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FOAM PROPERTY PREDICTION FROM PROCESS MODELING

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We are developing computational models to elucidate the injection, expansion, and dynamic filling process for polyurethane foam such as PMDI. The polyurethane is a chemically blown foam, where carbon dioxide is produced via reaction of water, the blowing agent, and isocyanate. In a competing reaction, the isocyanate reacts with polyol producing the polymer. A new kinetic model is implemented in a computational framework, which decouples these two reactions as extent of reactions equations. The model predicts the polymerization reaction via condensation chemistry and the foam expansion kinetics through a Michaelis-Menten approach. Both reactions are exothermic and temperature dependent. The conservation equations, including the equations of motion, an energy balance, and two rate equations for the polymerization and foaming reactions, are solved via a stabilized finite element method. The rheology is determined experimentally and is assumed to follow a generalized-Newtonian law where it depends on the degree of cure and temperature, but is not viscoelastic.

The conservation equations are combined with a level set free-surface algorithm to determine the location of the foam front as it expands over time similar to the model used in previous work [1]. The model predicts the velocity, temperature, viscosity, free surface location, and extent of polymerization of the foam. In addition, it predicts the local density and density gradients based on the Michaelis-Menten kinetics of foam expansion. Results from the model are compared to experimental flow visualization data and post-test CT data for the density. Recent work seeks to couple the fluid-thermal simulations with a nonlinear viscoelastic model for the structural response [2], giving us the means to predict dimensional changes during manufacture and aging. Property predictions from the fluid-thermal model are used to include density and cure gradients in the structural response, resulting in inhomogeneous material properties. This work will also be discussed.

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