K-Load: Thermal + Hydrolysis Aging

Case Study:

Predicting Relaxation and Shelf-Life of NBR Elastomers in Air/Oil Environment

Elastomer seals, gaskets, and packaging components often fail not by sudden fracture but by gradual loss of relaxation strength during service. This directly impacts shelf-life, storage stability, and long-term reliability across pharma, food, automotive, aerospace, and oil & gas.

K-Load Digital twin provides a powerful framework for predicting the long-term behavior of polymers by combining accelerated test data with physics-informed machine learning. In K-Load, the digital twin is established through five stages:
(1) experimental data acquisition,
(2) input and consistency checks,
(3) fine-tuning with material knowledge,
(4) post-processing and simulation, and
(5) output generation.

Valid for a Material Family

Once built, the digital twin is not limited to a single specimen; it is transferable across a material family, meaning a twin trained on one representative elastomer can be rapidly adapted to other formulations in the same class.

Minimized Training Data

A key advantage is the minimal training data requirement. For this study, the model was trained using only three relaxation datasets: 20% relaxation in air at 60 °C, 50% relaxation in air at 100 °C, and 25% relaxation in oil at 60 °C. Despite this small input, the model achieved high accuracy in predicting stress relaxation and constitutive behavior under a wide range of conditions: temperatures (60–100 °C), pre-stretch levels (20–50%), and surrounding media (air vs. oil).

Couple Theories & Computation

Beyond isolated stressors, the model allows coupling of multiple degradation pathways, such as thermal oxidation with hydrolysis, enabling reliable predictions of oil-induced aging. This capability provides a foundation for robust shelf-life and survivability assessments across industries.

K-Load with the Relaxation & DLO Modules provides a validated framework to simulate how materials lose integrity under thermal, chemical, and environmental exposures.

Stage 1: Experimental Data

- Continuous Relaxation Tests in air/oil at 60–100 °C were used to age samples.
- Three constitutive stress–relaxations curves were taken from [1,2] to train the model

- 20% relaxation (air, 60 °C)
- 50% relaxation (air, 100 °C)
- 25% relaxation (oil, 60 °C)
- - Validated for elastomers, adhesives, encapsulants, epoxies, and thin films.

CSV

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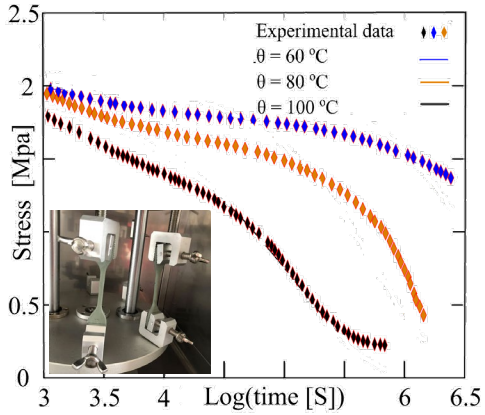

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1. Johlitz et al. 2014 International Journal of Plasticity 63
2. Musil et al. 2020 Continuum Mech. Thermodyn. 32,369

Stage 2: Data Input & Consistency Check

- Import accelerated test datasets in CSV/Excel.
- Normalize engineering stress P11 to initial stress.
- Outliers removed, master relaxation curves generated.
- Network shrinkage artifacts at 100 °C identified and filtered.

Stage 3: Fine-Tuning with Material Knowledge

- Model Trained based on the three curves provided.
- Incorporates oxidation kinetics, filler reinforcement, crosslink scission.
- Implemented in FE software and validated with tensile & tension set tests.
- Utilizes literature-based models for chain scission, free-volume evolution, and decay functions.
- Merges experimental data with polymer physics in a hybrid engine.

Relevance: For larger components, Diffusion-Limited Oxidation (DLO) must be considered → K-Load DLO module developed for heterogeneous oxidation (oxygen supply vs consumption imbalance).

Stage 4: Post-Processing & Simulation

4A. Thermal-Aging (air) baseline.
We first calibrate the thermal oxidation pathway using the air datasets (e.g., 20% @ 60 °C and 50% @ 100 °C). The model identifies the oxidative kinetics and shift laws—activation energy Ea, and the network-decay/relaxation coupling (e.g.,scission/crosslink terms). This yields master relaxation curves and checks DLO risk (oxygen supply vs. consumption). The thermal parameters are then frozen.

4B. Oil Infiltration via hydrolysis. We then retrain only the hydrolysis/solvent-ingress module using the oil dataset (e.g., 25% @ 60 °C), assuming non-corrosive oil (no additional chemical scission beyond ingress/plasticization). Parameters fitted: diffusion coefficient such as swelling/plasticization coefficient , and relaxation-time scaling with volume fraction ϕ. Oxidative kinetics from 4A remain fixed, so the oil prediction is a thermal + ingress superposition, not a new chemistry.

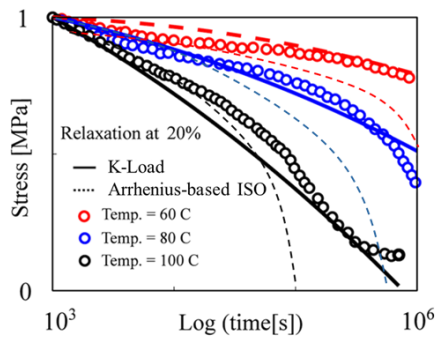
4C. Extrapolation & outputs.
With the two modules coupled, K-Load predicts relaxation and constitutive response across new conditions—air/oil, T={60,80,100}∘C, and pre-stretch levels {20,35,50}%—producing shelf-life curves, retention maps, and service envelopes.

4D. Higher-fidelity media.
Extending to brine, H_2S, fuels, blends adds reactive terms (e.g., hydrolysis/sulfidation kinetics, multi-species diffusion, salinity/pH effects). That fidelity requires more experimental inputs: at least 3–4 medium-specific datasets (sorption/mass change, FTIR/chemistry markers, relaxation/tension-set) plus one temperature sweep to pin down K, and reaction rates.

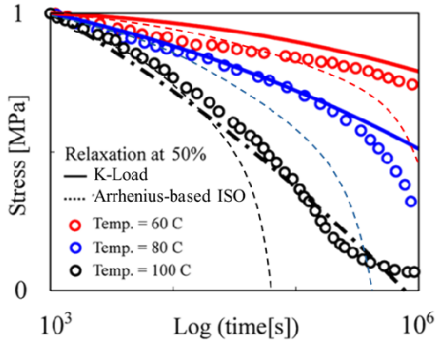
Stage 5: Output Data Generation

- Produces modulus–time plots, relaxation curves, and stress–strain envelopes.
- Multi-format export: Excel spreadsheets, CSV/JSON databases, PDF reports.
- API-ready outputs: tangent stiffness matrices for Abaqus, Ansys, COMSOL.
- Applications: (Oil & Gas): HPHT seals exposed to brine/H_2S. (Pharma/Food) Packaging/seals Shelf-life, (Automotive/Aerospace) Stress relaxation of gaskets, vibration isolators. (Energy): Cable insulation & O-rings in nuclear/renewables.

RELAXATION Air at ε= 20%



RELAXATION Air at ε= 50%



RELAXATION Oil at ε= 20%