Transition metals cations as EOR agents in carbonate reservoirs: an atomistic point of view

BRUNO F. ZORNIO[1], JAMES M. DE ALMEIDA[2], CAETANO R. MIRANDA[1]

[1] Instituto de Física - Universidade de São Paulo , São Paulo, SP – Brazil [cmiranda@if.usp.br]

[2] Universidade Federal do ABC, Santo André, SP – Brazil

Experimental observations indicate that the injection of cationic transition metals (TM) brine solution could assist oil desorption from carbonates. After a reference brine injection, by adding Copper II solutions, 5% to 10% of incremental recovery of original oil in place is observed, leading to a potential application on enhanced oil recovery (EOR) processes. However, the molecular mechanism involving Cu^{2+} and calcite/oil interactions are far from being well understood. Here, first principles simulations based on the Density Functional Theory (DFT) were performed to investigate the processes involved in the formation of a TM-oil complex [1] and the coverage of carbonate rocks with the respective TM minerals [2]. We have simulated octanoic acid (oct- deprotonated and octH protonated), to model the acidic oil components, the Cu(Oct)2 complex and the calcite (CaCO3) as matrix (Figure 1), to determine the structural properties and adsorption energies of the oil model and the formed Cu-oil complex, taking into account water as an implicit solvent.The adsorption energies for octanoic acid suggests interactions with the calcite surface (-0.6 eV for oct- and -1.3 eV for octH). However, in the presence of TM cations, the square planar complex formation energy is highly stable (-1.5 eV per TM-O bond), indicating that the complex formation is thermionically favorable. Besides, the adsorption of the TM-oil complex is favorable with the calcite surface in the aqueous phase; the nonacid fraction of the oil is capable of detaching the complex from the carbonate porous media.

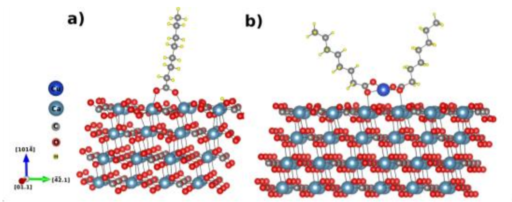

Figure 1: **a)** octanoic acid; **b)** $Cu(Oct)_2$ complex, adsorbed at calcite (10.14)

[1] Lee, Elzinga, and Reeder (2005) Geochimica et Cosmochimica Acta 69, 49-61.[2] Kitano, Kanamori and Yoshika (1976) Geochemical Journal 10,175-179.