ME Seminar

Flow and mixing dynamics of phase transforming multicomponent fluids using the van der Waals theory of capillarity

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ABSTRACT

Thermodynamic properties of fluids play a fundamental role in determining their phase behavior and transport phenomena. Traditionally, most thermodynamic modeling has focused on near-equilibrium properties, leveraging analytical and numerical results that become unreliable far from equilibrium. This gap arises because the governing equations for non-equilibrium thermodynamic behavior, when derived from first principles, are often highly complex and challenging to solve numerically. In this talk, we present a direct van der Waals simulation framework capable of capturing the intricate dynamics of phase-transforming fluids far from equilibrium. This approach goes beyond equilibrium-based approximations, enabling us to resolve the rapid processes and metastable states characteristic of non-equilibrium phase transitions. As an application, we investigate how dissolved air alters the characteristics of cavitation in water. Our results highlight that even small amounts of dissolved gas can fundamentally change cavitation thresholds and bubble dynamics.

Time permitting, I will talk about first-principles modeling combined with Bayesian parameter estimation to understand self-assembly of lipids during mRNA vaccine manufacturing.

ABOUT THE SPEAKER

I completed my B. Tech. from IIT Roorkee in 2016. After that, I worked at United Health Insurance in India for 2 years as an Associate Software Engineer. I started my PhD at Purdue University with Dr. Hector Gomez in 2018. We worked on phase field models for multiphase flows, using which we estimated the effect of dissolved air on cavitation in water. After finishing my PhD in 2023, I started working with Dr. Richard Braatz as a postdoc at MIT, where I work on mechanistic modeling of various manufacturing processes involved in making mRNA-based vaccines. My broad research areas include transport phenomena, fluid flows and uncertainty quantification.

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