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COMSOL CONFERENCE 2015 BOSTON

Constitutive Modeling of Polyethylene in COMSOL Multiphysics

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Outline

- Introduction
- Material model for MDPE
- Calibration to experimental data
- Implementation of material model in COMSOL Multiphysics
- Verification of developed material model

Introduction

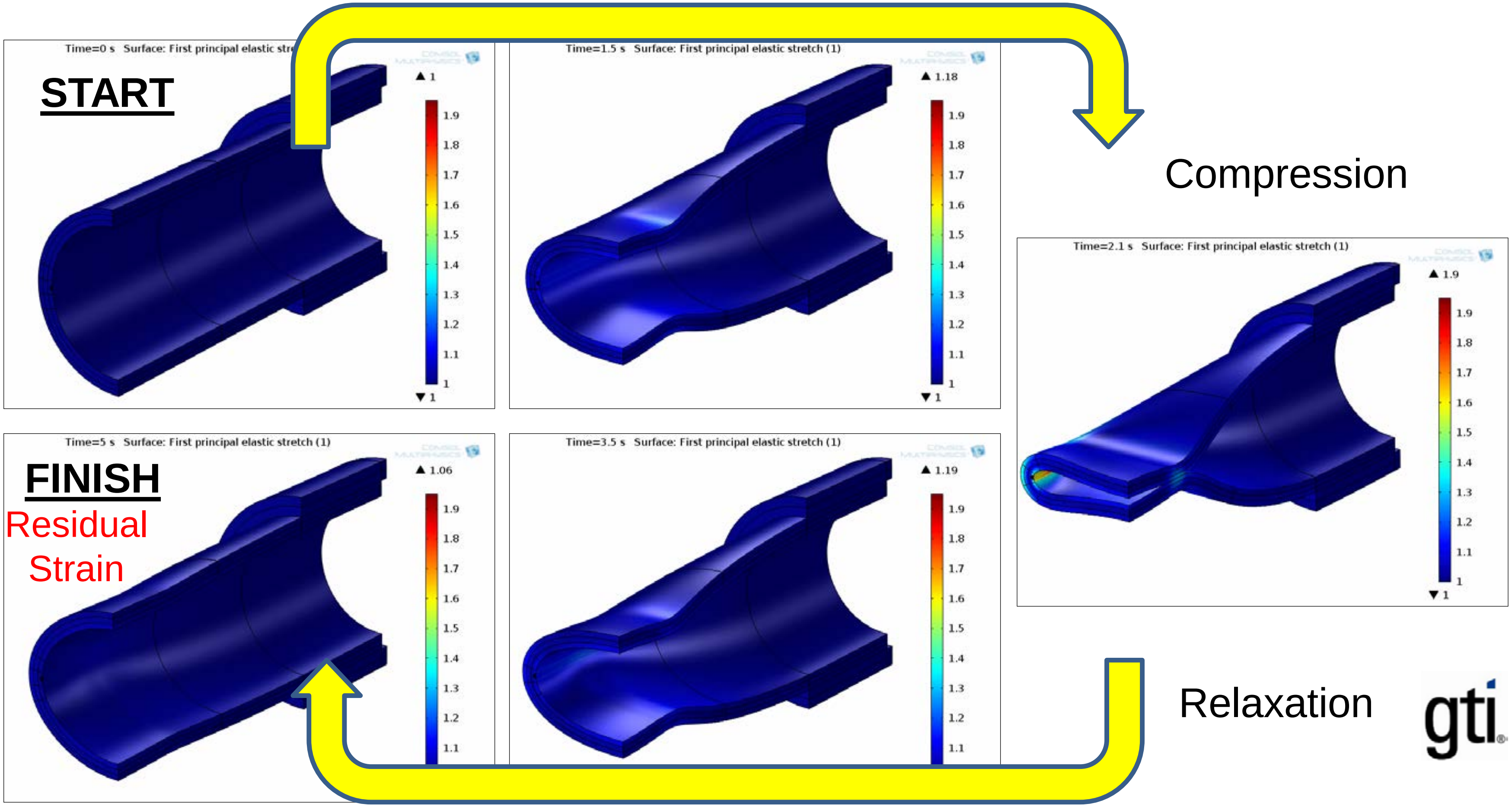
- Medium-density polyethylene (MDPE) is a thermoplastic commonly used in gas piping and fittings
  - MDPE pipe is flexible and can withstand deflection during subterranean installation, including full squeeze-off
  - Employed in a wide range of temperatures, from sub-freezing up to 60°C

(Performance Pipe)

Introduction

- Physical Properties of MDPE:
  - Density: 0.92 - 0.94 kg/m^3
  - Tensile Strength: 12-19 MPa
  - Young's Modulus: 170-600 MPa
  - Elongation at break: >150%
- Mixture of stiff, strong high density polyethylene (HDPE) and workable, flexible low density polyethylene (LDPE)
  - Very good crack resistance

End Use: Pipe Squeeze-Off



START

Compression

Relaxation

FINISH

Residual Strain

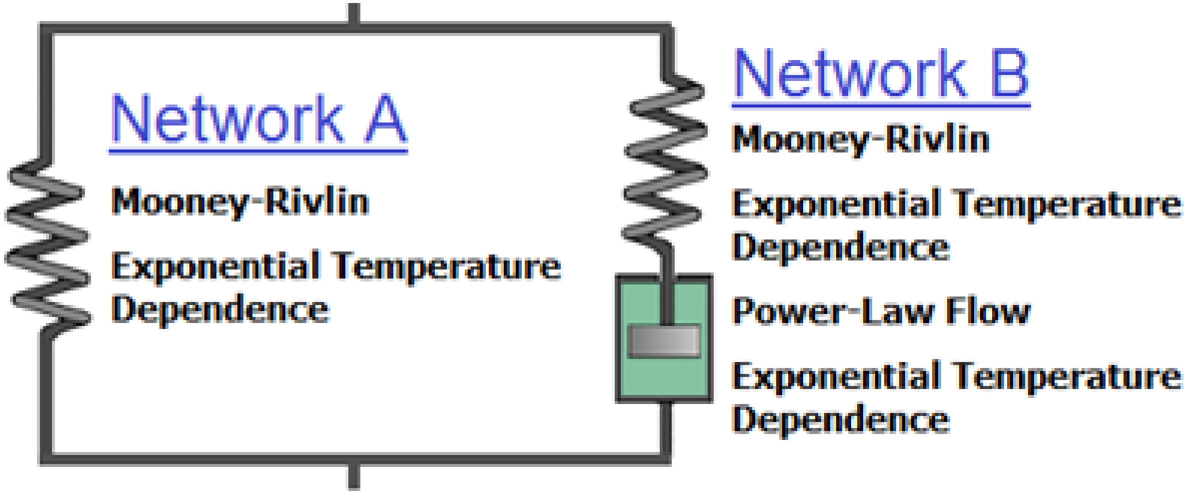
For more details:
Lever E, Lever O, Assessment of Squeeze-off Location for Small Diameter Polyethylene (PE) Pipe and Tubing, *COMSOL Conference 2015*, Newton MA.

Constitutive Modeling of MDPE

- MDPE behavior is nonlinear, strain rate and temperature-dependent
    - Cannot be accurately modeled with hyperelastic or elastic-plastic material models
- We selected a two-network nonlinear rate-dependent material model with exponential temperature dependence
    - More advanced material models suitable for MDPE are available in the PolyUMod® library from Veryst Engineering

Material Model

- Two parallel rheological networks with exponential temperature dependence



Network A

Mooney-Rivlin

Exponential Temperature Dependence

Network B

Mooney-Rivlin

Exponential Temperature Dependence

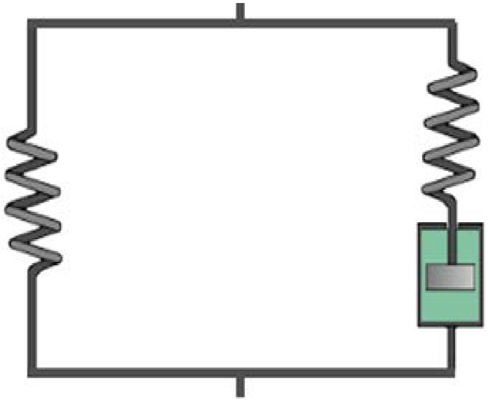
Power-Law Flow

Exponential Temperature Dependence

Material Model

- Deformation gradients

$$\mathbf{F}^A = \mathbf{F}^B = \mathbf{F}, \quad \mathbf{F}^B = \mathbf{F}_e \mathbf{F}_v$$



- Cauchy stress tensor

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^A + \boldsymbol{\sigma}^B$$

- Stiffness of both networks scale exponentially with temperature

$$f_\theta = exp\left[q * \frac{\theta - \theta_0}{\theta_0}\right]$$

Material Model

- Network A
  - Mooney-Rivlin hyperelastic element
- Network B
  - Mooney-Rivlin hyperelastic element
  - In series with viscoplastic power law damper

$$\mathbf{D}_v^B = \frac{\dot{\gamma}}{\tau}\mathrm{dev}[\boldsymbol{\sigma}^B] \quad \dot{\gamma} = \left(\frac{\tau}{\tau_{\mathrm{base}}}\right)^m$$

$\mathbf{D}_v^B$ is the rate of viscous deformation

τ is the effective shear stress

m, τ_{base} are material constants

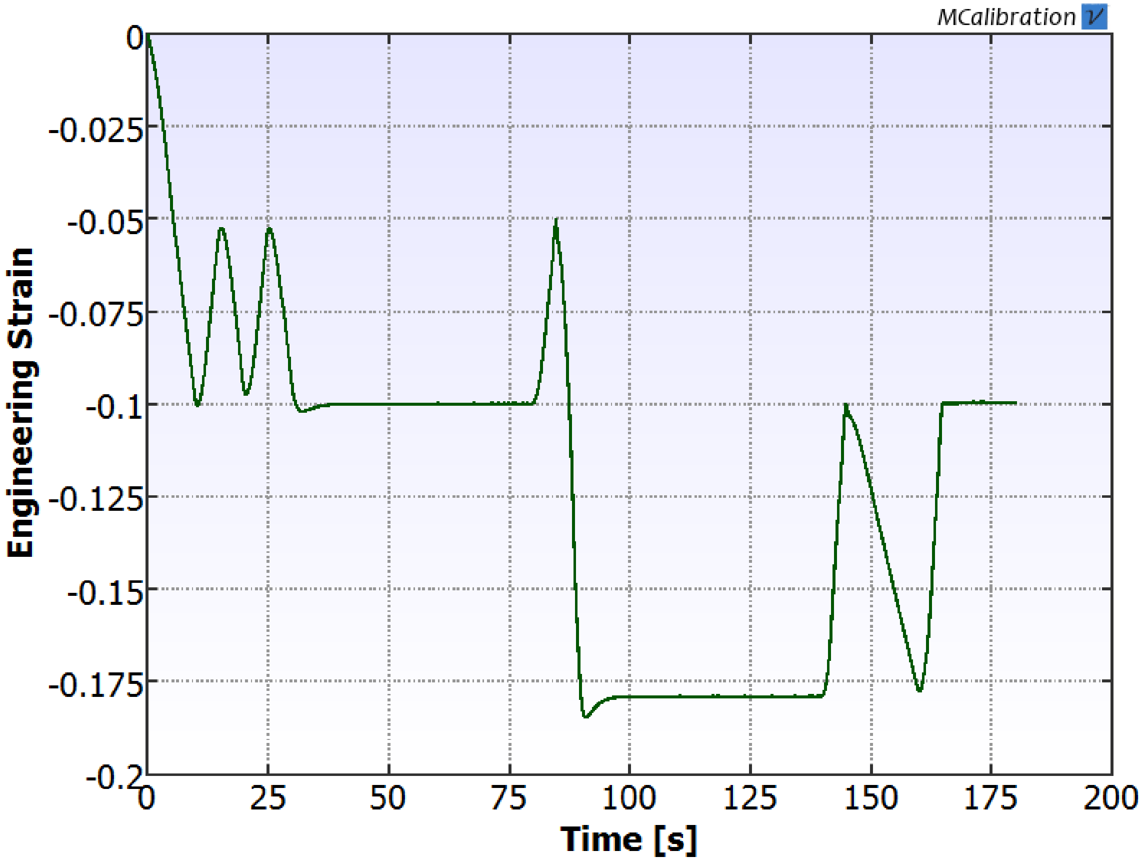
Material Model

- Parameters used in material calibration
  - Mooney-Rivlin Network A: C_{01}^{A}, C_{10}^{A}
  - Mooney-Rivlin Network B: C_{01}^{B}, C_{10}^{B}
  - Viscous part of Network B: τ_{base}, m
  - Three temperature scaling factors: q^{A}, q^{B}, q^{Bv}
- Bulk modulus (κ) set to a high value resulting in a nearly incompressible material

Experimental Data

- Gas Technology Institute (GTI) provided the experimental data used in calibration
  - Uniaxial tension tests at different
    - Temperatures (-20°C, 20°C & 60°C)
    - Strain rates (0.1 s^{-1}, 0.01 s^{-1} & 0.005 s^{-1})
  - Cyclic compression tests at different
    - Temperatures (-20°C, 20°C & 60°C)

Experimental Data – Cyclic Compression

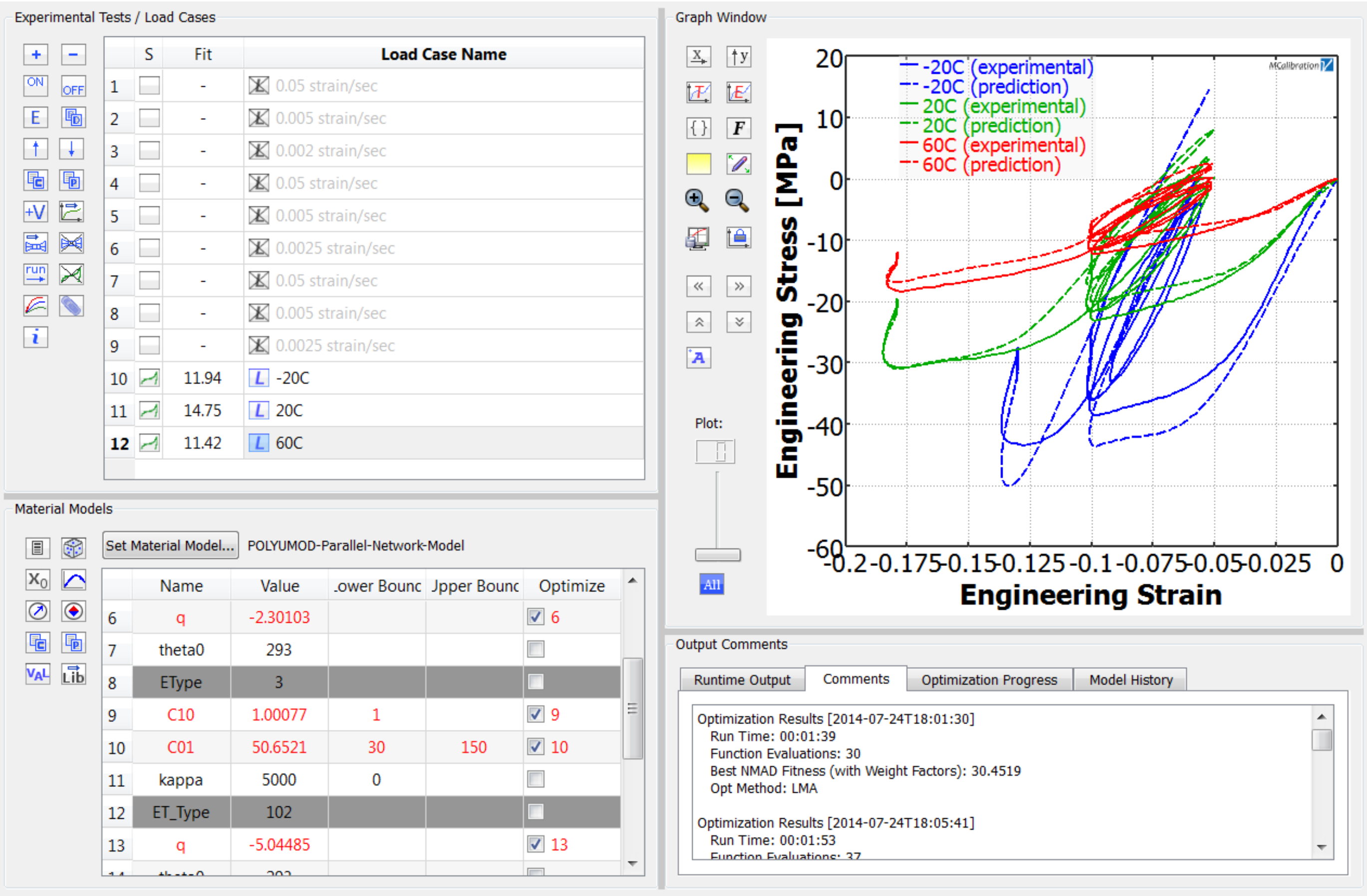


- Cyclic compression loading/unloading/hold profile includes segments at different strain rates

- Designed to capture more aspects of the material behaviour beyond monotonic loading or creep/relaxation tests

Material Model Calibration

- We used MCalibration® to fit the material parameters to experimental data



Experimental Tests / Load Cases

	S	Fit	Load Case Name
1	☐	-	0.05 strain/sec
2	☐	-	0.005 strain/sec
3	☐	-	0.002 strain/sec
4	☐	-	0.05 strain/sec
5	☐	-	0.005 strain/sec
6	☐	-	0.0025 strain/sec
7	☐	-	0.05 strain/sec
8	☐	-	0.005 strain/sec
9	☐	-	0.0025 strain/sec
10		11.94	-20C
11		14.75	20C
12		11.42	60C

Material Models

Set Material Model... POLYUMOD-Parallel-Network-Model

	Name	Value	.ower Bounc	Jpper Bounc	Optimize
6	q	-2.30103			☑ 6
7	theta0	293			☐
8	EType	3			☐
9	C10	1.00077	1		☑ 9
10	C01	50.6521	30	150	☑ 10
11	kappa	5000	0		☐
12	ET_Type	102			☐
13	q	-5.04485			☑ 13

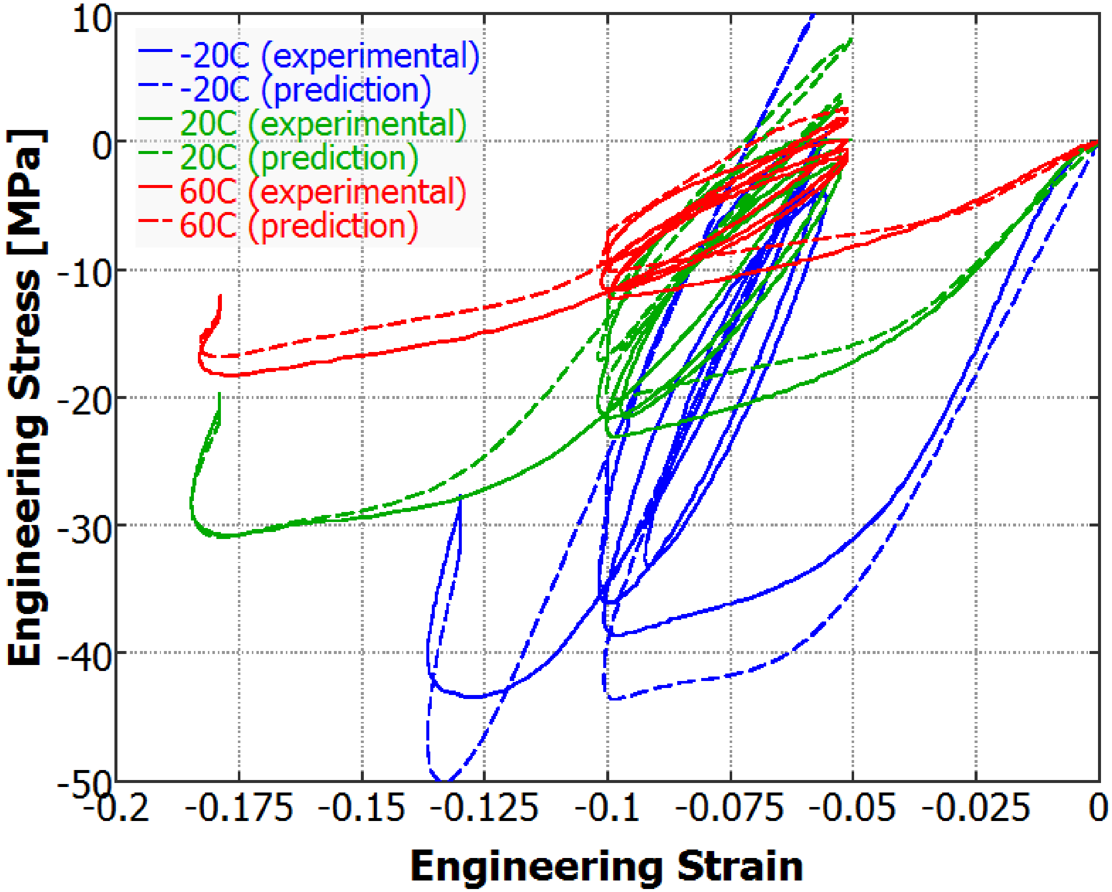
```
Optimization Results [2014-07-24T18:01:30]
   Run Time: 00:01:39
   Function Evaluations: 30
   Best NMAD Fitness (with Weight Factors): 30.4519
   Opt Method: LMA

Optimization Results [2014-07-24T18:05:41]
   Run Time: 00:01:53
   Function Evaluations: 37
```

MCalibration® is a product of Veryst Engineering

Material Model Calibration

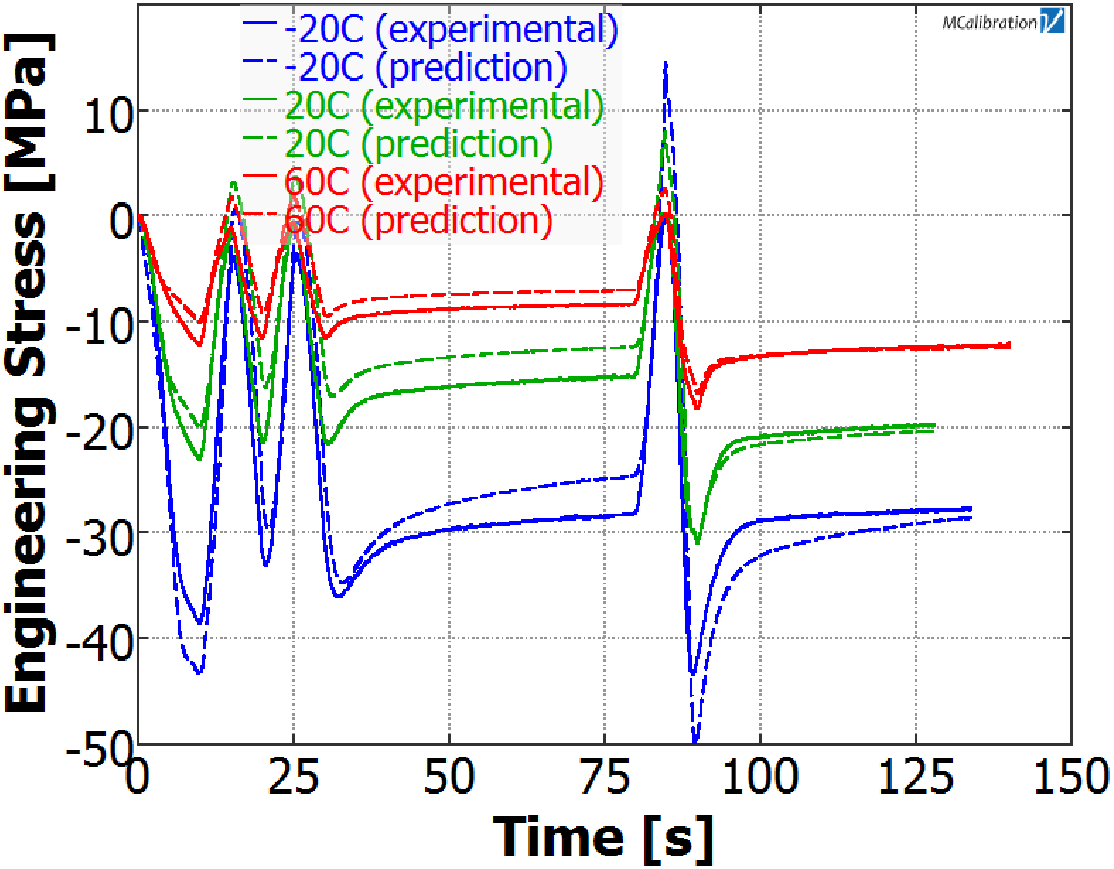
- Fit to cyclic compression data



- Solid lines are experimental results
- Dashed lines are material model predictions
- Good overall fit to compression data including behaviour at large strains, strain rate dependence and temperature dependence

Material Model Calibration

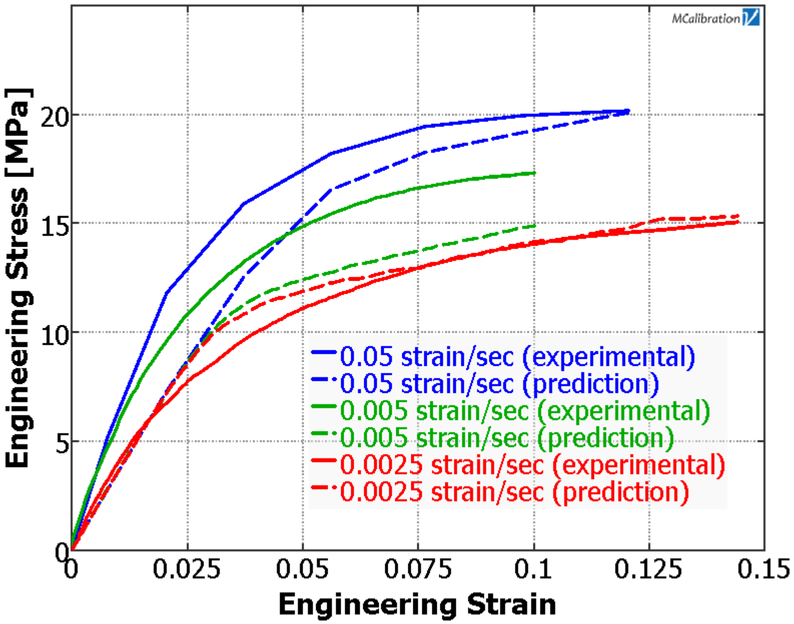
- Fit to cyclic compression data



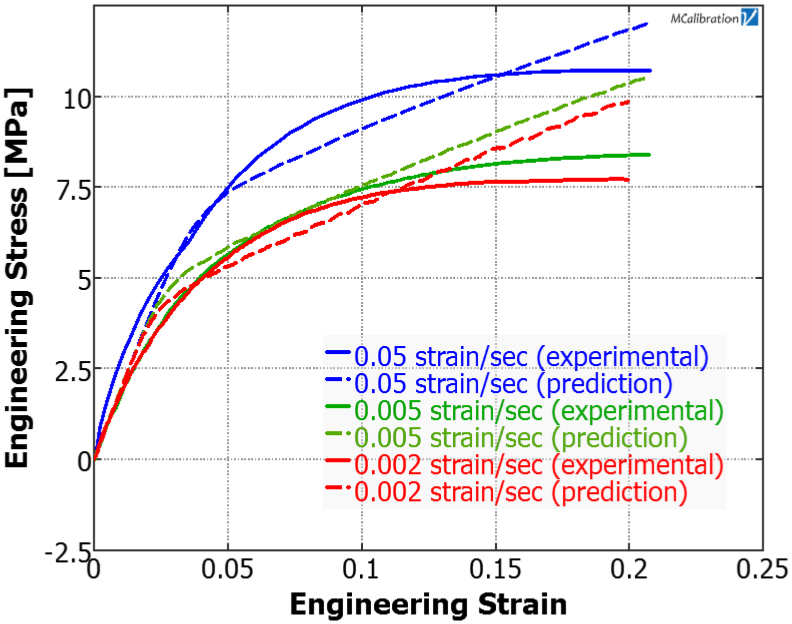
- Solid lines are experimental results
- Dashed lines are material model predictions
- Good overall fit to compression data including behaviour at large strains, strain rate dependence and temperature dependence

Material Model Calibration

- Relatively good fit also obtained for tension data at different temperatures



Tensile data at 20°C



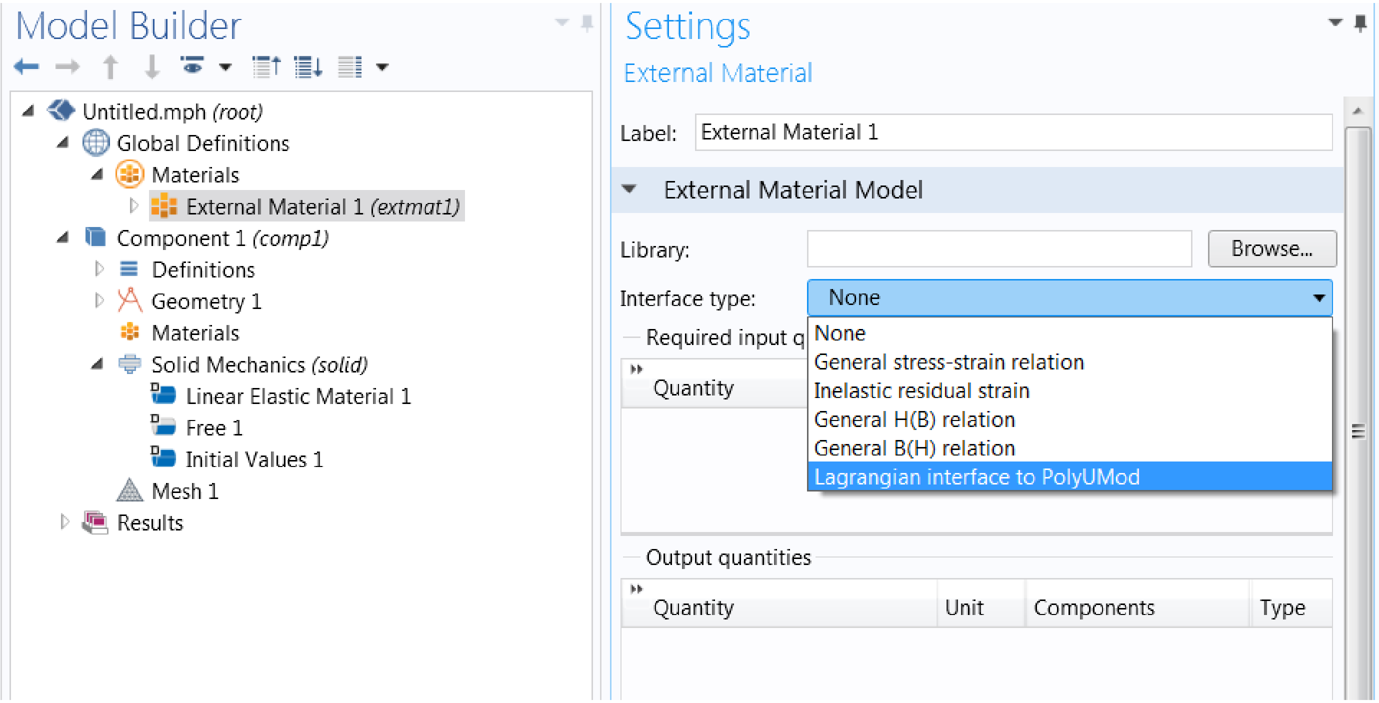
Tension data at 60°C

COMSOL Implementation

- The material equations are input directly to COMSOL Multiphysics
    - A weak form for the hyperelastic networks
    - Domain level ordinary differential equations (ODEs) for the viscous terms
- The implementation does not involve C or FORTRAN code linked to the FE program through pre-defined subroutines

COMSOL Implementation

- A different approach is now with the External Material functionality introduced in version 5.2!



Label: External Material 1

Library:

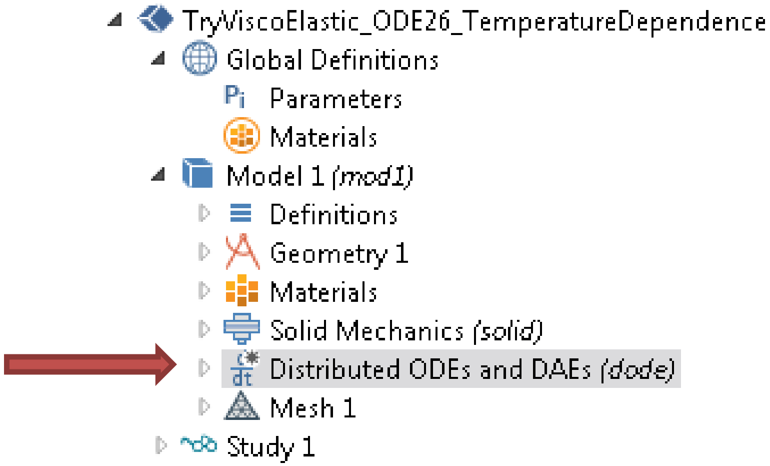
Interface type: None

COMSOL Implementation

- COMSOL supports general user-defined ODEs of the form

$$f(u, \dot{u}, \ddot{u}) = 0$$

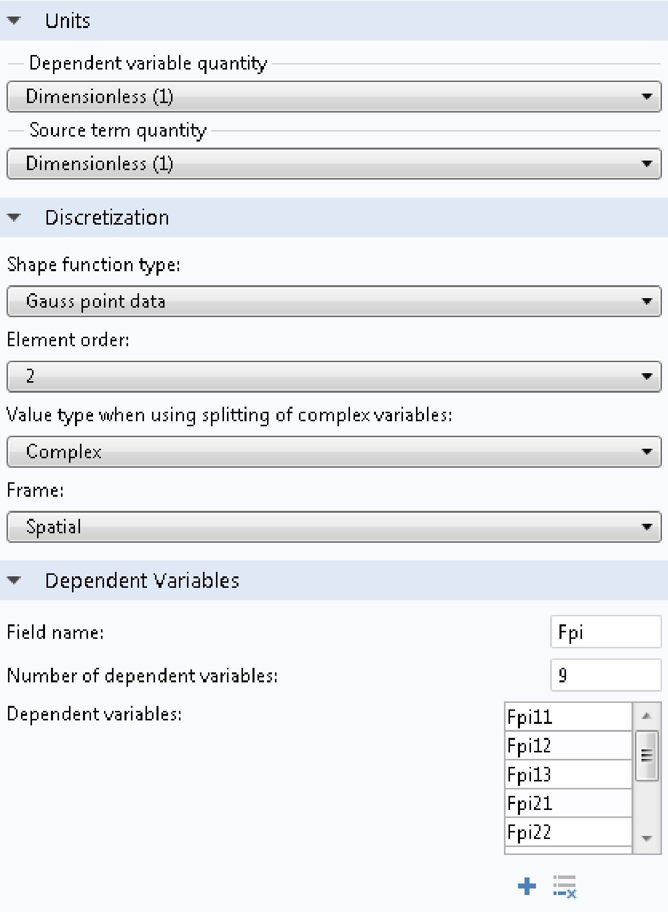
  - where u is an independent variable coupled directly and through its time derivatives to virtually any other variable in the finite element model



- TryViscoElastic_ODE26_TemperatureDependence
  - Global Definitions
    - Parameters
    - Materials
  - Model 1 *(mod1)*
    - Definitions
    - Geometry 1
    - Materials
    - Solid Mechanics *(solid)*
    - Distributed ODEs and DAEs *(dode)*
    - Mesh 1
  - Study 1

COMSOL Implementation

- Network B implementation
  - We selected the components of the inverse of the inelastic deformation gradient $\mathbf{F}_\mathrm{v}^{-1}$ as the independent variables for the ODEs
  - Selected element order and shape functions



Units

Dependent variable quantity

Dimensionless (1)

Source term quantity

Dimensionless (1)

Discretization

Shape function type:

Gauss point data

Element order:

2

Value type when using splitting of complex variables:

Complex

Frame:

Spatial

Dependent Variables

Field name: Fpi

Number of dependent variables: 9

Dependent variables:

Fpi11

Fpi12

Fpi13

Fpi21

Fpi22

COMSOL Implementation

- Network B implementation
  - Implemented the following deviatoric strain energy function

$$W_{Dev}(\mathrm{I}_{1e}^{*}, \mathrm{I}_{2e}^{*}) = C_{10}(\mathrm{I}_{1e}^{*} - 3) + C_{01}(\mathrm{I}_{2e}^{*} - 3)$$

  - where

$$\mathbf{C}_{\mathrm{e}} = \mathbf{F}_{\mathrm{v}}^{-\mathrm{T}}\mathbf{C}\,\mathbf{F}_{\mathrm{v}}^{-1}$$

$$\mathrm{I}_{1\mathrm{e}} = \mathrm{trace}(\mathbf{C}_{\mathrm{e}})$$

$$\mathrm{I}_{1\mathrm{e}}^{*} = \mathrm{J}^{-\frac{2}{3}}\mathrm{I}_{1\mathrm{e}}$$

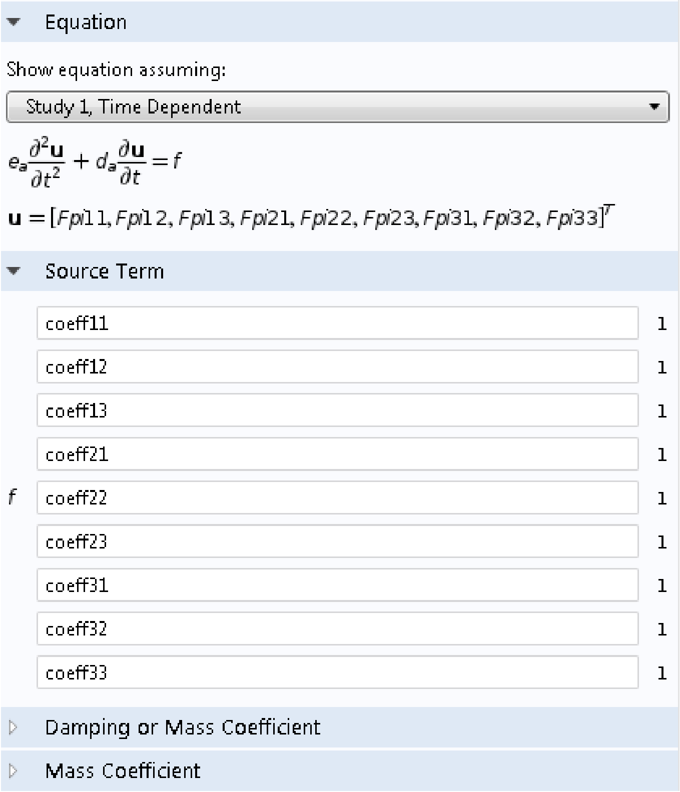
$$\mathrm{I}_{2\mathrm{e}} = \frac{1}{2}{\mathrm{I}_{1\mathrm{e}}}^{2} - \mathrm{trace}\left({\mathbf{C}_{\mathrm{e}}}^{2}\right)$$

$$\mathrm{I}_{2\mathrm{e}}^{*} = \mathrm{J}^{-\frac{4}{3}}\mathrm{I}_{2\mathrm{e}}$$

COMSOL Implementation

- Network B implementation
  - Evolution equation for $\mathbf{F}_v^{-1}$

$$\frac{d}{dt}[\mathbf{F}_v^{-1}] = -\dot{\gamma}\mathbf{F}_v^{-1}\frac{\mathrm{dev}[\mathbf{F}_v^{-T}\mathbf{U}^{*2}\mathbf{F}_v^{-1}]}{||\mathrm{dev}[\mathbf{B}_e^{*}]||}$$



Equation

Show equation assuming:

Study 1, Time Dependent

$$e_a\frac{\partial^2\mathbf{u}}{\partial t^2} + d_a\frac{\partial\mathbf{u}}{\partial t} = f$$

$$\mathbf{u} = [Fpi11, Fpi12, Fpi13, Fpi21, Fpi22, Fpi23, Fpi31, Fpi32, Fpi33]^T$$

Source Term

	coeff11	1
	coeff12	1
	coeff13	1
	coeff21	1
f	coeff22	1
	coeff23	1
	coeff31	1
	coeff32	1
	coeff33	1

Damping or Mass Coefficient

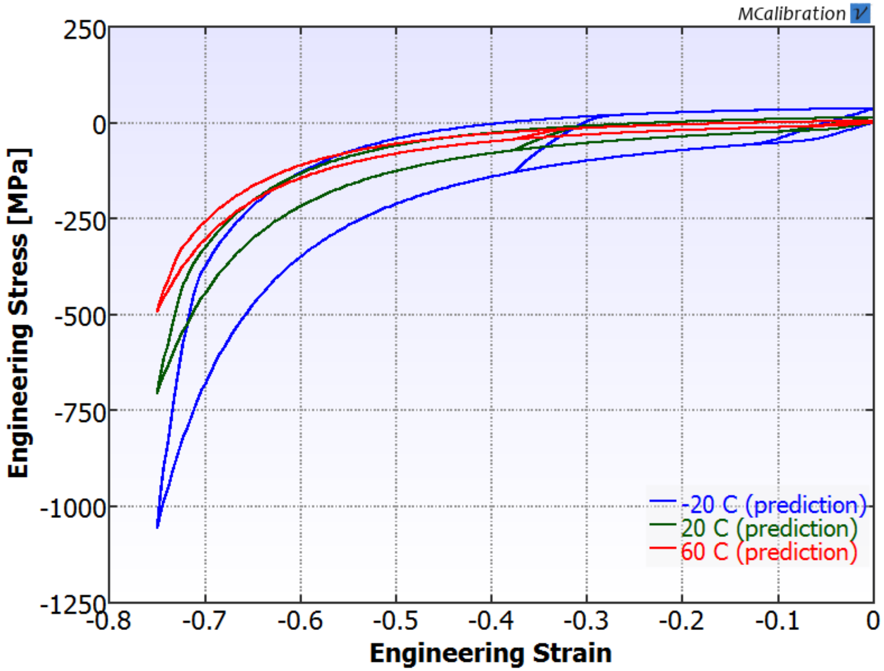
Mass Coefficient

Implementation Verification

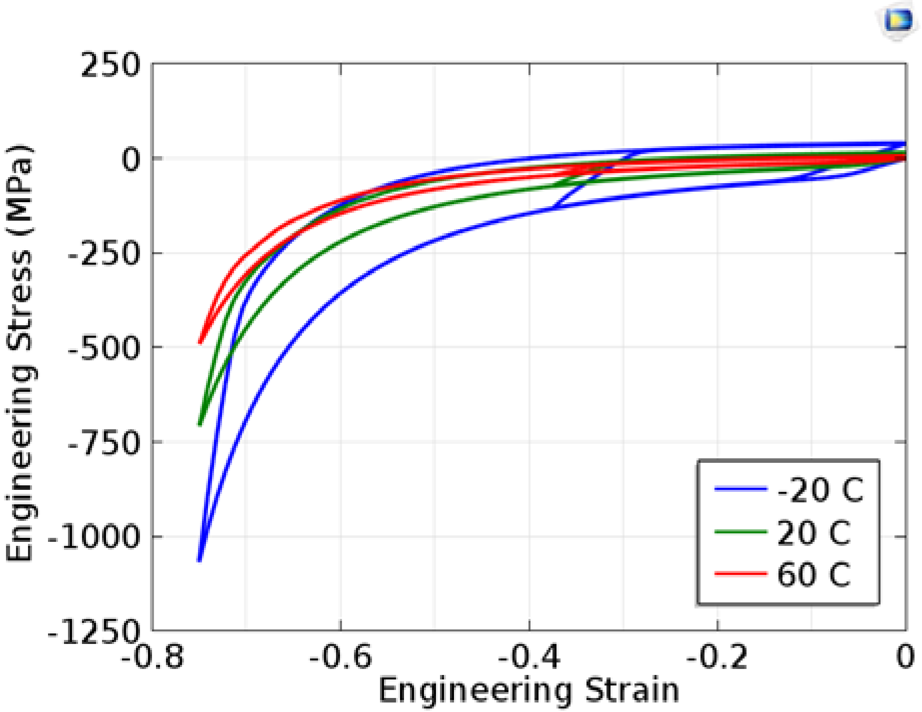
- Predictions from COMSOL model and MCalibration virtually identical for all experimental data
- We also performed numerous additional simulations for code verification, including the following:
  - Compressive loading/unloading at 3 temperatures to 37.5% and 75% compressive strain
  - Tensile loading/unloading at 3 temperatures up to 200% stretch
  - Tensile loading/unloading at 3 strain rates at 20°C up to 20% stretch

Verification: Cyclic Compression

- Loading/unloading cycles to 37.5% and 75% compressive engineering strain



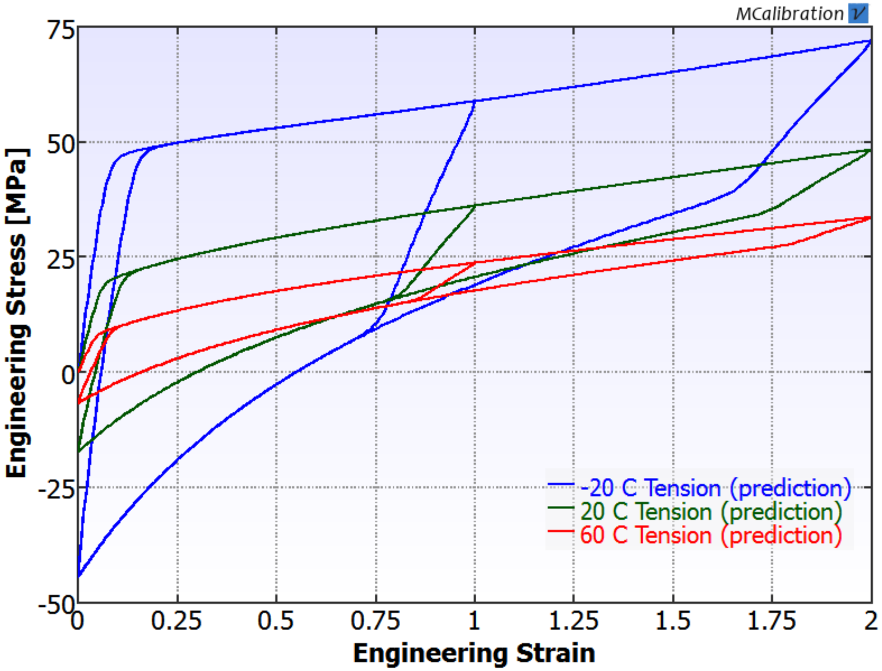
MCalibration



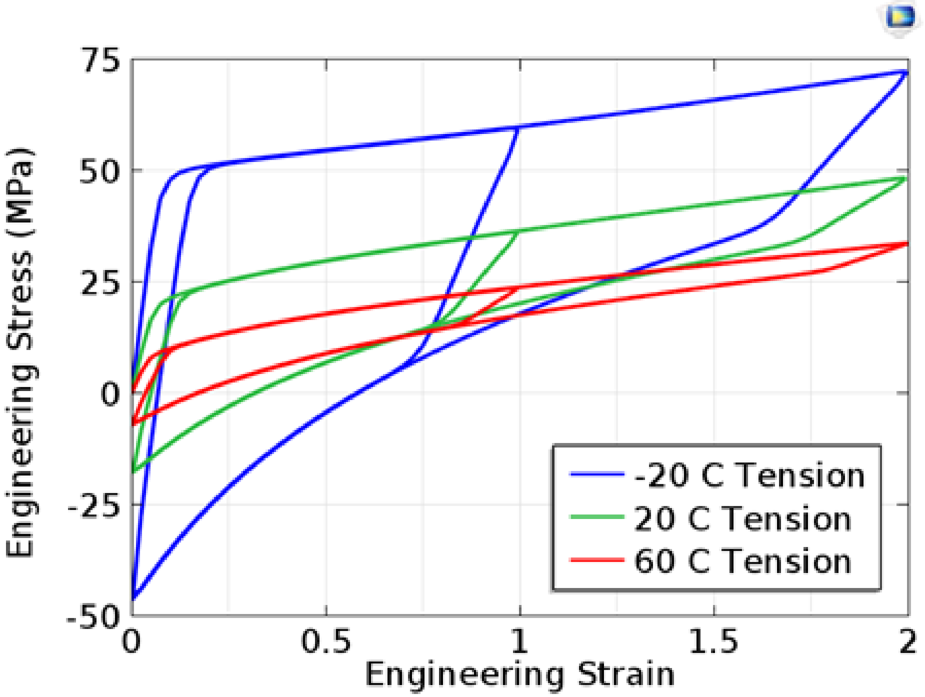
COMSOL model

Verification: Cyclic Tension

- Tensile loading/unloading cycles up to 100% and 200% stretch



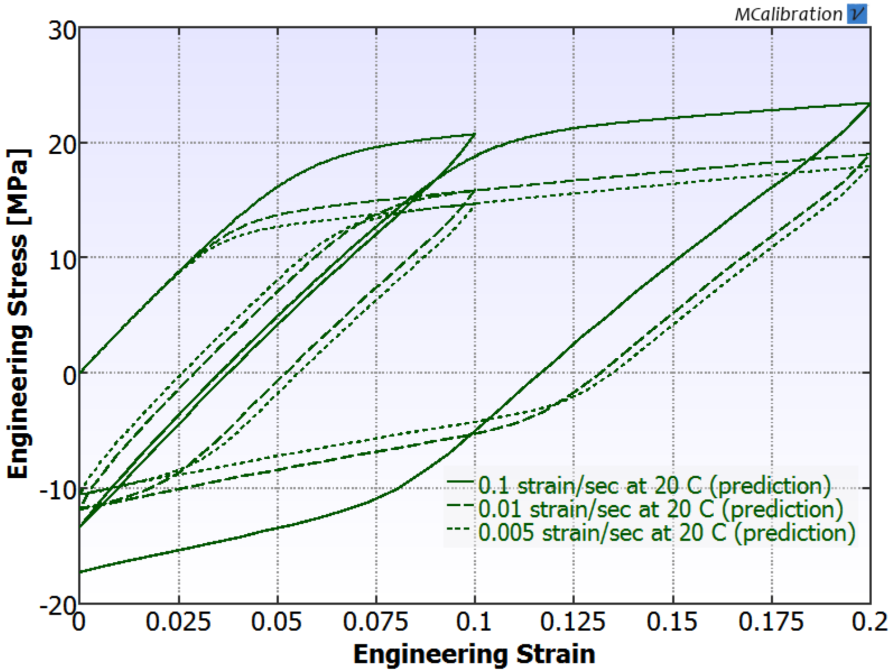
MCalibration



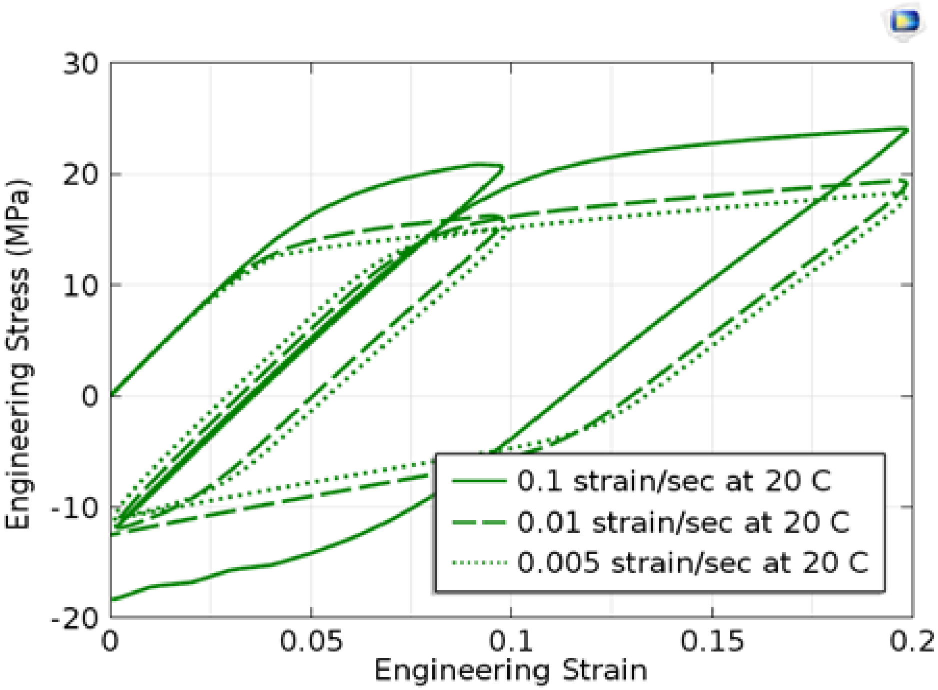
COMSOL model

Verification: Rate Dependence

- Tension at three strain rates at 20°C involving two loading/unloading cycles to 10% and 20% stretch



MCalibration



COMSOL model

Summary

- Selected a material model framework that captures the nonlinear, strain rate and temperature dependent behaviour of MDPE
- Calibrated the model calibrated to experimental tension and compression data at different temperatures and strain rates

Summary

- Implemented the material model in COMSOL Multiphysics as user-defined ordinary differential equations
- Partially verified the material model implementation for different loading modes
- COMSOL and MCalibration predictions for material behavior are virtually identical, indicating successful COMSOL implementation