Simulation of Droplet Breakup by Dissipative Particle Dynamics
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ABSTRACT

This project applies a new DPD simulation method developed by the Maia group with a tunable coarse-grained level to capture the physics of droplet breakup in micro- and nano-emulsions. The droplet breakup phenomenon is described based on the viscosity ratio of the phases and the capillary number, a ratio of shear stresses to pressure. Viscosity was modified by taking advantage of the Fluctuation-Dissipation theorem. We have found that DPD can qualitatively reproduce the Grace plot for Newtonian fluids under shear.

METHODS

• Dissipative Particle Dynamics (DPD)
  • Governed by Langevin
  • Fewer interactions
  • Coarse-grained
  • Cut-off radius
  • Can use long time step
  • Soft potentials
  • Study mesoscopic phenomena
• Droplet break-up
  • Important for any mixing operation
  • Food
  • Cosmetics
  • Pharmaceuticals
  • Oil recovery or clean-up
  • Experimentally described by Grace in the 1980s
  • Not yet fully described by simulation

RESULTS

Important Characteristics:
1) Gentle slope from left
2) Minimum near Viscosity Ratio = 1
3) Sharp increase on right

RESULTS

FUTURE WORK

• Improve “one parameter” (σ and γ) results
• Only change conservative force parameter
• Combine conservative force change with σ and γ
• Consider extensional flows
• Consider non-Newtonian fluids
• Consider polymeric materials

REFERENCES


CONCLUSIONS

• The material properties that we verified were
  • Newtonian fluid
  • Interfacial tension is shear independent
  • Viscosity fits to activation energy

• Ways to describe droplet breakup
  • 2 Parameter: Qualitatively correct behavior
  • 1 Parameter: Limited viscosity range