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Data-Driven Discovery of Thermodynamically Admissible Dissipation Potentials via Convexity-Preserving Symbolic Regression

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Abstract

Identifying dissipation potentials from experimental data remains a central challenge in rate-dependent constitutive modeling. Within the generalized standard materials framework, the dual dissipation potential $\varphi^*(A)$ governs internal variable evolution via the gradient flow $\dot{z} = \partial\varphi^*/\partial A$, where thermodynamic admissibility requires φ^* to be convex and non-negative. We develop a grammar-based symbolic regression methodology that enforces these constraints by construction rather than through penalty functions. The composition-extended grammar combines convex primitives—including quadratic, power-law, and hyperbolic terms—through operations proven to preserve convexity: positive scaling, summation, and composition of convex non-decreasing outer functions with convex non-negative inner functions. Genetic programming explores this thermodynamically constrained hypothesis space, with bounded L-BFGS-B optimization tuning coefficients and exponents at each generation. Fitness evaluation employs trajectory rollout of the evolution law, comparing predicted and measured storage/loss moduli under sinusoidal loading. Monte Carlo validation on synthetic generalized Maxwell data demonstrates near-exact recovery of Newtonian viscosity (100% success) and cubic power-law dissipation (97.8% success) across noise configurations combining Ornstein–Uhlenbeck process perturbations and Gaussian measurement noise. The framework is further validated on dynamic mechanical analysis measurements of carbon black-filled rubber. All discovered potentials are guaranteed thermodynamically admissible, enabling direct deployment in implicit finite element solvers without post-hoc verification.

Keywords:

symbolic regression dissipation potential Viscoelasticity Generalized standard materials