522f An Integrated Framework for the Computer-Aided Design of Engineering Rubbers

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The process of designing materials possessing desired engineering properties is an important endeavor with significant industrial benefits. Sulfur vulcanized rubber is a major industrial material with diverse engineering applications due to its unique combination of physical properties. A formulated engineering rubber is a complex mixture of several components that are involved in the vulcanization reactions. The life-performance of a rubber part is determined in a complex, coupled manner by vulcanization kinetics, part shape, thermal histories during part manufacture and service, and mechanical loading. The design challenge is then to appropriately adjust these features of the formulation chemistry, part geometry and manufacturing process to achieve the desired performance for a given end-use application. Due to this inherent complexity, the design process has traditionally been a heuristic, trial-and-error procedure which is, often time-consuming and expensive.

We propose a computer-aided design framework for the simultaneous formulation and part design driven by a fundamental understanding of the system. The framework requires the solution of two sub-problems: (1) the forward problem involving the prediction of the life-performance of the part given the starting formulation, processing details and service environment, and (2) the inverse problem, concerning the identification of the appropriate formulation, part shape and manufacturing conditions, given the desired part performance.

A complete forward model for part manufacture is currently under development. Our manufacturing model, integrates a transient heat conduction model, which describes the spatially heterogeneous temperature field in the part at the end of manufacture, with the kinetic model, which predicts the crosslink density profile in the part based on the local thermal history. After manufacture, the part is placed in active service, where it can experience a complex deformation field. The non-linear viscoelastic behavior of filled rubbers can lead to considerable heat buildup due to viscous dissipation, such that a significant spatially heterogeneous temperature field can result, affecting further vulcanization. A non-linear viscoelastic constitutive model has been implemented using Abaqus to describe the mechanical behavior of rubber part under sinusoidal loading. The energy dissipated per deformation cycle from this model, is then combined with the transient heat conduction model, to obtain the temperature rise due to viscous dissipation after a specified number of cycles. The resulting temperature field is then used with the full kinetic model to characterize the long term performance of the part expressed in terms of the evolution of crosslink density, or equivalently, modulus evolution with time. Now that a complete working forward model has been developed, inverse methods can then be used to design chemical formulations and part shapes for a particular engineering application.