How to Select and Calibrate an Accurate Material Model for Polymers

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***Abstract**: The non-linear mechanical response of thermoplastics, rubbers, foams, and biomaterials can be challenging to accurately represent in a FE simulation. Recent versions of Abaqus/Standard and Abaqus/Explicit support a number of different viscoelastic and viscoplastic material models, including the new Parallel Rheological Framework model. These material models can provide accurate predictions of the response of different material classes, but in many applications it can still be challenging to select an appropriate material model and to calibrate it to experimental data. This paper discusses what experimental data is necessary to use these models, illustrates the importance of model validation, and demonstrates how the material models can quickly be calibrated using the MCalibration software.*

***Keywords**: Constitutive Model, Creep, Damage, Experimental Verification, Implantable Medical Device, Optimization, Viscoelasticity*

1. Introduction

The mechanical response of thermoplastic materials is characterized by an initial elastic response followed by viscoplastic flow, large-scale yielding, and final strain stiffening before reaching failure. As will be shown in this paper, these non-linear behaviors can be accurately represented in Abaqus if a suitable material model is selected and calibrated to the correct type of experimental data. This paper focuses on polyether ether ketone (PEEK), which is a commonly used material for biomedical, aerospace, and automotive applications.

2. Experimental Testing

The mechanical response of an unfilled PEEK resin was experimentally determined using uniaxial compression and uniaxial tension experiments. The experimental setups that were used are shown in Figure 1. Cylindrical specimens (diameter=9 mm, height=9 mm) were tested in uniaxial compression at three different engineering strain rates ranging from -0.001/s to -0.1/s. Some of the tests included multiple loading and unloading segments, and some included 100 seconds of stress relaxation. The uniaxial tension response of the material was examined using dogbone-shaped tensile specimens, and the applied engineering strain rate was between 0.001/s and 0.1/s.

The high strain rate response of the material was determined using a Split Hopkinson Pressure bar test system, see Figure 1. Using this specialized testing system the compressive stress-strain response was determined at an applied engineering strain rate of -1000/s. Covering this wide range of strain rates, and multiple loading and unloading cycles is important for PEEK and other polymers in order to determine their non-linear viscoelastic response.

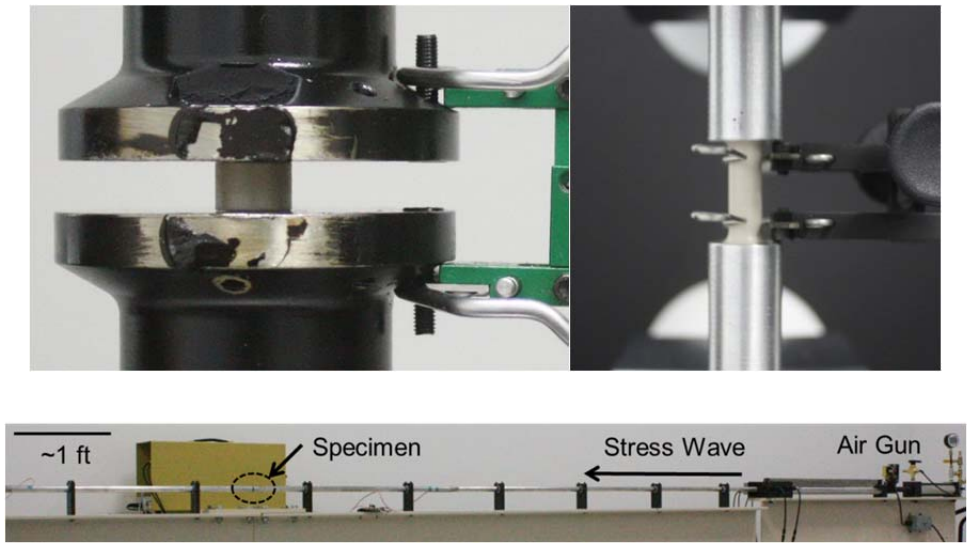

Figure 1. The PEEK material was tested using uniaxial compression, tension, and using a split Hopkinson pressure bar system.

To validate different material models we also performed two types of multiaxial experiments: small punch tests, and spherical indentation tests. Figure 2 shows photos of the experimental test systems and exemplar specimens. The purpose of the multiaxial testing was to get experimental data that can be used for material model validation. All tests were performed at room temperature.

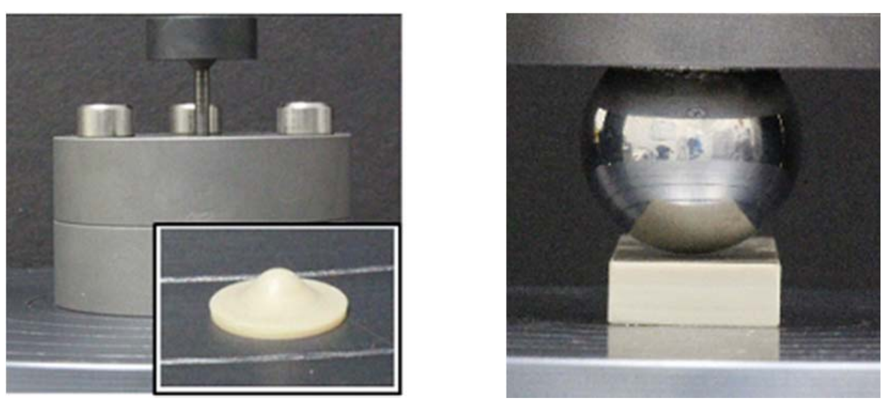

Figure 2. Experimental validation tests. Left: small punch test following ASTM F2638. Right: spherical indentation test.

3. Material Model Calibrations

The Abaqus native Parallel Rheological Framework (PRF) model and the Three Network (TN) model from the PolyUMod® library [1,2] were calibrated to all uniaxial test data from the nine compression tests and the two tension tests. In the calibration, experimental test cases from repeated experiments at the same strain rate were given a reduced fitness weight in order to not bias the calibration for any given strain rate. The Poisson's ratio for each material model was assumed to be 0.4.

The calibration was performed using the MCalibration® software [3], which can quickly calibrate all material models in Abaqus and the PolyUMod library in a fully automatic way.

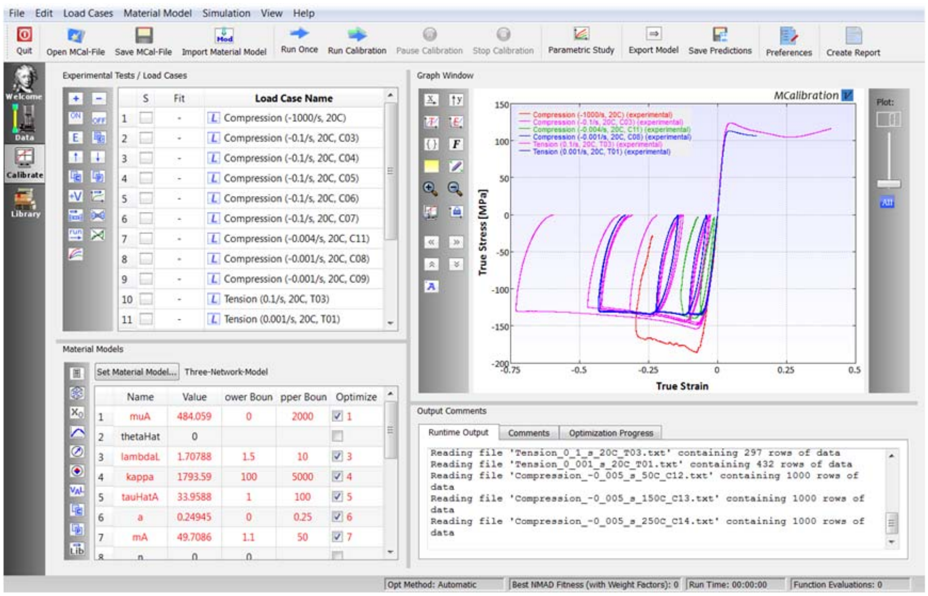

Figure 3. Screenshot of material model calibration performed using the MCalibration software from Veryst Engineering [3].

The Parallel Rheological Framework model that was selected was based on Yeoh hyperelasticity and the viscoelasticity was given by the power-law strain hardening model. The Yeoh hyperelastic model was selected since it is a simple I_1-based model that can capture the non-linear hyperelastic response of many polymers. The Three Network (TN) model is based on the Arruda-Boyce eight-chain hyperelastic model that is also I_1-based but is using a specific micromechanism inspired hyperelastic energy function. The difference between these two hyperelastic models is small in this application.

The results from the calibrations are shown in Figures 4 and 5. Each of these figures shows both the experimental data (in solid lines) and the final calibration results (in dashed lines). Figure 4 shows that the Three Network Model captures the experimental data very well. The R^2 value of the prediction is 0.912 for strain rates covering 6 orders of magnitude.

The calibration results for the Parallel Rheological Framework (PRF) model are summarized in Figure 5. The calibrated response of the PRF model is slightly less accurate with an R^2 value of 0.719.

The reason these material models do not capture all aspects of the experimental data is due to the highly non-linear response of the material under the applied uniaxial loading.

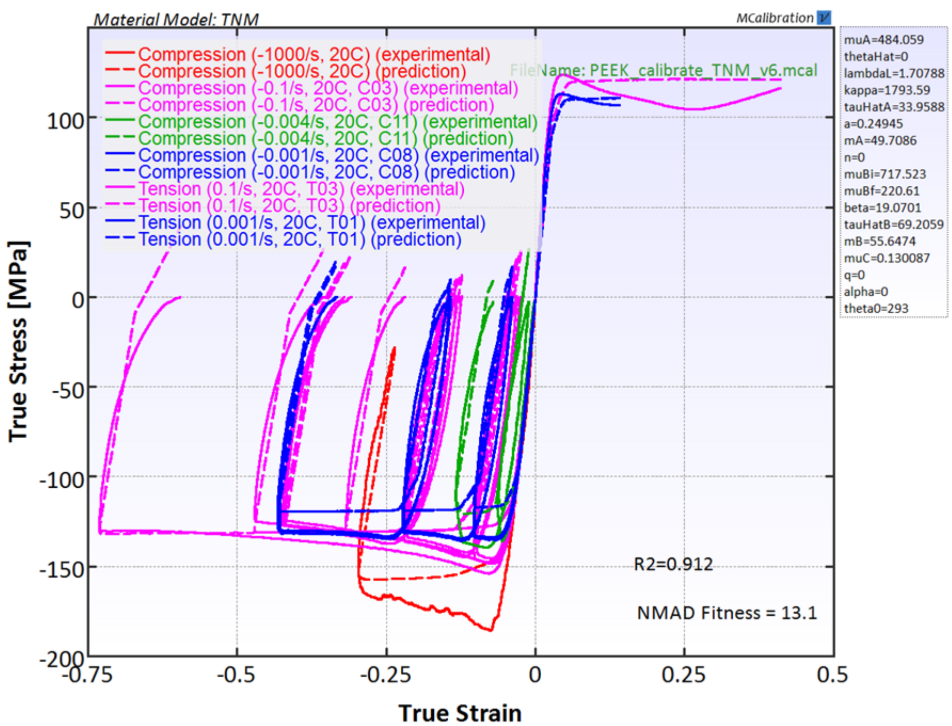

Figure 4. Calibration results for the Three Network (TN) model.

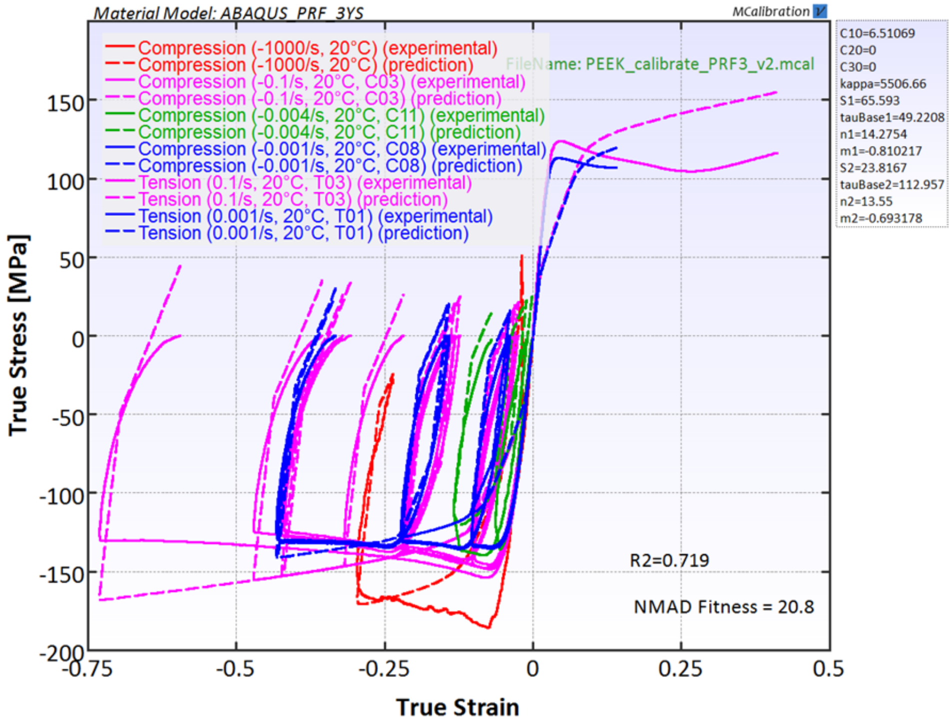

Figure 5. Calibration results for the 3-network Parallel Rheological Framework (PRF) model.

4. Material Model Validations

When working with non-linear material models it is important to examine if a calibrated material model also works for more general multiaxial deformations. Frequently, it is easier to match uniaxial data than multiaxial data. However, since virtually all industrially important problems involve of multiaxial loading it is important to verify that the material model also gives accurate predictions for loading modes other than what was used for the calibration.

In this case we created Abaqus/Standard FE simulations of the small punch test and of the spherical indentation test. The results from the FE simulation of the small punch test are shown in Figure 6. The solid black line in this figure shows the experimental force-displacement results, the blue curve shows the predictions from the TN model, and the red curve shows the predicted response from the PRF model. Both material models capture the trends in the experimental data, but the TN model is more accurate than the PRF model.

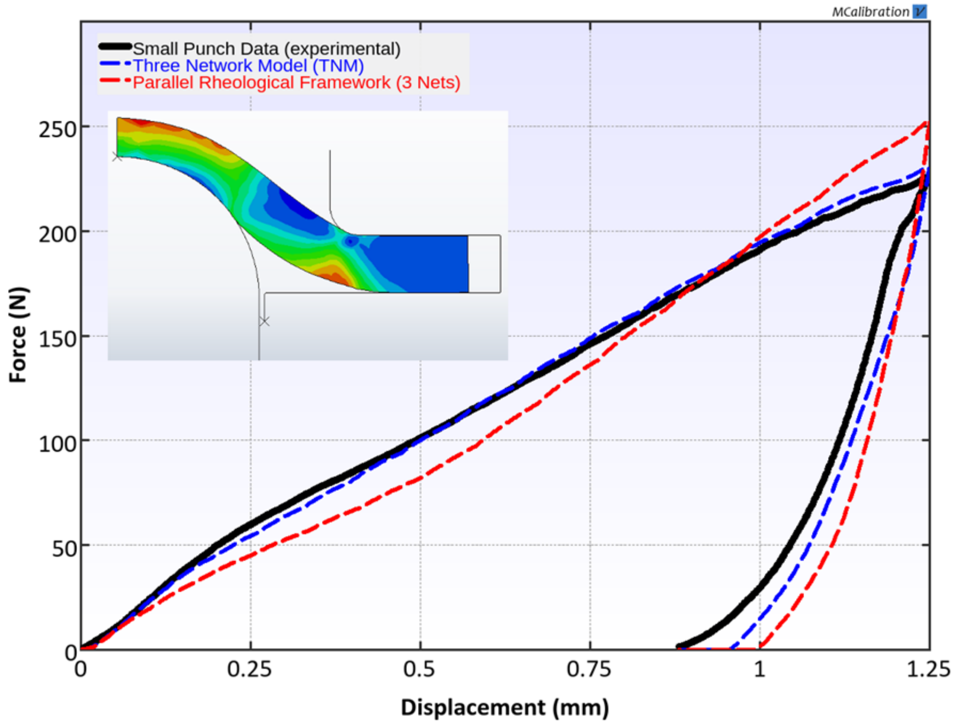

Figure 6. Comparison between experimental data from the small punch test and predictions from the TN and PRF models.

The results from the FE simulations of the spherical indentation test are summarized in Figure 7. In this case the indenter was applied in three loading-unloading cycles of increasing displacement magnitude. Both material models capture the trends in the experimental data, but also in this case the TN model is more accurate than the PRF model.

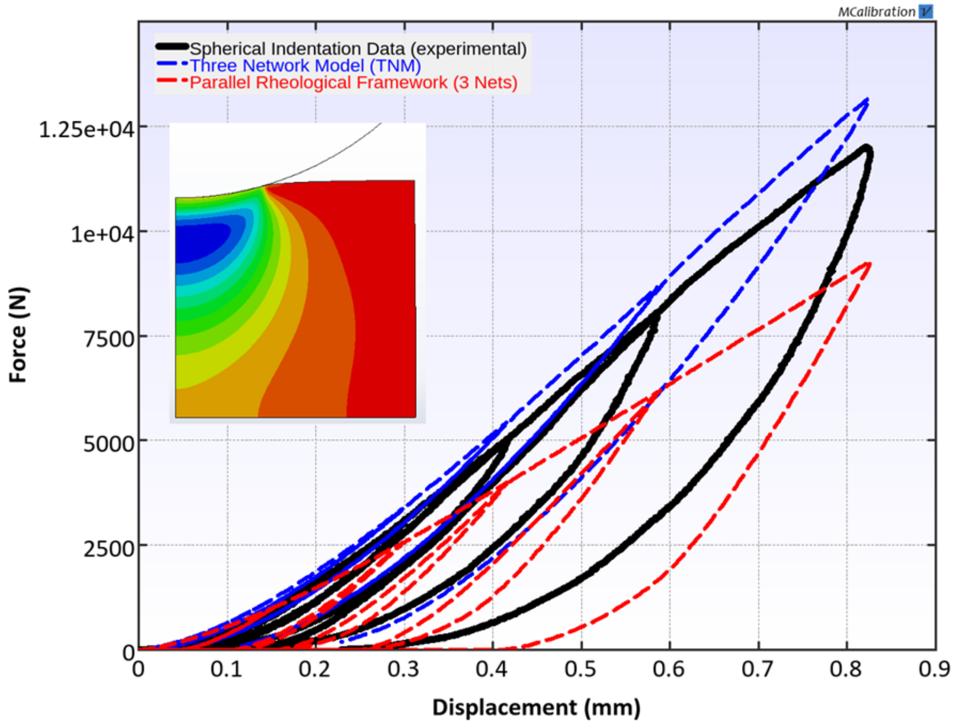

Figure 7. Comparison between experimental data from the spherical indentation test and predictions from the TN and PRF models.

5. Conclusions

As shown above, Abaqus can very accurately capture the response of highly non-linear thermoplastics, such as PEEK. Table 1 summarizes the accuracy of the model predictions and lists the FE simulation run times for the small punch and spherical indentation tests. The overall R^2 value for the Three Network (TN) model is 0.902, and the overall R^2 value for a 3-network Parallel Rheological Framework (PRF) model is 0.806. Both of these models have similar run times for the test cases examined here.

Table 1. Summary of model predictions and FE run times.

Loading Mode	Three Network Model	Parallel Rheological Framework (3 Networks)
Uniaxial Calibration	R^2=0.912	R^2=0.719
Small Punch	R^2=0.984 Run time: 88 s	R^2=0.927 Run time: 83 s
Spherical Indentation	R^2=0.809 Run time: 1028 s	R^2=0.772 Run time: 1200
Average	**R^2=0.902**	**R^2=0.806**

6. References

1. PolyUMod Material Subroutine Library, Veryst Engineering, LLC.
2. Bergstrom, J. S., and J.E. Bischoff, "An Advanced Thermomechanical Constitutive Model for UHMWPE," Int. J. Structural Changes in Solids, Vol 2, No 1, pp. 31-39, 2010.
3. MCalibration Material Calibration Software, Veryst Engineering, LLC.