Molecular simulations of surfactant-modified interfaces: numerical tools and analysis

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Abstract

Carbon dioxide is one of the two main components of the alternating water/CO2 flooding technique which has proven highly effective for improving the efficiency of enhanced oil recovery (EOR). However, carbon dioxide from smaller sources, such as CO2 separated from hydrocarbon streams originating in CO2 rich fields, is still considered to be a waste and often released into atmosphere.

It is our belief that we can achieve a similar effect via injecting emulsion-like mixture of water, CO2, and a "dual-action" emulsifying agent. The dual nature of the surface-active component refers to its affinity towards both water/CO2 and water/hydrocarbon interfaces. A portion of injected CO2 will remain inside the reservoir and thus safely stored underground, with remaining injected fluids contributing to enhanced petroleum recovery. The proposed approach will be financially feasible for small carbon dioxide sources, while effectively combining CO2 storage with EOR. The success of this technology will rely on pinpointing surfactant candidates with desired properties, ie identifying components exhibiting interfacial activity for both interfaces.

We have chosen molecular dynamics (MD) as our main scientific tool for evaluation of various surfactant structures, their behavior and relative impact on the interfaces of interest. MD simulations are computationally intensive at relevant system sizes, so we have established a computational framework allowing a desktop to perform at speeds until recently only possible for supercomputers. Benchmarks showed that our consumer-grade desktop with eight core Intel CPU and two Nvidia GPUs routinely outperformed four Cray XE6m supercomputer nodes.

Evaluation of surfactants involves sophisticated analysis of MD data describing the interfacial systems. Traditional techniques involving density profiles have proven to be insufficient to capture the structure of roughened interfaces. We have implemented a more advanced method providing a more accurate description of interfaces involved, allowing us to study their structure in detail.

Recent Publications

1. J. Selvåg, T. Kuznetsova, B. Kvamme (2017) Molecular dynamics study of surfactant-modified water-carbon dioxide systems, *Molecular Simulation*, in press.
2. J. Selvåg, T. Kuznetsova, B. Kvamme (2017) Molecular Dynamics Study of N-formyl Morpholine Surfactant in CO2/H2O/Oil Interfacial System. Paper presented at the 13th International Conference of Computational Methods in Sciences and Engineering.
3. G. Tóth, J. Selvåg, B. Kvamme (2017) Phenomenological Continuum Theory of Asphaltene-Stabilized Oil/Water Emulsions. *Energy & Fuels* 31:1218-1225.
4. G. Tóth, B. Kvamme, (2015) Phase field modelling of spinodal decomposition in the oil/water/asphaltene system. *Physical Chemistry, Chemical Physics* 17:20259-20273.
5. B. Kvamme, M. Qasim, K. Baig, P. Kivelä, J. Bauman (2014) Hydrate phase transition kinetics from Phase Field Theory with implicit thermodynamics and heat transport. *International Journal of Greenhouse Gas Control* 29:263-278.



Biography

Bjørn Kvamme obtained his MSc in Chemical Engineering (1981) and PhD in Chemical Engineering (1984) from the Norwegian University of Technology and Natural Sciences. After a short period with SINTEF and two years at Bergen University College, he was appointed as full Professor in 1987 and started education of MSc and PhD in Process Technology in Telemark. He is appointed as a Professor in Gas Processing at the Department of Physics, University of Bergen in March 2000. He is the author/co-author of 422 publications during last 25 years, of which 148 are in good international scientific journals. He has 2270 citations as per May 1, 2017, and has presented numerous papers at international conferences.

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