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PHYSICS AND CHEMISTRY-BASED PHASE-FIELD CONSTITUTIVE FRAMEWORK FOR THERMO-CHEMICALLY AGED ELASTOMER

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ABSTRACT

We propose a novel physics and chemistry-based constitutive framework to predict stress and brittle failure responses in thermo-chemically aged elastomers. Aging at high temperatures, especially in the presence of oxygen, induces chemical reactions causing significant changes in the elastomer's macromolecular network. Our work uniquely connects the evolution of the macromolecular network, namely effective crosslink density in this case, to the elastomer's mechanical properties. Using Arruda-Boyce hyperelastic constitutive equations and a phase-field approach, we predict stress-strain responses and brittle failure due to aging. Four material properties in the constitutive equations evolve with aging and capture its detrimental effects. These properties are characterized by changes in effective crosslink density based on chemical tests. The framework is analytically solved for uniaxial tension, demonstrating interconnections between material properties. It is then numerically implemented in Abaqus, validated against experimental results, confirming its accuracy.

Additionally, we address the computational cost issue in current phase-field algorithms, particularly the staggered solution scheme. This scheme requires small time increments for crack advancement, resulting in elevated computational costs. In our study, we compare two solution strategies: the quasi-Newton Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS) and the full Newton-based alternating minimization (AM/staggered) algorithm. Our analysis demonstrates that the BFGS algorithm is a more efficient alternative to the traditional AM/staggered approach for solving large-deformation solid-mechanics-phase-field problems. This finding suggests that the BFGS algorithm can significantly reduce computational costs while maintaining the accuracy and robustness of the phase-field method in predicting crack propagation in hyperelastic materials.