Molecular simulations of surfactant-modified H_2O/CO_2 and H_2O/hydrocarbon interfaces

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Abstract

Phenomenological continuum theories of Ginzburg-Landau type have been successfully applied before to address complex interfacial phenomena involving emulsion formation in aqueous systems relevant for Enhanced Oil Recovery (EOR). Molecular simulations were proven crucial for calibration of model parameters required to both validate the theory and produce reasonable equation of state.

Our molecular simulation work focused on surfactant-modified H_2O/CO_2 and H_2O/oil systems central for an earlier proposed technique that combines EOR and safe storage of carbon dioxide. Viscosity contrast between asphaltenes and the bulk liquids will heavily influence the coalescence of oil droplets and thus offer an alternative, kinetically driven mechanism for emulsion formation and reformation triggered by dual-action surfactants. Analysis needed to evaluate the structural details and fluctuations dominating the interfacial regions requires knowing the exact locations of interfaces between all the relevant liquid phases. We have deployed an intuitive technique allowing us to find intrinsic surfaces defining liquid-liquid interfaces through the analysis of instantaneous and time averaged molecular configurations. While fairly straightforward in case of simple liquids, such approach becomes more complicated when the size and the shape of molecules start playing a significant role. We have thus augmented our analysis of large-scale multicomponent systems by studying several smaller ternary systems with the non-aqueous component varying in size and molecular complexity from carbon dioxide to asphaltenes to investigate the possible impact of different broadening parameters.

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 CO_2/H_2O/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.

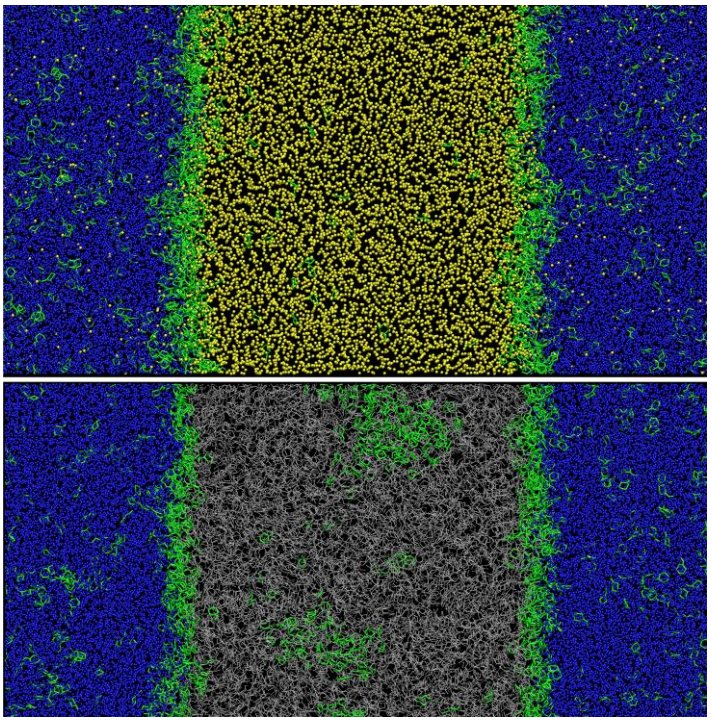


Figure 1. Snapshots of surfactant modified H_2O/CO_2 and H_2O/hydrocarbon molecular interfacial systems. Blue: H_2O, yellow: CO_2, gray: hydrocarbon and green: surfactant molecules.



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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