Simulation of Anaerobic SOM Biodegradation and Biogenic Methane Production for Basin Modeling

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ABSTRACT

Methanogenic biodegradation of Sedimentary Organic Matter (SOM) has recently focused the interests of the O&G industry following the growing demand on natural gas, the discovery of giant biogenic methane accumulations (Levant, Tamar field, …) and the growing interests towards gas hydrates (biogenic gas accounts for as much as 20% of the world's natural gas resource (Rice, 1993)). Nevertheless, the complex microbial mechanisms involved in the anaerobic degradation of organic matter (fermentative and methanogenic degradation of SOM) is comparably less understood than the surface and shallow oxidative biodegradation of SOM or the deep thermal cracking of kerogen. Therefore, new tools are at present required to guide the exploration of biogenic gas resources, with potential applications to conventional resources, unconventional resources and gas hydrates, taking into account both physical and biological processes of gas generation and migration. In this context, basin models need to incorporate new functionalities to take into account the biodegradation of SOM and the associated production and fate of biogenic methane.

The equation given by Middleburg (1989), derived from the initial work of Berner (1980), as remained until now as a favored model for the very early diagenesis evolution of the SOM (e.g. Wallman *et al.*, 2006). However, the lack of geochemical data to depths below several tens of meters precludes any validation of this law to deeper diagenetic conditions. Several studies have proposed conceptual models based on experimental data to consider the organic matter diagenetic evolution at greater depths, where the thermally-induced evolution and the biodegradation of SOM are coupled (Burdige *et al.*, 2011). Indeed, it is suggested that a fraction of the SOM available for biodegradation, also referred to as labile organic matter (or LSOM), might be delivered from the so-called refractory fraction of the SOM (RSOM) with depth as a consequence of the temperature increase (Wellsburry *et al.*, 1997). Furthermore, given the shallow conditions of biogenic methane generation, the effect of dissolved methane advection in a sedimentary basin seems to play a key role in the formation of gas accumulations.

In order to study biogenic gas generation and migration, new functionalities have been developed by IFP Energies nouvelles within TemisFlow™. First the total SOM was split into three distinct fractions: (1) a labile fraction that micro-organisms can directly metabolize and degraded following a rate law which is a function of temperature and organic matter aging, (2) a labilizable fraction that may be converted to the labile fraction through a thermal transformation, controlled by an Arrhenius equation, and (3) a refractory fraction, which may not be degraded. Consequently, temperature has a strong impact on biogenic methane generation fraction degradation since it controls both the bacterial activity and the transformation rate from labilizable to labile organic matter. The methane produced in the model is allowed to be distributed in three states: 1) adsorbed onto RSOM (Langmuir equation, e.g. Romero-Sarmiento *et al.* (2013)), 2) dissolved in formation water (or brine) (model of Duan & Mao (2006)) and 3) as a free gas phase. The methane is transported in the model by the effects of burial and compaction, whereby the production of biogenic methane is fully coupled with dissolution, and is then allowed to migrate as a dissolved compound in water but also as a free gas phase.

Since the model parameters reported in the literature have been determined at the meter scale, an upscaling is essential to use this model at the basin scale. The effects of the different parameters given in the Middleburg (1992) and Burdige (2011) rate laws within reasonable ranges suitable for basin modeling are submitted to a sensitivity analysis. Recommended values are defined based on natural 1D cases. Using data from Wefer *et al*. (1998), we have been able to build a simple 1D case corresponding to the geological history of LEG175 (Benguela upwelling, offshore Namibia). Based on the results of Hatcher et al. (2014), it has been possible to tune the rate law variables. It appears that the nominal rate (r_{bio}), which controls the amount of labile SOM degraded at each time step must be increased to meet the kinetics observed at basin scale. On the other hand, the effect of SOM age has been neglected because it was found to be redundant with the fractionation of the SOM into three fractions. The optimal temperature for bacterial activity was shown to be of primary importance because it will control at which depth the main event of degradation occurs. Moreover, the Monod parameter seems to be of little influence at the basin scale and has been thus neglected. It appears that simulation results obtained with this set of parameters fit published results of LEG175.

However, although these results seem very promising, the implemented model could certainly be improved. Some of these improvements are not directly correlated to the biodegradation model but totally basin related. It appears, in particular, that the conditions of methane preservation in the top layer seem to be biased by the default surface boundary conditions (no capillary pressure), and may induce significant artificial (numerical) loss of gaseous methane to the surface. The effect of the boundary condition is thus examined using different gridding and time step resolutions and corrected for by tuning different parameters of the rate law and of the lithological description of the top layer.