

## Multiphysics modeling for structural polyurethane foams: from foam filling and curing to nonlinear viscoelastic deformations and 30 years of aging

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### Abstract:

Polyurethane foams are used in many industries to provide protection from impact, structural support and thermal insulation. Complex physical processes during both manufacturing and aging of these materials can cause part shape changes to occur over timescales of hours (during manufacturing) to years (part aging). A good understanding of what drives these deformations and the ability to model foam behavior is essential to enable production of parts with tight dimensional tolerances that remain acceptable over time. In this talk, we present a computational modeling platform that predicts shape change of foam parts from birth to thirty years of service. The model is based on new experimental observations of aging mechanisms in polyurethane foams, which include water uptake-based swelling/deswelling and water reactions with isocyanate that releases carbon dioxide gas and leads to shrinkage over long time scales (years), complementing our work on modeling foaming, curing, and manufacturing warpage during polymerization and cool down. A new theoretical representation of the solid foam matrix constitutive behavior that couples water uptake and chemical species evolution with strain is developed. This model is based on a nonlinear viscoelastic formalism developed for manufacturing with the additional solution fields of water concentration and post-cure chemical reaction extent. Computational implementation uses the finite element method with an arbitrary Eulerian/Lagrangian representation of the transport phenomena including energy conservation and reaction kinetics that is loosely coupled with the Lagrangian momentum balance. The model is calibrated using small-scale fiber Bragg gratings embedded in cylindrical polymer parts. The model is then used to predict long-term aging behavior and shape changes of a complex foam part that requires over 2 million elements to resolve.

### Bio:

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 130 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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