Veryst Engineering | Engineering Through The Fundamentals

COMSOL CONFERENCE 2016 BOSTON

Non-Linear Mechanical Modeling of Thermoplastics using COMSOL Multiphysics

Jorgen Bergstrom, Ph.D.
Nagi Elabbasi, Ph.D.

jbergstrom@veryst.com
www.veryst.com

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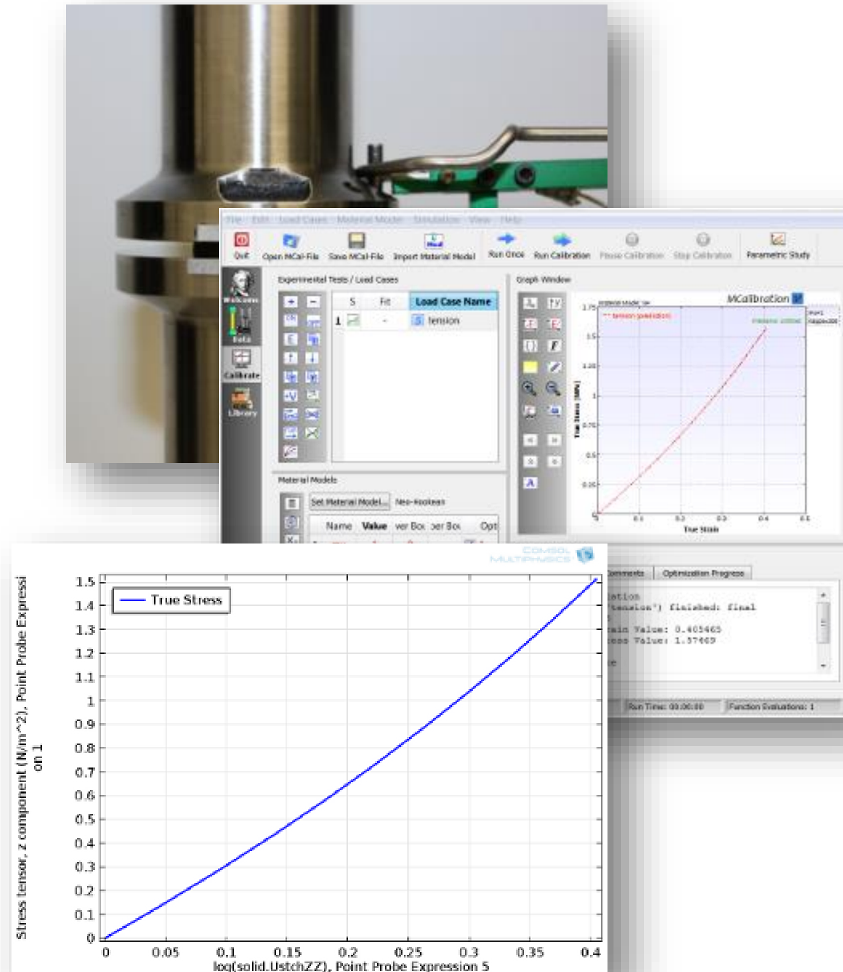
Outline

- Introduction to material models for structural FEA
- COMSOL External Material Functionality
- Example Problem: modeling of PEEK
  - Experimental data
  - Material model calibration
  - Material model validation using COMSOL
- Summary



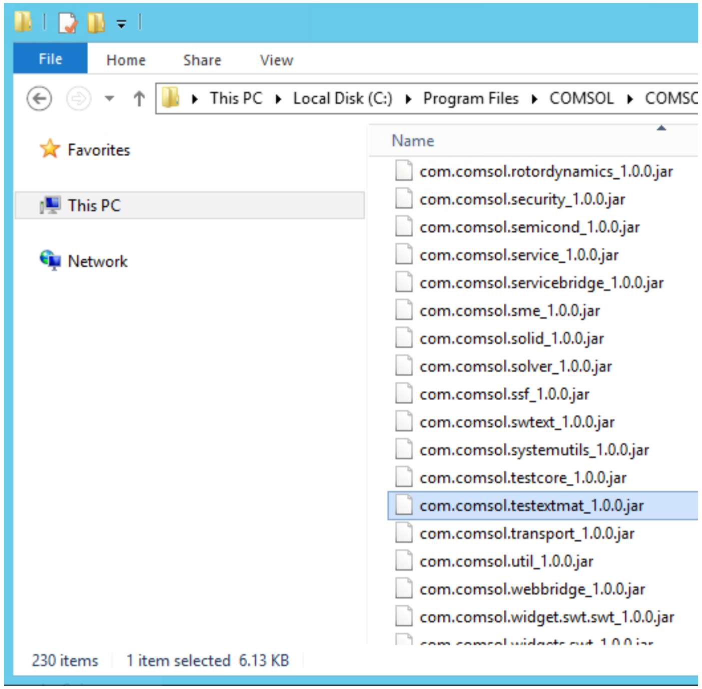
COMSOL Solid Mechanics Materials

- Elastoplastic Material
- Fatigue
- General Stress-Strain Relation
- Geomechanics Material
- Hyperelastic Material
- Linear Elastic Material
- Linear Viscoelastic Material
- Nonlinear Elastic Material
- Poroelastic Material
- External Material Functionality

Commonly used to represent polymer behavior

External Material Model with COMSOL

```
EXPORT int
eval(double *time0,          // Time at previous step, sca
     double *time1,          // Time at current step, scal
     double *temp0,          // Temperature at previous st
     double *temp1,          // Temperature at current ste
     double *F0,             // Deformation gradient at pr
     double *F1,             // Deformation gradient at cu
     double *PK2_stress,     // Second Piola-Kirchoff stre
     double *Jac,            // Jacobian d(PK2_stress[i],F
     double *elastEner,      // Elastic energy, scalar, st
     double *plastEner,      // Plastic energy, scalar, st
     int *nProps,            // Number or material model p
     double *props,          // Material model properties,
     int *nStates,           // number of states, scalar,
     double *states)         // States, nStates vector
{
    int res = 0;
    COMSOL_POLYUMOD(time0, time1, temp0, temp1, F0, F1,
            PK2_stress, Jac, elastEner, plastEner, nProps,
            props, nStates, states, &res);
    return res;
}
```

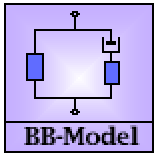


1. Write code for user-material model
2. Compile code to shared-library format
3. Copy jar-file to COMSOL plugins directory
4. Define the material parameters in COMSOL

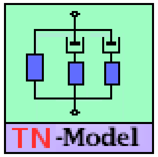
The PolyUMod library is available for COMSOL

PolyUMod Library

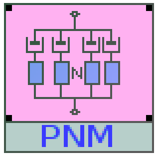
- Commercially available library available from Veryst Engineering
- More than 15 different highly accurate non-linear viscoplastic material models, e.g.:
  - Bergstrom-Boyce (BB) Model
    - *Suitable for rubbers and elastomer-like materials*
    - *Captures: strain rate effects, hysteresis*



  - Three Network (TN) Model
    - *Suitable for isotropic thermoplastics*
    - *Captures: strain rate effects, viscoplastic flow and recovery*



  - Parallel Network (TN) Model
    - *Suitable for highly non-linear and/or anisotropic materials*
    - *Captures: strain rate effects, viscoplastic flow and recovery*



Polyether Ether Ketone (PEEK)

- Good mechanical properties ($E \approx 4$ GPa, $\sigma_{ut} \approx 100$ MPa)
- Good wear resistance
- Inert, generally biocompatible
- Orthopedic applications:
  - Spinal implants/spacers
  - Fixation (screws, plates, etc.)
  - Biomedical textiles (wovens, braids)
- Sealing applications (HPHT)

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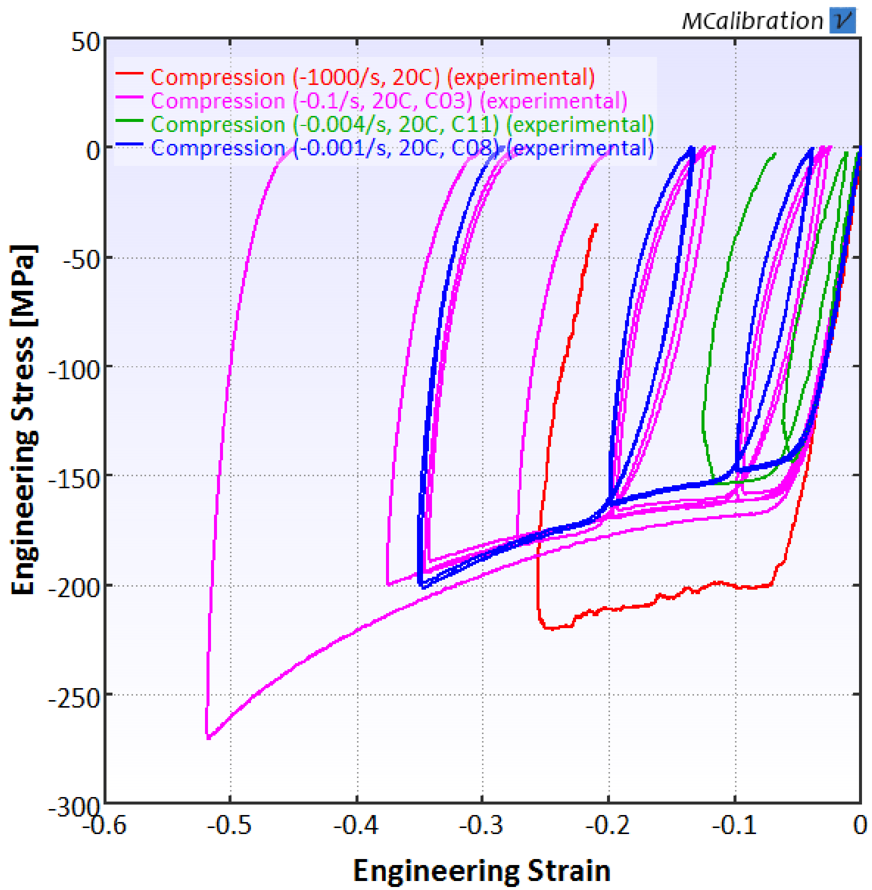
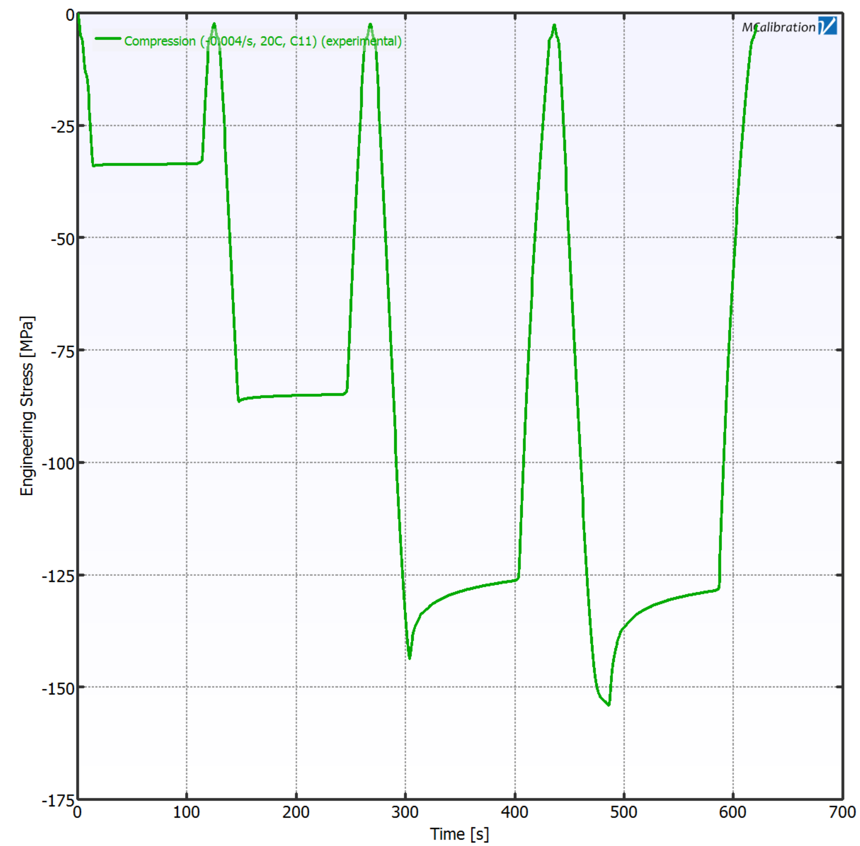
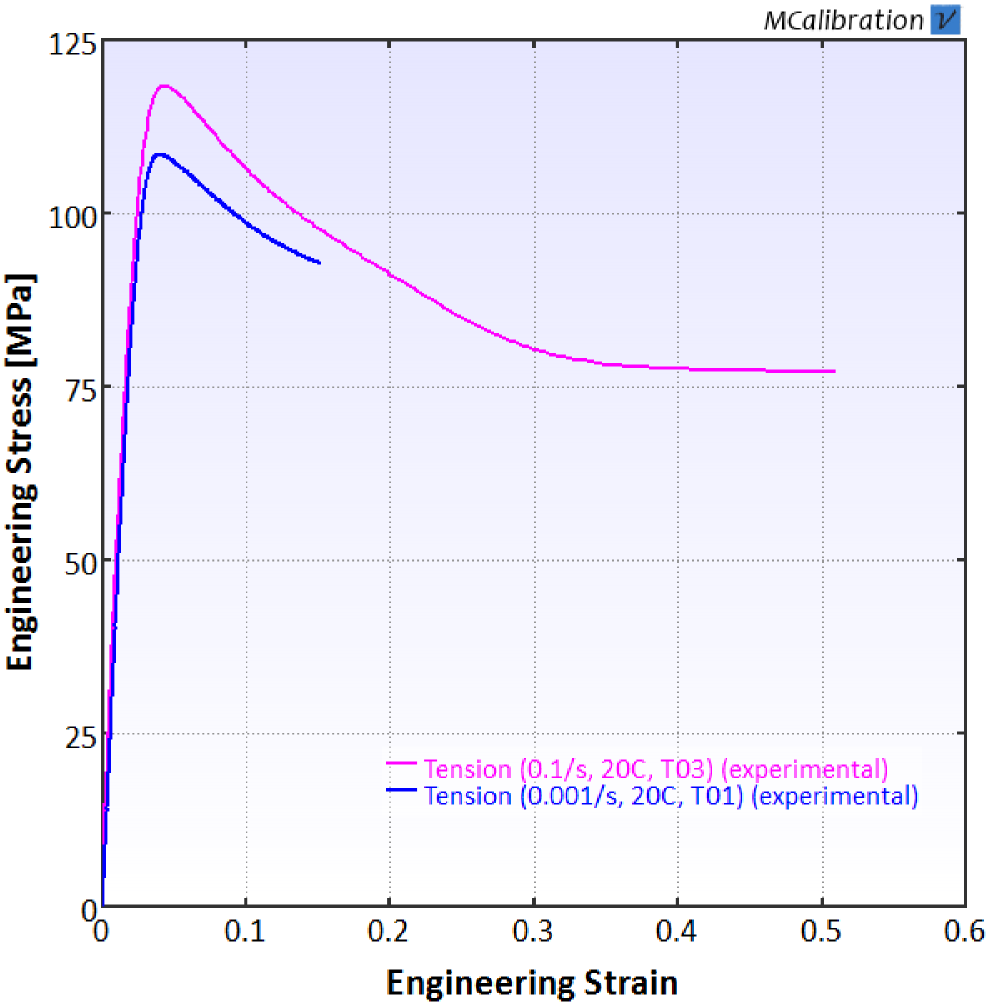
Experimental Test: Uniaxial Compression





Uniaxial Compression

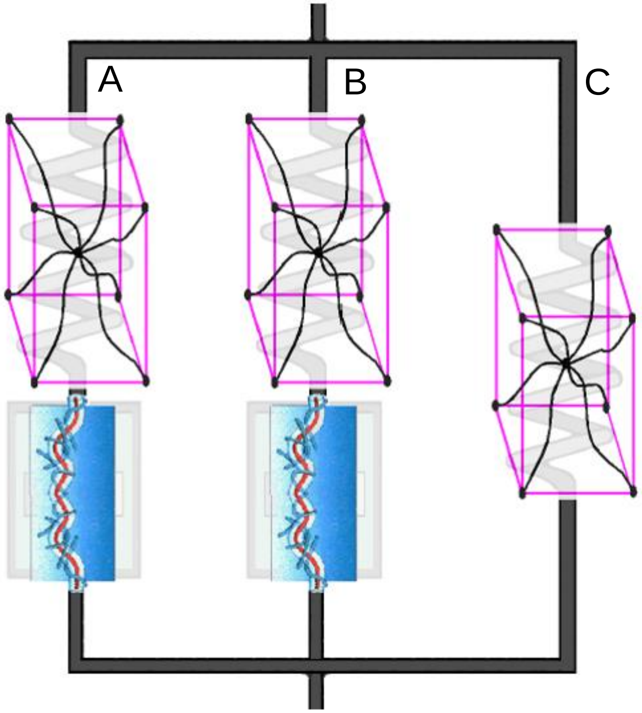
Experimental Test: Uniaxial Tension

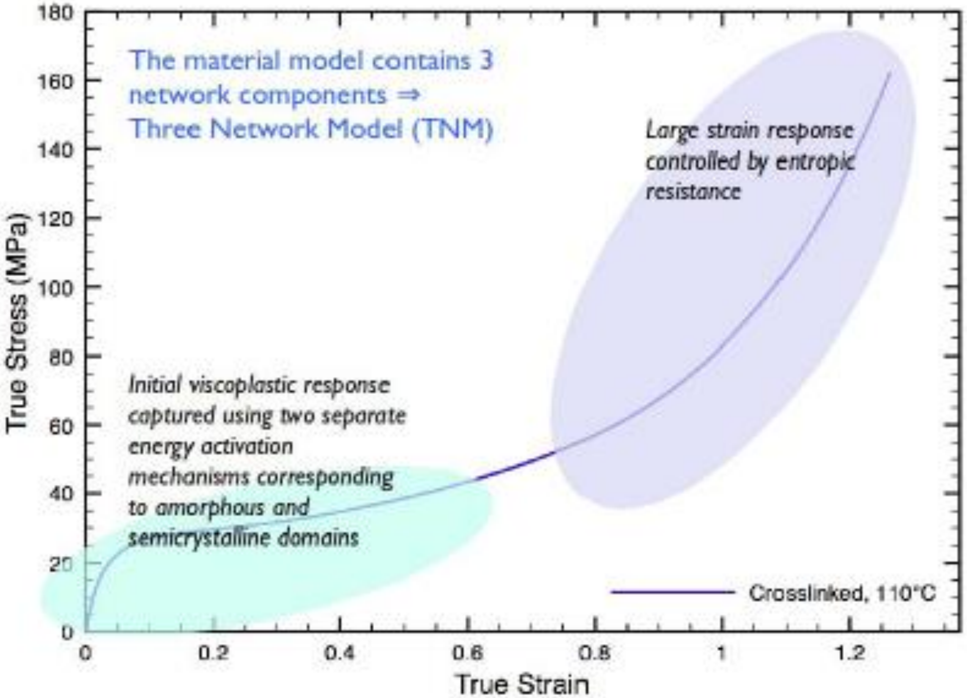


Viscoplastic response with slight softening after yield

Uniaxial Tension

Three Network (TN) Model

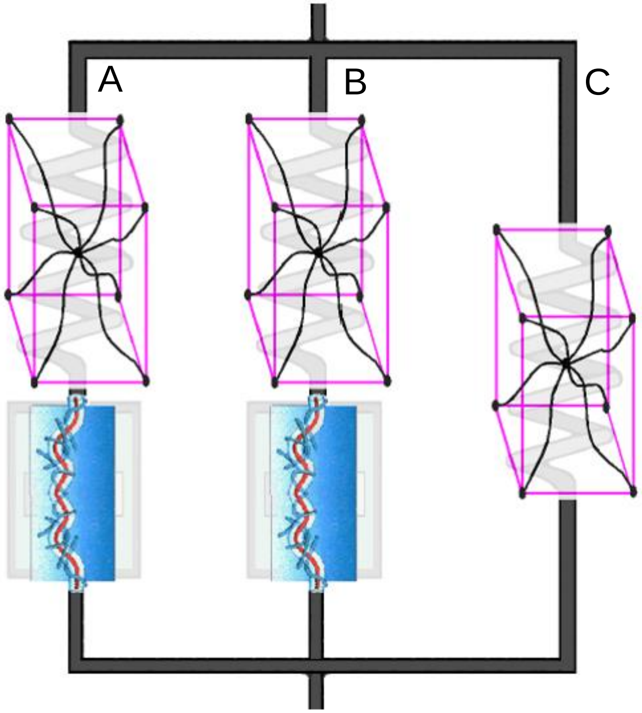




The **Three Network (TN) model** is a micromechanism inspired modeling framework suitable for thermoplastics. The TN model is available in the PolyUMod library.

Bergstrom, Bischoff, "An Advanced Thermomechanical Constitutive Model for UHMWPE," Int. J. Structural Changes in Solids, Vol 2, No 1, pp. 31-39, 2010

TN Model Theory



- The stress in each network is defined by the Arruda-Boyce Eight Chain model:

$$\sigma = \frac{\mu_A}{J^e \overline{\lambda^e}} \frac{\mathcal{L}^{-1}\left(\overline{\lambda^e}/\lambda_L\right)}{\mathcal{L}^{-1}(1/\lambda_L)} \mathrm{dev}[b^e] + \kappa(J^e - 1)\mathbf{1}$$

- The shear modulus in Network 2 evolves with the plastic strain:

$$\dot{\mu} = -\beta\left[\mu_i - \mu_f\right]\dot{\gamma}$$

- The flow in each network is defined by a reptation inspired equation:

$$\dot{\gamma} = \dot{\gamma}_0 \left(\frac{\tau}{\hat{\tau} + aR(p)}\right)^m$$

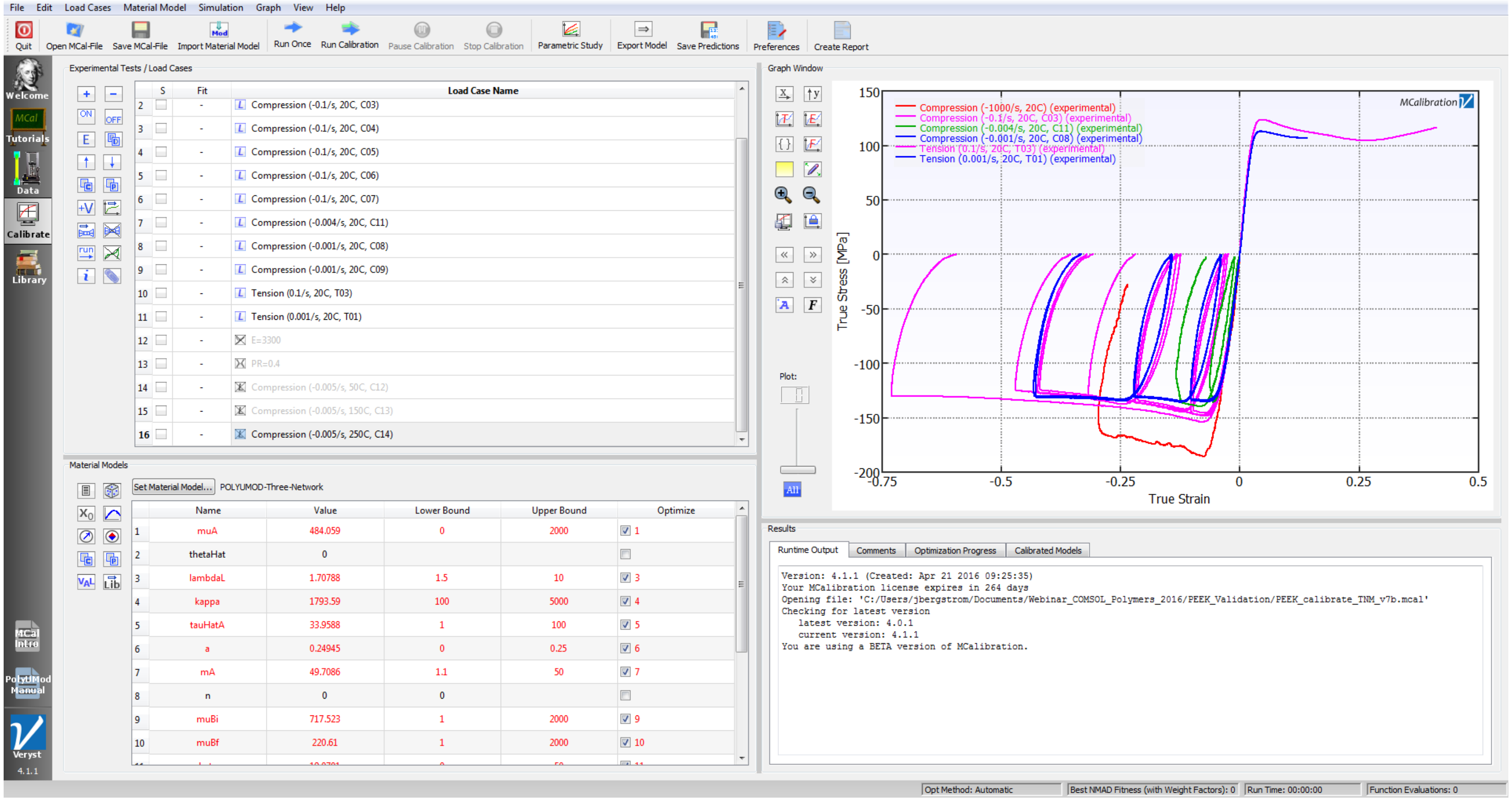
TN Model Parameters

Index	Symbol	Parameter 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, f = frequency

- The TN model needs up to 17 parameters that need to be determined from experimental data

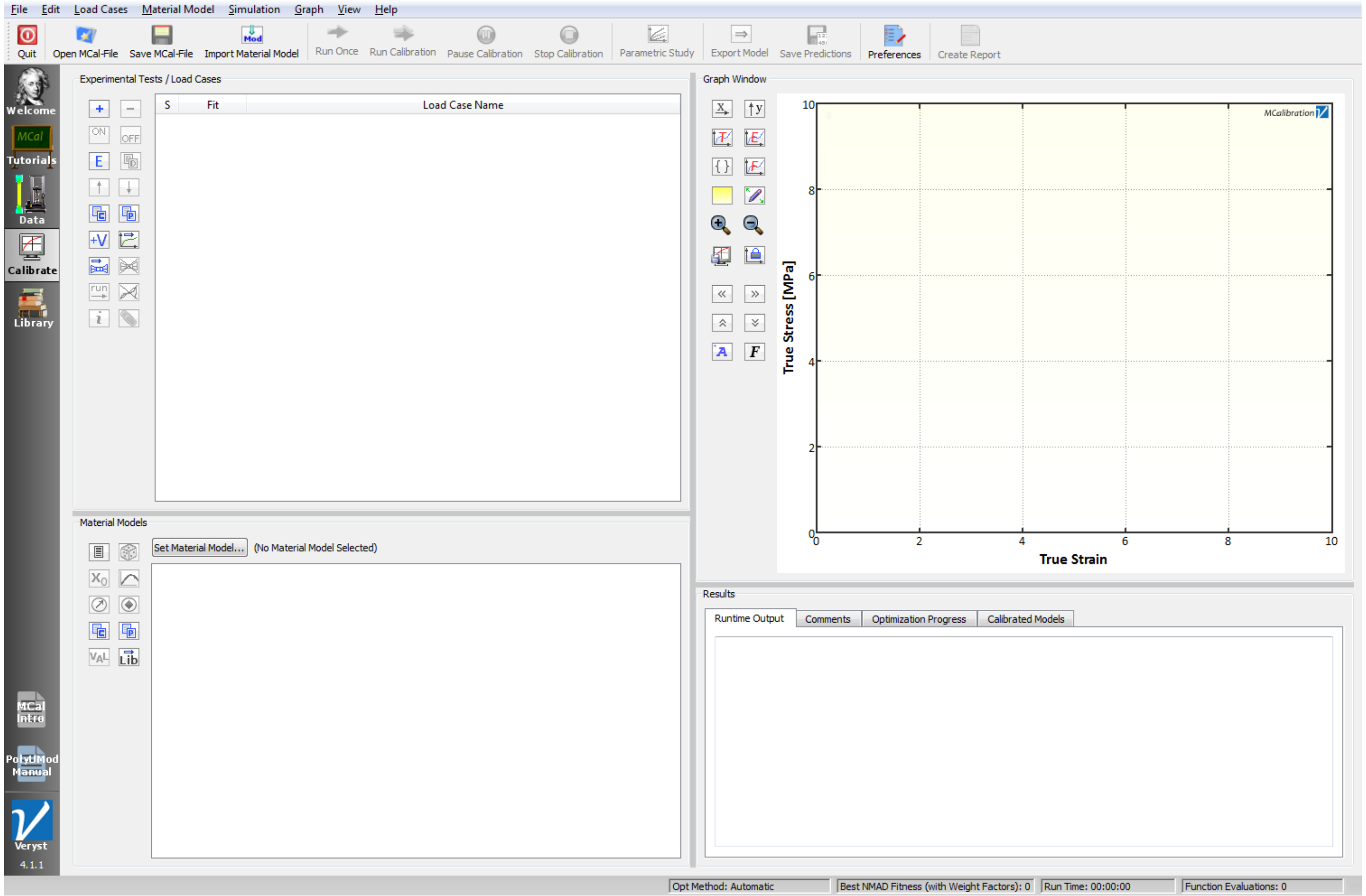
Material Model Calibrations



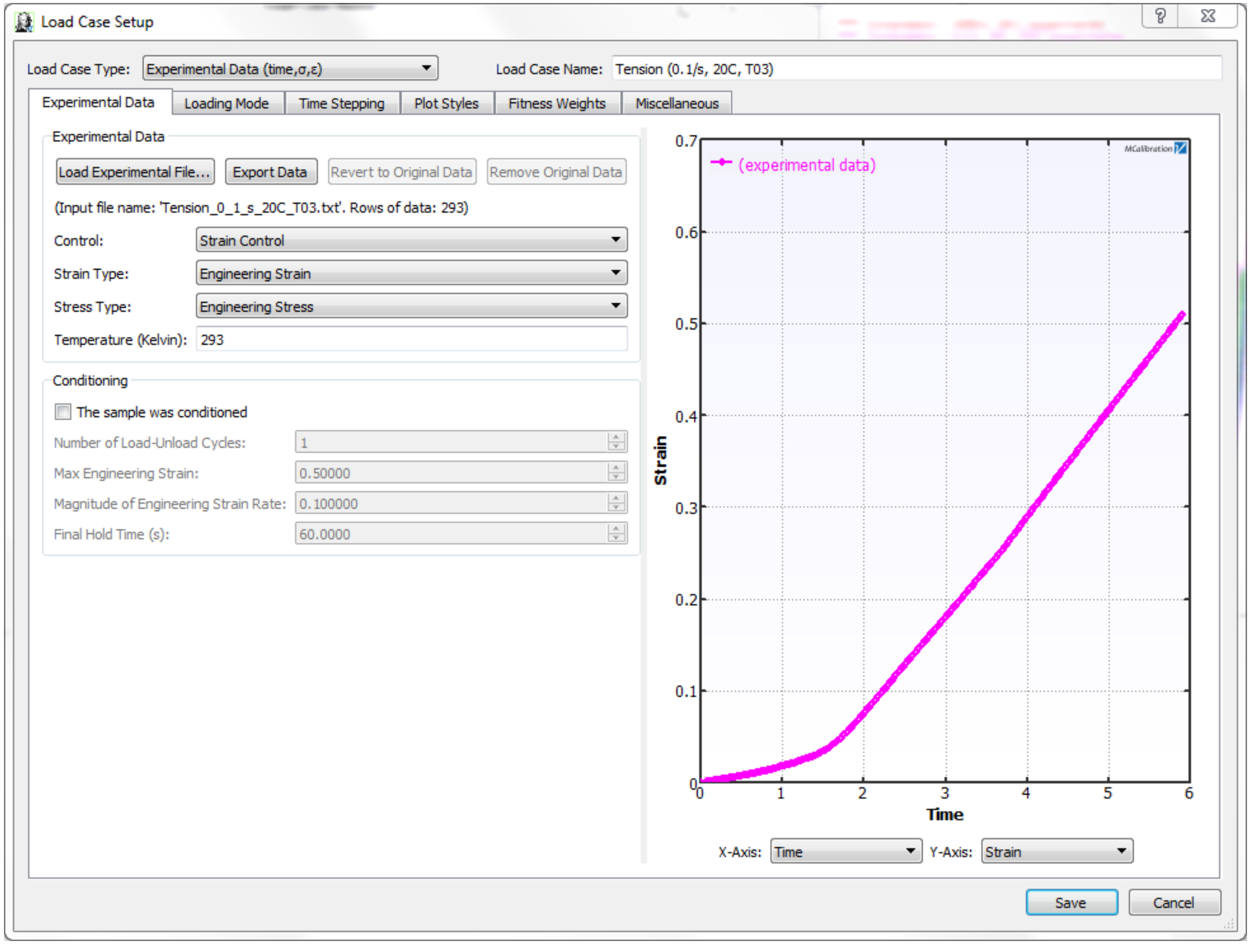
The TN model was calibrated using the MCalibration® software from Veryst Engineering.

MCalibration Example - 1

- Start the software and read in the experimental data

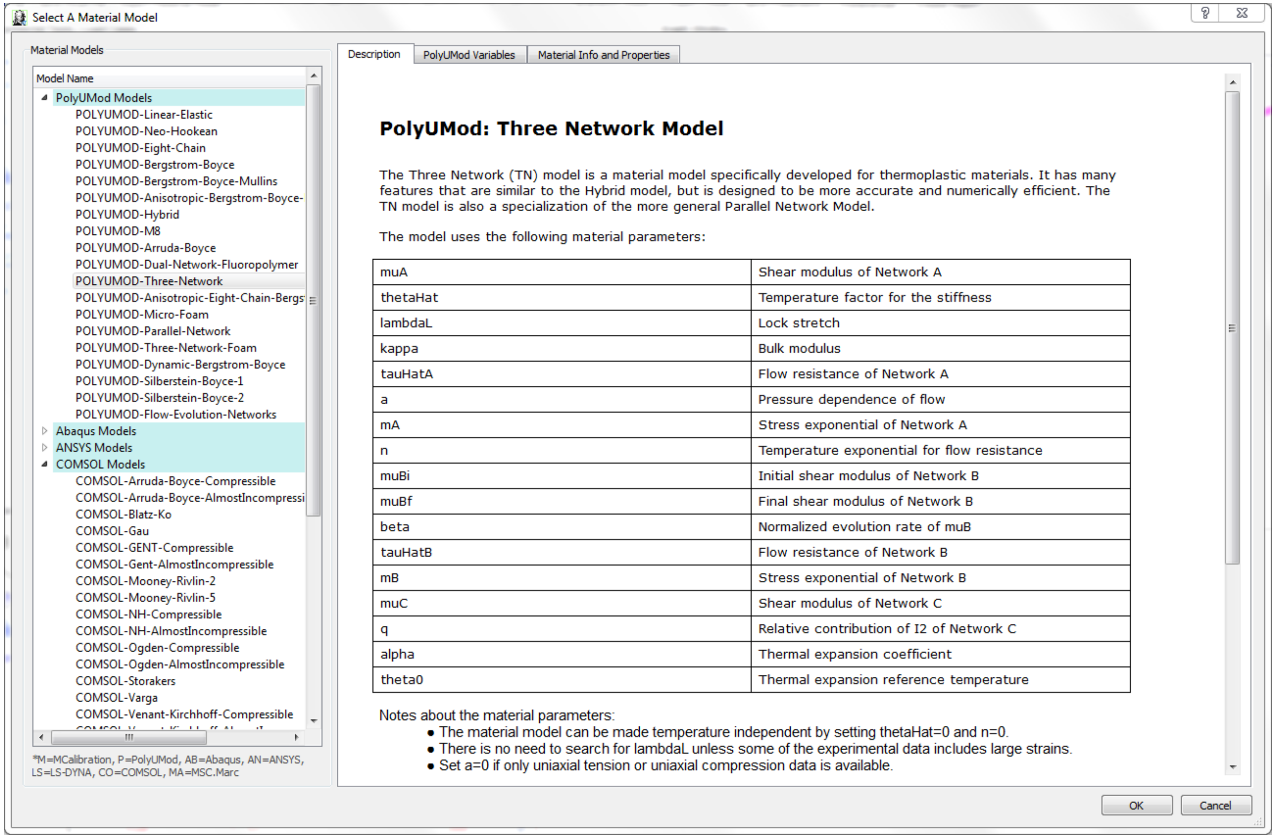


MCalibration Example – 2



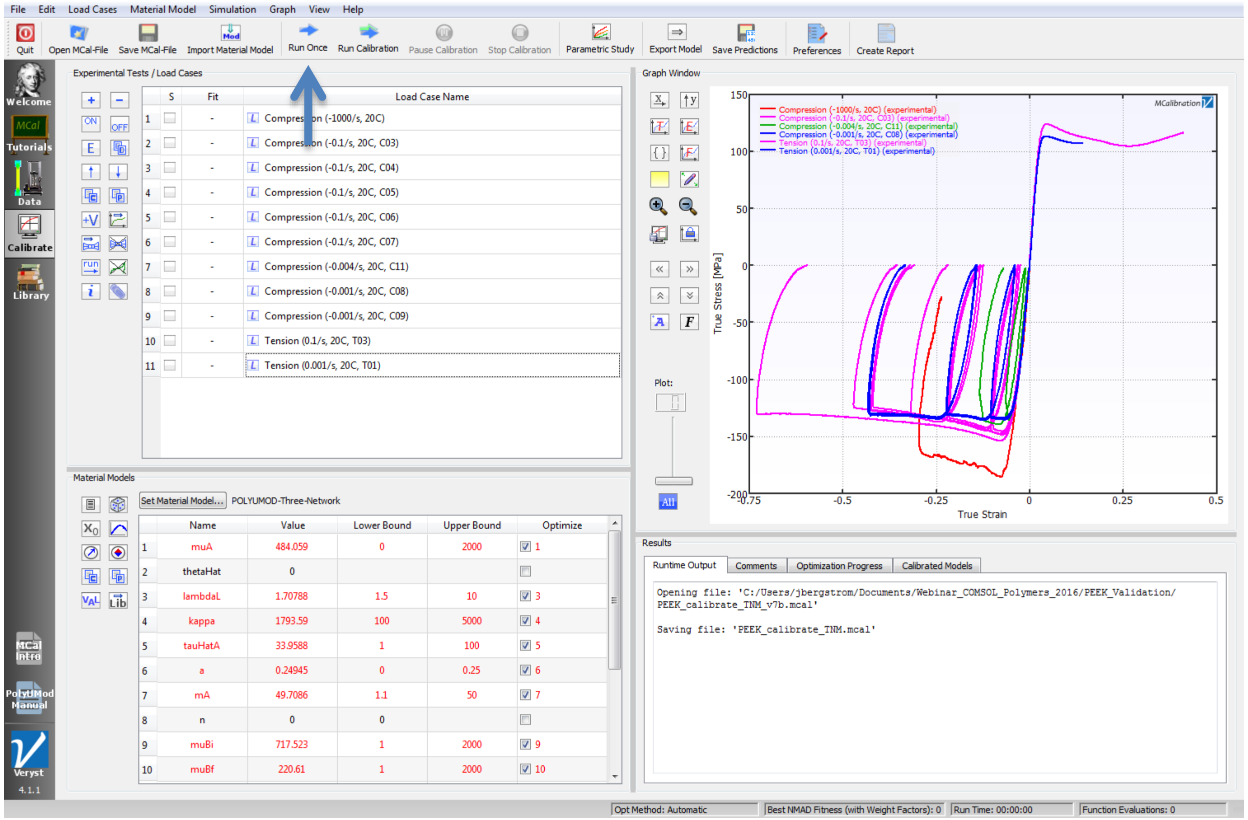
- The experimental data is loaded using a Load Case dialog
- This figure shows a tension load case
- Repeat this step for all experiments

MCalibration Example – 3



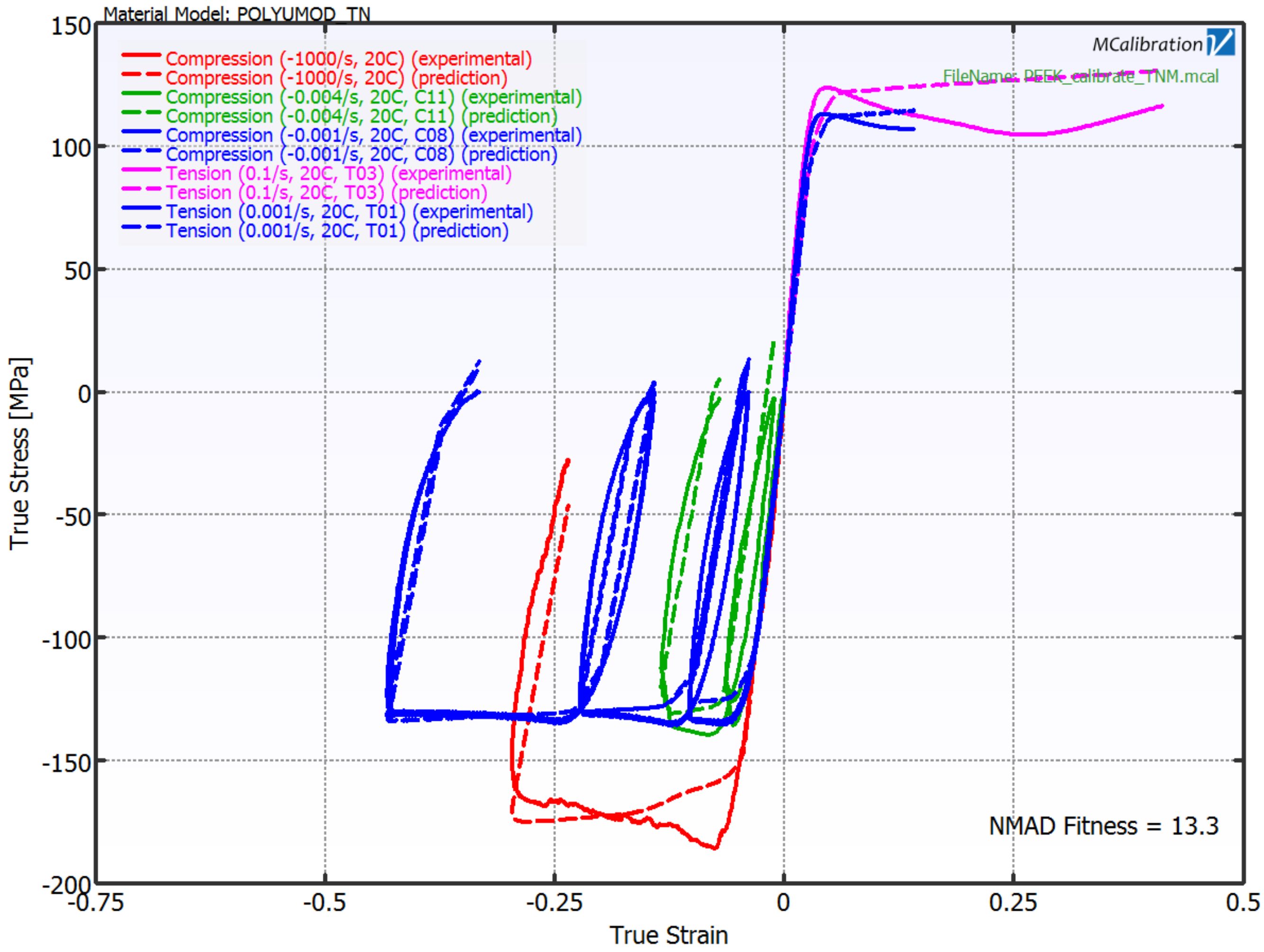
- Then select a material model to calibrate
- In this example we will select the TN model

MCalibration Example – 4



- Then simply click “Run Calibration” to automatically adjust the material parameters to best match the experimental data
- The stress calculations are performed within MCalibration

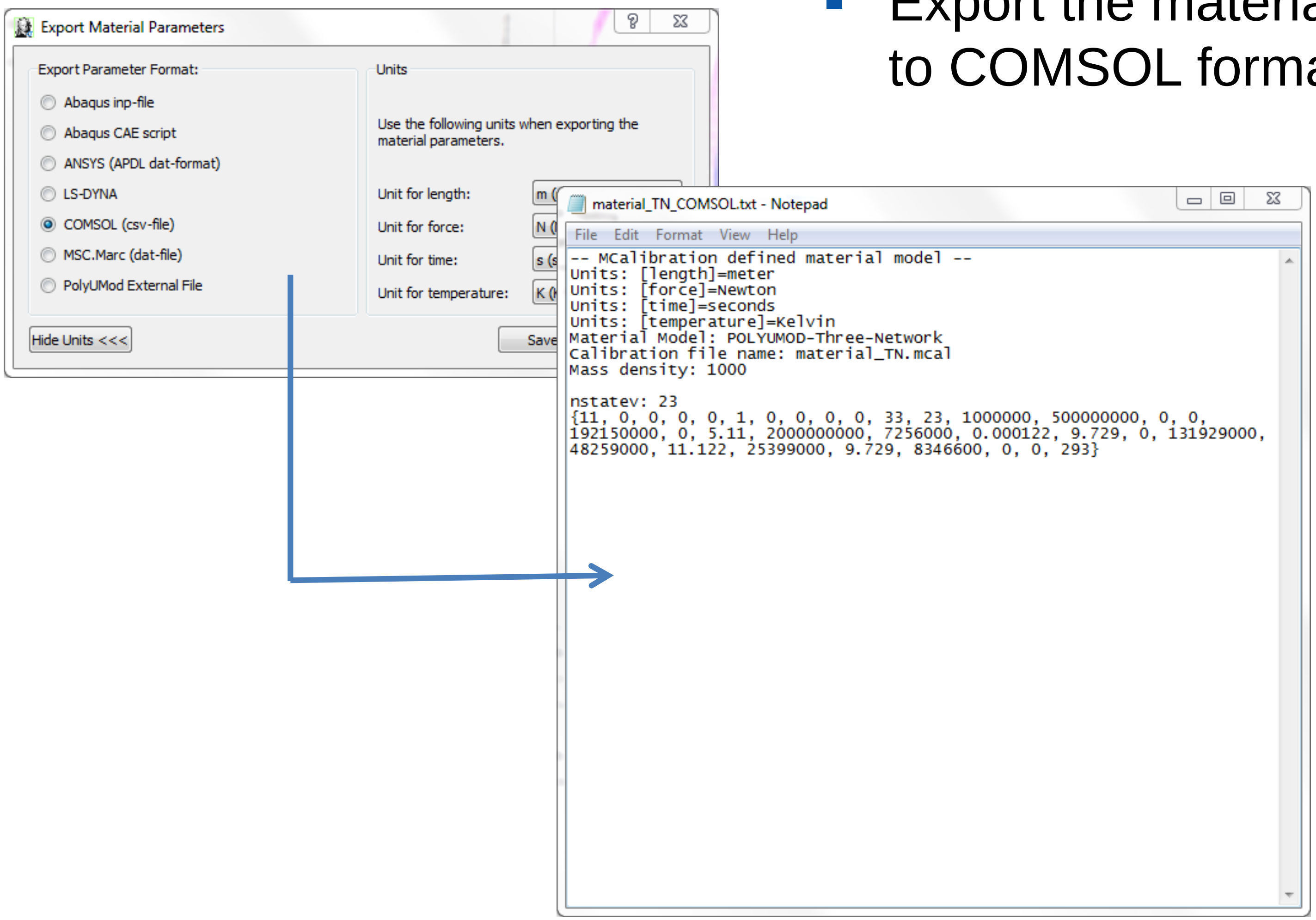
MCalibration Example – 5



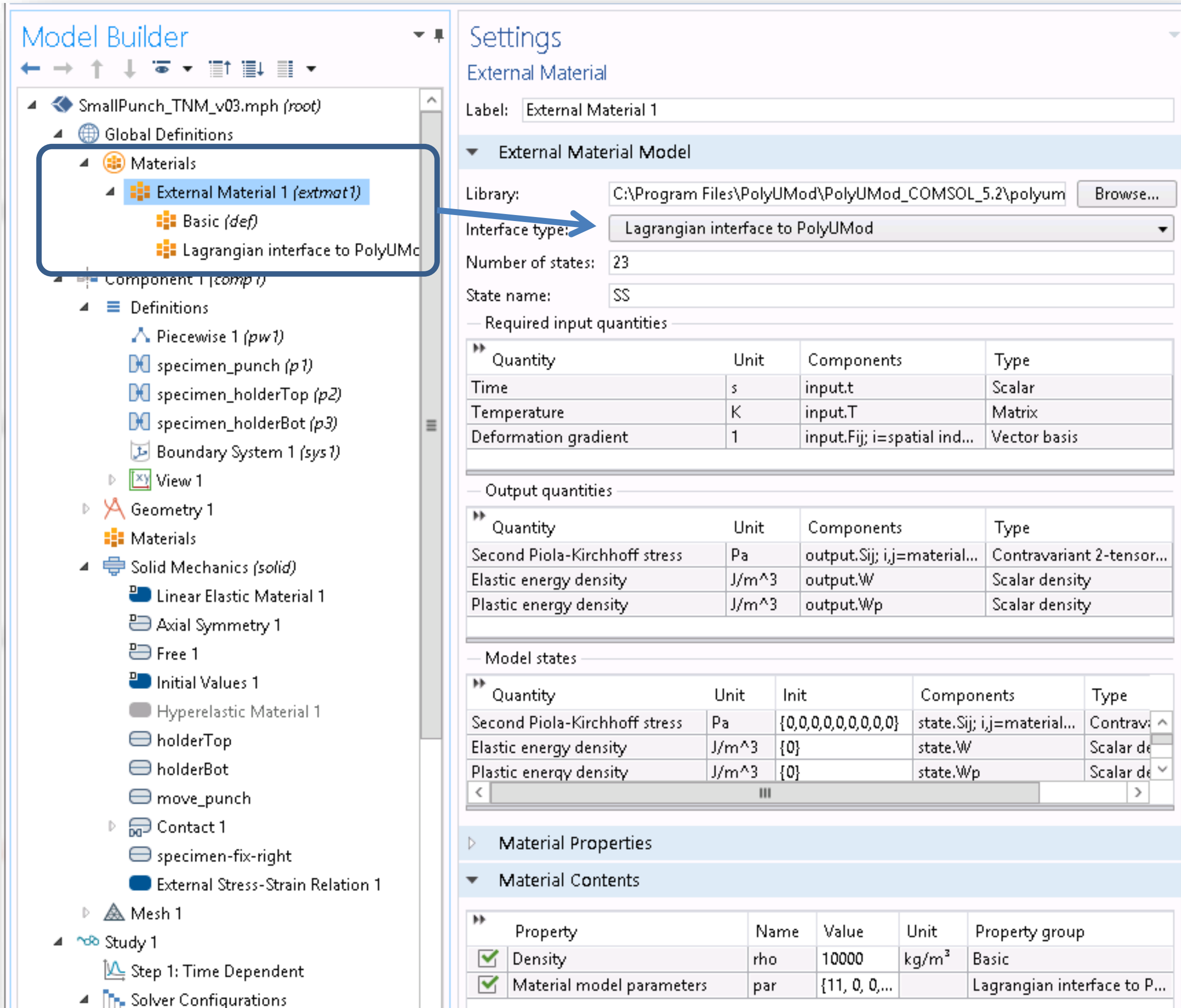
- Comparison between experimental data and material model predictions
- The TN model accurately captures the uniaxial tension and compression response

MCalibration Example - 6

- Export the material model to COMSOL format

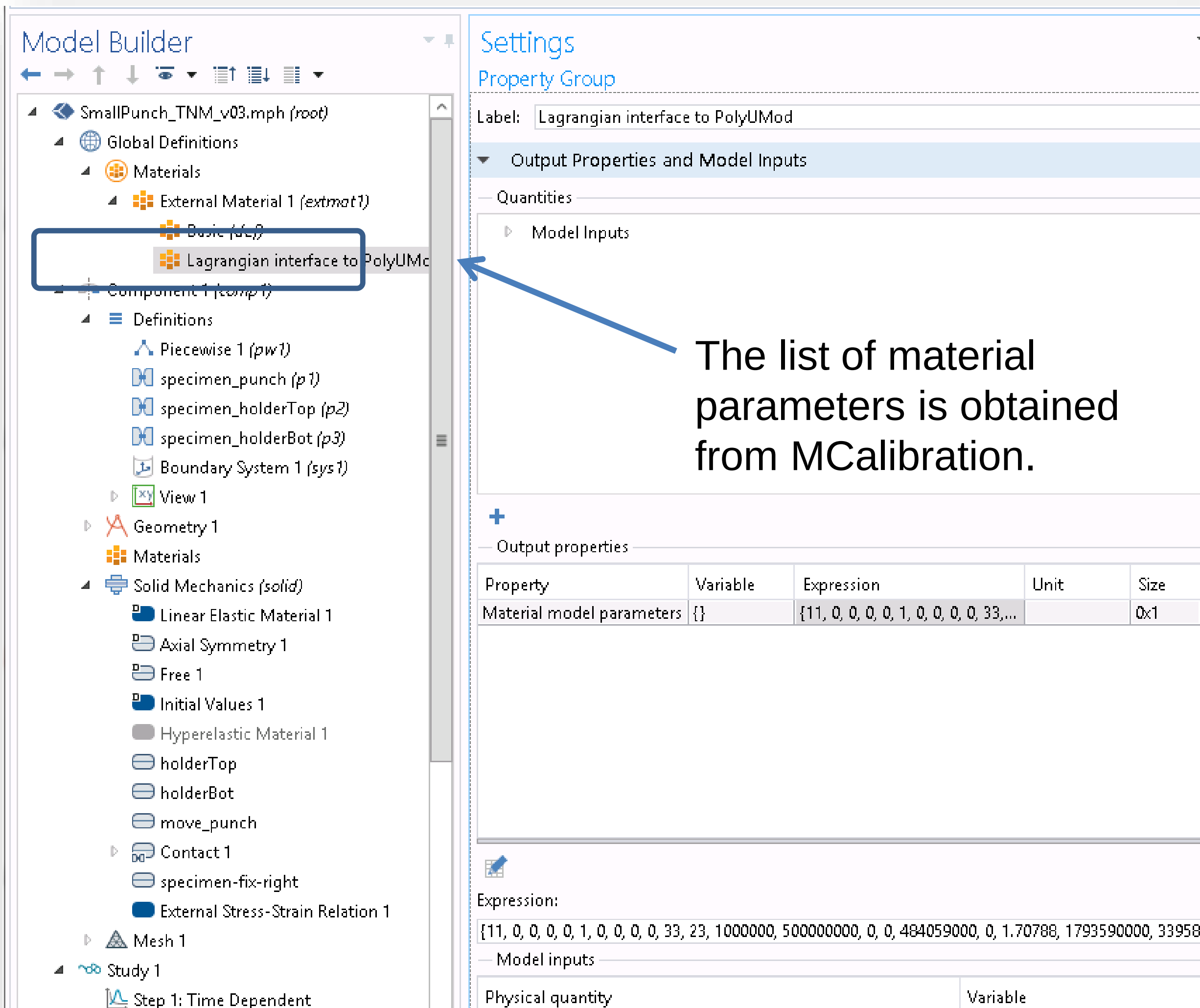


MCalibration Example - 7



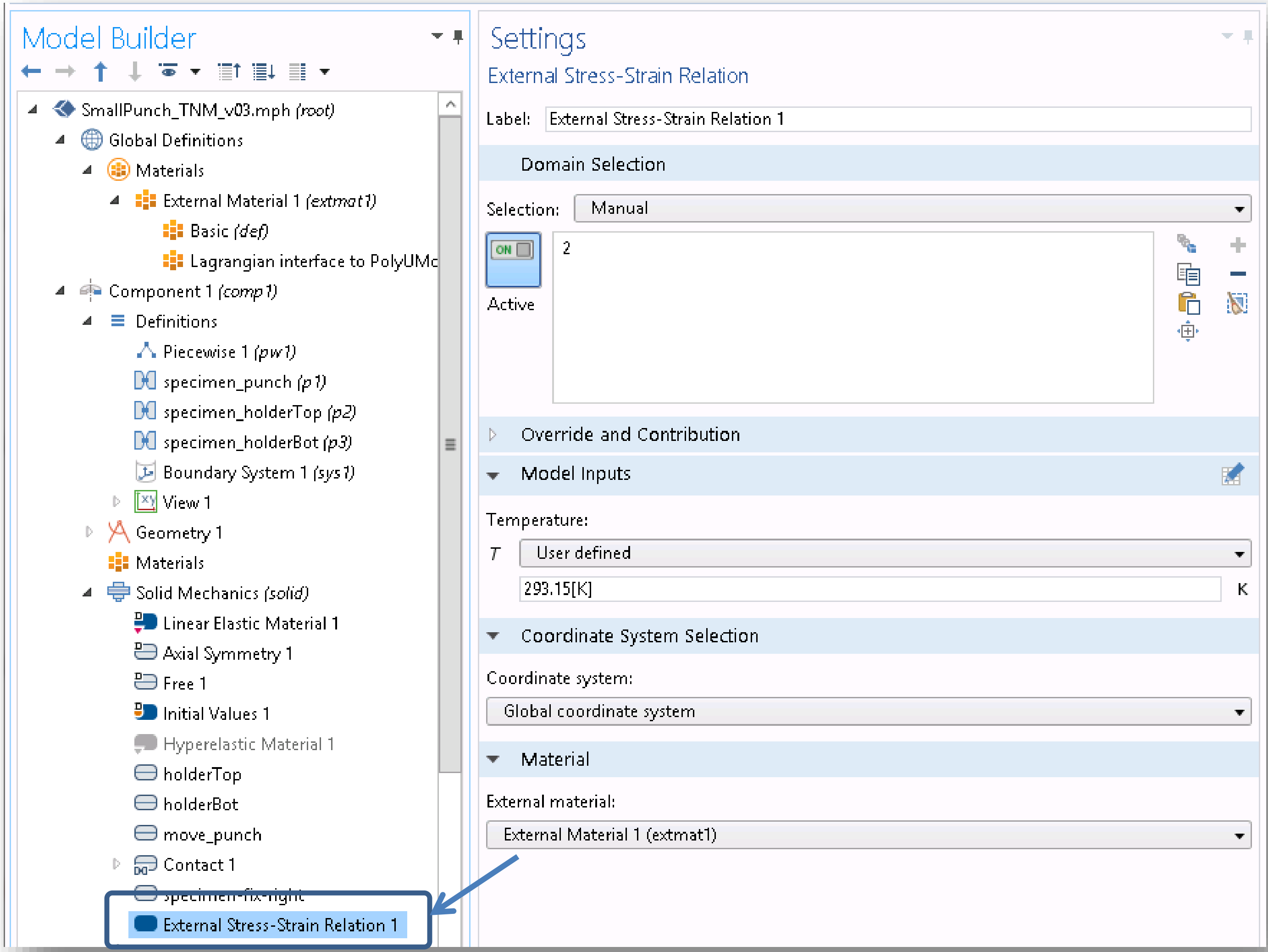
- The calibrated material model can then be entered into COMSOL Version 5.2 (and later) using the interface for external material models
- This interface can be used to model advanced nonlinear viscoplastic material models using the PolyUMod® library from Veryst Engineering

COMSOL External Material Functionality

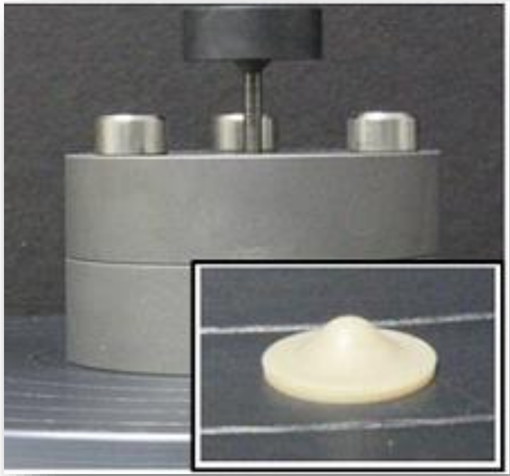


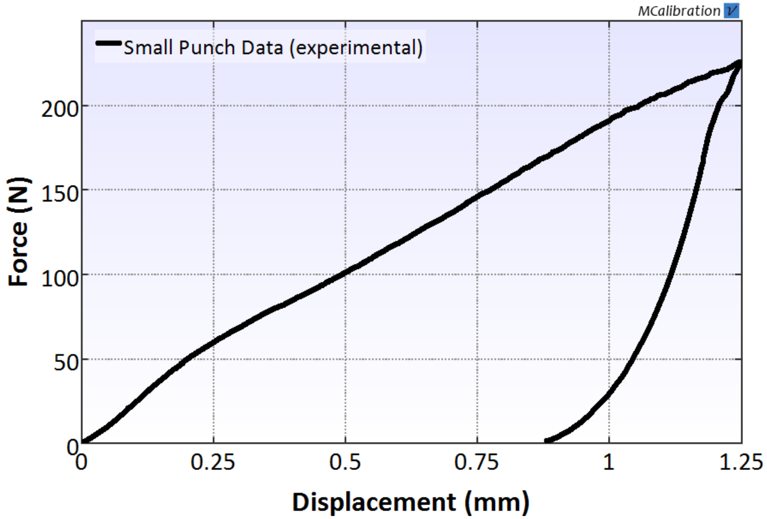
The list of material parameters is obtained from MCalibration.

COMSOL External Material Functionality

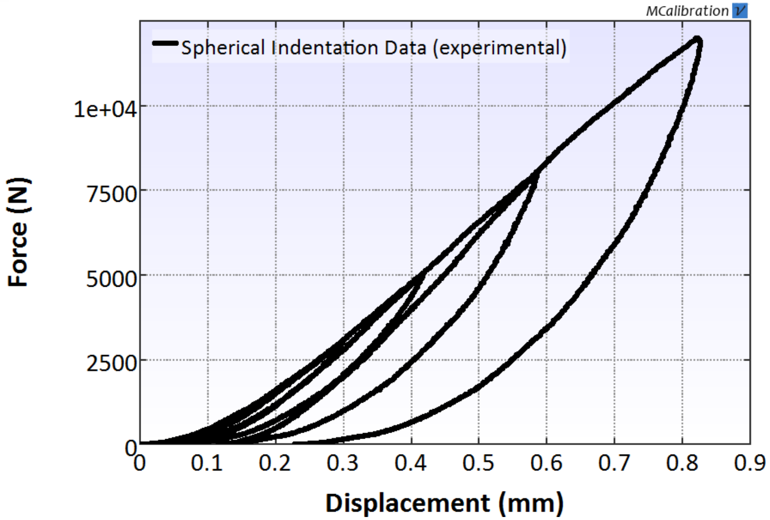


Multiaxial Validation Testing



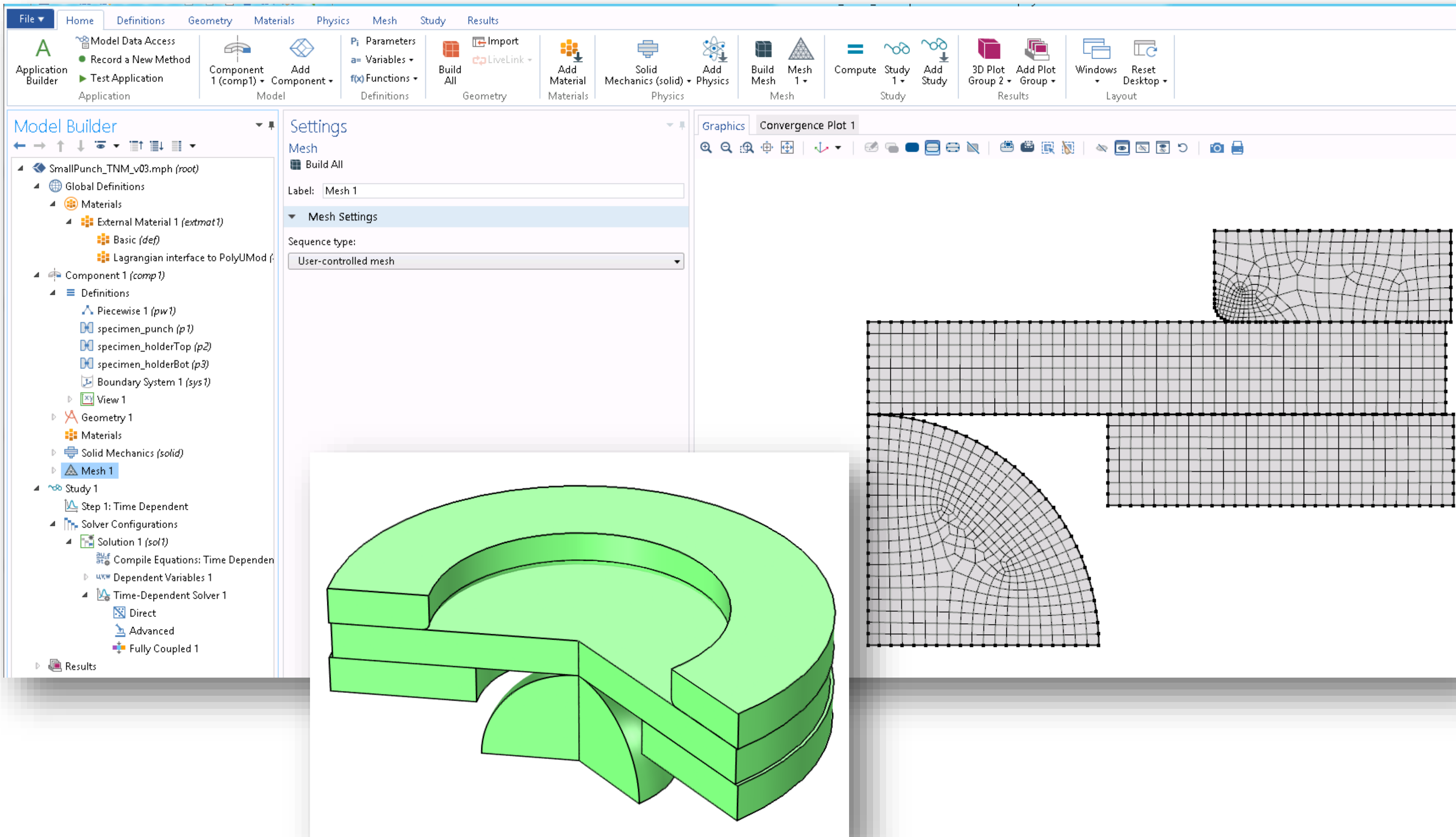


Small punch testing (ASTM F2183)

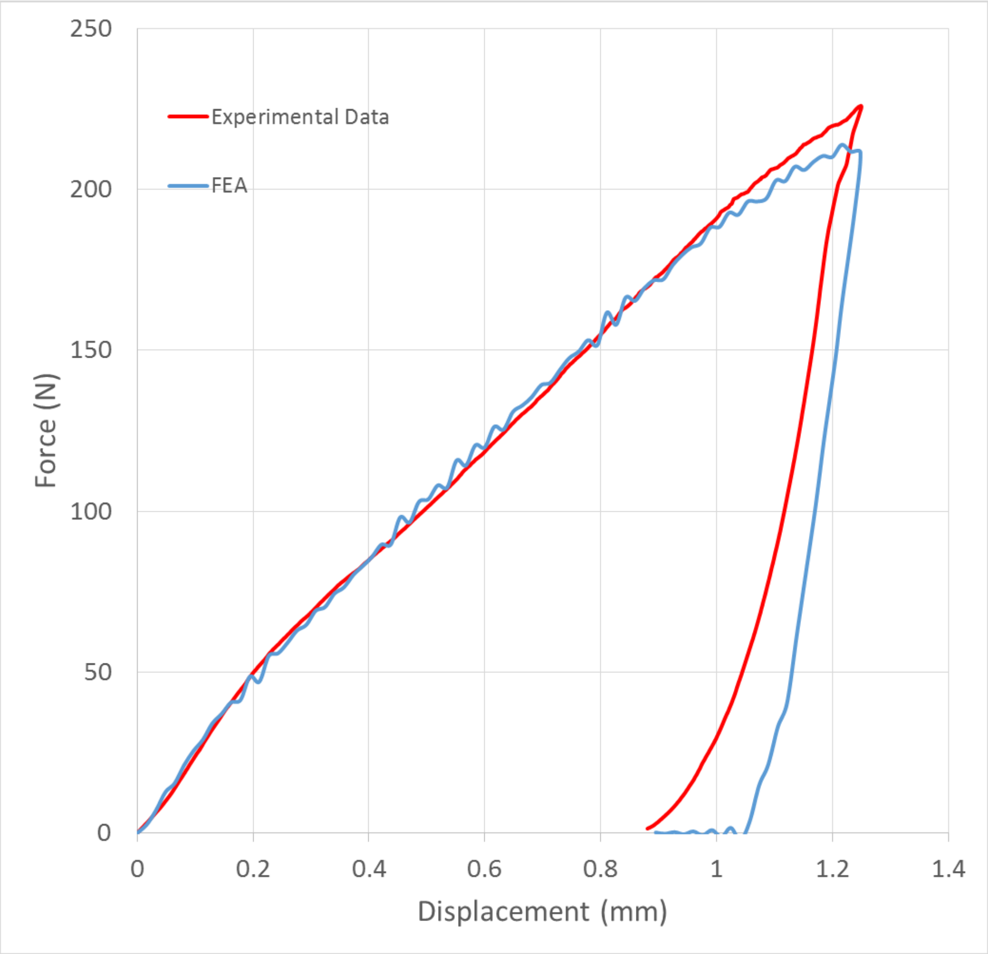


Spherical Indentation Testing

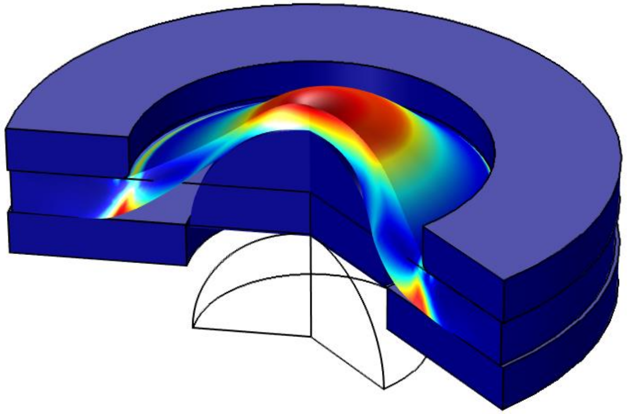
COMSOL: Small Punch Simulation



COMSOL: Small Punch Test

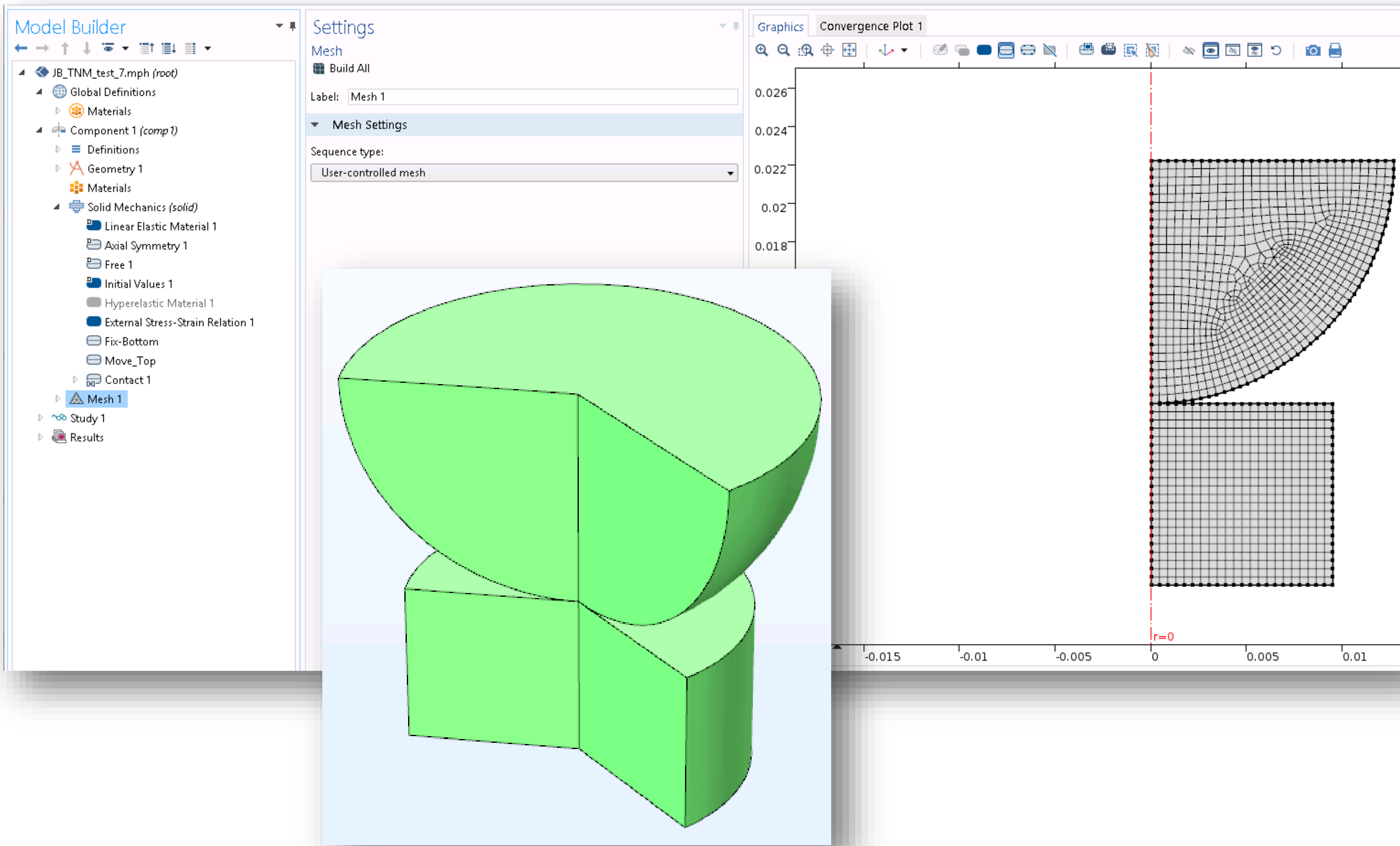


- The COMSOL model is in excellent agreement with the experimental data

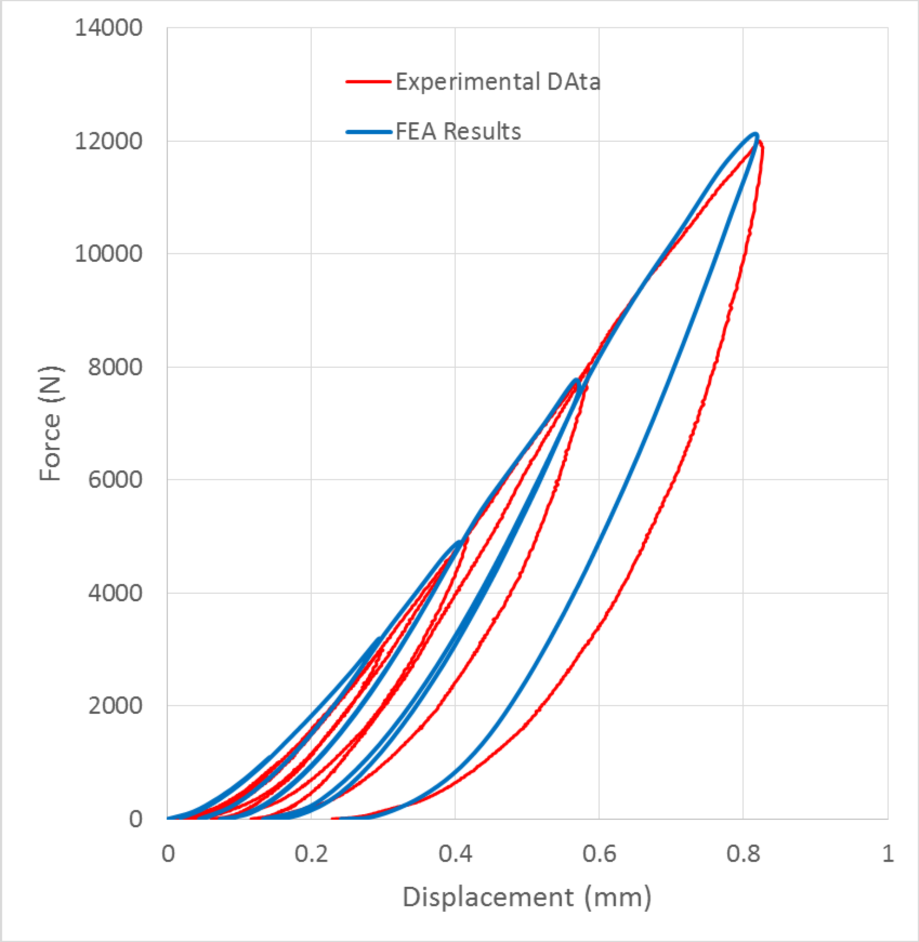


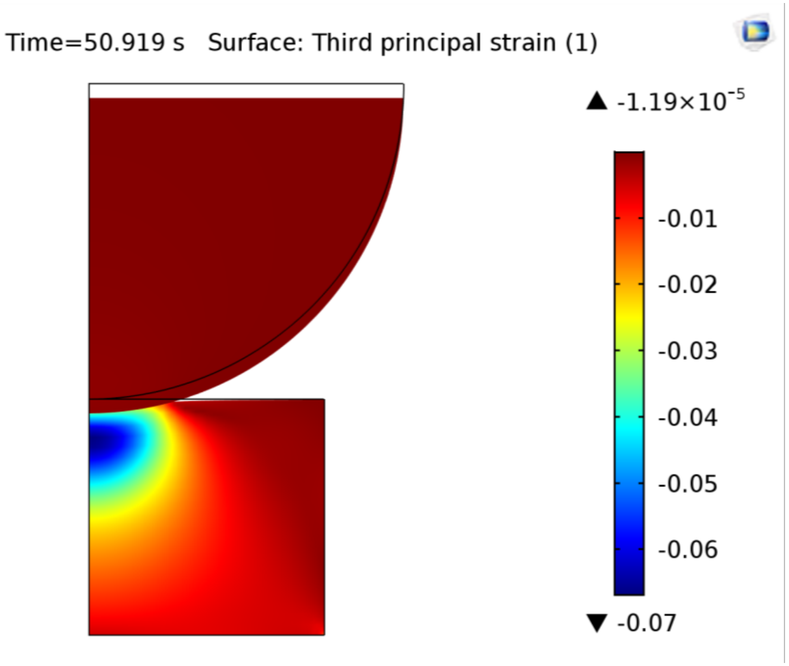
Axisymmetric model

COMSOL: Indentation



COMSOL: Indentation





- The TN model is in excellent agreement with the experimental validation data

Summary

Accurate COMSOL non-linear structural FE analysis requires:

- Careful experimental testing
- Selection of an appropriate material model
  - The External Material Functionality in COMSOL can be used to introduce very accurate viscoplastic material models
- Material model calibration
  - The MCalibration software is very useful for model calibration
- Material model validation (optional)
- FE model setup and simulation