Simulating the Spontaneous Emulsification of Oil/Water/Surfactant Mixtures

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Goals:

Understanding the fundamental mechanisms in spontaneous emulsification, exploring the growth laws of internal interfaces in the forming microemulsion.

Computer Simulation Method:

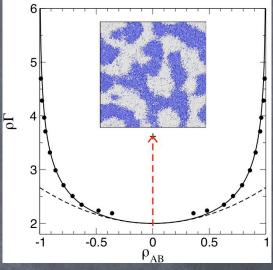
A mesoscale, particle-based method called Multi-Particle Collision Dynamics with explicit surfactant, consistent thermal fluctuations and hydrodynamics.

E. Tuzel et al, Europhys. Lett. 80 (2007) 40010.

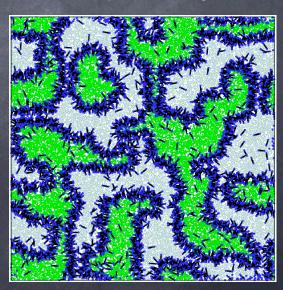
Results in 2009:

Exact derivation of the constitutive relation for the algorithm of a one-component fluid directly from the microscopic collision rules by means of Chapman-Enskog kinetic theory.

T. Ihle, Phys. Chem. Chem. Phys. (2009) DOI: 10.1039/b910356b.



Binary phase diagram



Snapshot of a fluctuating microemulsion in equilibrium