Entropy Reduced Time Non-Linear Viscoelastic Model

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Plastic and rubber are notoriously difficult to simulate, because their viscoelastic mechanical properties change with time, temperature and environment. Psylotech's polymer FEA solution combines mechanics, thermodynamics, materials science and heat & mass transfer. To understand our entropy reduced time (ERT) model, first consider polymers at atomic length scales (Figure 1), where microstructure is an entanglement of long chain carbon backbone molecules. Consider how macroscopic stress affects this entanglement in the context of the glass transition temperature (Tg):

Glassy below Tg: the material is purely elastic with no hysteresis; interlocked entanglements transfer mechanical stress directly to inter-atomic bonds within chains.

Viscoelastic Transition through Tg: Thermal expansion increases the space around the chains (*a.k.a.* "Free Volume"). As entanglements disengage, chains slide passed each other, causing internal friction. Detangling means less load carried by inter-atomic bonds.

Rubbery or Melt above Tg: Free Volume replaces interlocked entanglements. In thermoplastics, the material melts and flows. In thermosets, cross-links carry stress. In elastomers, entropic elasticity carries stress; deformation aligns chains and the 2^{nd} Law drive to maximize randomness causes macro-scale elasticity.

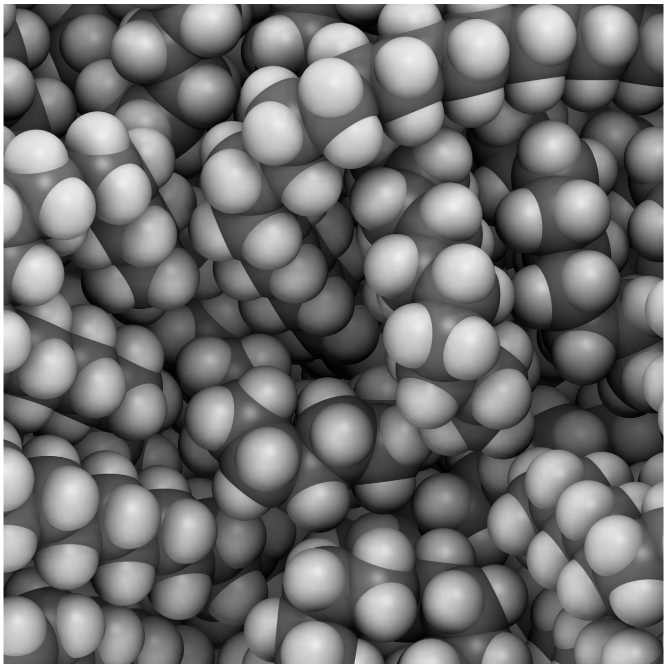

Figure 1: *Entangled polyethylene molecule chains on the atomic level.*

Temperature dependence can be transformed into time dependence through time-temperature superposition (TTS). Mathematically, TTS is a form of reduced time, meaning modulus is a function of time, and time is a function of temperature. Psylotech's ERT replaces temperature with entropy. Modulus is still a function of time, but now time is a function of entropy.

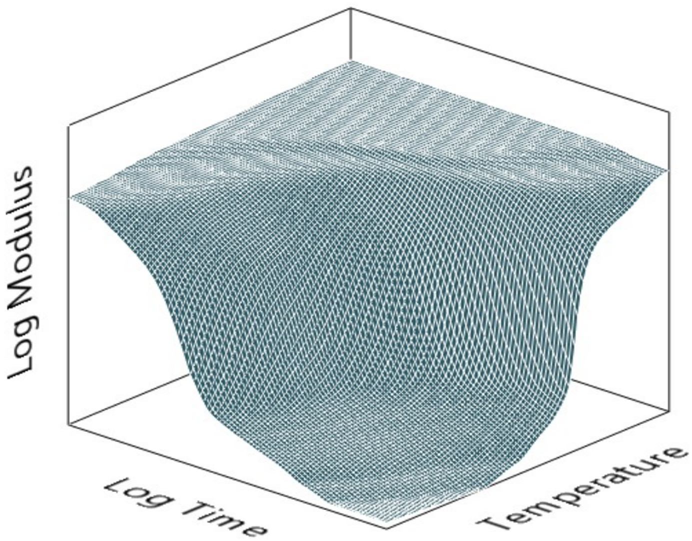

Figure 2: *Experimental data from Psylotech's contract test: Modulus vs. Time & Temperature Master Surface*

Entropy provides a unifying parameter to define the glassy, rubbery and viscoelastic states. At each FEA time step, Psylotech's ERT tracks entropy change from large deformation, temperature and pressure. The ERT incorporates heat transfer from viscous dampening, entropic elasticity, and external boundary conditions. Grounded in thermodynamics, ERT also accommodates solvent absorption, chemical aging and damage.

Reduced time models require the full 3D viscoelastic material property matrix. Psylotech produces this data on a novel, proprietary instrument. Instead of master curves normally associated with TTS, Psylotech produces master surfaces of moduli as functions of time and temperature (Figure 2).

As an example result, consider the analysis of an Ashland polyurethane adhesive, published in Arzoumanidis & Liechti, 2003. In that work, the displacement controlled load/unload/reload ramp test was the most difficult to simulate for the shear modified Free Volume reduced time model. In particular, Free Volume is not able to capture the steep drop in stress during unloading. Replacing Free Volume with Entropy produces much better agreement.

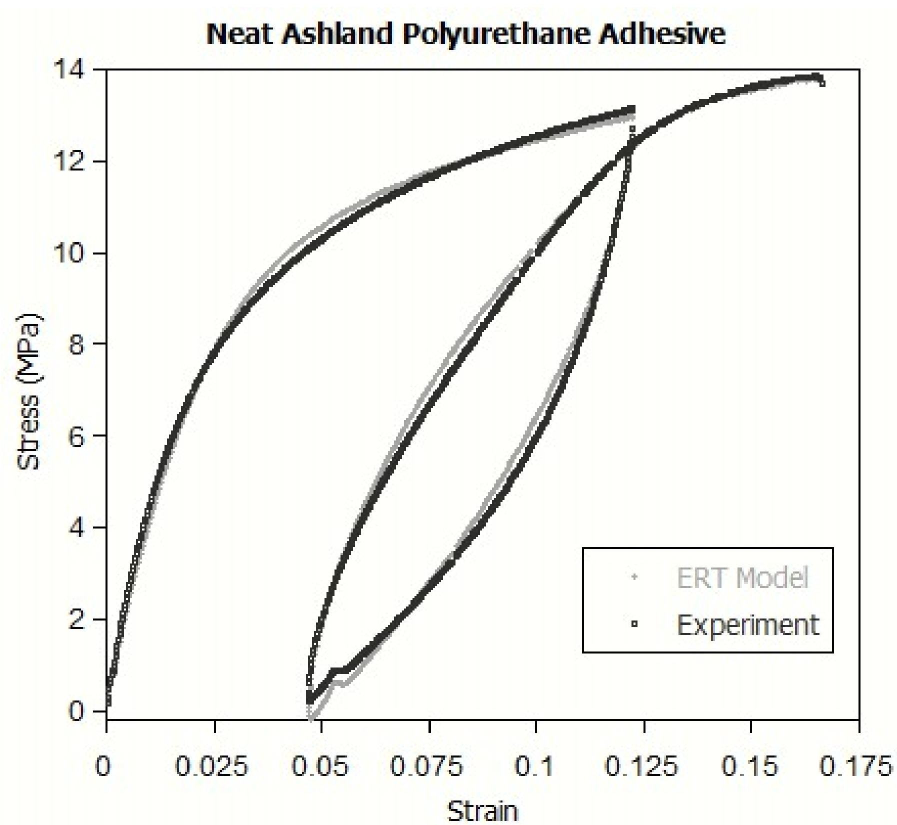

Figure 3: *ERT model compared to experiment for load-unload-load displacement controlled ramp. Unloading is particularly difficult to simulate.*

Psylotech's Entropy Reduced Time model builds on decades of development in the technical literature. Reduced time has been shown to effectively simulate temperature, pressure, large deformation, solvent absorption and even damage. Users need not be experts in polymer physics to implement this advanced nonlinear viscoelastic simulation solution. Psylotech provides data and software needed for companies to quickly and cost-effectively benefit add value to their current simulation process. Psylotech provides **1/**contract testing services to produce the data and **2/**a UMAT for ABAQUS.