

## Multiscale modeling of industrial emulsions: fundamentals and applications of random chemistry in asphaltene dispersions

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Emulsions are at the heart of many a soft material of practical industrial interest; one finds them in such frivolous systems as ice-creams, but also in food and cosmetics and, as we discuss here, in crude oils. Invariable, what is the same in all these systems is the enormous diversity in chemical signatures of the constituent chemicals. Such 'random chemistry' is commonly overlooked in simulation and modeling, due to the seemingly impenetrable complexity, but the inevitable randomness has very serious consequences for dispersion morphology and stability, foremost the formation of compound core-shell structures in which layers of molecules produce, what could best be described as, 'gradient droplets' (Figure 1).

We present an in depth analysis of such behaviors for asphaltene emulsions in crude oils. By way of multiscale modeling, including scales from molecular to mesoscopic (microns), we discovered a common thermodynamic footing of sometimes bizarre behavior. In particular, the analysis suggests that core-shell structures should be the rule, not the exception, with in-droplet phase separation into at least a few phases. Conditions apply where the core shell structures are spherically symmetric, or of broken symmetry with buds and lens formation. The new insight immediately leads to alternative rational design strategies for emulsion modifiers, that are meant to stabilize or inversely break the emulsion systems, such as asphaltene blockers; whether in crude oil or in oil-in-water emulsions.

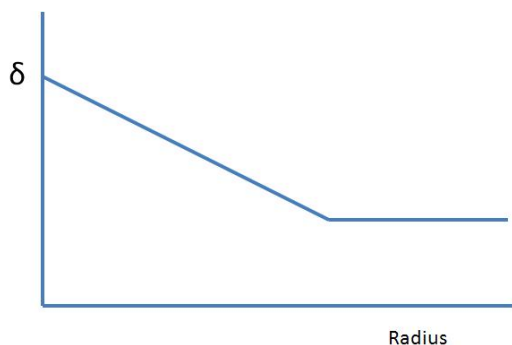


Figure 1 Solubility parameter distribution in asphaltene aggregate

All simulations are with the novel CULGI (Chemistry Unified Language Interface) scripted software library, that was designed especially for industrial multiscale modeling. The Culgi consortium is sponsored by a number of companies and EU projects, including chemical, pharmaceutical, petrochemical, and oil industries. In this setting, it is especially important that modeling assists the industrial researcher by offering practical solutions, with a powerful scripting interface, and easy and trustworthy access to the most powerful simulation algorithms to date. Moreover, the interdisciplinary approach allows porting of concepts from one industrial domain to the other. In this case, the gradient droplets were first discovered (by us) in polyolefin blends; that have very different chemical process backgrounds, but quite some analogies to asphaltene emulsions in molecular thermodynamics.