Numerical Modeling of Non-Isothermal Viscoelastic Flow

Phan-Thiên-Tanner (PTT) Model for Rubber Compounds

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Challenges in Rubber Characterisation

- Numerical simulation of SBR requires both clever numerical strategy and physical model
- PTT model: accurate but requires difficult-to-obtain parameters for rubber materials
- Challenge: Parameter characterization for complex viscoelastic behavior
- Solution: Integrated approach combining numerical methods + material characterization

Two-Stage Characterization Strategy

Stage 1: Linear Parameters

Oscillatory RPA

Extract G', G" vs frequency

Define viscosity and relaxation spectrum

Stage 2: Nonlinear Parameters

Continuous shear RPA

Extract steady shear viscosity

Determine extensibility parameters

Phan-Thiên-Tanner (PTT) Model

- Inkompressible **Stokes:**

$$\frac{\partial \boldsymbol{u}}{\partial t} - 2\eta_s \nabla \cdot \boldsymbol{D}(\boldsymbol{u}) - \nabla \cdot \boldsymbol{\sigma} + \nabla p = (1-\gamma\theta) \cdot g, \qquad \nabla \cdot \boldsymbol{u} = 0, \qquad \sigma = \sum_i {}^{\eta_i}/_{\lambda_i} (\tau_i - I)$$

- Constitutive equation in each mode i: $f\big(tr(\boldsymbol{\tau})\big)\,\boldsymbol{\tau} + \lambda\boldsymbol{\tau}' = \boldsymbol{2\eta D}$

$$\boldsymbol{\tau}' = \frac{\partial \boldsymbol{\tau}}{\partial t} + (u \cdot \nabla)\,\boldsymbol{\tau} - (\nabla u)^T \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot (\nabla u), \qquad f\big(tr(\boldsymbol{\tau})\big) = \exp\left(\frac{\varepsilon\lambda}{\eta} tr(\boldsymbol{\tau})\right)$$

- Temperatur: $\frac{\partial \theta}{\partial t} + (\boldsymbol{u} \cdot \nabla)\theta = \eta_T \Delta\theta + Q_{\boldsymbol{\Theta}}$

Parameters needed for each relaxation mode:

- η = viscosity of mode i
- λ = relaxation time of mode i
- ε = extensibility parameter of mode i (nonlinear)

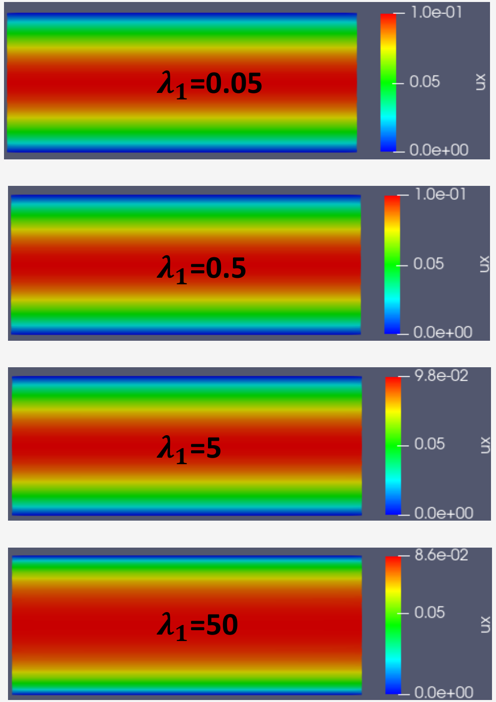
Numerical Strategy: Relaxation Mode Selection

Pre-optimization identifies optimal number of relaxation modes

Result: i = 4 modes proven optimal

Balance between physical accuracy and computational efficiency

This determines the size of all parameter sets: {η}, {λ}, {ε} where i = 1, 2, 3, 4



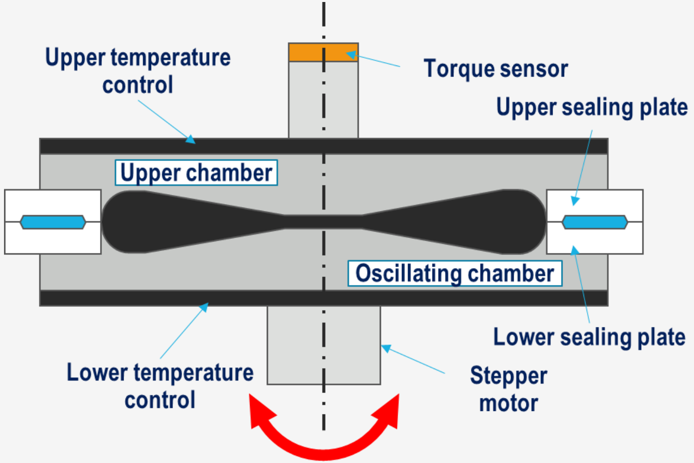
Stage 1: Linear Viscoelastic Parameters

Oscillatory RPA Testing

- Multiple frequencies and temperatures
- Varying amplitudes within linear regime
- Measure: Storage modulus G' and loss modulus G"

Output: Relaxation spectrum

{η, λ} for i = 1 to 4 modes

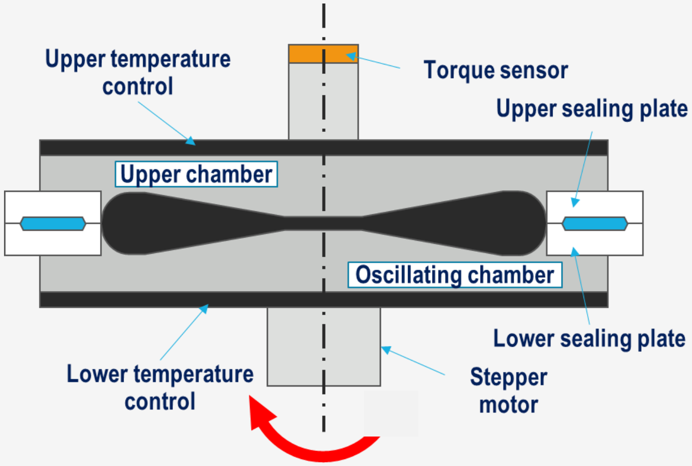


Stage 2: Nonlinear PTT Parameters

Continuous Shear RPA Testing

- Range of constant shear rates
- Measure: Torque → derive steady shear viscosity $\eta(\dot{\gamma})$
- Extract nonlinear behavior beyond first mode

Linear parameters $\{\eta, \lambda\}$ from Stage 1 are inputs to Stage 2



PTT Tensor Decomposition: τ_{12} Component

Reduce PTT `Constitutive equation` to 4-mode 1st-order ODE

`For` τ_{12} `component solve:`

Simple shear

Yields 1st-order ODE in $\tau_{12}(\dot{\gamma})$

$$\frac{d\tau_{12i}}{dt} = \frac{2\eta_i\dot{\gamma} - \exp\left(\frac{\epsilon_i\lambda_i}{\eta_i}\tau_{12i}\right)\tau_{12i}}{\lambda_i}$$

Given constant $\dot{\gamma}$ Solves numerically via Runge-Kutta method

Stage 2: Parameter Extraction

- Set up PTT τ_{12} 1st-ODE with known {η, λ} from stage 1
- Vary ε values iteratively for 4 modes
- Match numerical solution to experimental torque → viscosity
- Converge on optimal {ε} for each shear rate

Output: Nonlinear parameters

{ε} for i = 1 to 4 modes

Final PTT Parameter Set

From Stage 1 (Linear):

$\{\eta_1, \eta_2, \eta_3, \eta_4\}$ and $\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$

From Stage 2 (Nonlinear):

$\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4\}$

Ready for numerical flow simulations

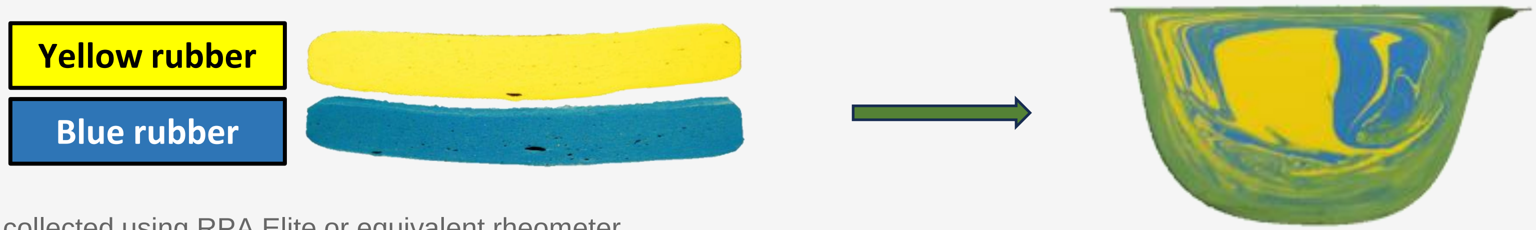
Test Case: SBR Material

Material: Styrene-Butadiene Rubber (SBR)

- Temperature range: 60°C – 120°C
- Frequency range (oscillatory): 0.05 – 70 Hz
- Shear rate range (continuous): 1 – 100 s^{-1}
- Strain amplitude (linear regime): γ = 0.1-10%

D-RPA 3000, MonTech, Germany

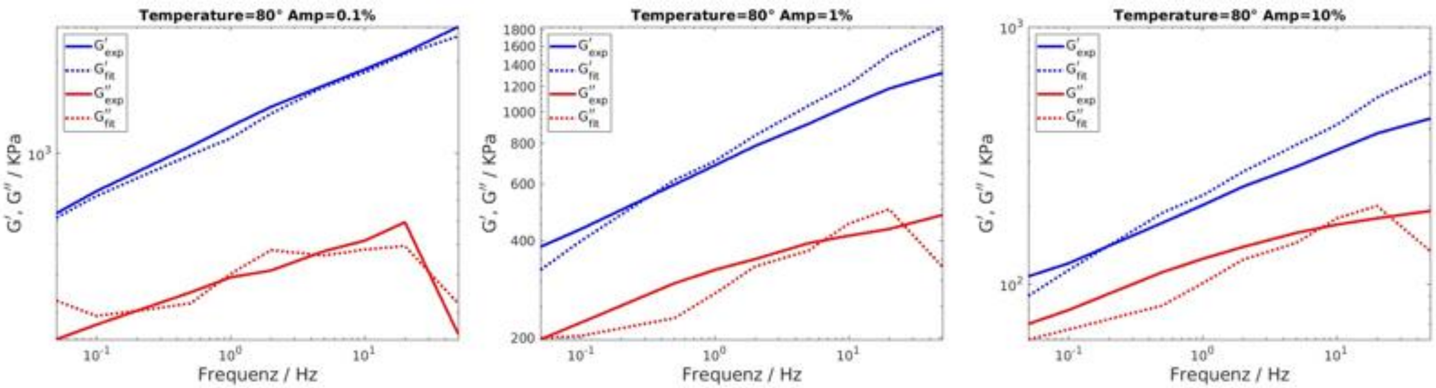
Parameter	Parameter Setting
Temperature	60 / 80 / 90 / 100 / 120 °C
Strain	0.1%, 1%, 10%
Frequency	0.05 / 0.07 / 0.1 / 0.2 / 0.5 / 0.7 / 1 / 2 / 5 / 7 / 10 / 20 / 50 / 70 Hz



Data collected using RPA Elite or equivalent rheometer

Stage 1 Results: G', G" vs Frequency

Storage (G') and loss (G") moduli



From curve fitting: {η, λ} extracted

Stage 1 Results: G', G" vs Frequency

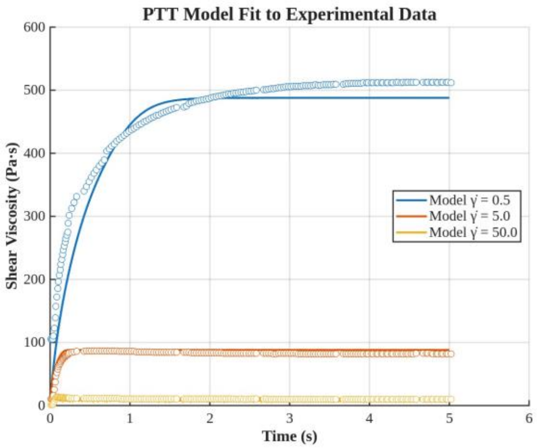
Storage (G') and loss (G") moduli

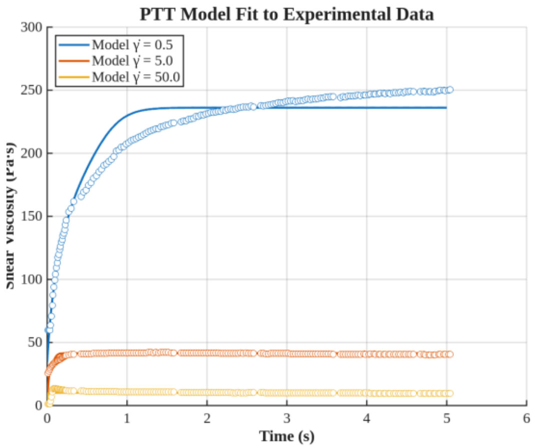
Ampl.	0.1%	1%	10%	0.1%	1%	10%	0.1%	1%	10%
	T=80°			T=100°			T=120°		
λ	G_{fit}	G_{fit}	G_{fit}	G_{fit}	G_{fit}	G_{fit}	G_{fit}	G_{fit}	G_{fit}
0,05	840,318	911,285	369,933	859,174	595,419	314,506	816,805	581,944	305,580
0,5	720,902	424,682	154,430	308,855	267,793	114,402	258,644	239,995	99,081
5	295,600	271,294	95,453	126,344	112,156	60,302	96,938	94,825	51,753
50	689,810	358,0189	97,491	307,439	212,196	68,903	344,907	212,463	60,675

From curve fitting: {η, λ} extracted. Go to Mastercurve

Stage 2 Results: Shear Viscosity $\eta(\dot{\gamma})$

shear viscosity vs shear rate





Nonlinear fit yields {ε} values

Stage 2 Results: Shear Viscosity $\eta(\dot{\gamma})$

shear viscosity vs shear rate

$\dot{\gamma}$	NMSE	NMSE
0.5	0.005	0.0027
5	0.0086	0.0016
50	0.036	0.0243
{ε} values	3.7705 6.2691 8.3551 6.6879	4.9258 9.9769 9.9969 9.8255

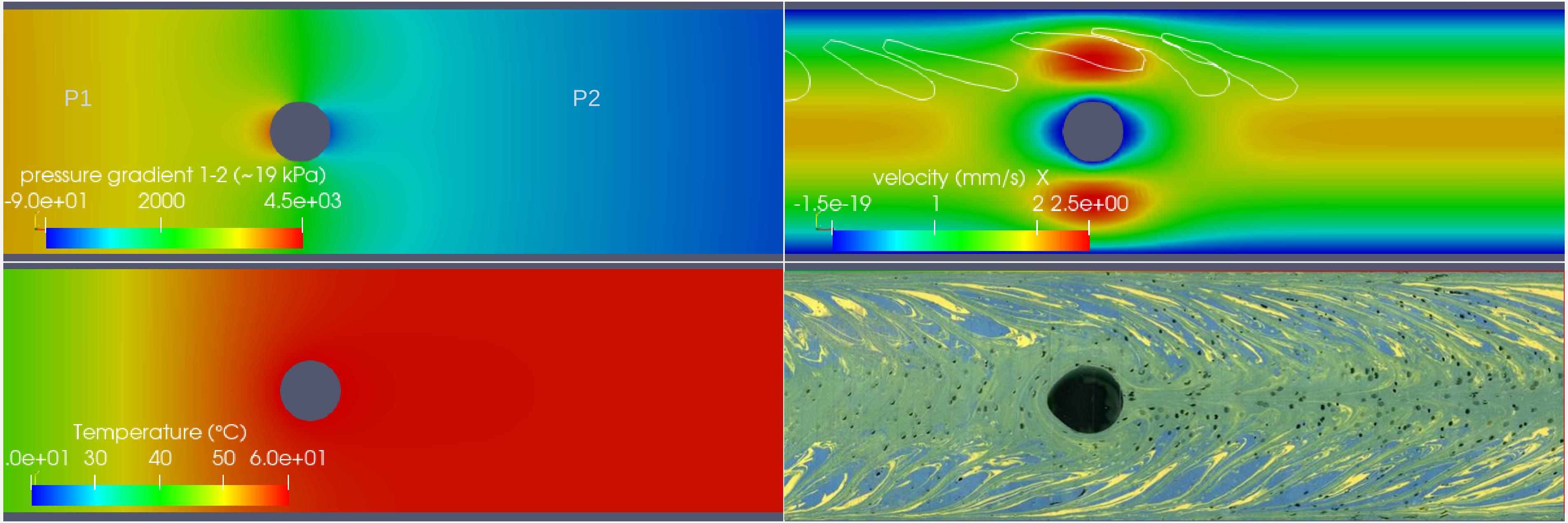
Nonlinear fit yields {ε} values

Validation: Numerical Flow Simulation

Using complete parameter set:

Model: PTT equation with {η, λ, ε}

Test geometry: pipe flow



Key Points

- Systematic approach: Clear separation of linear and nonlinear characterization
- Componentwise solver: Reduced complexity via τ_{12} 1st-order ODE formulation
- Informed optimization: Numerical strategy pre-selects optimal modal structure
- Industrial relevance: Uses standard RPA equipment and data

Conclusions

Integrated methodology enables accurate characterization of PTT model parameters for SBR

Combines rigorous material science with efficient numerical modeling

Applicable to wide range of rubber formulations and processing conditions

Thank You!

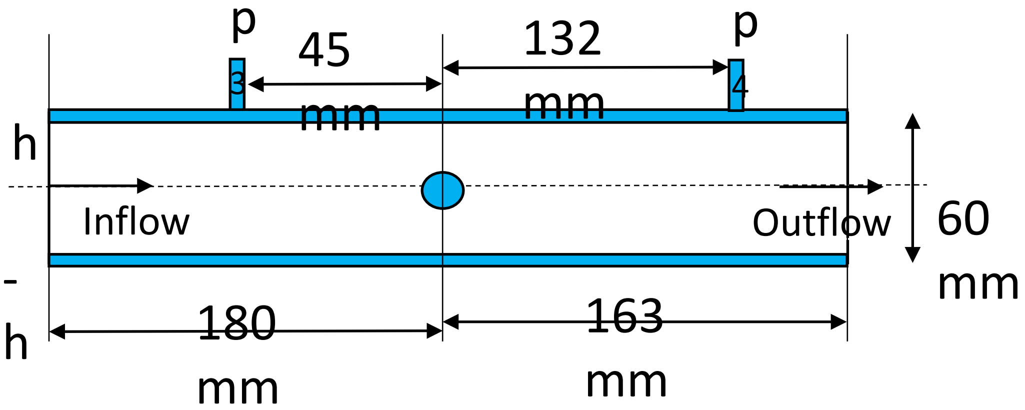
Online Questions? hdamanik@math.tu-dortmund.de

Normalized Mean Squared Error (NMSE):

$$NMSE = \frac{\text{mean}(\text{ymodel} - y_{exp})^2}{\text{mean}(y_{exp}{}^2)}$$

- NMSE > 1 indicates poor fit
- NMSE ~ 0 indicates excellent fit

Component	Amount [phr]
SBR	**90**
NR	**10**
Plasticizer	**41.18**
Silica	**64.71**
Kaolin	**64.71**
Pigment	**3.82**
Minor chemicals	**19.71**



- λ_1 =5, λ_2=0.5
- ϵ_1 =0.4, ϵ_2=0.5
- Rotations/min=10 U/sec

- Flow rate=28.5kg/h
- Velocity=2.2mm/sec
- Pressure difference (P3-P4)= 16.52