSM since on one hand it can greatly impact the reservoirs potential and the prospect evaluation and on the other hand PSM provides most of the parameters controlling biodegradation (oil composition and oil quantity, temperature,...) to rigorously describe biodegradation processes.

Even if biodegradation processes are better understood thanks to recent works (e.g. Zengler *et al.*, 1999; Head *et al.*, 2003; Jones *et al.*, 2008; Dolfing *et al.*, 2008), the controlling parameters, at basin scale, of the mechanisms involved are still not clearly known. Although some authors consider that nutrients supply can be a limiting factor of biodegradation processes (Head *et al.*, 2003) there is still no clear evidence of such effects at the basin scale. In that context we adopted an approach based on several concepts commonly accepted corresponding to the description of macro scale consequences (loss of hydrocarbon) of micro scale biodegradation processes (decomposition of hydrocarbons into methane and carbon dioxide by a pool of micro-

organisms working in association). Biodegradation being a microbial process, it only works within the range of temperatures within which micro-organisms can live. When temperature exceeds the micro-organisms living temperature (pasteurization temperature) the rock is pasteurized and no more biodegradation can occur. Therefore, at a given time, biodegradation processes are restricted to the zones where the pasteurization temperature has never been reached and where oil saturation is in a limited range. This saturation range where oil alteration can take place corresponds to the transition zone between water saturated and oil saturated zone, often referred to as the reservoir oil-water contact, but it can also correspond to low hydrocarbon velocity migration paths. As biodegradation is restricted to a zone where hydrocarbon is abundant, it has been assumed that microbial population is not limited by the hydrocarbon quantity but by a parameter (such as nutrient concentration) which is related to the deposited rock property. There is therefore a reference microbial population corresponding to the deposition conditions that evolves during burial as a function of the available space. Microbial consumption is assumed to be a zero order mechanism which relies only on the microbial population and to the microbial activity, closely linked to the temperature. Biodegradation being a compositional process, differential consumption rates are assigned to chemical compounds as a function of their biodegradability. As the products of the biodegradation reactions (mostly methane and carbon dioxide) are not found in much higher quantities in biodegraded fields than in nearby non degraded fields (Head *et al.*, 2003), they are not taken into account in the approach followed in this work. Thus, biodegradation is considered as being only destructive.

From the petroleum system point of view, the close integration of biodegradation mechanisms in basin models directly improves the modeling of the petroleum properties such as density or viscosity giving more accurate results in terms of reservoirs filling, spilling and migration timing what would not be achieved with a post-processing approach.

2.1 Biodegradation location

Previous works have demonstrated that biodegradation processes occur mostly at the oil-water contact (e.g. Head *et al.*, 2003; Larter *et al.*, 2003). However some authors have also admitted that it could not be restricted only to reservoirs oil-water contact but that it could also occur in migration paths (Larter *et al.*, 2003). In order to account for the locations where biodegradation can take place, the solution mainly adopted (Larter *et al.*, 2003; Blumenstein *et al.*, 2008) consists in determining the surface area of the oil-water contact within the reservoir and using a biodegradation rate per unit area of this oil-water contact (e.g. Larter *et al.*, 2003; Blumenstein *et al.*, 2008). This approach oversimplifies the problem because the oil-water contact is in fact a transition zone whose thickness depends on the capillary pressure and on the oil density. So, using the surface of the base of the oil accumulation in the reservoir as a controlling parameter of biodegradation does not account accurately for the global biodegradation rate. Secondly biodegradation process are restricted to reservoir oil-water contact described on the base of arbitrary criteria, though they can also occur the migration paths.

In the model developed during this work, to account for micro-organisms requiring both water and hydrocarbon to develop, we assumed that microbial population is optimal (and limited by the available space as we will described it in the following section) only

in a restricted range of oil saturations. This latter range leads to the restriction of biodegradation process to the oil-water transition zone in reservoirs and potentially to some parts of the migration path where hydrocarbon movements are slowed down. We adopted this new approach to precisely control locations and involved volumes where biodegradation processes can take place. This is done based on a range of oil saturation and without any hypothesis on the definition of a potential trap or on the way the reservoir is filled.

Generally mesh thicknesses used in basin modeling are too coarse to represent properly the oil-water transition zone, especially in good reservoirs. Grid cells are usually tens of meters thick while oil-water contacts are several meters thick. In order to be able to determine the volume of the oil-water transition zone independently of the mesh geometry we used the capillary pressure and the oil density to compute its thickness. This transition zone, also referred to in the following as the oil-water contact zone, is used to determine the zone where biodegradation can take place (Fig. 1). In a general formulation, the thickness of the transition zone (the thickness in which the saturation is assumed to vary linearly from the maximum oil saturation in the rock to the irreducible oil saturation at the base of the oil-water contact) is given by the following expression:

$$Thick_{owc} = \frac{\Delta Pc}{\Delta \rho g} \quad (1)$$

Where $Thick_{owc}$ is the thickness of the oil-water contact (transition zone), ΔPc is the variation of capillary pressure between the top and the base of the transition zone, g is the gravity and $\Delta \rho$ is the difference of density between the water and the petroleum phase. As it has been assumed that biodegradation takes place in a restricted range of

205 saturations, thickness of the biodegradation interval is smaller than that of the transition
206 zone.

207 One of the great advantages of this method relies on the fact that no assumption other
208 that the presence of reactants is needed for determining the location of the
209 biodegradation processes.

211 **2.2 Micro-organisms density and oil consumption**

212 Some authors have investigated the microbial population density in sediments (e.g.
213 Cragg *et al.*, 1999). Thanks to the extensive amount of data provided by the Ocean
214 Drilling Program (ODP), a lot of microbial population measurements have been
215 performed and analyzed. Cragg *et al.* (1999) for instance derived a microbial population
216 law from ODP data (e.g. Cragg *et al.*, 1997; Parkes *et al.*, 2000) given by the following
217 expression:

$$218 \quad \text{Log}_{10}(\text{bacterial number}) = 7.95 - 0.64\text{Log}_{10}(\text{depth in m}) \quad (2)$$

219 As measurements were not performed in hydrocarbon reservoirs, corresponding
220 microbial pools are surely not exactly the same as the one responsible for hydrocarbon
221 biodegradation. However the evolution of the microbial pool, at geological time-scale,
222 can be considered as responding instantaneously to changes on environmental
223 conditions. Therefore, it is assumed that information on the evolution of microbial
224 population through burial obtained in ODP programs could be extrapolated to microbial
225 population responsible for hydrocarbon biodegradation.

226 The model proposed by Cragg *et al.* (1997) which reproduces the measurements
227 performed during the ODP is based on a relationship between the microbial population

and the depth. Thus it relies more on empirical observations than on a real deterministic concept. In order to express the evolution of the microbial population in sediments we assumed that, at the pore scale, micro-organisms are located at the oil-water interface. We use a simple model of the rock micro-structure in which pores are represented by spheres and where the number of pores per unit of solid volume depends on the lithology and remains constant during burial. Thus porosity reduction during the burial is accounted for through pore volume reduction and not through pore number decrease. The oil present in the pores is also represented as a bubble totally surrounded by water (Fig. 2). With these hypothesis we can express the evolution of the microbial population as a function of the lithology and of the porosity.

The number of pores in the rock (m^{-3} of bulk rock) is given by the following expression:

$$n_{pores} = d(1 - \varphi) \quad (3)$$

where d is the pore density for the given rock (m^{-3} of solid rock) and φ is the rock porosity.

Using this micro-structure rock model, the rock porosity can be expressed as follows:

$$\varphi = d(1 - \varphi) \frac{4}{3} \pi R^3 \quad (4)$$

where R is the pore radius as illustrated in Fig. 2. Thus the corresponding pore radius can be deduced:

$$R = \sqrt[3]{\frac{3\varphi}{4d\pi(1 - \varphi)}} \quad (5)$$

The hypothesis on oil distribution within porosity leads to the following expression of the contact area between oil and water in the porosity (m^2/m^3 of bulk rock):

$$a = 4d\pi(1 - \varphi)r^2 \quad (6)$$

where r is the oil drop radius as illustrated in Fig. 2 and a the oil-water surface area by unit of rock volume.

The oil saturation can be expressed as follows:

$$S = \frac{r^3}{R^3} \quad (7)$$

where S is the oil saturation. Combining the previous equations, the oil-water interface area in the porosity can be expressed as a function of the oil saturation:

$$a = 4d\pi(1 - \varphi)R^2 S^{2/3} \quad (8)$$

Then, using the hypothesis of vertical linear saturation profile (which is a handy and reasonable approximation of the true saturation profile), S , along the oil-water contact ($h = 0$ at the base of the oil-water contact and $h = Thick_{OWC}$ at the top of the oil-water contact):

$$S(h) = \frac{h}{Thick_{OWC}} \quad (9)$$

and assuming that the porosity does not change significantly within the oil-water contact zone (which can be considered as being homogeneous and too thin to experience significant porosity variations), the mean oil-water interface area in the transition zone can be approximated as follows:

$$\bar{a} = \frac{1}{Thick_{OWC}} \int_0^{Thick_{OWC}} a(h)dh \quad (10)$$

thus

$$\bar{a} = \frac{1}{Thick_{OWC}} \int_0^{Thick_{OWC}} 4d\pi(1-\varphi)R^2 \left(\frac{h}{Thick_{OWC}} \right)^{2/3} dh \quad (11)$$

Then, using equation (5), the cumulated area of contact surface between oil and water in the transition zone is given by the following formula:

$$\bar{a} = 2.9\sqrt[3]{d}(1-\varphi)^{1/3}\varphi^{2/3} \quad (12)$$

Finally an expression can be proposed to compute the microbial population by unit of rock volume in the oil-water contact zone:

$$N(\varphi) = N_0 \left(\frac{1-\varphi}{1-\varphi_0} \right)^{1/3} \left(\frac{\varphi}{\varphi_0} \right)^{2/3} \quad (13)$$

Where N_0 corresponds to a reference microbial population at a reference porosity φ_0 .

Assuming a classical porosity versus depth function $\varphi = \varphi_{surface} e^{-kz}$ a comparison can be made between the resulting microbial population determined through this new approach with the one proposed by Cragg *et al.* (1999). Imposing the same microbial population at a depth of 1000m (equation 14) leads, for typical values of $k = 7 \times 10^{-4}$ and $\varphi_{surface} = 0.5$, to $C = 1491640$.

$$C(1 - \varphi_{surface} e^{-1000 \cdot k})^{1/3} e^{2/3 \cdot 1000 \cdot k} = 10^{(7.95 - 0.64 \log_{10}(1000))} \quad (14)$$

The comparison of the evolution of microbial population with the Cragg *et al.*'s (1999) formula and the one derived from the approach proposed in this work is illustrated in Fig. 3. It demonstrates a close behavior of the two models between 800 and 2500m. The differences observed at shallower depths are not important in regard of the dispersal of measurements. The model based on the evolution of porosity proposed in this work

falls in the 95% confidence interval of the model derived by Cragg *et al.* (1999). This comparison should be interpreted with caution since the two considered microbial populations can be very different, the first one corresponding to a global population and the second one to the microbial population responsible for methanogenesis in petroleum reservoirs. However, if one considers the hypothesis that microbial pool is constantly adapting to its environmental conditions, the model is in agreement with ODP measures and uses parameters available in basin modeling.

The model relating microbial population with porosity proposed in this work assumes that micro-organisms are located at the interface between the water and the drops of oil. However following the same reasoning but assuming that micro-organisms are located at the surface of the rock would lead to proportional results. Indeed, the surface available for micro-organisms would be in that case:

$$a^* = 4d\pi(1-\varphi)R^2 \quad (15)$$

Thus the mean oil-water interface area in the transition zone can be expressed as follows:

$$\bar{a}^* = \frac{1}{Thick_{OWC}} \int_0^{Thick_{OWC}} 4d\pi(1-\varphi)R^2 dh \quad (16)$$

Resulting again in:

$$\bar{a}^* = 4.8\sqrt[3]{d}(1-\varphi)^{1/3}\varphi^{2/3} \quad (17)$$

Considering that microbial individual capacity to degrade hydrocarbons is mainly dependent on the temperature, the global biodegradation capacity can then be approximated by the following equation:

$$M_{hb} = M_0 \left(\frac{1-\varphi}{1-\varphi_0} \right)^{1/3} \left(\frac{\varphi}{\varphi_0} \right)^{2/3} \quad (18)$$

where M_{hb} is the mass of hydrocarbon degraded by the microbial population in kg/My/m³ of rock and M_0 is the reference mass in kg/My/m³ of hydrocarbons degraded by the microbial population at the reference porosity φ_0 of rock.

The choice of the texture (Fig. 2) was made arbitrarily to obtain evolutions of microbial population versus porosity simple to compute using basin model parameters. However even with alternative models of texture the resulting evolutions of microbial population would not lead to drastically different biodegradation results.

2.3 Microbial activity

In the previous section, the variation of microbial population as a function of the available space in rock has been described. It is also known that some factors can have impacts on the microbial activity. Previous works already emphasized for instance the importance of temperature as a controlling parameter of the biodegradation rate (Wilhelms *et al.*, 2004; Adams *et al.*, 2006; Larter *et al.*, 2006). Some authors also pointed out that salinity (Bernard *et al.*, 1992), water flux (Head *et al.*, 2003; Larter *et al.*, 2003) or nutrients presence (Head *et al.*, 2003) can also significantly control the biodegradation rate. However impacts of these latter parameters are not well constrained and there is still not a consensus on their importance. Thus, it makes sense to assume that these factors have a second order control on microbial activity.

In the approach presented here, on a first order approximation, only the role of temperature and of available space on hydrocarbon consumption rate are considered:

$$M_{hb} = M_0 \left(\frac{1-\varphi}{1-\varphi_0} \right)^{1/3} \left(\frac{\varphi}{\varphi_0} \right)^{2/3} \quad (19)$$

where $R(T)$ is the coefficient of microbial activity whose value is between 0 and 1 and which depends on temperature (see section below).

Besides controlling the microbial activity, temperature can also pasteurize rocks. Even if the threshold temperature is not well constrained (e.g. Wilhelms *et al.*, 2001; Head *et al.*, 2003), it is commonly admitted that a rock that would have experienced temperature above a threshold around 90°C should be pasteurized. The algorithm designed during this work takes into account this concept of paleo-pasteurization. If temperature reaches the temperature threshold corresponding to pasteurization, biodegradation rate is permanently set to 0 for the given cell even if the cell temperature drops below the threshold afterwards. The underlying hypothesis is that there is no movement of micro-organisms at basin scale after sedimentation, even by water advection.

2.4 Consumption preferences and compositional description of petroleum

Biodegradation modelling requires a compositional description of the hydrocarbon phase in order to be able to represent the differential biodegradability of the different hydrocarbon molecules (e.g. Haeseler *et al.*, 2010). It also needs a model of thermogenic transformation of organic matter and of hydrocarbon fluids in order to be able to simulate the complete petroleum system history including migration from source rock to reservoirs. Consequently, the description of the hydrocarbon fluids must account for PVT, for thermogenic transformation of the organic matter and for biogenic aspects.

This detailed petroleum model is also essential to simulate properties changes in the hydrocarbon fluid such as viscosity or density.

The numerical approach proposed in this work to account for biodegradation is similar to the post-processing tool proposed by Haeseler *et al.* (2010) with the additional notion of degradation rate. The global mass of hydrocarbon biodegraded by micro-organisms is calculated at each time step using equation (19). This mass is then distributed between the biodegradable compounds according to the microbial consumption preferences. When one of the biodegradable compounds has completely disappeared, consumption preferences are normalized on the remaining biodegradable compounds so that all the biodegradation capability of the micro-organisms is used. This means that it is assumed that microbial species evolved in parallel with the change in composition in order to adapt to their new environment, conserving their overall consumption capability.

2.5 Biodegradation index

In a natural system, defining of a biodegradation index which measures the biodegradation advancement of a given hydrocarbon mixture is quite difficult for two reasons at least, as it has to integrate the effects of mixing between fresh and degraded oil and the effects of secondary cracking. However, such a criterion is necessary for comparing estimated losses from in-situ measurements and from numerical models. Although the petroleum system model gives access to the final composition of the hydrocarbon fluids and thus to a complete information about its economical value, a biodegradation index integrating information about the complete evolution of the

hydrocarbon composition to be compared to measurements would strengthen the prediction and help to evaluate the reliability of the model.

Nickel and vanadium concentrations have proved to provide good indications of hydrocarbon losses due to biodegradation (Magnier *et al.*, 2001; Kowalewski *et al.*; 2001). Even if some authors are reluctant to use this methodology (Head *et al.*, 2003), it remains one of the most common and accessible method to quantify these losses. A method to compute a concentration index which would give an information directly comparable with the nickel/vanadium variations of concentration between non-degraded and degraded oils was added to the biodegradation calculation developed during this work.

Thus, besides the quantitative description of the effects of biodegradation on migration velocity through viscosity changes and on oil quality, a tracer concentration index is calculated. It is used to define a quantitative indicator of the biodegradation magnitude, in addition to the oil composition which is calculated by the simulator.

The biodegradation index is designed to account for the same processes as those which control the concentration of biodegradation resistant compounds such as nickel and vanadium into the petroleum phase. Thus, a fictitious tracer was numerically introduced in the hydrocarbon phase generated by the source rock. The increase of its concentration due to secondary cracking effects and biodegradation effects (main phenomenon that leads to loss of hydrocarbons in the petroleum phase) enables to compute the hydrocarbon mass loss. The value of the concentration index is then defined as follows:

$$CI = 1 - \frac{[T]_{generated}}{[T]_{current}} \quad (19)$$

where CI is the concentration index, $[T]_{generated}$ is the tracer concentration in the generated oil and $[T]_{current}$ is the tracer concentration in the current oil phase.

3. Application: The Potiguar Basin (Brazil)

3.1 Geological setting

The Potiguar Basin is the most northeastern basin of the Brazilian equatorial margin, covering part of the states of Rio Grande do Norte and Ceará. Around 30% of its 70,000km² area is located onshore (Behar *et al.*, 2006), whereas the offshore area extends beyond the continental platform to water depths of at least 2000m (Bertani *et al.*, 1990). (Fig. 5)

The Potiguar Basin is typical of most Brazilian marginal rifted basins that formed during the breakup between South America and Africa during the Neocomian age. It can be considered as a rift basin that evolved to a passive margin. Sedimentary filling of the basin took place from the Early Cretaceous to the present days and the sedimentary sequences can be 8 kilometers thick. The major structural features and sedimentary bodies of the Potiguar Basin are closely related to the processes and tectonic mechanisms occurring during the opening of the Atlantic ocean.

Bertani *et al.* (1990) recognized 3 main tectono-stratigraphic sequences that characterize the evolution of the Potiguar Basin: rift, transitional and drift stages of continent separation. The rift period corresponds to ages from the Early Neocomian to the Early Aptian in the offshore portion of the basin. Deep asymmetric grabens were formed where the Pendência Formation, one of the two main source rock of the Potiguar Basin, deposited. The unit is later overlain by syntectonic sandstones followed by a general

uplift that occurred at the end of the rift phase. The transitional stage corresponds to a change from a rifting regime to a thermally subsiding basin (Bertani *et al.*, 1990). During this period, the subsidence is slow and is characterized by the deposition of sandstones, limestones and lagoonal rich shales of the Alagamar Formation, which constitutes the second main source rock. Drift-phase sedimentation occurred during a long period of thermal subsidence under marine conditions that lead to the formation of stratigraphic and structural traps.

3.2 The petroleum system

The Potiguar Basin contains two main source rocks: the Pendência formation, a type I lacustrine organic matter deposited during the rift phase, and the Alagamar formation, a mixed organic rich carbonates and shales interbedded with deltaic sandstones, deposited during the transitional period. The hydrocarbon formed from the Alagamar source rock is mostly found in structural traps of the Açú sandstones formation.

The petroleum system in the Carnaubais trend is characterized by migration of hydrocarbons generated in the offshore part of the basin towards the inland in low depth reservoirs of the Açú formation sandstones. Long distance migration of the oil from the offshore kitchen to the southern part of the basin was possible along the updip trend through Aptian carrier beds.

There are a lot of evidences of biodegradation processes such as high NSO (resins and asphaltenes) contents in the majority of the trapped hydrocarbons along the Carnaubais trend in Açú formation reservoirs. Although there are slight differences between oil fields that are close from each other, the Carnaubais trend clearly shows an increasing

intensity of biodegradation (Behar *et al.*, 2006, de Barros Penteadó *et al.*, 2007) in a direction from the deeper and most offshore reservoirs in the northeast, to the most shallowest and onshore reservoirs in the southwest. As the hydrocarbons migrated over a long distance, the differences in the biodegradation magnitudes were mostly explained by the residence time (de Barros Penteadó *et al.*, 2007; Haeseler *et al.*, 2010) and the differences of hydrocarbons generated during the maturation of the organic matter (England *et al.*, 1991).

As explained in the previous section, the hydrocarbon fluid composition is controlled by PVT, thermal and biogenic factors. Thus the selected compositional approach is derived from a previous work of Behar *et al.* (2008) about the kerogen thermal cracking and from previous works of de Barros Penteadó *et al.* (2007), Behar *et al.*, (2006) and Haeseler *et al.* (2010) on biodegradation rates and on microbial preferences.

Consequently, a 12 classes description of the kerogen cracking was selected to account for both thermal and microbial effects (Table 1). The main changes brought to the kerogen cracking model proposed by de Barros Penteadó *et al.* (2007) to account for the biogenic aspects concern the splitting of the saturated C₁₄₊ fraction into 3 classes (n-alkanes, iso-alkanes and cyclo-alkanes) due to critical differences in their biodegradability. Their respective fractions was derived from the composition of the oil composition of the non-biodegraded oil from the ARG2 field (Haeseler *et al.*, 2010).

3.3 2D Numerical model

Numerous studies have already been dedicated to the investigation of the biodegradation processes in the Potiguar basin (Behar *et al.*, 2006; de Barros Penteadó

et al., 2007; Haeseler *et al.*, 2010) and aimed at modelling the petroleum system history (de Barros Penteado *et al.*, 2007). The 2D numerical model of the Potiguar basin that is used in the present study is derived from the model previously proposed by de Barros Penteado *et al.* (2007) and has been updated to improve the thermal history of the basin. Although this model is in 2D, it has been considered as significant enough to account for the migration at the basin scale since hydrocarbon migration in the basin is assumed to follow the axis of the Carnaubais trend from the offshore kitchen in the northeast to the Açu oil fields in the southwest (Fig. 5).

As explained in the section describing the mechanisms that control biodegradation processes, temperature plays a key role in the biodegradation rate. This is why a special care has been taken to adjust the temperature fields in the Potiguar basin. The results of the thermal calibration obtained with the 2D model are illustrated in Fig. 6 and reported in the following table (Table 2).

The thermally calibrated model show a very good match (less than 3.0°C misfit) between measured and simulated present day temperatures. This calibration step is very important to insure a realistic description of the biodegradation rates within the Potiguar basin since temperature plays also an important role in the description of the organic matter maturation. Kinetic schemes elaborated by Behar *et al.* (2007) from source rock samples of the Potiguar basin are adapted for describing the PVT and the thermogenic transformation of the organic matter. They were adjusted to be also consistent with a compositional description useful for biodegradation processes. The stoichiometric coefficients used in the Potiguar source rock kinetic scheme are described in table 1.

Table 3 illustrates the results of oil composition in the ARG2 field obtained using the thermally calibrated 2D model previously described with a simulation including

maturation and migration of the hydrocarbons. In this simulation, the biodegradation processes were not modeled so that simulated petroleum composition can be compared with petroleum composition in fields that are known to contain non-biodegraded oil such as in the ARG2 field. These results, obtained after some minor adjustments of the parameters of the kinetic scheme proposed by Behar *et al.* (2007) for the NSO cracking, show a very good match between observed and simulated composition. The model can be considered as well calibrated for the thermal aspects as well as for the compositional aspects. The module describing the biodegradation processes can then be activated.

Calibration parameters of this biodegradation module are mainly the microbial activity versus temperature and compositional microbial preferences (relative biodegradation rates). The selected microbial activity curve as a function of the temperature (Fig. 2) is taken and adapted from Wellsbury *et al.* (1997). The biodegradation rate in the temperature range of 40°C and 50°C was slightly increased. Concerning relative biodegradation compositional rates, a first try has been made using coefficients resulting from the work of Haeseler *et al.* (2010). They were later adjusted in order to better match the composition observed in the biodegraded fields. Differences between coefficients determined for the BioClass approach of Haeseler *et al.* (2010) and the values used in this work are due to the fact Bioclass is a static 0D concept not fully coupled to the migration processes whereas a dynamic approach is followed in this work. Indeed BioClass assumes that, for all reservoirs, the initial oil composition is the same. Our model shows that hydrocarbons reaching the most southwestern reservoirs have already been biodegraded during their migration. The relative biodegradation rates used in the Potiguar simulation are presented in the following table (Table 4). All the

other chemical compounds such as NSO (resins and asphaltenes) or non-hydrocarbon gases are considered as non-biodegradable.

The other parameters corresponding to biodegradation aspects chosen for the Potiguar model are listed here below:

- Pasteurization temperature: 90°C
- Interval of saturations associated with biodegradation processes: [20%; 80%]
- Reference porosity (φ_0): 30%
- Hydrocarbon degradation rate (M_0): 155kg/My/m³ of rock

The first important result is that the activation of the biodegradation module does not prevent from filling the known fields with oil (Fig. 7). Then, the simulated compositions in the biodegraded fields are illustrated in Fig. 8 and compared with measured compositions. A very good match can be observed all along the Carnaubais trend with very altered oil in the shallowest fields of the South western part of the basin and less biodegraded fields towards the offshore part of the Potiguar basin. Variations of oil composition in terms of API gravity in the Potiguar basin are represented in Fig. 9.

The field for which the results are not as good as for the other fields is the ARG2 field. The obtained results predict a more biodegraded oil that was actually measured. However this field is known to have compartments with non-biodegraded oil. So the difference between simulated and measured compositions of the ARG2 field could be explained by mixing of biodegraded and fresh. This hypothesis is consistent with the observation that fresher oil is coming in the last stages of the basin history from deeper layers (Fig. 9 and 10).

Using the formalism described in section 2.5, a biodegradation index was computed during the simulation of the Potiguar basin. Results, presented in Fig. 10, emphasize the fact that the hydrocarbon mass loss is at least of 25% in the considered fields and can be as high as 65% in the most biodegraded oils of the basin. These results which give a complete picture of the state of biodegradation along the Carnaubais trend are consistent with those of Behar *et al.* (2006).

4 Results and Discussions

A new approach consistent with general observations on key controlling factors of the biodegradation processes such as the relationship of microbial activity versus temperature and the concept of paleo-pasteurization has been developed. It provides a quantitative and predictive solution for modeling biodegradation processes in a fully coupled way with migration and accumulation processes. This is a major step in the correct description of petroleum systems where biodegradation plays a key role on the quality and quantity of hydrocarbon in place in the reservoirs. Till now only post-processing methods were available and the application on natural cases should demonstrate the great importance of accounting for all migration mechanisms in a fully coupled way to correctly assess prospects potential.

This new approach goes a step forward than the Biodexx method (Blumenstein *et al.*, 2008), since the oil-water contact is precisely localized. Thus temperature, microbial activity and degradation rate can be accurately computed and are directly consistent with the whole petroleum system history. No assumption has been made on the

mechanisms that drive the reservoir filling. The complete description of hydrocarbon saturation in the migration paths as well as in the reservoirs relies on the Darcy's law. The application of the new approach on the Potiguar basin leads to very good results consistent with measured compositions and oil qualities. The Potiguar basin shows no evidence of paleo-pasteurization. The comparison of the evolution of temperatures of fields covering a wide range of biodegradation degrees demonstrates that even if biodegradation processes are very dependent on temperature, this latter cannot explain by itself the variation of biodegradation in the Potiguar basin. The migration history shows that hydrocarbons undergo successive steps of biodegradation while migrating along the migration path emphasizing the importance to tightly link biodegradation and migration processes. The basin model was able to simulate very fine lateral and vertical variations of oil quality even in the reservoirs. It has been possible to explain the difference of oil quality as well as the presence of non-biodegraded oil in the ARG2 field by the arrival of fresh oil from a deeper carrier bed latter in the basin history.

Some of the results obtained are less intuitive and should lead to further investigations. For instance the results obtained on the Potiguar basin model show that gaseous fractions increase with increasing biodegradation due to the loss of a great part of liquid fractions. Thus, even if the API gravity increases with biodegradation, contrary to what could have been expected the viscosity of the hydrocarbon phase does not increase. This explains the fact that even if the oil is biodegraded it can still migrate which is consistent with observations on the Potiguar basin. This effects could be even more important than expected as the products of the biodegradation processes (carbon dioxide, methane...) are not taken into account in this approach. Further work should investigate the effect of these gases produced during biodegradation of hydrocarbon

fluids on oil properties (quality, viscosity, density...) taking into account dissolution into water and changes in fluid phase. Results of work still in progress, which focuses on biodegradation rates and microbial consumption preferences through laboratory experiments, could also be integrated in the approach.

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References

- Adams, J., Riediger, C., Fowler, M.G. & Larter, S.R. (2006) Thermal controls on biodegradation around the Peace River tar sands: Palaeopasteurization to the west. *J. Geochem Explor.*, 89 (1-3), 1-4.
- Behar, F., Lorant & F. Mazeas, L. (2008) Elaboration of a new compositional kinetic schema for oil cracking. *Organic Geochemistry*, 39, 764-782.
- Behar, F., Budzinski, H., de Barros Penteado, H.L. & Lorant, F. (2006) Study of the biodegradation processes along the Carnaubais trend, Potiguar Basin (Brazil) - Part I. *Organic Geochemistry*, 37-9, 1042-1051
- Bernard, F.P. & Connan, J. (1992) Indigenous microorganisms in connate waters of many oilfields: a new tool in exploration and production techniques. SPE 24811. In: 67th Annual Technical Conference and exhibition of the Society of Petroleum Engineers, Washington D.C., October 1992, 467-476.
- Bertani, R.T., Costa, I.G. & Matos, R.M.D. (1990) Evolução tectono-sedimentar, estilo estrutural e "habitat" do petróleo na Bacia Potiguar. In: Gabaglia, J.P.R., Milani, E.J. (Eds), *Origem e evolução de bacias sedimentares*. Rio do Janeiro, Petrobras, 291-310.

603 Blanchet, D., Kowalewski, I., Magnier, C., Marchal, R., Grabowski, A. & Huc, A.Y.
 604 (2005) In: Vandecasteele, J.P. (Ed.), Microbiologie pétrolière, concepts,
 605 implications environnementales, applications industrielles, vol. 2. Editions
 606 Technip, Paris, 629-675.

607 Blumenstein, I.O., Kross, B.M., di Primio, R., Rottle, W., Muller, E., Westerlage, C. &
 608 Littke, R. (2008) Biodegradation in numerical basin modeling a case study from
 609 the Gifhorn Trough, N-Germany. *Int. J. Earth Sci (Geol Rundsch)*, 97, 1115-1129.

610 Carpentier, B., Behar, F., de Barros Penteado, H.L. & Lorant, F. (2005) New approach
 611 for predicting biodegradation in a basin modeling perspective. AAPG – American
 612 Association of Petroleum Geologists international conference and exhibition,
 613 Paris, September 11th-14th, 2005.

614 Connan, J. (1984) Biodegradation of crude oils in reservoirs. In: Brooks, J. Welte D.H.
 615 (eds) *Advances in petroleum geochemistry*. Academic, London, 299-335.

616 Cragg, B.A., Law, K.M., O'Sullivan, G.M. & Parkes, R.J. (1999) Bacterial profiles in
 617 deep sediments of the Alborean sea, Western Mediterranean, sites 976-978. In
 618 Zahn, R., Comas, M.C., Klaus, A., (Eds), *Proceedings ODP Scientific Results*,
 619 161; College Station, Texas (Ocean Drilling Program), 433-438.

620 Cragg, B.A., Law, K.M., Cramp, A. & Parkes, R.J. (1997) Bacterial profiles in Amazon
 621 fan sediments, Sites 934, 940. In Flood, R.D., Piper, D.J.W., Klaus, A., Peterson,
 622 L.C. (Eds), *Proceedings ODP Scientific Results*, 155; College Station, Texas
 623 (Ocean Drilling Program), 565-571.

624 de Barros Penteado, H.L., Behar, F., Budzinski, H. & Lorant, F. (2007) Study of the
 625 biodegradation processes along the Carnaubais trend, Potiguar Basin (Brazil) -
 626 Part I. *Organic Geochemistry*, 38-8, 1197-1211.

627 Dolfing, J., Larter, S.R. & Head, I.M. (2008) Thermodynamic constraints on
 628 methanogenic crude oil biodegradation. *ISME Journal*, 2, 442-452.
 629 Dzou, L. & He, D. (2009) The advantages of Interactive Fluid Property modeling.
 630 AAPG Hedberg Conference on: "Basin and Petroleum System Modeling: New
 631 Horizons in Research and applications". May 3rd-7th, 2009, Napa, California,
 632 USA.
 633 England, W.A., Mann, A.L. & Mann, D.M. (1991) Migration from source to trap.
 634 AAPG Special Bulletin, 3, 23-47.
 635 Haeseler, F., Behar, F., Garnier, D. & Chenet, P.Y. (2010) First stoichiometric model of
 636 oil biodegradation in natural petroleum systems. Part I – The BioClass 0D
 637 approach. *Organic Geochemistry*, 41, 1156-1170.
 638 Head, I.M., Jones, D.M., & Larter, S.R. (2003) Biological activity in the deep
 639 subsurface and the origin of heavy oil. *Nature*, 426 (6964), 344-352.
 640 Johns, R.B. (1986) *Biological Markers in the Sedimentary Records*. Elsevier,
 641 Amsterdam, 364 pp.
 642 Jones, D.M., Head, I.M., Gray, N.D., Adams, J.J., Rowan, A.K., Aitken, C.M., Bennett,
 643 B., Huang, H. Brown, A., Bowler, B.F., Oldenburg, T., Erdmann, E. & Larter,
 644 S.R. (2008) Crude oil biodegradation via methanogenesis in subsurface petroleum
 645 reservoirs. *Nature*, 2008 Jan 10; 451 (7175), 176-180.
 646 Kowalewski, I., Carpentier, B., Huc, A.Y., Magnier, C. & Delamaide, E. (2001)
 647 Geochemical study of biodegraded heavy oils of Wabasca sand deposits (Canada).
 648 In: 20th International Meeting on Organic Geochemistry, September 10th-14th,
 649 Nancy, p. 87.

650 Larter, S.R., Huang, H., Adams, J., Bennet, B., Jekanola, O., Oldenburg, T., Jones, M.,
 651 Head, I.M., Riediger, C. & Fowler, M. (2006) The Controls on the composition of
 652 biodegraded oils in the deep subsurface. Part 2 – geological controls on subsurface
 653 biodegradation fluxes and constraints on reservoir-fuils property prediction.
 654 AAPG Bulletin, 90, 921-938.

655 Larter, S.R., Wilhelms, A., Head, I.M., Koopmans, M.P., Aplin, A. di Primio, R.,
 656 Zwach, C., Erdmann, M. & Telnaes, N. (2003) The controls of the composition of
 657 biodegraded oils in the deep surface – Part 1: biodegradation rates in petroleum
 658 reservoirs. Organic Geochemistry, 34, 601-613.

659 Magnier, C., Kowalewski, I., Carpentier, C. Huc, A.Y., Delamaide, E. & de Barros
 660 Penteado, H.L. (2001) Tentative quantification of the extent of biodegradation in
 661 oil fields using heavy metal content. In: 20th International Meeting on Organic
 662 Geochemistry, September 10th-14th, Nancy, 413-414.

663 Moldowan, J.M., Albrecht, P. & Philp, R.P. (1992) Biological Markers in Sediments
 664 and Petroleum. Prentice Hall, New Jersey, 411 pp.

665 Parkes, R.J., Cragg, B.A. & Wellsbury, P. (2000) Recent studies on bacterial
 666 populations and processes in subseafloor sediments: a review. Hydrogeol. Journal,
 667 8, 11-28.

668 Peters, K.E., Walters, C.C. & Moldowan, J.M. (2005) The Biomarker Guide, 2nd ed.
 669 Biomarkers and Isotopes in Petroleum Exploration and Earth History, vol. 2.
 670 Cambridge University Press, New York, NY, 1155 pp.

671 Roadifer, R.E. (1987) Size distribution of the world's largest oil and tar accumulations.
 672 In: Meyer, R.F. (Ed.), Exploration for Heavy Crude Oil and National Bitumen.

673 AAPG Studies in Geology, Vol. 25, American Association of Petroleum
 674 Geologists, Tulsa, 3-23.
 675 Trindade, L.A.F., Brassell, S.C. & Santos Neto, E.V. (1992) Petroleum migration and
 676 mixing in the Potiguar Basin, Brazil. AAPG Bulletin, 76, 1903-1924.
 677 Walters, C.C., Freund, H., Kelemen, S.R., Braun, A.L. & Wenger, L.M. (2009)
 678 Predicting Oil Quality - Simulating Reservoir Alteration Processes. AAPG
 679 Hedberg Conference on: "Basin and Petroleum System Modeling: New Horizons
 680 in Research and applications". May 3rd-7th, 2009, Napa, California, USA.
 681 Wellsbury, P., Goodman, K., Barth, T., Cragg, B.A., Barnes, S.P. & Parkes, R.J. (1997)
 682 Deep marine biosphere fuelled by increasing organic matter availability during
 683 burial and heating. Nature, 388, 573-576.
 684 Wenger, L.M., Davis, C.L. & Isaksen, G.H. (2001) Multiple Controls on Petroleum
 685 Biodegradation and Impact on Oil quality. SPE 71450, Society of Petroleum
 686 Engineers.
 687 Wilhelms, A., Erdmann, M. & Larter, S.R. (2004) Easy-Fest versus BDI uncertainties in
 688 Predrill prediction of biodegradation degree in subsurface petroleum reservoirs.
 689 AAPG Bulletin, 88, (13) (Supplement).
 690 Wilhelms, A., Larter, S.R., Head, I.M., Farrimond, P., di Primio, R. & Zwach, C. (2001)
 691 Biodegradation of oil in uplifted basins prevented by deep-burial sterilization.
 692 Nature, 411, 1034-1037.
 693 Yu, A.Z., Cole, G., Grubitz, G. & Peel, F. (2002) How to predict biodegradation risk
 694 and reservoir fluid quality. World Oil, April 1st-5th 2002.

695 Zengler, K., Richnow, H.H., Rossello-Mora, R., Michaelis, W. & Widdel, F. (1999)
696 Methane formation from long-chain alkanes by anaerobic microorganisms.
697 Nature, 401, 266-269.
698

Figures and tables captions

Table 1 Stoichiometric coefficients for kerogen cracking (mg/g).

Compound class	PT beds	Upanema Mb.
CO ₂	92	90
C ₁ -C ₅	36	20
C ₆ -C ₁₄ sat	22	22
C ₆ -C ₁₄ aro	6	6
C ₁₄₊ n-alkanes	11	12
C ₁₄₊ iso-alkanes	16	17
C ₁₄₊ cyclo-alkanes	24	26
C ₁₄₊ aro	12	15
C ₁₄₊ NSO	15	9
C ₁₄₊ NSO-retained	138	83
Kero2	628	700
Dead kerogen	0	0

Table 2 Comparison of measured and simulated present-day temperatures in the Potiguar basin.

Field	Measured temperature (°C)	Simulated temperature (°C)
GMR	47.5	47.2
FP	42.9	45.7
MAG1	39.8	40.8
ARG2	38.1	36.4
ET	38.6	37.2

Table 3 Comparison of simulated and measured oil composition of a non-biodegraded oil from the ARG2 field.

Compound class	Measured composition in non-biodegraded oil of the ARG2 field (%)	Simulated composition in non-biodegraded oil of the ARG2 field (%)
C ₆ -C ₁₄	32	32
C ₁₄₊ n+iso alkanes	23	22
C ₁₄₊ cyclo-alkanes	21	20
C ₁₄₊ aro	9	10
C ₁₄₊ NSO	15	14

Table 4 Relative biodegradation rate of the biodegradation compound classes used to describe the hydrocarbon phase.

Compound	Relative biodegradation rate
C ₆ -C ₁₃ sat	0.630
C ₆ -C ₁₃ aro	0.140
C ₁₄₊ n-alkanes	0.121
C ₁₄₊ iso-alkanes	0.078
C ₁₄₊ cyclo-alkanes	0.031
C ₁₄₊ Aro	0.000

Saturation computed in a low resolution mesh (1 cell)

Saturation computed in a high resolution mesh (7 cells)

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Figure 2

Figure 3

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