Development and Experimental Validation of an Advanced Non-Linear, Rate-Dependent Constitutive Model for Polyether Ether Keytone (PEEK)

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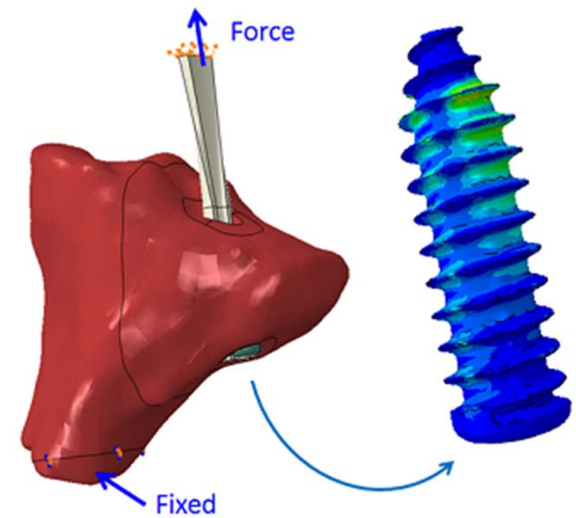
Outline

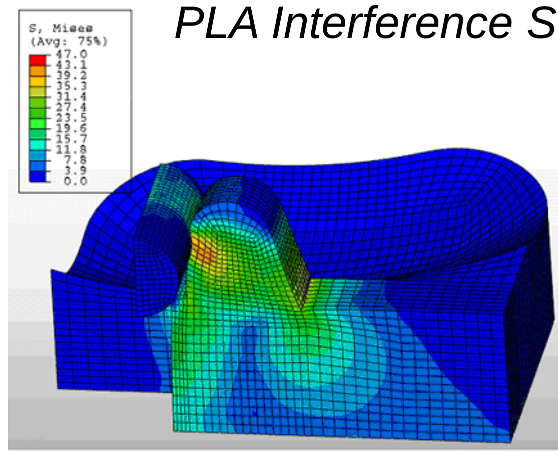
- Motivation: The need for advanced constitutive models of polymers in medical devices.
- Case Study: Calibration and validation of an advanced material model for PEEK.
- Discussion of material model validation.
- Conclusions and future work.

Why do we need an advanced material model?

- Polymers (thermoplastics, rubbers, foams) are not linear, especially above small strains (1-2%)
- Many medical device applications have localized high stresses and strains
- Multiple loading-unloading cycles
- Wide range of time-scales and strain rates



PLA Interference Screw



UHMWPE Knee Replacement

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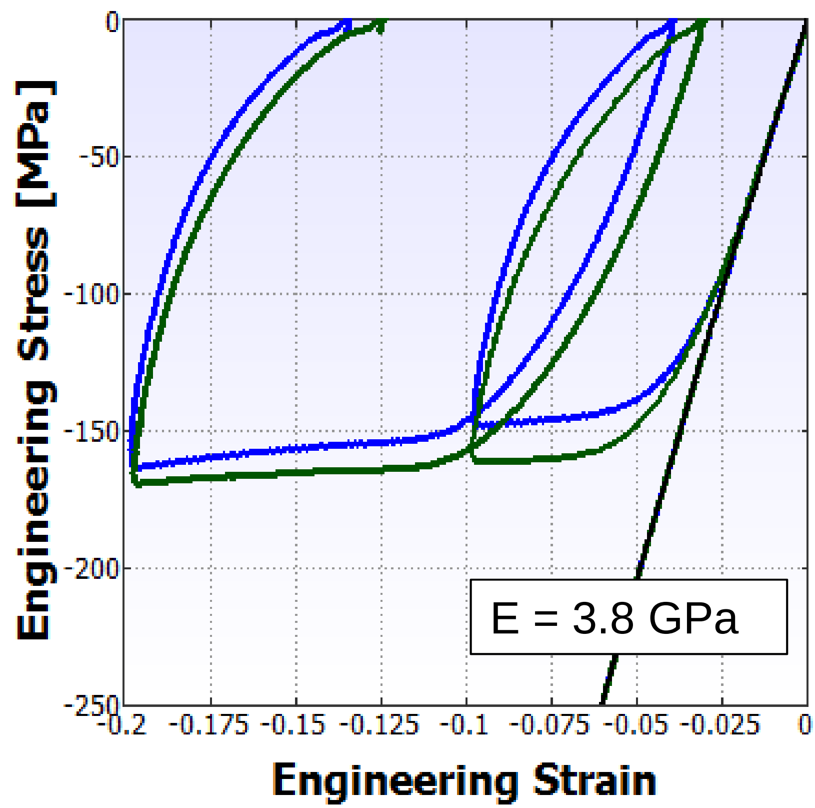
Unfilled PEEK, Uniaxial Compression

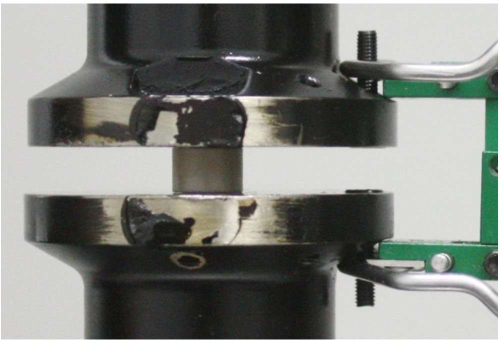


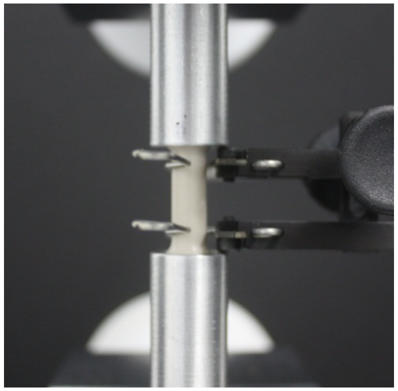
Polyether Ether Ketone (PEEK)

- Good mechanical properties (E ~ 4GPa, σ_{ut} ~ 100 MPa)
- Good wear resistance
- Inert, generally biocompatible
- Orthopedic applications
  - Spinal implants/spacers
  - Fixation (screws, plates etc.)
  - Biomedical textiles (wovens, braids)

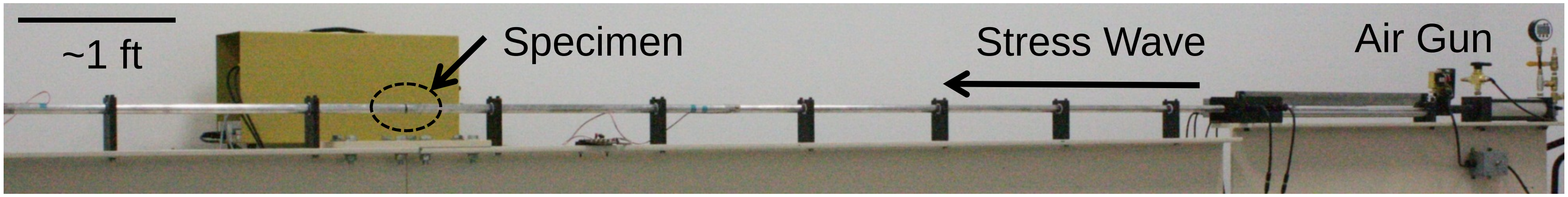
Experimental Testing

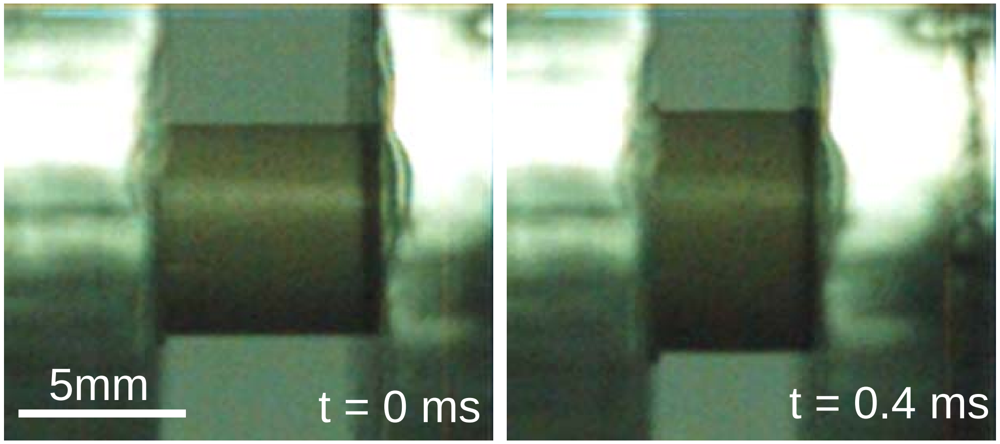
- Unfilled PEEK
- Uniaxial compression and tension testing (up to ~0.1/s)





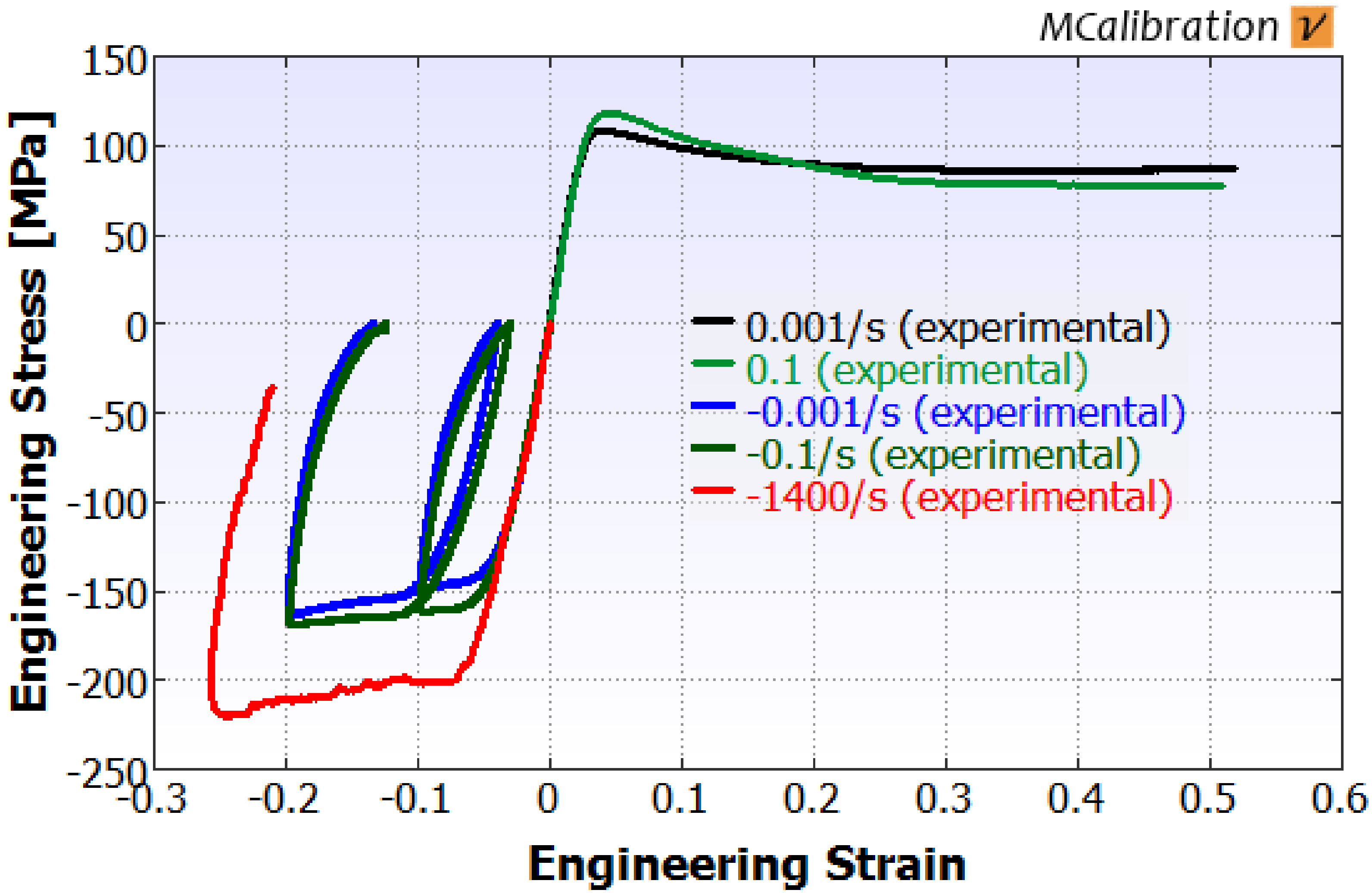
- Split Hopkinson pressure bar (SHPB) (up to ~ 1500/s)





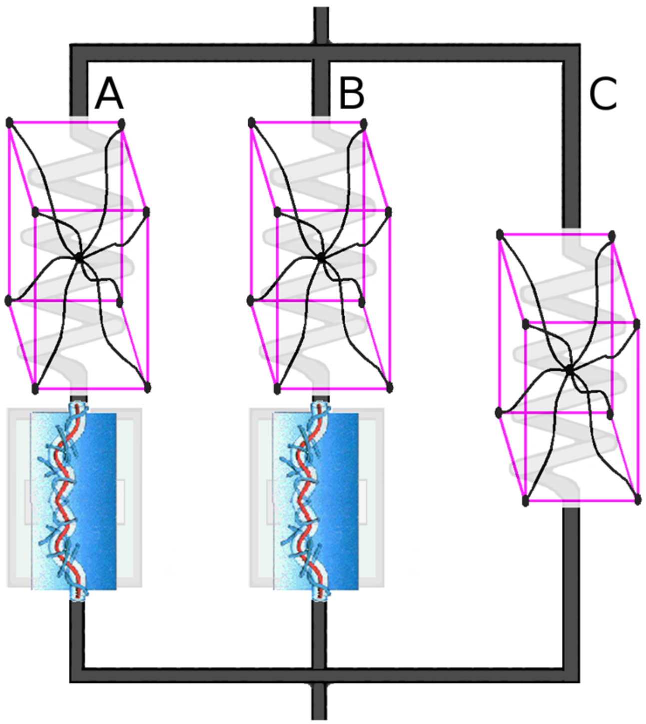
Experimental Results

- Clear rate dependent yield and post-yield behavior

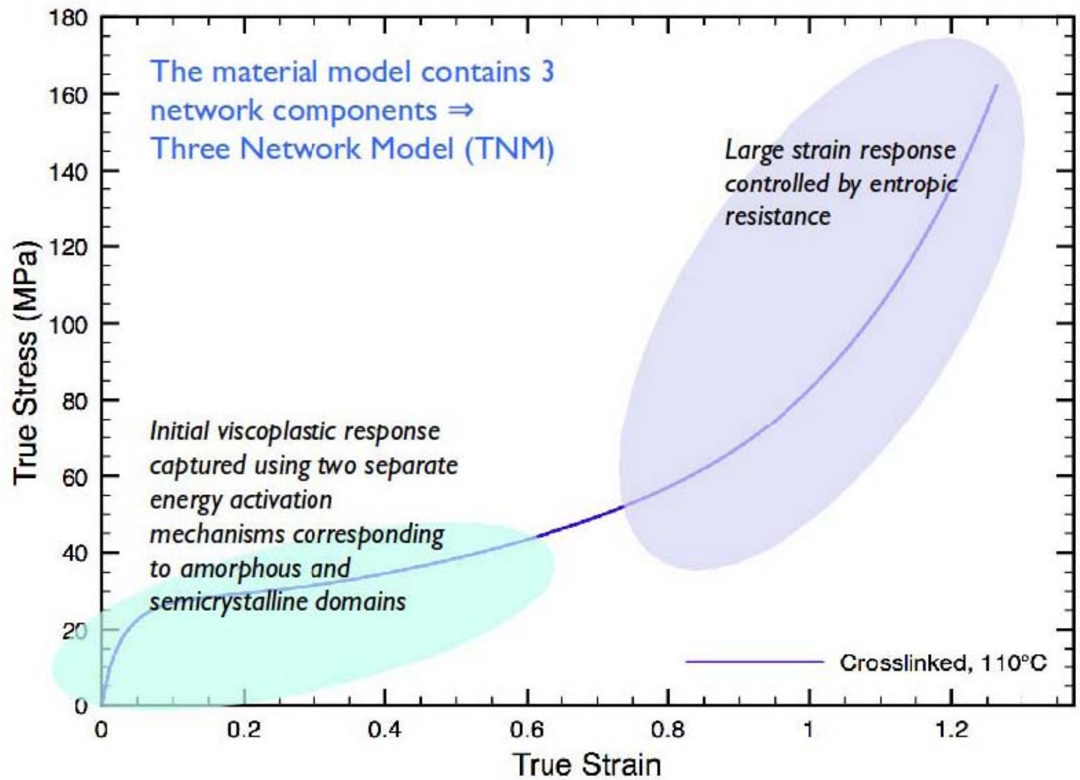


The Three Network Model (TNM)

- Polymer physics-driven modeling framework
- Previously used for modeling UHMWPE
  - Low strain rate over limited range: ~0.001 – 0.01/s



Rheological Representation of the TNM



Bergstrom, J.S., Bischoff, J.E., "An Advanced Thermomechanical Constitutive Model for UHMWPE" *Int. J. of Structural. Changes in Solids,* 2(1): 31-39, 2010.

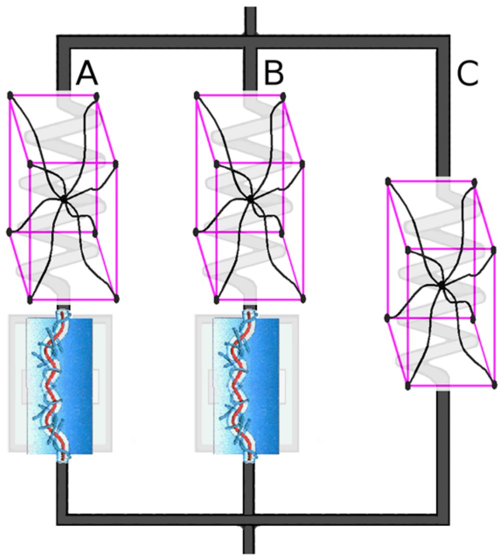
Stress in Networks A & B

Cauchy Stress from Arruda-Boyce 8-chain model (with temp. dependence):

$$\sigma_A = \frac{\mu_A}{J_A^e \overline{\lambda_A^{e*}}} \left[1 + \frac{\theta - \theta_o}{\hat{\theta}}\right] \frac{\mathcal{L}^{-1}\left(\overline{\lambda_A^{e*}}/\lambda_L\right)}{\mathcal{L}^{-1}(1/\lambda_L)} dev[\mathbf{b}_A^{e*}] + \kappa(J_A^e - 1)\mathbf{1}$$

Material Parameters:

μ_A – initial shear modulus
κ – bulk modulus
$\hat{\theta}$ – material temp. dependence
λ_L – locking stretch



Where:

$\mathcal{L}^{-1}$ - inverse Langevin function
θ, θ_o – current, reference temperature
$\overline{\lambda_A^{e*}} = (tr[\mathbf{b}_A^{e*}]/3)^{1/2}$ - effective chain stretch
$J_A^e = \det[\mathbf{F}_A^e]$
$\mathbf{b}_A^{e*} = (J_A^e)^{-2/3}\mathbf{F}_A^e(\mathbf{F}_A^e)^T$ - Cauchy-green deformation tensor

Controls the initial modulus and the plastic flow behavior

Rate Kinematics – Networks A & B

Shear Modulus Evolution: $\dot{\mu}_A = -\beta\left[\mu_A - \mu_{Af}\right] \cdot \dot{\gamma}_A$

Viscoplastic flow rate:

$$\dot{\gamma}_A = \dot{\gamma}_o \cdot \left(\frac{\tau_A}{\hat{\tau}_A + aR(p_A)}\right)^{m_A} \cdot \left(\frac{\theta}{\theta_o}\right)^n$$

$$\tau_A = \|\sigma'_A\|_F \equiv (tr[\sigma'_A \sigma'_A])^{1/2}$$

Viscoelastic velocity gradient: $\dot{\mathbf{F}}^v{}_A = \dot{\gamma}_A \mathbf{F}^{e-1}{}_A \frac{\mathrm{dev}[\sigma_A]}{\tau_A} \mathbf{F}$

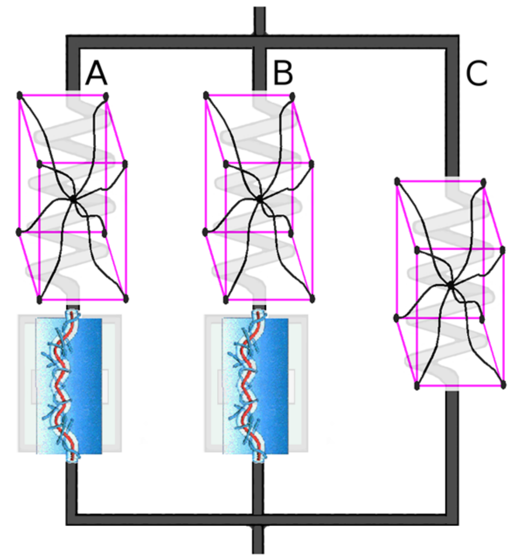
Material Parameters:

μ_{Af}, μ_{Bf} – final shear moduli
κ – bulk modulus
$\hat{\theta}$ – material temp. dependence
λ_L – locking stretch

Stress in Network C

Cauchy Stress from eight-chain model with first order I_2 dependence:

$$\sigma_C = \frac{1}{1+q}\left\{\frac{\mu_c}{J\bar{\lambda}^*}\left[1+\frac{\theta-\theta_o}{\hat{\theta}}\right]\frac{\mathcal{L}^{-1}\left(\bar{\lambda}^*/\lambda_L\right)}{\mathcal{L}^{-1}(1/\lambda_L)}dev[\mathbf{b}^*]+\kappa(J-1)\mathbf{1} + q\frac{\mu_c}{J}\left[I_1^*\mathbf{b}^*-\frac{2I_2^*}{3}\mathbf{I}-(\mathbf{b}^*)^2\right]\right\}$$



Controls the large strain response

Total Stress: $\sigma_{Tot} = \sigma_A + \sigma_B + \sigma_C$

TNM – Material model parameters

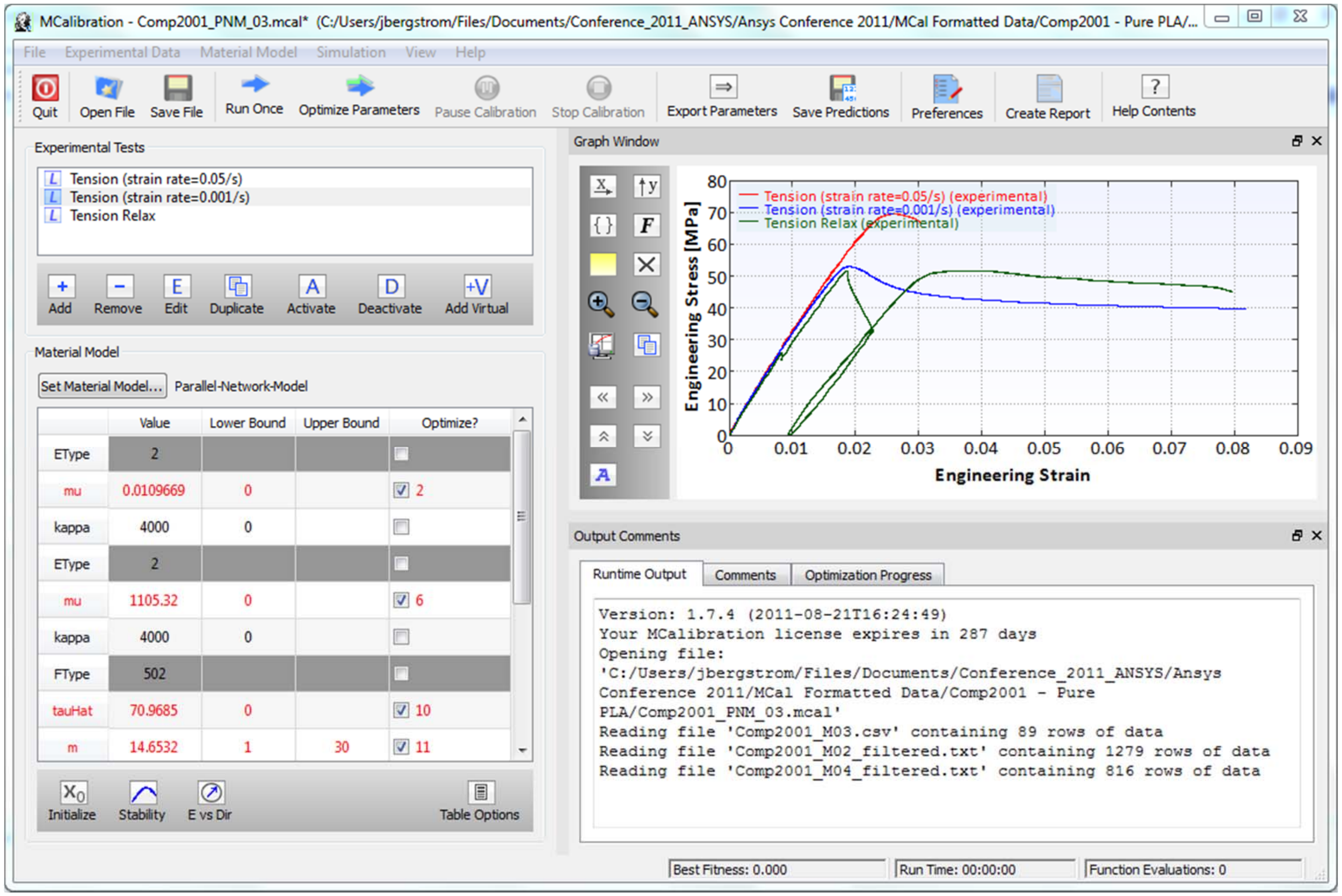
- The TNM is implemented as a user-material model (UMAT) in FEA codes (Abaqus, Ansys)
- Up to 17 material parameters specified or calibrated.
- Calibration requires:
  - Experimental data over range of time-scales
  - Automated process using an optimization method ("Guess and check" will not work)

Table 1: Material parameters used by the three-network model.

Index	Symbol	Umat Name	Unit*	Description
1	μ_A	muA	S	Shear modulus of network *A*
2	$\hat{\theta}$	thetaHat	T	Temperature factor
3	λ_L	lambdaL	-	Locking stretch
4	κ	kappa	S	Bulk modulus
5	$\hat{\tau}_A$	tauHatA	S	Flow resistance of network A
6	a	a	-	Pressure dependence of flow
7	m_A	mA	-	Stress exponential of network A
8	n	n	-	Temperature exponential
9	μ_{Bi}	muBi	S	Initial shear modulus of network B
10	μ_{Bf}	muBf	S	Final shear modulus of network B
11	β	beta	-	Evolution rate of μ_B
12	$\hat{\tau}_B$	tauHatB	S	Flow resistance of network B
13	m_B	mB	-	Stress exponential of network B
14	μ_C	muC	S	Shear modulus of network C
15	q	q	-	Relative contribution of I_2 of network C
16	α	alpha	T^{-1}	Thermal expansion coefficient
17	θ_0	theta0	T	Thermal expansion reference temperature

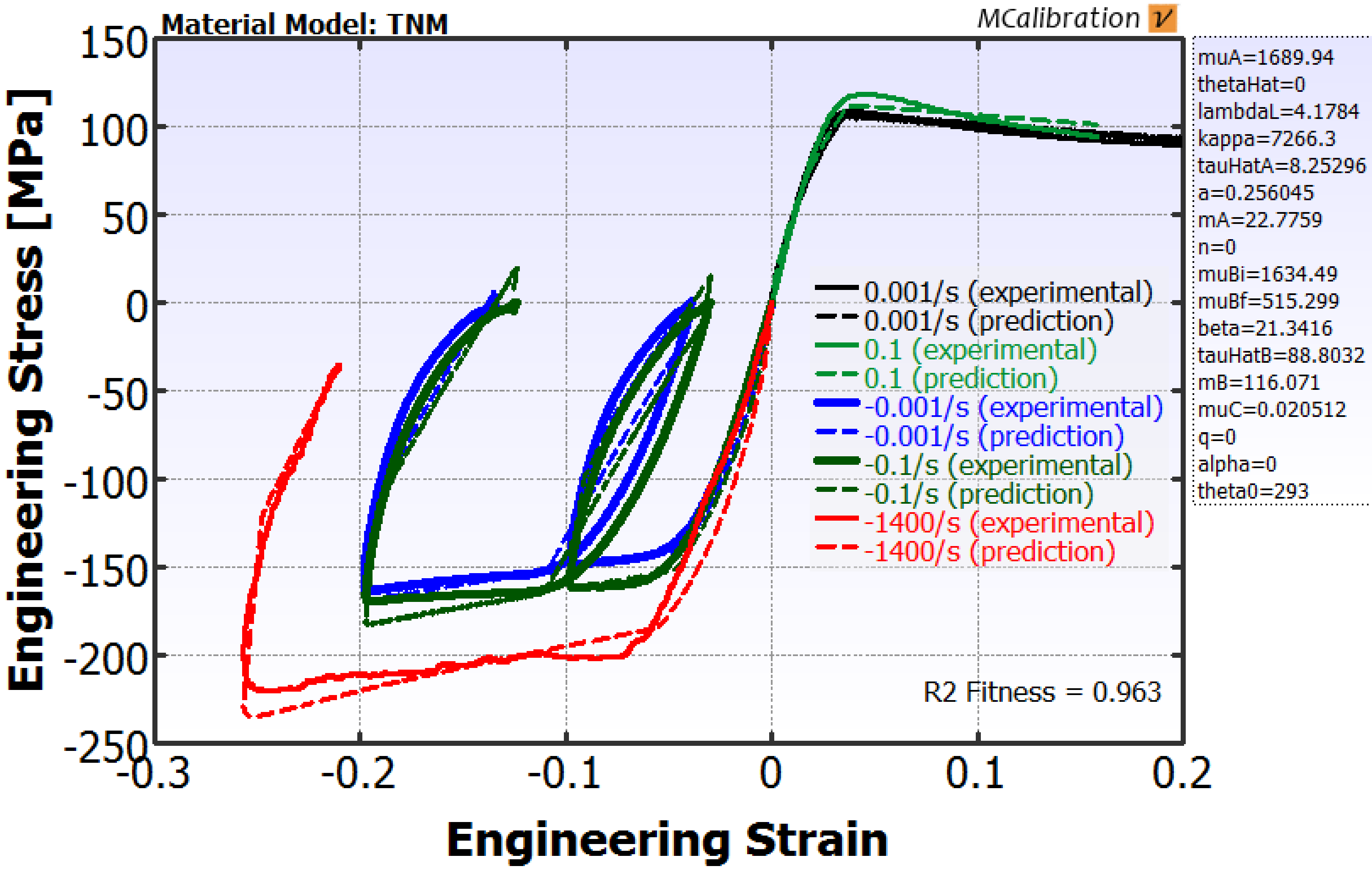
*where: - = dimensionless, S = stress, T = temperature

Material Model Calibration



- The material model calibration was performed using MCalibration.
- MCalibration is commercially available from Veryst Engineering.
- The calibrated material model can be exported for use in Abaqus, Ansys, LS-Dyna with Veryst's PolyUMod Library.

Calibrated Material Model



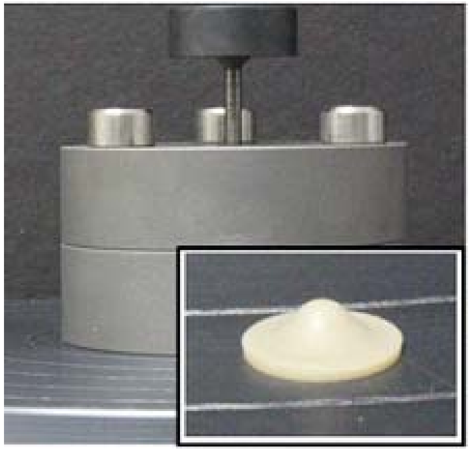
- The calibrated material model shows good agreement with experimental data in tension and compression over 6 decades of strain rate!

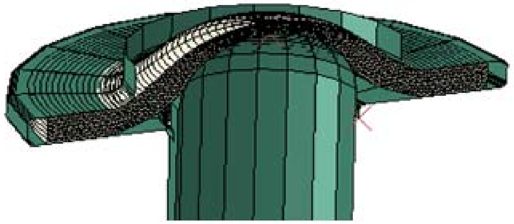
The Need for Model Validation Experiments

- Constitutive models are typically calibrated using uniaxial tension/compression.
- However, in most applications the material is subjected to multiaxial loading (tension, compression, biaxial, shear).
- Independent experiments should be used to assess the predictive capability of the model in the relevant loading conditions.

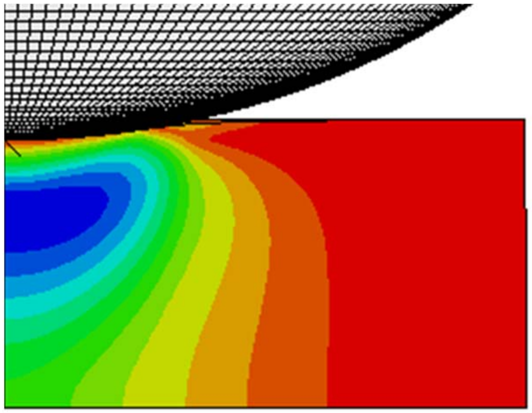
Model Validation Experiments

Small Punch Test (ASTM F2638)

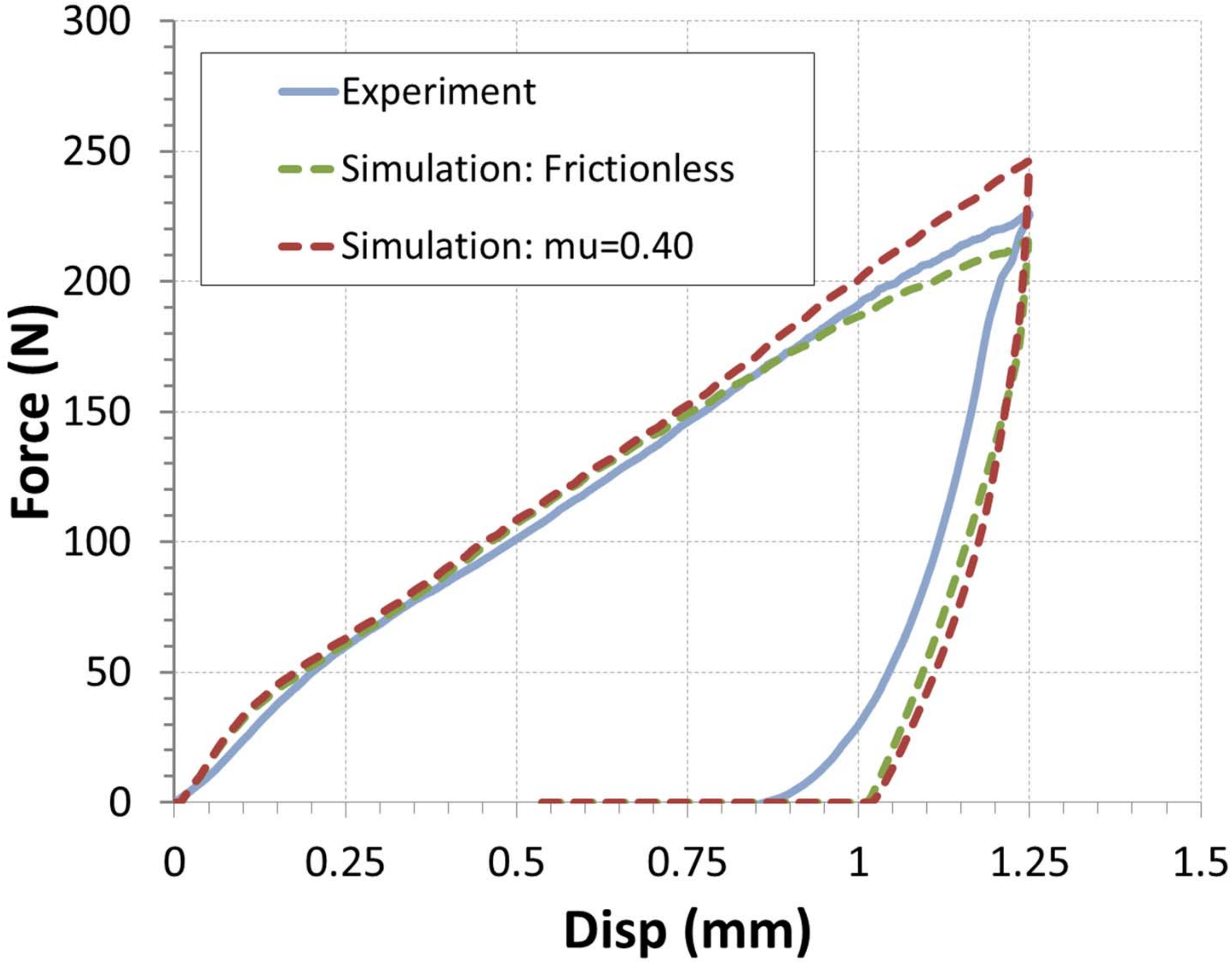




Spherical Indentation

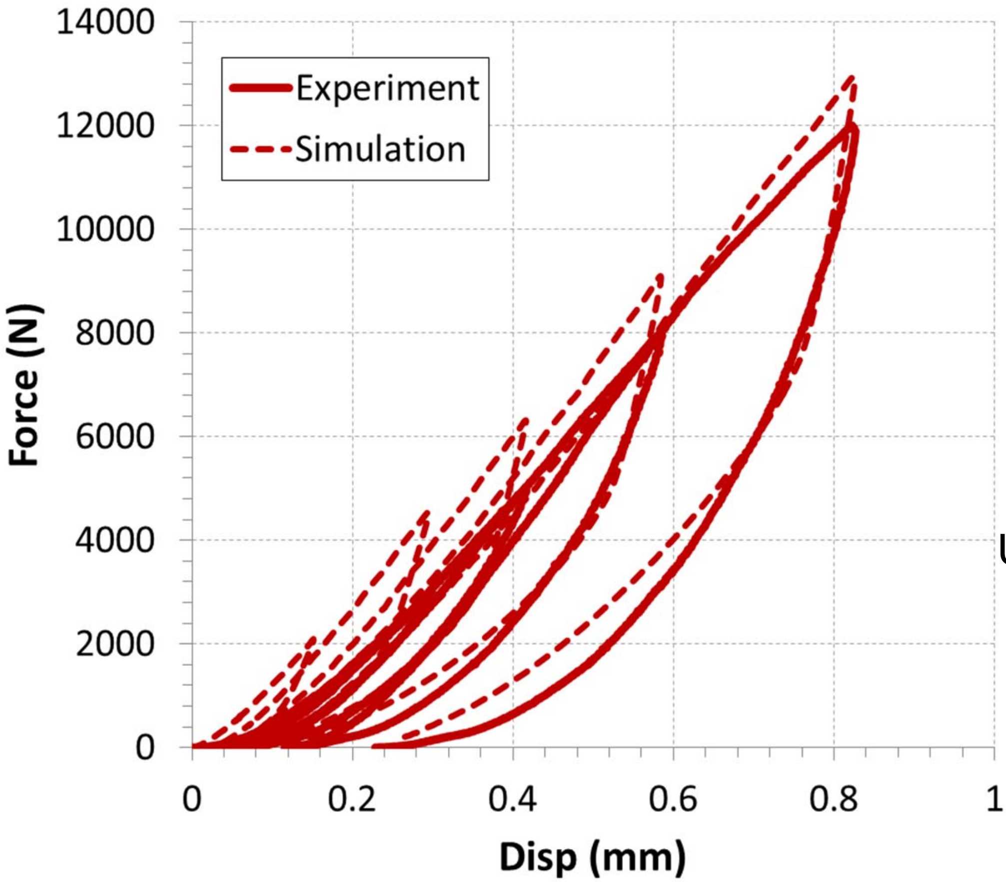


Small Punch Test Results

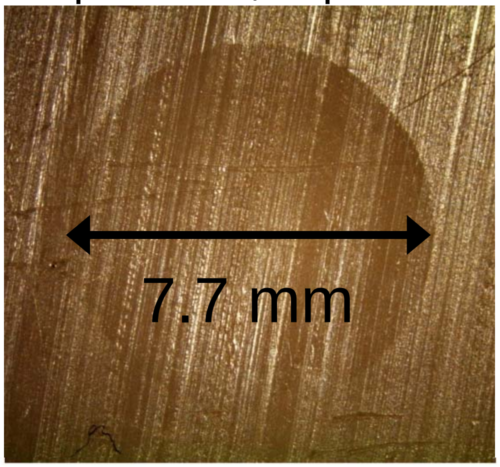


- Accurate predictions of force, displacement and permanent deformation.
- Results are sensitive to friction at higher loads.

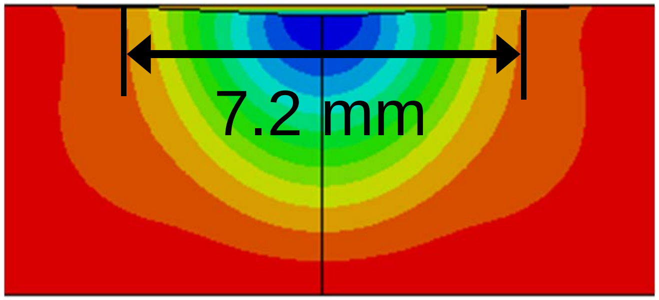
Spherical Indentation Test Results



Experiment, Top View



Unloaded Displacement Field (Side View)



- Accurate predictions of peak force, displacement and deformation.
- Simulation is in-sensitive to frictional effects over these conditions.

When is the Material Model Valid?

Device or Application Specific Questions to Ask:

- What is the dominant stress state and range of stresses/strains in the device/application?
- How do the material model predictions compare over that range ***and slightly beyond***?
- How closely does the validation experiment mimic the anticipated loading environment?
- What is the validation criteria? Total deformation/displacement? “Failure” load?
- How do uncertainties in the material model propagate to the simulation of the device?
- What is the risk (to the patient) of being wrong?

Conclusions

- Accurate simulations of polymeric systems in medical device applications frequently require an advanced, rate-dependent material model.
- When calibrated using an advanced optimization routine, the three network model (TNM) will give accurate stress-strain predictions for PEEK over a large range of strain rates.
- The calibrated TNM can be experimentally validated using independent, multiaxial loading experiments.
- Validation criteria is application and device-specific.

Future Work

- Device-specific application – orthopedics (spinal spacers, bearing surfaces in hip/knee, biomedical textiles).
- Validate model over longer time-scales and strain rates.
- Include damage and failure mechanisms in material model for failure and wear predictions.
- Sensitivity studies and uncertainty predictions.