Quantitative Prediction of CO2 and H2S in the Gulf of Gabes, Offshore Tunisia

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Introduction
Within the Gulf of Gabes, offshore Tunisia, the inert gases CO2 and H2S are an important exploration risk. A quantitative prediction of occurrence of these gases at locations of interest is difficult. We present new developments in basin and petroleum systems modeling to improve the understanding on the behavior of such inert gases. A number of CO2 and H2S specific processes have newly been integrated in a coupled modeling approach, which accounts for the interactions of those with geological processes. Finally, this method was applied to an already existing model of the area (Grimmer et al., 2011) to better analyze and quantitatively predict generation and migration amounts of inert gases.

Method
The key mechanism for the generation of H2S in the basin is Thermochemical Sulfate Reduction (TSR) which occurs mainly in the carbonate reservoir intervals. A reaction scheme developed by Tang (Tang et al., 2009) has been used for modeling of this geological process (Kauerauf et al., 2012).

\[ C_n H_m^+ + SO_4^{2-} + H^+ \rightarrow H_2 S + CO_2 + H_2 O \]

Helium isotope analysis indicates that generation of CO2 is mainly from the thermal destruction of deeply buried carbonates (Grimmer et al., 2011). The corresponding reaction

\[ CaCO_3 \rightarrow CaO + CO_2 \]

is modeled by a kinetic equation based on Arrhenius law which yields huge amounts of CO2, cmp. Fig. 1.

Figure 1. Transformation ratio of carbonates in layer Lower Serdj (Late Triassic)

Under subsurface conditions, both gases are highly soluble in water and a mutual solubility model, based on work of Duan et al., 2006 and Duan et al., 2007, has been implemented into petroleum systems modeling. Excess inert gas amounts dissolve in liquid or vapor phases of the petroleum.

Migration of the inert gases, which are dissolved in water, was modeled with a diffusion equation based on Fick’s law with diffusion coefficients determined according to an Eyring type equation

\[ D_{eff} = D_0 \phi \delta / \tau, \quad D = D_0 \exp(-E_a / RT) \]

with \( D_0 \) the pure component diffusion coefficient, \( D_{eff} \) the effective diffusion coefficient, \( \phi \) porosity, \( \delta \) constrictivity, \( \tau \) tortuosity, \( E_a \) the activation energy, \( R \) the universal gas constant and \( T \) the temperature. It has been observed, that, according to these equations, high temperatures allow for a significant migration due to diffusion inside the water phase. Especially, CO2 originating from deeply buried carbonates might pass quite long distances.

The migration of CO2 and H2S dissolved in liquid or vapor petroleum phases was performed with separate phase flow such as Darcy flow or Invasion Percolation (Hantschel and Kauerauf 2009). Herein, the gases are dissolved within migrating petroleum phases. The equilibrium between dissolution into water and the petroleum phases was continuously updated in the entire model at all locations and geological times.

Finally, a modeling method with a full coupling of all relevant processes, namely generation of CO2 and petroleum, destruction of petroleum with subsequent generation of H2S, mutual dissolution of inert gases into water and petroleum phases, and migration via diffusion and separate phase flow has been used.

Results and Discussion
This method has been applied to a basin model in the Gulf of Gabes, offshore Tunisia (Grimmer et al., 2011). It already contained an overall thermal analysis with generation and migration of hydrocarbons, performed with established methods of petroleum systems modeling. It has been found that large amounts of CO2 dissolve in the water, Table 1, and diffuse into reservoir layers which are of interest for exploration.

<table>
<thead>
<tr>
<th></th>
<th>CO2</th>
<th>H2S</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Generation</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Mass Losses</td>
<td>35%</td>
<td>35%</td>
</tr>
<tr>
<td>Dissolved in Water</td>
<td>40%</td>
<td>60%</td>
</tr>
<tr>
<td>Free Phase</td>
<td>5%</td>
<td>5%</td>
</tr>
</tbody>
</table>

Table 1. Mass Balance of CO2 and H2S.

Due to a limited capacity of water to dissolve both inert gases, dissolved CO2 inhibits dissolution of H2S. Significant amounts of H2S are thus not dissolved into water and kept in the petroleum phases. In total, measured concentrations of both inert gases could be reproduced, see Table 2.
Table 2. CO2 and H2S concentrations at some specific locations.

<table>
<thead>
<tr>
<th></th>
<th>Area 1</th>
<th>Area 2</th>
<th>Area 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2 - Measured</td>
<td>10 – 20 %</td>
<td>15 – 21 %</td>
<td>55 – 85 %</td>
</tr>
<tr>
<td>CO2 - Modeled</td>
<td>40 – 90 %</td>
<td>55 %</td>
<td>55 %</td>
</tr>
<tr>
<td>H2S - Measured</td>
<td>500 – 1000 ppm</td>
<td>4000 – 1000 ppm</td>
<td>570 ppm</td>
</tr>
<tr>
<td>H2S - Modeled</td>
<td>1000 – 2000 ppm</td>
<td>5000 ppm</td>
<td>5500 ppm</td>
</tr>
</tbody>
</table>

Conclusions
Measured concentrations of both inert gases, H2S and CO2, could be approximately reproduced by modeling. Mutual water dissolution of inert gases and diffusion in deeply buried layers are important processes, which are necessary for a quantitative prediction of these gases. As such the overall workflow of basin and petroleum systems modeling with incorporation of inert gas processes has given a better understanding of the distribution of H2S and CO2 in the Gulf of Gabes.

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References