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Finite-strain Thermomechanics of Viscoelastic-Viscoplastic Model for Thermoplastic Polymers

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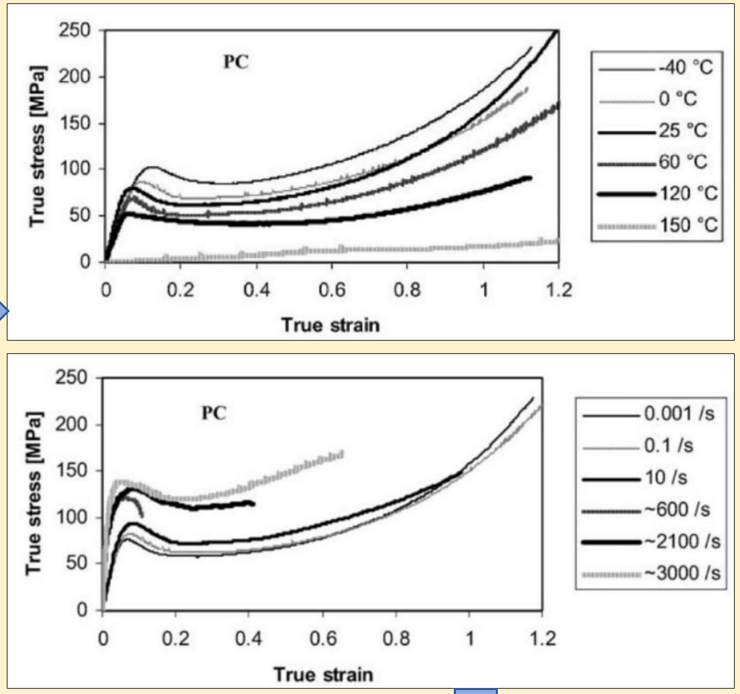
Introduction

Motivation

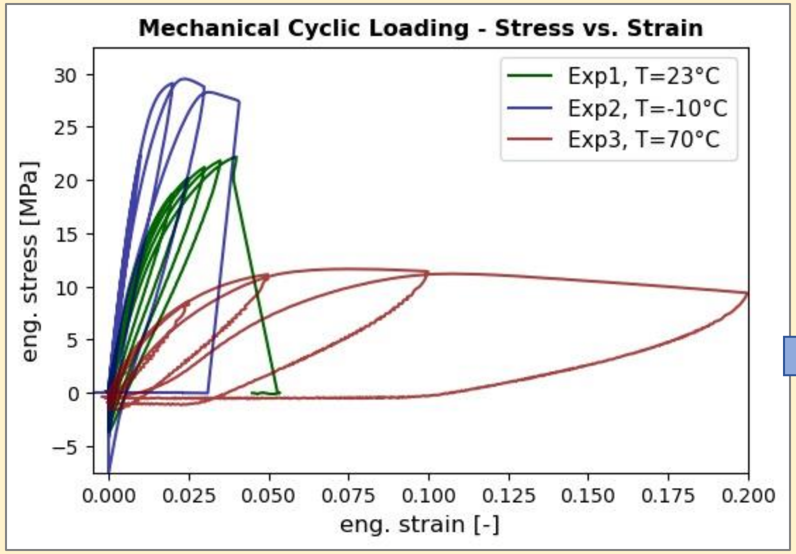
- Thermoplastic composites with remolding capabilities [1 Burgoa 2023]
- High mechanical loads and temperatures (~200 ◦C)
- **Need for a finite strain thermoviscomechanical model for polymers - Geometric and Material nonlinearities!**

Literature



Uniaxial compression or polycarbonate (PC) at strain rate of $0.01s^{-1}$ (top) and temperature of 25 ̊C (bottom) [2 Richeton 2006].

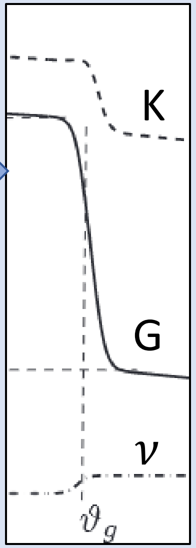
Experimental Data



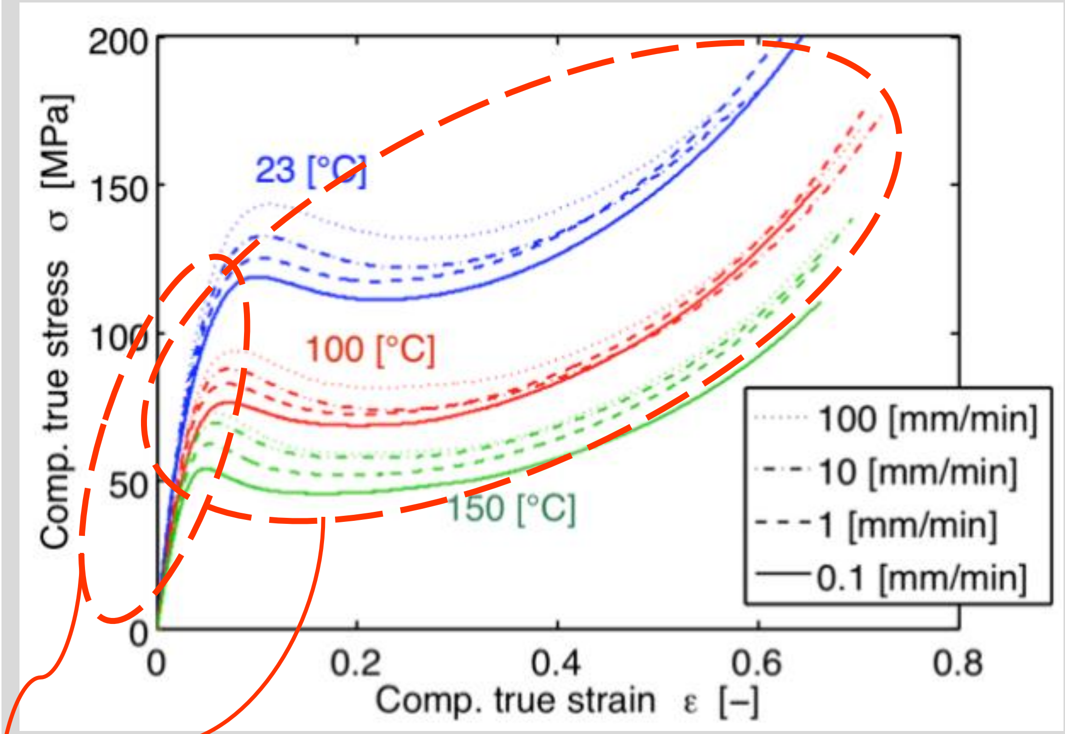
Cyclic Loading Experiments
(Provided by Experimental Partner - Leartiker)

Modelling Requirements

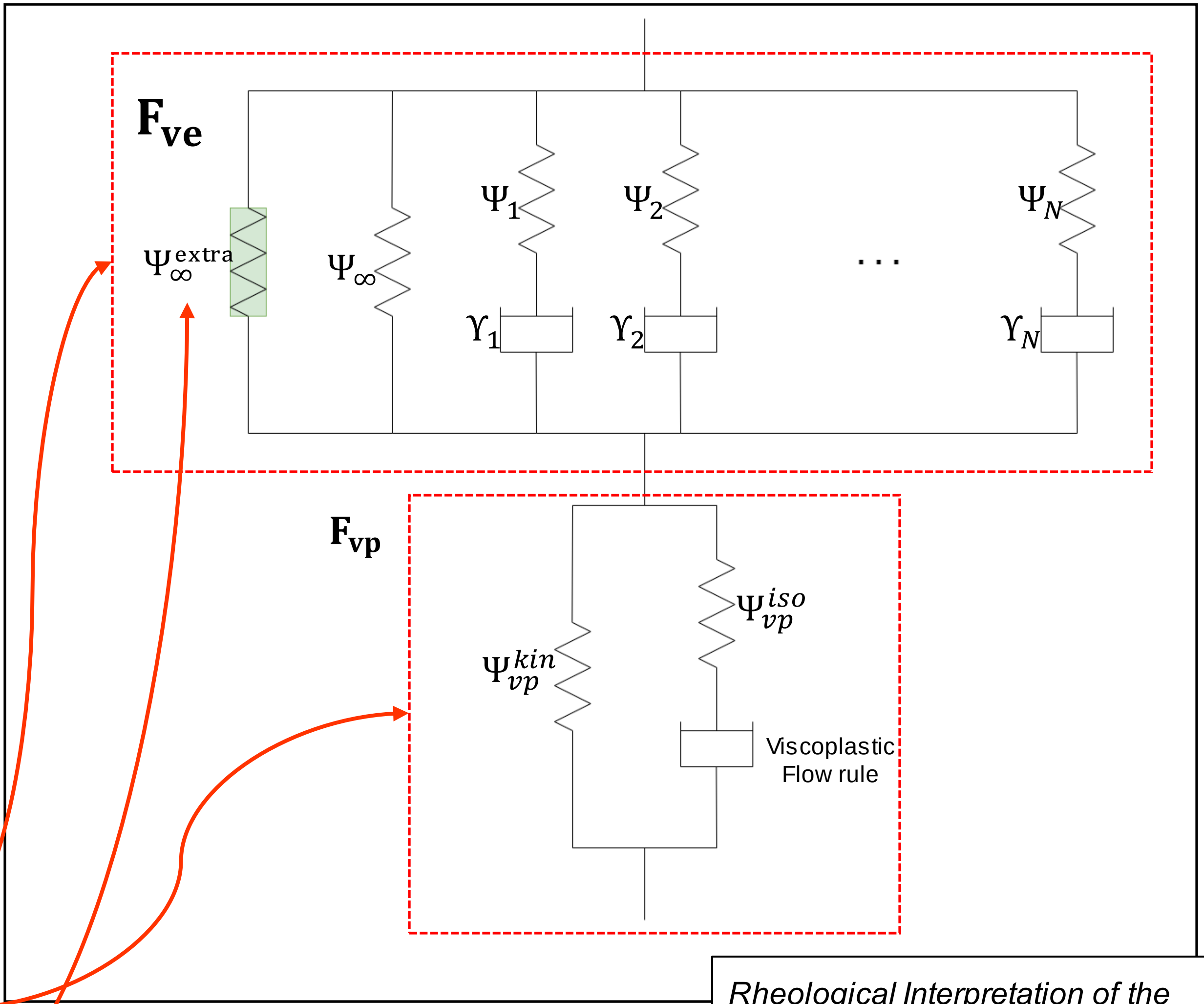
- Adaptability to high strain rates
- Glass Transition Phenomena (Glass <-> Rubber)
  - Steep decline in material moduli and strengths
  - Range of temperatures
  - Variable Tg range
- Material dependency
  - Calibration -> Experiments



Generalised Thermo(visco)mechanics



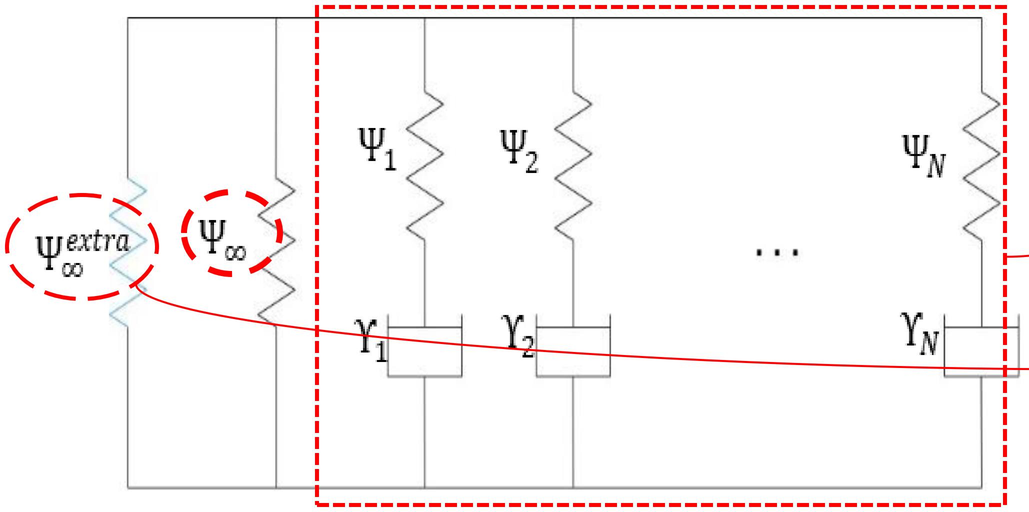
Compression Tests on RTM6 Epoxy [3 morelle 2017]



Rheological Interpretation of the Constitutive Model

- Thermo(Visco)Elasticity (TVE) – Maxwell Model + TTSP
- Thermo(Visco)Plasticity (TVP) – Power Law YF + Perzyna Flow
- Additional Effects – Elastic Hardening [4 Srivatsava 2010]

Thermo(Visco)Elastic Model



Generalised Maxwell model

- Hookean Hyperelastic term (ψ_∞) - Bilogarithmic in <u>logarithmic strain tensor</u> ($\mathbf{E_e}$) .

$$\mathbf{E}_e = \frac{1}{2} \ln \mathbf{C}_e$$

- Hookean Viscoelastic Free Energy (ψ_{ve}) – Bilogarithmic in log strain tensor ($\mathbf{E_e}$) and internal variable tensor ($\mathbf{\Gamma}_i$).

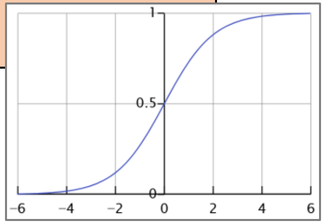
$$\psi_{ve} = \psi_{ve}(\mathbf{E}_e, T, \mathbf{\Gamma}_i)$$

- Consistent Corotational Kirchhoff stress ($\boldsymbol{\tau}$) in volumetric and deviatoric terms.

$$\frac{1}{3} \operatorname{tr} \boldsymbol{\tau}_e = K_\infty (1 + a) \operatorname{tr} \mathbf{E}_e - 3K_\infty \alpha_\infty (T - T_0) + \sum_{i=1}^{N_i} K_i \operatorname{tr} (\mathbf{E}_e - \mathbf{\Gamma}_i)$$

$$\operatorname{dev} \boldsymbol{\tau}_e = G_\infty (1 + b) \operatorname{dev} \mathbf{E}_e + \sum_{i=1}^{N_i} G_i \operatorname{dev} (\mathbf{E}_e - \mathbf{\Gamma}_i)$$

- Hyperelastic extra branch (ψ_∞^{extra}) -> a and b scalars as <u>sigmoid functions</u> of the log strain.



ODEs for internal variable ($\mathbf{\Gamma}_i$). To solve for $\mathbf{\Gamma}_i$ using **TTSP**!

$$\dot{\mathbf{\Gamma}}_i = f(\mathbf{E}_e, \mathbf{\Gamma}_i, k_i, g_i)$$

Assuming, k_i = g_i and constant Poisson's ratio.

TVE - Time Temperature Superposition Principle (TTSP)

- Convolution Integrals for stress.

$$\frac{1}{3}\,\mathrm{tr}\,\boldsymbol{\tau}_e = K_\infty (1 + a)\,\mathrm{tr}\,\mathbf{E}_e - 3K_\infty \alpha_\infty (T - T_0) + \ldots$$
$$\ldots + \sum_{i=1}^{N} K_i \int_{0^+}^{t} \exp\left(-\frac{(t-s)}{k_i}\right) \frac{d}{ds}\left[\mathrm{tr}\,\mathbf{E}_e(s)\right] ds$$

- Solution with recursive addition for previous time steps.

$$\frac{1}{3}\,\mathrm{tr}\,\boldsymbol{\tau}_e = (aK_\infty + K_e)\,\mathrm{tr}\,\mathbf{E}_e - 3K_\infty\alpha_\infty (T - T_0) - \ldots$$
$$\ldots - (K_e - K_\infty)\left[\mathrm{tr}\,\mathbf{E}_e^n\right] + \sum_{i=1}^{N} B_i^n \exp\left(-\frac{\Delta t}{k_i}\right)$$
$$\text{where,}\quad K_e = K_\infty + \sum_{i=1}^{N} K_i \exp\left(-\frac{\Delta t}{2k_i}\right)$$

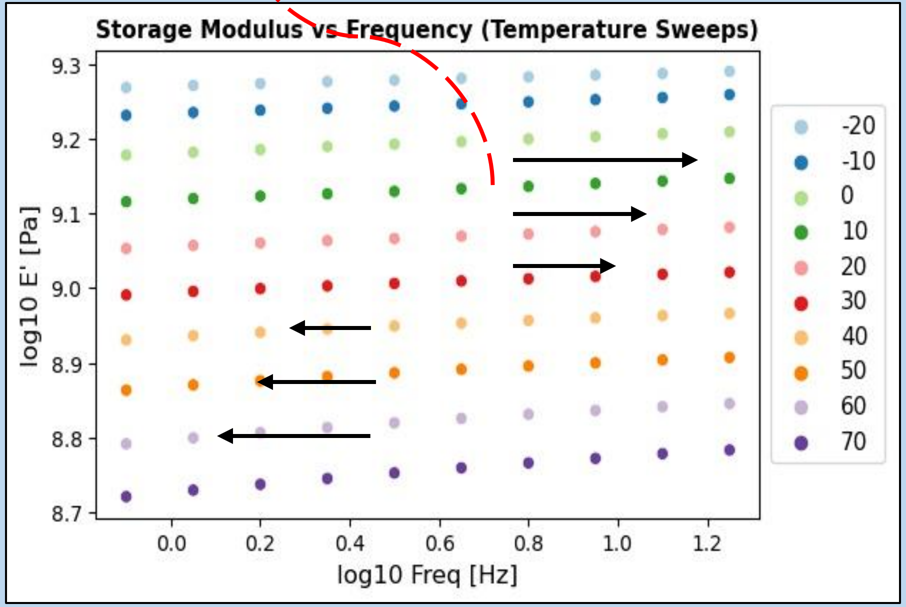
Integrations are instead performed in material time -> shifted laboratory time. Implemented using TTSP.

- Stress relaxation in shifted laboratory time.

$$\Delta t_n^* = \int_{t_n}^{t_{n+1}} \frac{1}{a_T(\epsilon)} d\epsilon$$

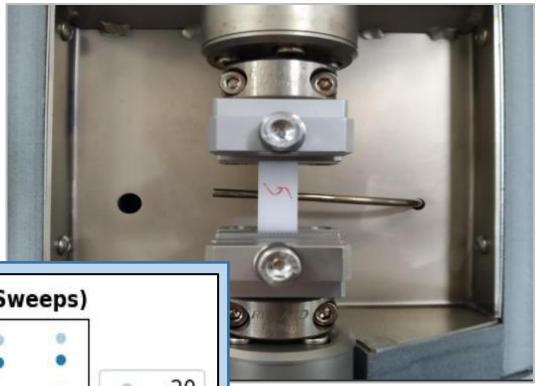
- WLF Shift Factor (a_T), T_{ref} is taken a little lower than Tg.

$$a_T = exp\left(-\frac{C_1(T - T_{ref})}{C_2 + T - T_{ref}}\right)$$



Shift factor obtained from DMA.

Experimental Campaign (with Leartiker)

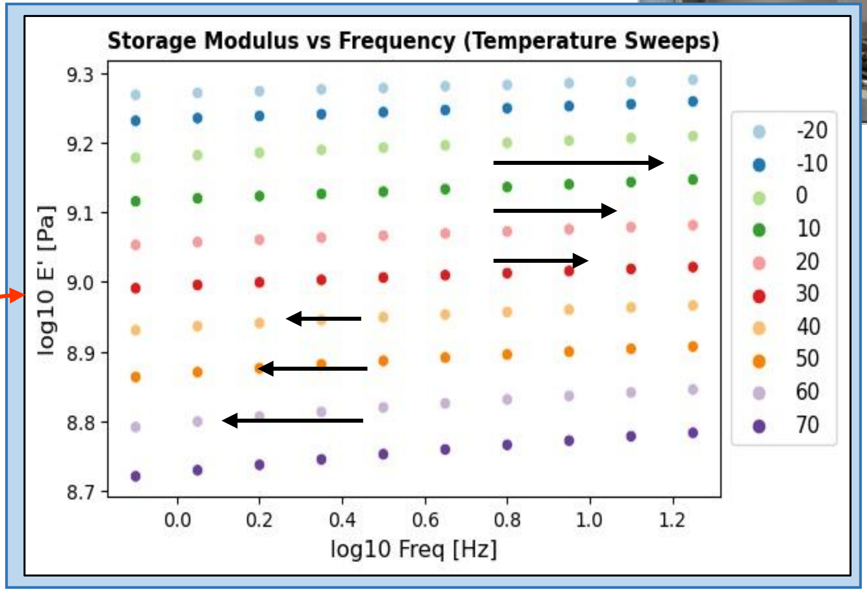


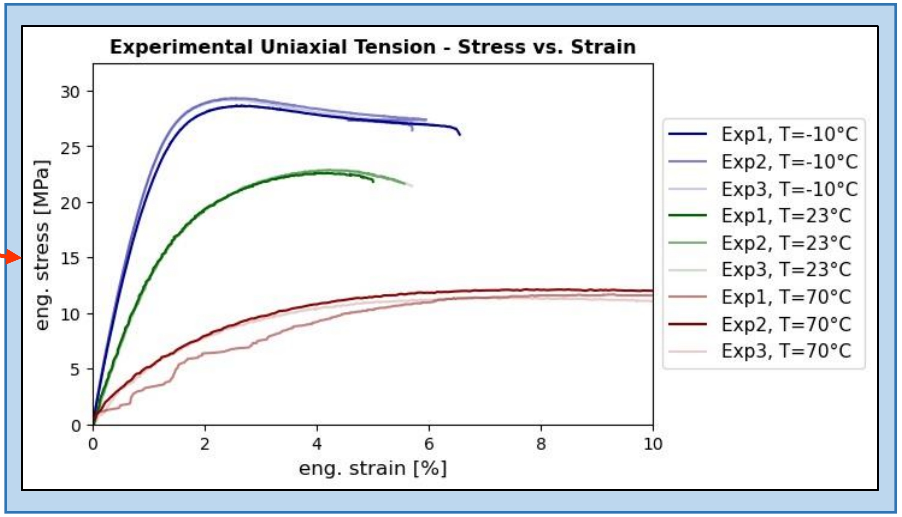
Choice of Polymer – Polypropylene

- Thermoplastic - reversible glass transition, recyclable.
- Stiffer relative to PEs.
- Sufficiently high melting point - broader temperature sweeps into rubbery region.

Planned Experiments

1. DMA Tension Mode - TVE shift factor and relaxation spectrum.
2. QS Tension Tests - Stress strain isotherms for TVP calibration.
3. Thermal Property Tests
   - DSC -> Specific Heat (Cp)
   - TMA -> Coefficient of Thermal Expansion (CTE) – zero/small force
4. QS Compression Tests – Tension-compression asymmetry.
5. Cyclic Loading Tests - Stress strain isothermal cycles at different temperatures.



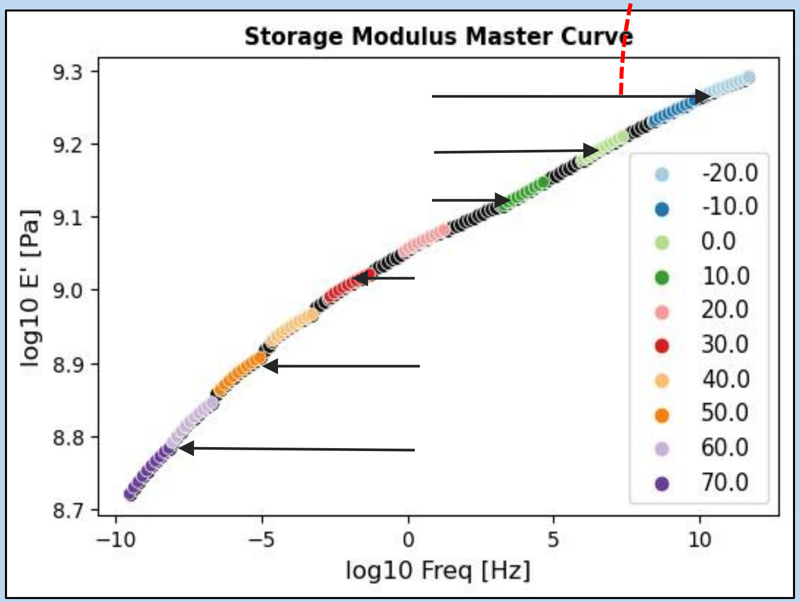


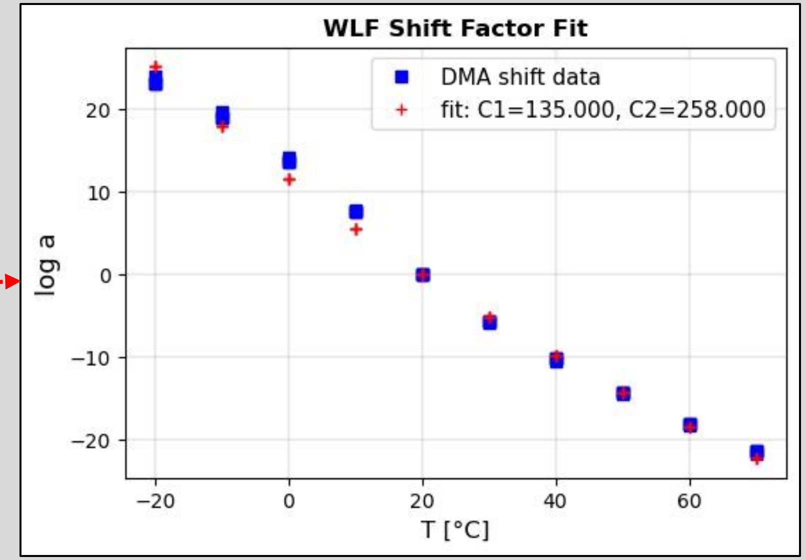
Experimental Data – DMA Tension Mode

Shift factor and Relaxation Spectrum Data from DMA Tension Master Curve

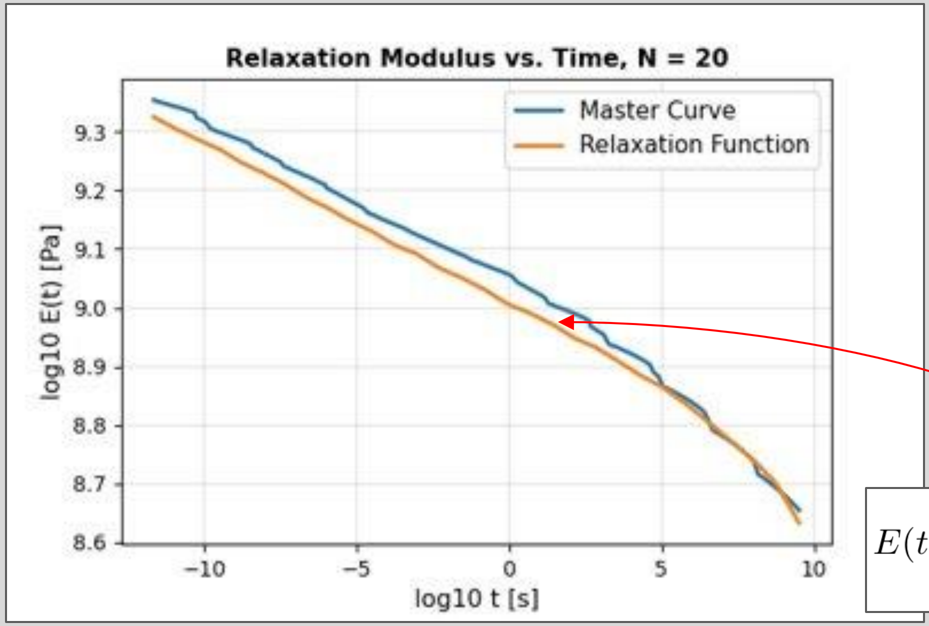
$$E'(\omega, \mathrm{T}) = E'(\mathrm{a_T}\ \omega\ , \mathrm{T_{ref}})$$

where, $\mathrm{T_{ref}}$ is the reference temperature. Rigid shifts in the log-log plot. WLF shift factor calibrated using the above relation.





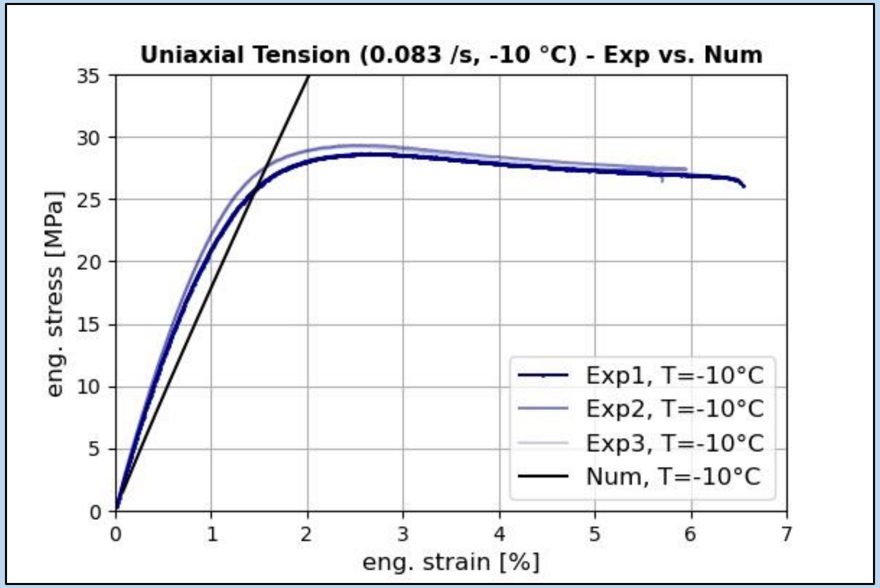
Negative exponential fit of horizontal shifts -> WLF shift factor

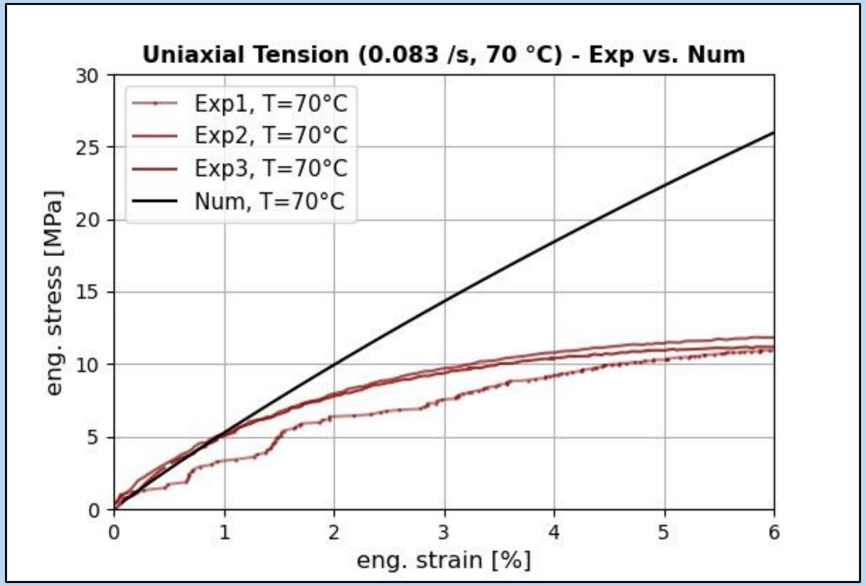


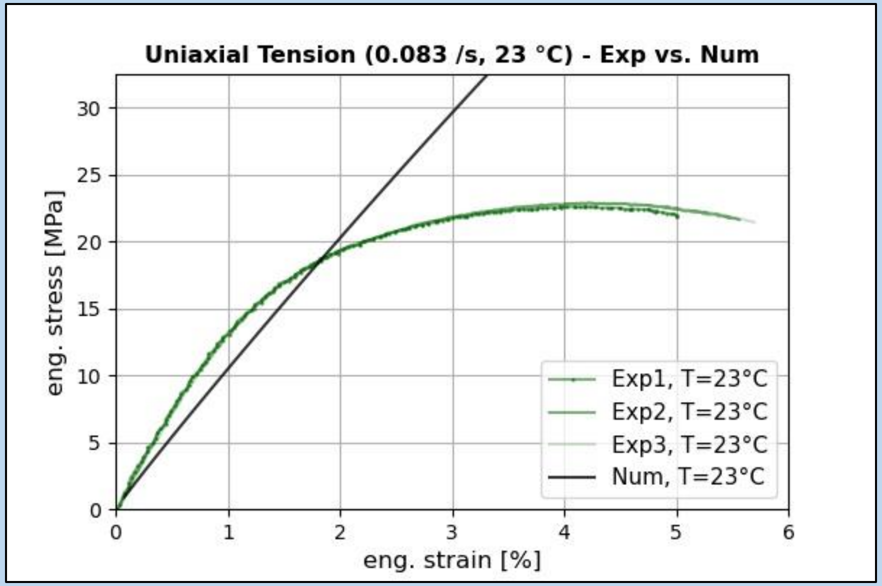
Master Curve data of Storage Modulus-> least squares optimization for 2*N+1 terms in <u>Relaxation Spectrum</u>

$$E(t) = E_\infty + \sum_{(i)} E_i\ \exp(-\frac{t}{\tau_i})$$

TVE Preliminary Results – Uniaxial Tests







- Tg assumed to be ~293 K.
- Possibility to improve the slope using N = 30 terms.
- Over-stiff and linear viscoelasticity at low elongations.

TVP Model Elements

Elements

- <u>Extended Drucker-Prager Power Yield Function</u> ($\bar{F}$) – **pressure dependency,** a_2, a_1, a_0 - functions of tensile and compressive yield strength.

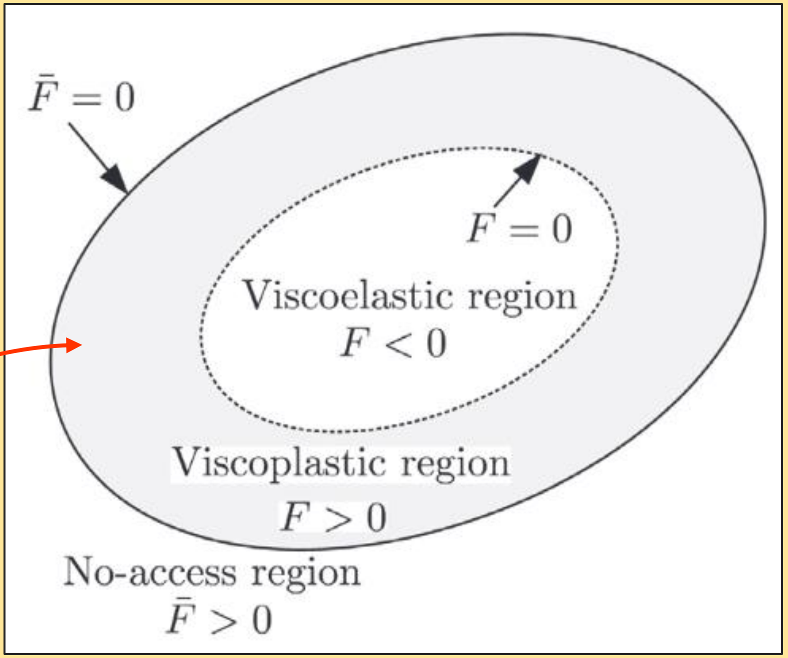
$$\bar{F}(\Gamma, \Delta\gamma, T) = a_2\boldsymbol{\phi}_{\boldsymbol{e}}^{\alpha} - a_1\boldsymbol{\phi}_{\boldsymbol{p}} - a_0 - \left(\eta\frac{\Gamma}{\Delta t}\right)^{p}$$

- <u>Perzyna Flow Rule</u> with temperature-dependent viscosity (η), quadratic plastic potential (P).

$$\mathbf{D}_p = \frac{1}{\eta(T)}\langle \boldsymbol{F}\rangle^{\frac{1}{p}}\frac{\partial P}{\partial \mathbf{M}_e}$$

Flow Normal (**Q**)

- <u>Chaboche NLKH</u> – for backstress.



Extended yield surface with various regimes [5 Nguyen 2016 – Session Wednesday morning A4-206].

Extended yield surface ($\bar{F}$) defined using regular yield surface (F) and <u>viscous (rate-dependent) term.</u>

Temperature Dependency:

Yield strengths, kinematic hardening modulus (H_X) and viscosity (η) scaled with temperature dependent negative exponential functions like WLF shift factor (a_T).

$$\eta(\gamma, T) = a_T(T)\eta(\gamma)$$

TVP – Loss of Commutavity

- Solution to convolution integrals with recursive addition for previous time steps.

$$\frac{1}{3}\operatorname{tr}\boldsymbol{\tau}_e = (aK_\infty + K_e)\operatorname{tr}\mathbf{E}_e - 3K_\infty\alpha_\infty(T - T_0) - \ldots$$
$$\ldots - (K_e - K_\infty)[\operatorname{tr}\mathbf{E}_e^n] + \sum_{i=1}^{N} B_i^n \exp\left(-\frac{\Delta t}{k_i}\right)$$
$$\text{where,} \quad K_e = K_\infty + \sum_{i=1}^{N} K_i \exp\left(-\frac{\Delta t}{2k_i}\right)$$

- Loss of commutativity of corotational Kirchhoff stress ($\boldsymbol{\tau}_e$) with log strain (**$\mathbf{E}_e$**) -> 2nd PK Stress (**$\mathbf{S}_e$**) does not commute with left Cauchy strain (**$\mathbf{C}_e$**) -> Loss of symmetricity of Mandel Stress (**$\mathbf{M}_e$**)

$$\mathbf{M}_e = \mathbf{C}_e\mathbf{S}_e \neq \mathbf{S}_e\mathbf{C}_e$$

- Loss of thermomechanical consistency (δ<0) in finite isotropic plasticity

$$\delta = \underbrace{\mathbf{M}_e : \mathbf{D}_p}_{\text{Plastic Power}} \geq \mathbf{0}$$

Solution: Modified stress measure -> **$\mathbf{S}_e$** and **$\mathbf{C}_e$** commute.

$$\mathbf{S}_e = \boldsymbol{\tau}_e : (\boldsymbol{\mathcal{I}} \cdot \mathbf{C}_e^{-1}) \rightarrow = \frac{1}{2}\left(\boldsymbol{\tau}_e\mathbf{C}_e^{-1} + (\boldsymbol{\tau}_e\mathbf{C}_e^{-1})^T\right)$$

- New Definition of Mandel Stress

$$\mathbf{M}_e = \frac{1}{2}\left(\boldsymbol{\tau}_e + \mathbf{C}_e\boldsymbol{\tau}_e\mathbf{C}_e^{-1}\right)$$

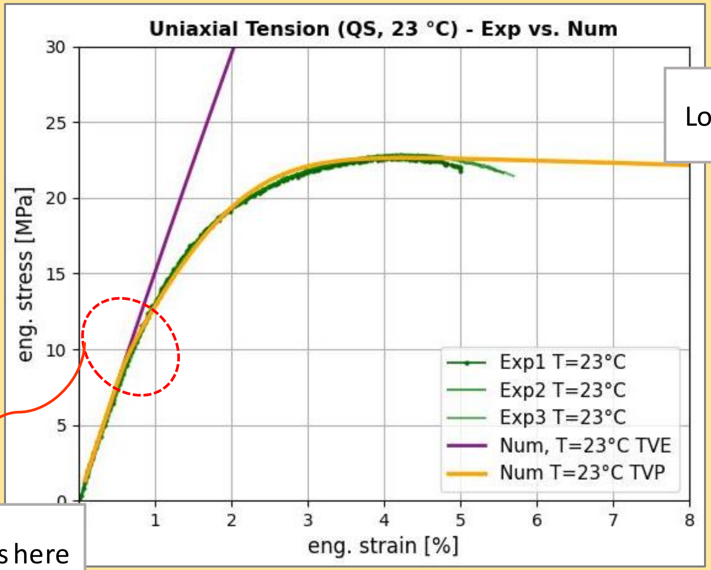
Non-linear Equation of Effective Stress

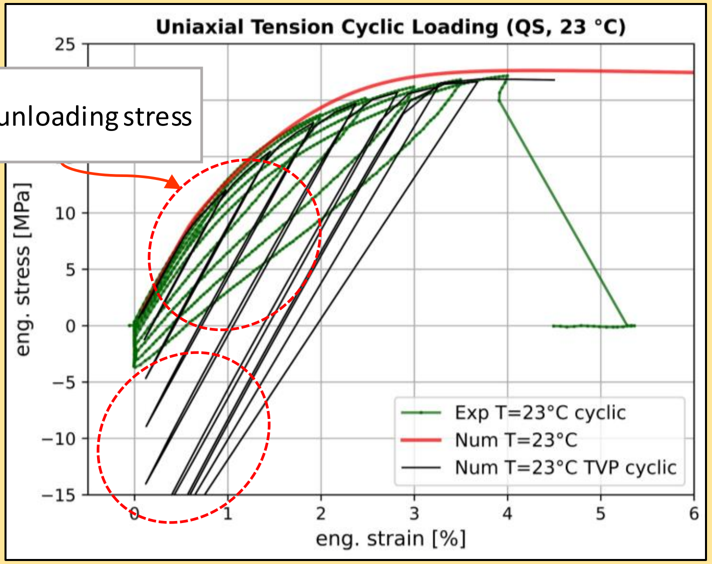
- Resolving commutativity requires implicit solution of effective stress (**$\boldsymbol{\phi}$ = $\mathbf{M}_e$ - $\mathbf{X}$**) –> additional internal Newton-Raphson loop.

$$\phi = \bar{\tau}_\infty + \hat{\phi}^{pr} + \underbrace{\frac{1}{2}\left(\mathbf{C}_e\hat{\boldsymbol{\tau}}_e^{pr}\mathbf{C}_e^{-1} - \mathbf{C}_e^{pr}\hat{\boldsymbol{\tau}}_e^{pr}\mathbf{C}_e^{pr-1}\right)}_{\mathbf{D}(\phi)} - \mathbf{B} - \mathbf{X}_{n+1} + \mathbf{X}_n$$

Where, **B** is the corrector tensor and $\bar{\tau}_\infty$ is the extra-branch stress.

Numerical Results – Significance of Extra Branch

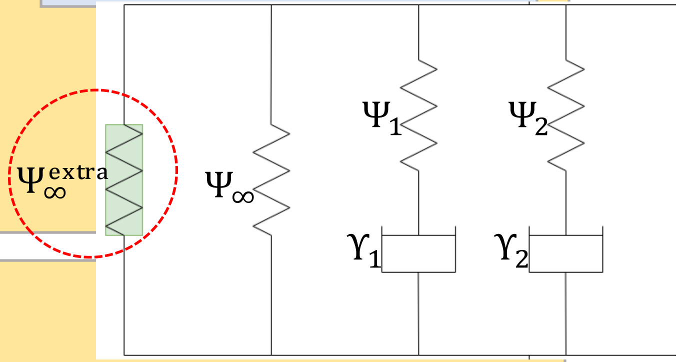


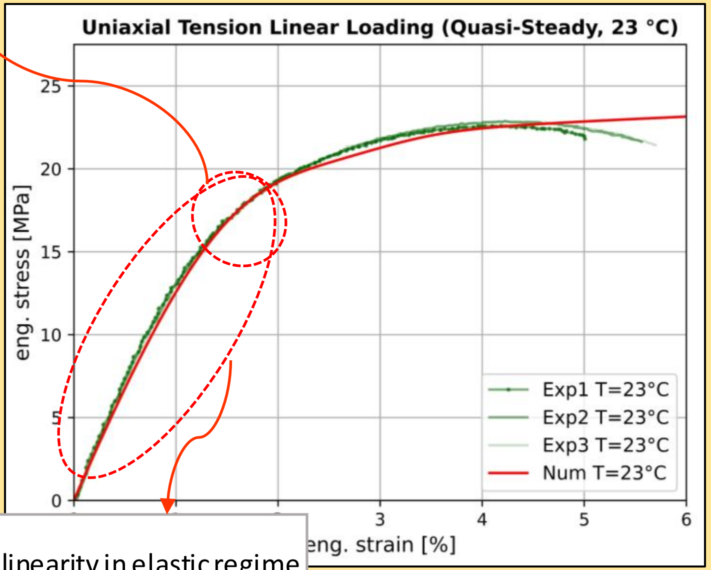


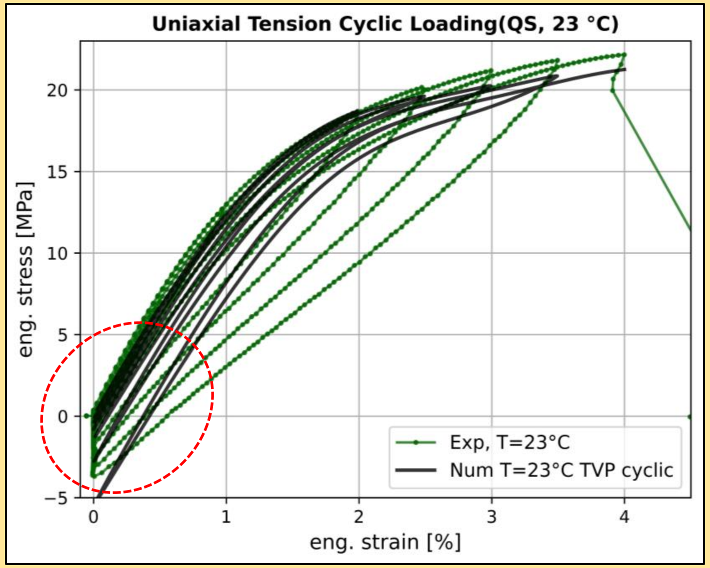
Low unloading stress

Yielding starts here

- Works for Uniaxial loading using TVE+TVP!
- Inaccurate unloading curves in Cyclic loading.
- **Fix using extra branch functionality**!



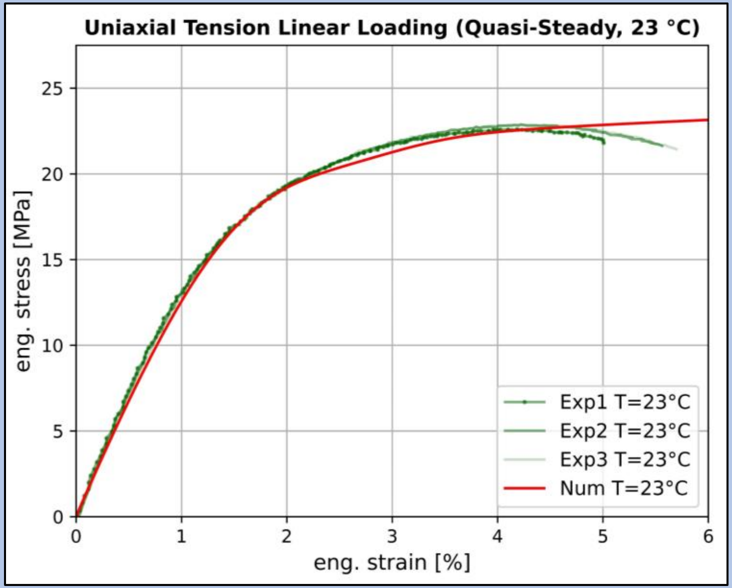


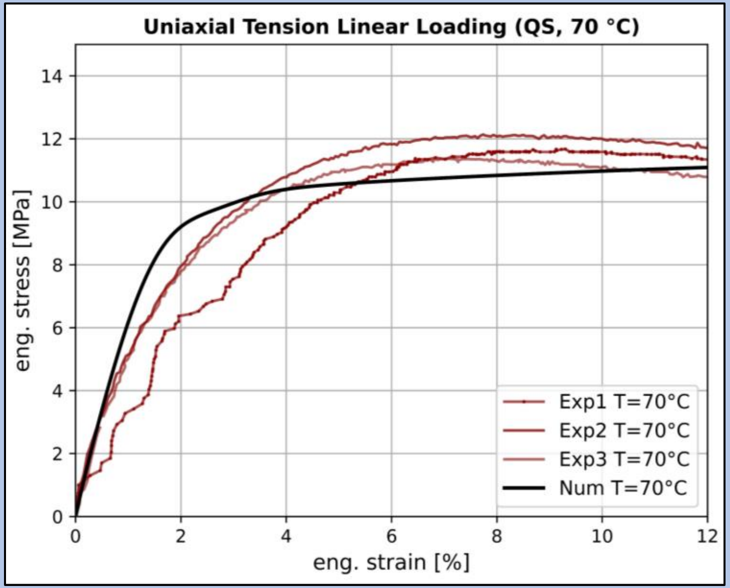


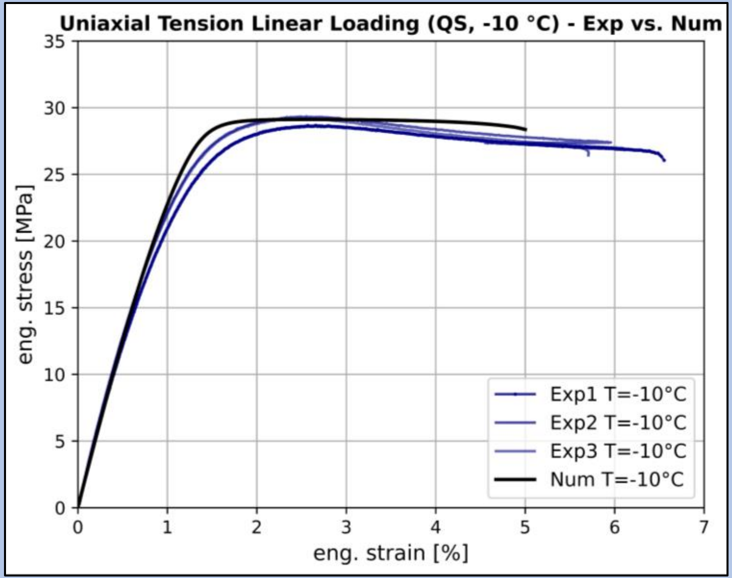
Sigmoid non-linearity in elastic regime

- Better cyclic loading results. Sigmoid non-linearity in the elastic regime

Numerical Results – Extra Branch



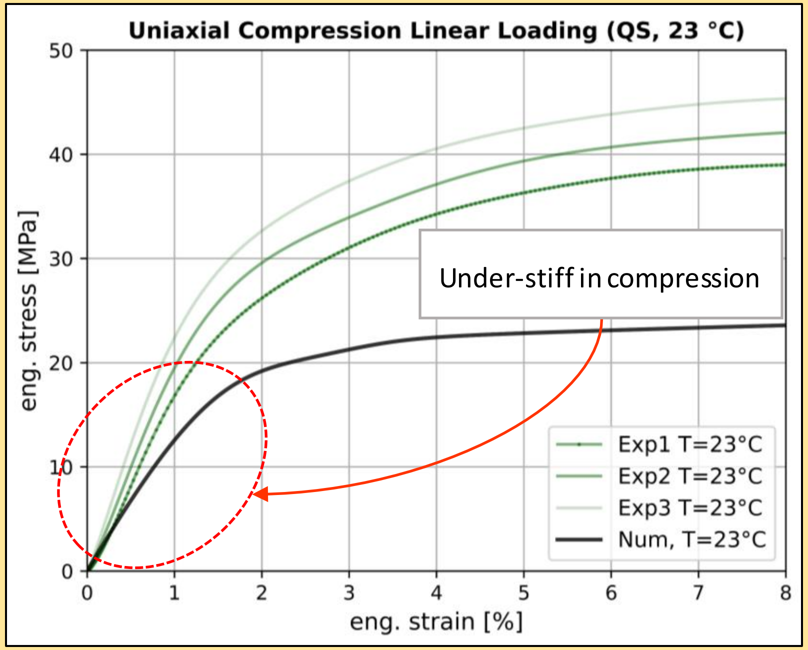




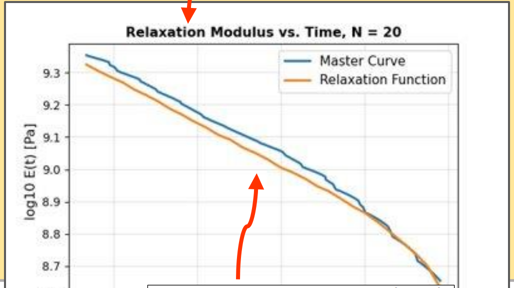
- TVE + sigmoid non-linearity followed by saturated isotropic hardening.
- Good results obtained in linear loading.

Future Developments

Compression Linear Loading



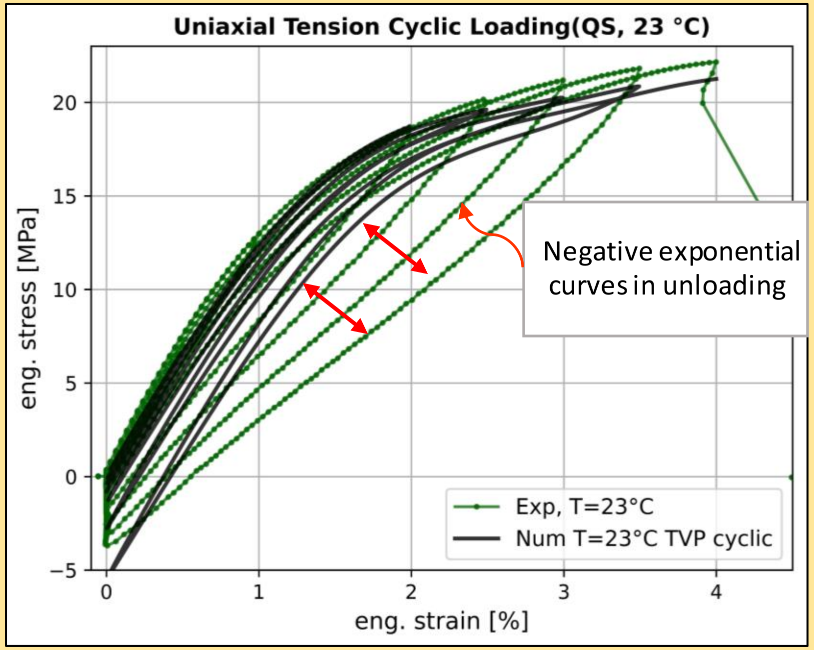
- Compression asymmetry in elastic regime!
- Can be fixed using different bulk and shear relaxation times. Remove assumption of $k_i = g_i$ and variable Poisson's ratio [6 Wu 2023].



$$K(t) = K_\infty + \sum_{(i)} K_i \exp\left(-\frac{t}{k_i}\right)$$

$$G(t) = G_\infty + \sum_{(i)} G_i \exp\left(-\frac{t}{g_i}\right)$$

Mullin's Effect in Unloading



- Mullin's effect to lower the stress in unloading using a damage variable (η -> 1 to η_{min}) functional of deformation energy [7 Ricker 2021].

$$\boldsymbol{\tau}_e = \eta\left(\psi\right)\hat{\boldsymbol{\tau}}_e$$

Thank You for your attention

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Appendix 0 - Mechanical Source

Elements

- Self Heating: Heat generated by elasticity and irreversible processes. Mechanical source is intended as the resulting heat flux.
- TVE: Heat generated by viscoelasticity.
- TVP: Heat generated by plastic power and isotropic hardening.

$$W_m = \underbrace{-\rho_0\, \mathbf{C}_d(T)\,\dot{T}}_{\text{Thermal Source}} + \underbrace{T\frac{\partial}{\partial T}\left(\rho_0 \frac{\partial \Psi}{\partial \mathbf{C}_e}\right) : \dot{\mathbf{C}}_e}_{\text{Gough-Joule Effect}} + \ldots$$

$$\ldots + \underbrace{\rho_0 R}_{\text{Ext. Heat Source}} + \underbrace{\mathbf{P} : \mathbf{F}_e \dot{\mathbf{F}}_p}_{\text{Plastic Power}} - \ldots$$

$$\ldots - \underbrace{\sum_{i=1}^{N_i} \rho_0 \frac{\partial}{\partial \boldsymbol{q}_i} (\Psi + TS) : \dot{\boldsymbol{q}}_i}_{\text{TVE}} + \underbrace{\sum_{j=1}^{N_j} \rho_0 \frac{\partial}{\partial \boldsymbol{\xi}_j} (\Psi + TS) : \dot{\boldsymbol{\xi}}_j}_{\text{TVP}}$$

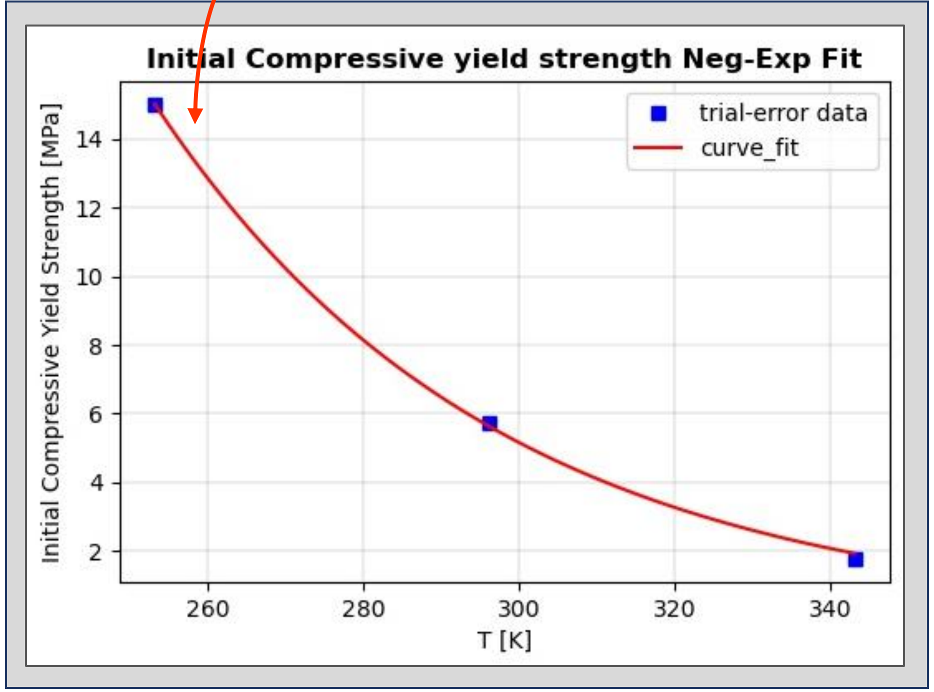
Specialized Definition of Hardening Stress

- Isotropic Hardening Stress (R): Using negative exponential functions for temperature dependency of hardening coefficients.

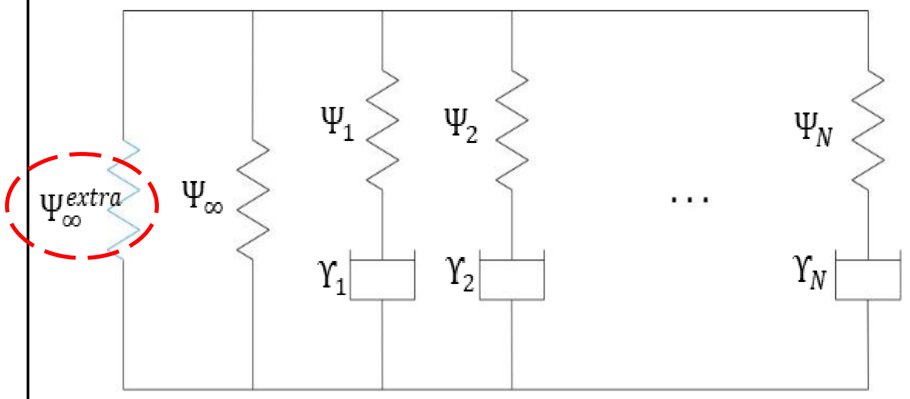
$$R = a_T\,(\sigma_c - \sigma_{c0})$$

$$\sigma_c = \sigma_{c0} + h_1\gamma + h_2 \exp(-h_3\gamma)$$

Where, σ_{c_0} is the initial yield stress,



Appendix 1 – TVE Equations



Generalised Maxwell model with N+1 branches - Ψ is the free energy, Υ is the coefficient of viscosity, extra is the additional hyperelastic branch

- Hookean Viscoelastic Free Energy (ψ_{ve})

$$\psi_{ve}(\mathbf{E}_e, T, \mathbf{\Gamma}_i) = \sum_{i=1}^{N_i}\left[\frac{K_i}{2}\left[\mathrm{tr}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)\right]^2 + \ldots \right.$$
$$\left. \ldots + G_i\,\mathrm{dev}\,(\mathbf{E}_e - \mathbf{\Gamma}_i) : \mathrm{dev}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)\right]$$

- Consistent Corotational Kirchhoff stress ($\boldsymbol{\tau}$) conjugated to logarithmic strain tensor ($\mathbf{E}_e$).

$$\frac{1}{3}\,\mathrm{tr}\,\boldsymbol{\tau}_e = K_\infty\,(1 + a)\,\mathrm{tr}\,\mathbf{E}_e - 3K_\infty\alpha_\infty\,(T - T_0) + \sum_{i=1}^{N_i}\underbrace{K_i\,\mathrm{tr}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)}_{\mathrm{tr}\,(\boldsymbol{\tau}_i - \mathbf{Q}_i)}$$

$$\mathrm{dev}\,\boldsymbol{\tau}_e = G_\infty\,(1 + b)\,\mathrm{dev}\,\mathbf{E}_e + \sum_{i=1}^{N_i}\underbrace{G_i\,\mathrm{dev}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)}_{\mathrm{dev}\,(\boldsymbol{\tau}_i - \mathbf{Q}_i)}$$

Viscous Overstress = $\boldsymbol{\tau}_i$ - Q_i

- ODEs for internal variable ($\mathbf{\Gamma}_i$). To solve for $\mathbf{\Gamma}_i$.

$$\mathrm{tr}\,\dot{\mathbf{\Gamma}}_i = \frac{1}{k_i}\,\mathrm{tr}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)$$
$$\mathrm{dev}\,\dot{\mathbf{\Gamma}}_i = \frac{1}{g_i}\,\mathrm{dev}\,(\mathbf{E}_e - \mathbf{\Gamma}_i)$$

Solve using TTSP

- Maxwell model + Hookean Free Energy with log strain -> Stresses decrease with temperature.

$$\mathbf{E}_e = \frac{1}{2}\ln\mathbf{C}_e$$

- Thermal coupling -> Heat flux definition from Fourier's law, temperature dependent CTE and thermal conductivity.

ψ_∞^{extra} such that a and b are sigmoid functions of the log strain -> exponential non-linearity in elastic regime. Temperature dependence in V and D parameters only.

$$a = V\frac{\left(\frac{\xi}{3}\mathrm{tr}\,\mathbf{E}_e \cdot \mathrm{tr}\,\mathbf{E}_e - \zeta\right)}{\sqrt{1 + \left(\frac{\xi}{3}\mathrm{tr}\,\mathbf{E}_e \cdot \mathrm{tr}\,\mathbf{E}_e - \zeta\right)^2}}$$
$$b = D\frac{(\theta\mathrm{dev}\,\mathbf{E}_e : \mathrm{dev}\,\mathbf{E}_e - \pi)}{\sqrt{1 + (\theta\mathrm{dev}\,\mathbf{E}_e : \mathrm{dev}\,\mathbf{E}_e - \pi)^2}}$$

Appendix 2 – TVP Equations

Elements

- Extended Drucker-Prager Power Yield Function ($\bar{F}$) – **pressure dependency** and temperature and equivalent plastic strain ($\Delta\gamma$) dependent coefficients (a_2, a_1, a_0), and the flow parameter (Γ). a_2, a_1, a_0 - functions of tensile and compressive yield strength.

$$\bar{F}(\Gamma, \Delta\gamma, T) = a_2 \phi_e^{\alpha} - a_1 \phi_p - a_0 - \left(\eta \frac{\Gamma}{\Delta t}\right)^p$$

- Perzyna Flow Rule with temperature-dependent viscosity (η), quadratic plastic potential (P).

$$\mathbf{D}_p = \frac{1}{\eta(T)} \langle \boldsymbol{F} \rangle^{\frac{1}{p}} \frac{\partial P}{\partial \mathbf{M}_e}$$

Flow Normal (**Q**)

- Chaboche NLKH – coefficients are functions of equivalent plastic strain for cyclic loading performance; temperature term for performance under high temperatures.

$$\dot{\mathbf{X}} = k^2 H_{\mathbf{X}} \mathbf{D}_p + \left(m_\gamma(\gamma) \dot{\gamma} \mathbf{X} + m_T(\gamma, G(\mathbf{X})) \right) + \frac{1}{H_{\mathbf{X}}} \frac{\partial H_{\mathbf{X}}}{\partial T} \dot{T} \mathbf{X}$$

For cycling loading

Static Recovery

Temperature term

TVP Internal Variables:

- Equivalent plastic strain ($\Delta\gamma$): Solved using a rate equation. (k is a material parameter)

$$\dot{\gamma} = k \sqrt{\mathbf{D}_p : \mathbf{D}_p}$$

- Flow parameter (Γ): Solved using $\bar{F}$.

Two Equations: yield function ($\bar{F}$=0) and $\Delta\gamma$ rate equation **!**

Two unknowns: Γ and $\Delta\gamma$ **!**

Temperature Dependency:

Yield strengths, kinematic hardening modulus (H_X) and viscosity (η) are scaled with temperature dependent negative exponential functions like the WLF shift factor (a_T). For a parameter:

$$\eta(\gamma, T) = a_T(T)\eta(\gamma)$$

Appendix 3 - Elasto-Plastic Algorithm

Summary

1. Initialise elastic predictor step, get predictor stresses (**τ_e**, **M_e**).
2. Check Yield Function ($\bar{F}$). If $\bar{F} \leq 0$, **exit**.
3. If $\bar{F}$ >0, get derivatives with respect to equivalent plastic strain (γ) and flow parameter (Γ), solve simultaneously. Solve the effective stress equation (**J(ϕ)**). Iterate until $\bar{F}$ convergence.
4. Update the stresses (**τ_e**, **M_e**). Get Piola-Kirchhoff stress (**P**).

Then, get the stress derivatives with respect to deformation and temperature, get thermal flux term and its derivatives, sources ….