Nano-pore scale dynamics of surfactant flooding in asphaltene containing oils using coarse-grained Molecular Dynamics simulations

Edo S. Boek,[a,*] Patrice Ligneul,[b] John P. Crawshaw,[a] and Mikhail Stukan[b]

[a] *Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ United Kingdom*
[b] *Schlumberger Dhahran Carbonate Research Center, Dhahran Techno Valley - KFUPM, P.O. Box 39011, Dammam / Doha Camp 31942, Kingdom of Saudi Arabia*

(corresponding author: e.boek@imperial.ac.uk)*

The re-emergence of interest in enhanced oil recovery (EOR) has recently illuminated the complexity and importance in understanding recovery processes in varying pore types and wetting states. Multi-scale reservoir heterogeneity plays a key role, and in particular the displacement of hydrocarbon reserves from oil-wet micropores poses significant challenges due to capillary effects. Methods to overcome these include reducing interfacial tension or altering the wetting state to more hydrophilic by means of addition of suitable chemicals (for example surfactants).

However, a critical controlling process in transporting the chemical agent to the targeted pore fluids is diffusion. Molecular Dynamics (MD) simulation is particularly suited to describe the diffusion effects at the sub-pore, even nano-scale, level and has the potential to emerge as a powerful analytic tool in the industry.

This study investigates the use of coarse-grained MD techniques in determining the impact of surfactants on modifying capillary forces from small oil-wet pore spaces with or without asphaltenic fractions. Two different wetting states are modeled:

1. initially oil-wet
2. water-wet altered to oil-wet by the presence of asphaltenic components adsorbing to the pore surface

As a result, two different mechanisms of surfactant physico-chemical process are illustrated:

1. surfactant adsorption at the pore surface making the wall more hydrophilic, aiding water imbibition;
2. in the second case, surfactant action on specific components of asphaltene molecules is demonstrated, also leading to improvement in water imbibition.

This study presents the modeling set up, the investigation and demonstrates the potential use of these modeling techniques in oil recovery research. This type of approach can be also considered as a tool to estimate effectiveness, and selection of the most applicable additives given the geological and chemical characteristics at the reservoir pore scale. After experimental verification of modeling scenarios, the data can be used in up-scaled models for reservoir simulations.

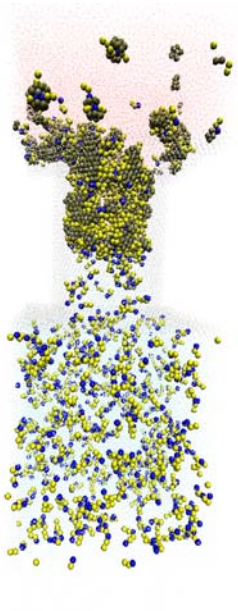

Figure 1: Snapshot of coarse-grained MD simulation of a aqueous surfactant solution (bottom) imbibing in a nano-pore (top), rendered oil-wet by the adsorption of asphaltenes. Surfactants are yellow and blue, asphaltenes are black. Note emulsification in the top part

References

[1] E.S. Boek, D.S. Yakovlev, T.Headen, "Quantitative Molecular Representation of asphaltenes and Molecular Dynamics simulation of their aggregation", *Energy & Fuels* 23, 1209-1219 (2009).
[2] Headen, T. F.; Boek, E. S.; Skipper, N. T.; Energy and Fuels, 2009, 23, 1220 - 1229