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Seminar

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A Coupled Computational Fluid Dynamic/Population Balance Method to Understand Microstructure: From Foam Manufacturing to Polymer Upcycling

Abstract

Understanding the rheology and microstructure of foams and emulsions is important for a number of applications from enhanced oil recovery to polymer upcycling and advance manufacturing methods. We are developing a coupled computational fluid dynamics/population balance method to understand bubble/droplet size distribution during flow in complex geometries. In this presentation, we focus on PMDI polyurethane foams, which are chemically blown foams used for electronic encapsulation and lightweight structural parts. A published kinetic model is extended with a population balance equation using the Quadrature Method of Moments (QMOM) to predict bubble size evolution as well as density variations during mold filling. We use a stabilized finite element method to solve the conservation equations; equations of motion, energy balance equation, species conservation with reaction, and transport of moments for QMOM. We combine these equations with the level set method to track the free surface between the foam and the surrounding gas. This model is used to predict final foam properties including density, thermal conductivity, and bubble size evolution in a three-dimensional foam bar geometry. Results for final densities are compared to experimental X-ray CT data. Bubble size evolution and final distributions are compared to optical and SEM data. In a complementary project on polymer upcycling with Case Western Reserve University, we extend these population balance models to understand emulsion formation during hybrid chemical-mechanical upcycling of polymer blends of PET and PE. The material mixtures are melted and blended in an extruder, forming nanodomains of PET which grow over time due as coalescence dominates over droplet breakup. Once the droplets are large enough, they can be filtered out from the PE melt. Experimental results from Case are discussed and compared with preliminary results from the model.

Biography

Dr. Rekha Rao is a Distinguished Member of Technical Staff at Sandia National Laboratories. She came to Sandia in 1990 after earning her BS from UC Berkeley and Ph.D. from the University of Washington, both in Chemical Engineering. Rekha is an expert in the computational mechanics of complex fluids, including theoretical development, numerical algorithms, and finite element implementation. She is one of the founding authors of Goma, an R&D 100 winning open-source software package for process flow modeling. She has authored or coauthored over 125 peer-reviewed journal articles, reports, and conference proceedings. Rekha's research has spanned model development in support of energy-production, environmental issues, polymer processing, and manufacturing. Her work on foam process models have led to publications, collaborations with industry, and to a production computational capability impacting manufacturing yields. Rekha is the President of the US Association of Computational Mechanics and the Chair of the Female Research Committee of the International Association of Computational Mechanics, mentoring and encouraging women in computational mechanics.

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