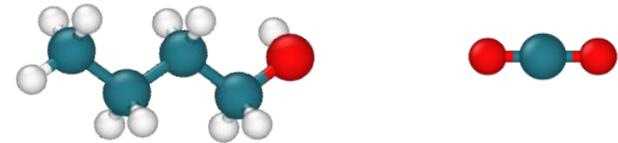


Interfacial Tension of Binary Mixtures of Alcohols with Carbon Dioxide Using Molecular Dynamics (MD) Simulations

Motivation

- Mixtures of alcohols and CO₂ are of great importance in process engineering, such as separation technology and catalysis
- Interfacial tension affects phenomena like wetting, bubble formation, and mass transport across interfaces
- Molecular Dynamics (MD) simulations of mixtures of alcohols and CO₂ at process-relevant conditions are very scarce

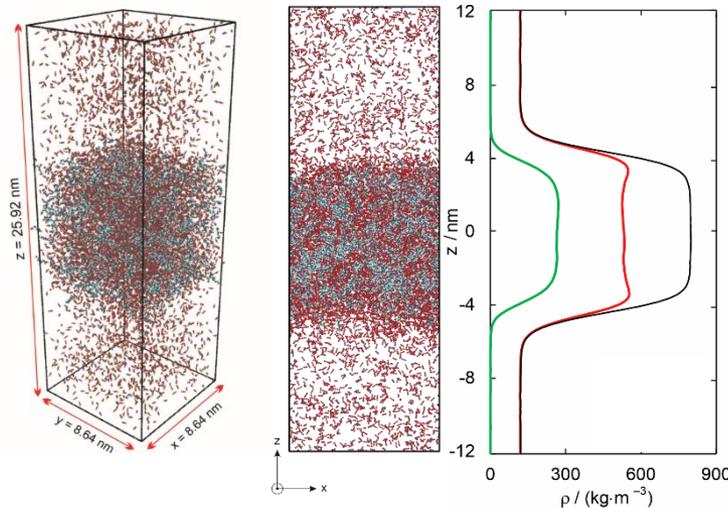
Simulation	×	Modeling	×
Experiment		Construction	



Focus

- MD simulation of interfacial tension of binary mixtures of 1-alcohols and CO₂ using existing models
- Variation of chain length of 1-alcohols: ethanol, 1-butanol, 1-octanol
- Effect of temperature (298-338 K) and pressure (0.1-20 MPa)
- Analysis of density profiles and surface enrichment
- Comparing simulation results with experimental data

We are looking for students who are motivated to learn and implement MD simulations for master's theses.



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