Accurate Finite Element Simulations of PTFE Components

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Abstract: *Fluoropolymers is an import class of thermoplastics that is used in many different applications, e.g. seals, insulators, vascular grafts, coatings, etc. Fluoropolymers, as well as other thermoplastics, exhibit a complicated non-linear response when subjected to external loads. At small deformations, the material response is linear viscoelastic. At larger strains, the material undergoes distributed yielding, unrecoverable deformation, viscoplastic flow, and finally, gradual material stiffening at large deformations until ultimate failure occurs. It is also known that the material response is strongly dependent on strain-rate and temperature: higher deformation rates and lower temperatures increase the stiffness of the material. In this presentation I will demonstrate how all of the experimentally observed behaviors of this important material can be accurately simulated using Abaqus. Particular emphasis will be placed on the material model selection and calibration.*

Keywords: *Constitutive Model, Thermoplastics, Creep, Temperature-Dependence, Damage, User material, UMAT, VUMAT.*

1.   Introduction

Thermoplastic materials are increasingly used in many important engineering applications. The mechanical response of thermoplastic materials is characterized by a number of nonlinearities: initial strain-rate dependent stiffness, distributed yielding that evolves into large-scale yielding, large-strain stiffening due to entropic resistance, and final failure. The response is further complicated by significant strain-rate and temperature dependence. These experimental observations can be modeled in Abaqus Standard and Explicit using either built-in material models and external user-material subroutines.

In this work we calibrated a few of the built-in material models in Abaqus/Standard and the Dual Network Fluoropolymer (DNF) model and the Three Network (TN) model from the PolyUMod library [1] to a set of experimental data for a PTFE fluoropolymer. The following sections present the selected material models, the techniques and tools used to calibrate the material models, and an exemplar finite element small punch simulation is presented to demonstrate the use of the calibrated material models.
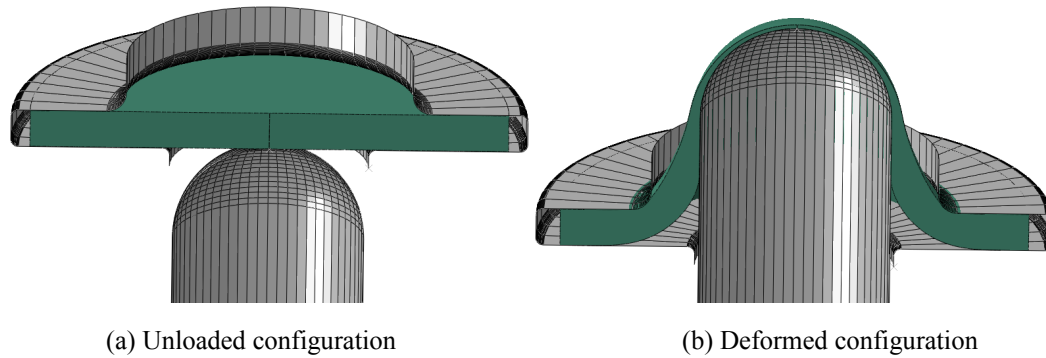
2. Experimental Data

In this study we have focused on a 15 vol% fiberglass filled PTFE fluoropolymer material. This material was experimentally tested in different loading modes: (1) cyclic uniaxial compression, (2) cyclic and monotonic uniaxial tension, (3) stress relaxation in tension, (4) cyclic volumetric compression, and (5) small punch testing. Figure 1 summarizes the experimental data.
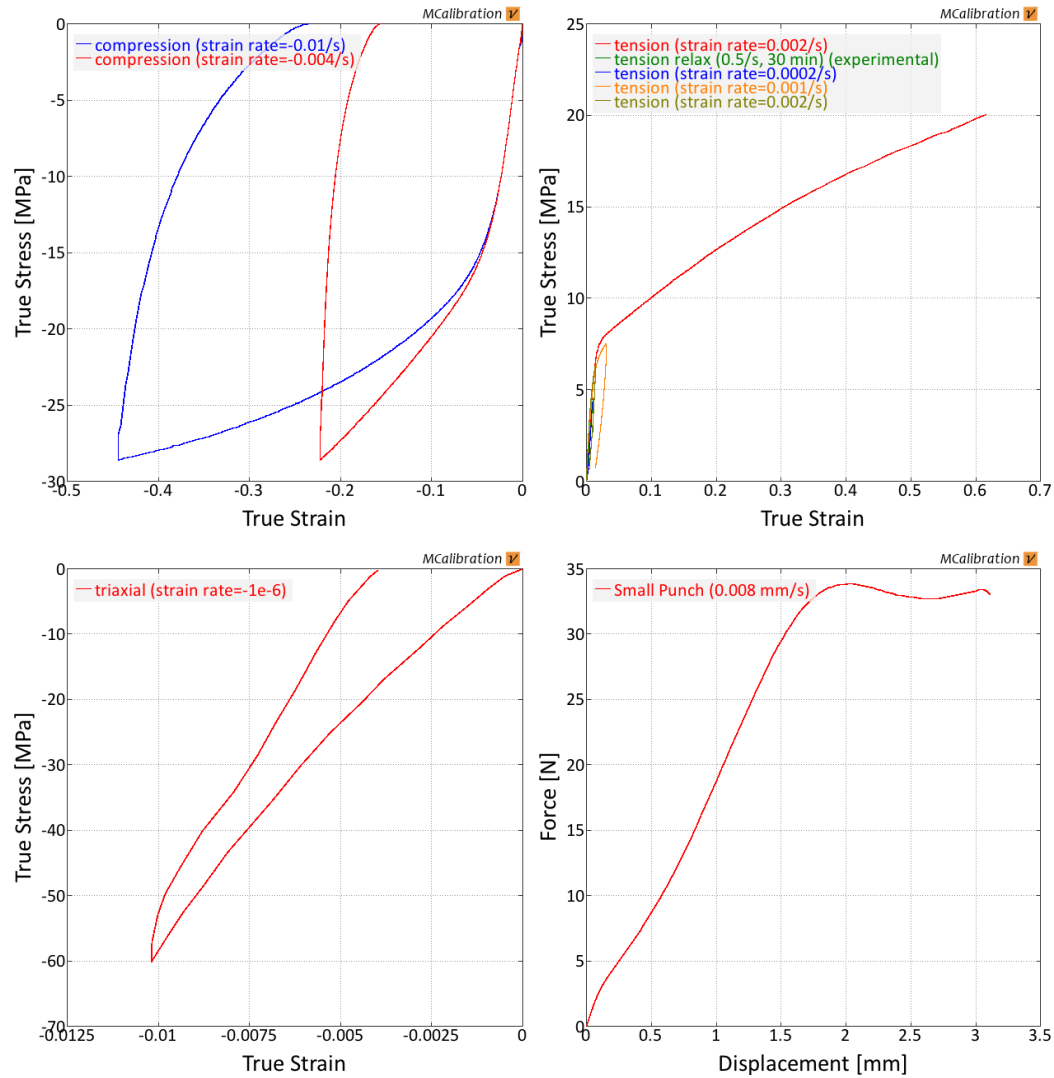
Figure 1. Experimental stress-strain data for a PTFE fluoropolymer in different loading modes.

The small punch tests [2] were performed on a small disc-shaped specimens with a diameter of 6.4 mm and a thickness of 0.5 mm, see Figure 2. The small punch test measures the force-displacement response of the punch.


(a) Unloaded configuration   (b) Deformed configuration

Figure 2. Abaqus finite element representation of the small punch experimental test.

3.   Material Models

The experimentally observed behavior of the PTFE fluoropolymer, presented in the previous section, can be modeled using either a built-in material model is Abaqus, or one of the material models in the PolyUMod library [1]. In this study we focused on the following material models: (1) Neo-Hookean hyperelasticity, (2) Isotropic hardening plasticity, (3) Drucker-Prager plasticity, (4) Dual Network Fluoropolymer model [3], and (4) the Three Network Model [4].

The Drucker-Prager material model was selected as once of the candidate material models since the PTFE material has significantly higher yield stress in uniaxial compression compared to uniaxial tension.

The rheological representation of the Dual Network Fluoropolymer (DNF) model and the Three Network (TN) model are illustrated in Figure 3. The details of these constitutive theories are given in other references [3-4].

|(a) DNF Model|(b) TN Model|
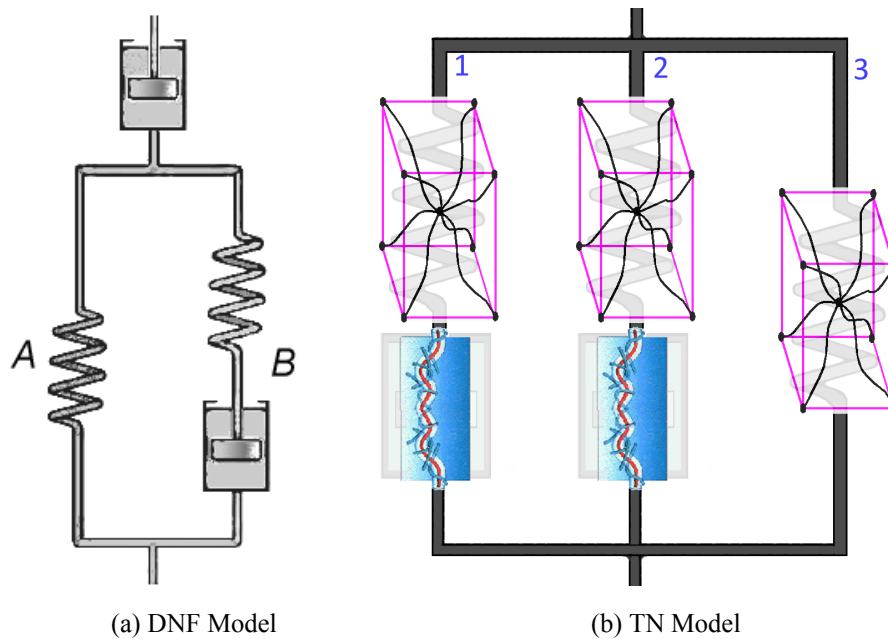
Figure 3. Micromechanical rheological representations of the DNF and TN models.

4. Material Model Calibrations

All material models were calibrated to the experimental tension, compression, relaxation, and small punch data using the MCalibration software [1]. The MCalibration software defines a "load case" for each experimental data file, and then use iterative algorithms to optimize the necessary material parameters for each selected material model. The calibration procedure is fully automatic. The uniaxial loading data is calculated using an internal solver in MCalibration, and the small punch data is determined by running an Abaqus/Standard FE simulation of the small punch experiment.

Once the MCalibration software has found the optimal material parameters the calibrated material model can then be exported to Abaqus/CAE or inserted into an inp-file for further FE analysis.
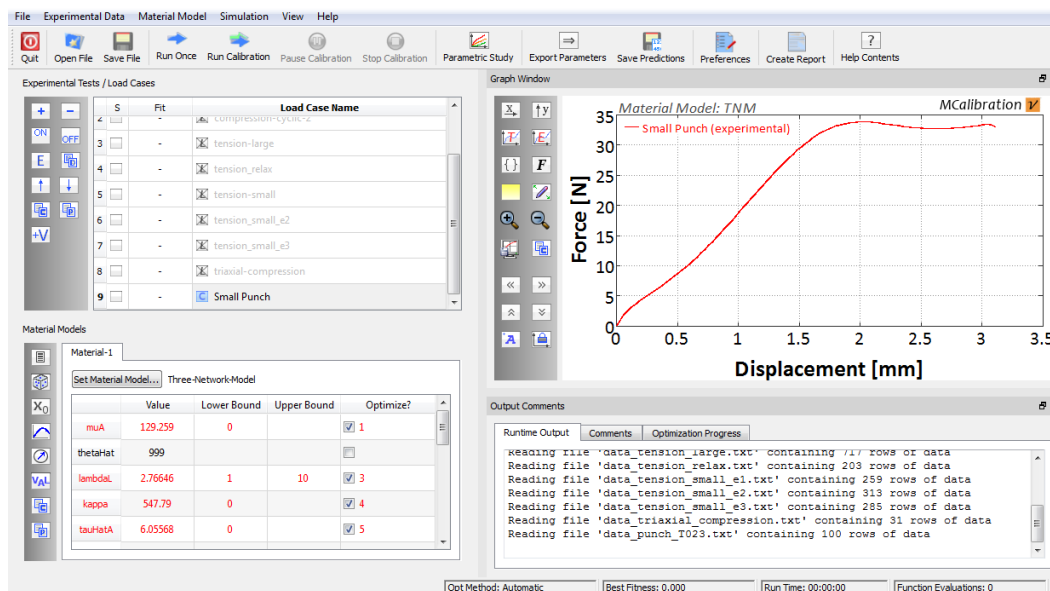
Figure 4. Screen shot of the MCalibration software that was used to calibrate all material models.

5. Results

The results from the material model calibrations are shown in Figures 5 to 9. These figures show the predicted stress-strain and small punch responses for each of the material models that were investigated.

Figure 5 shows that, as expected, the Neo-Hookean hyperelastic model should not be used to simulate the large deformation response of PTFE fluoropolymers. Is was included in the study as a numerically efficient baseline case.
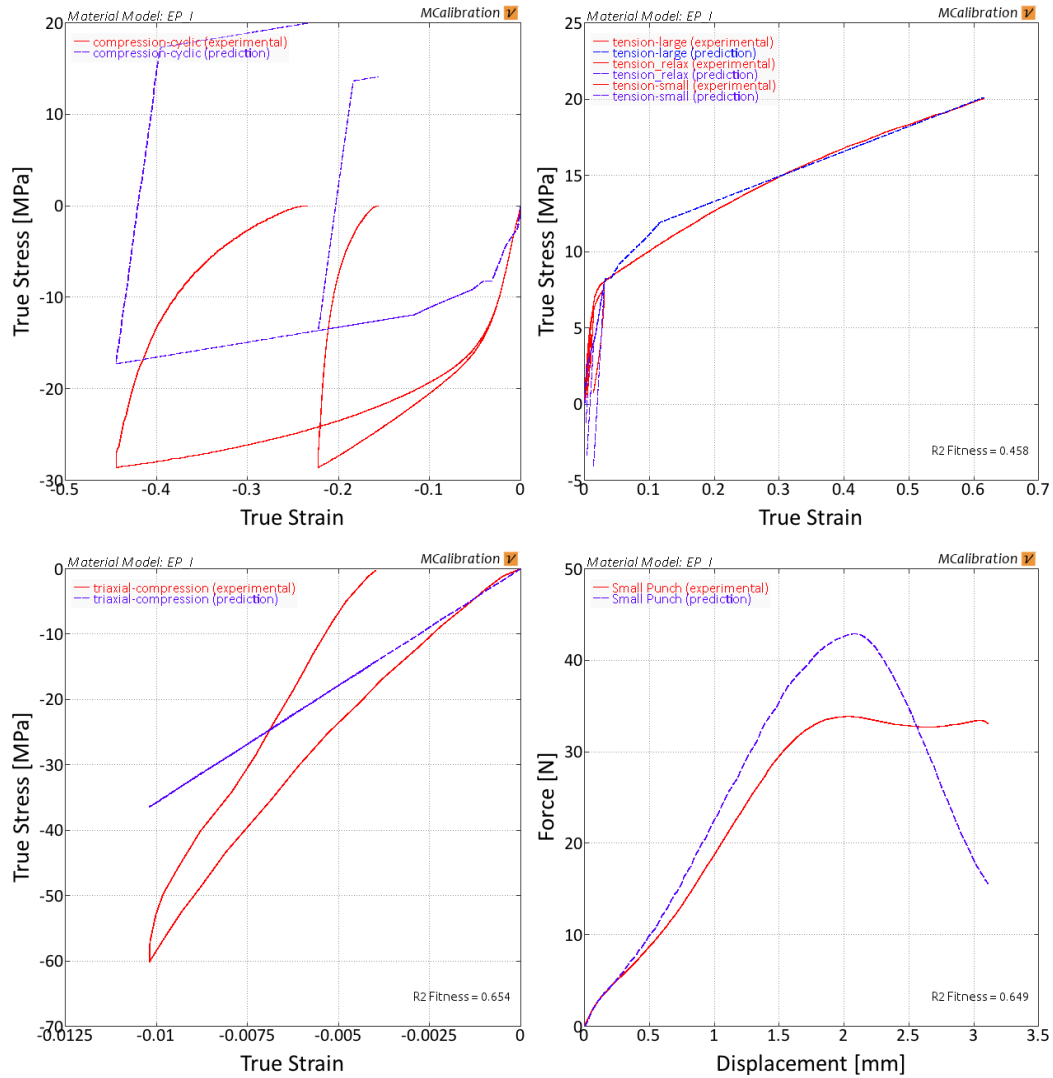
Figure 6 shows that the isotropic hardening plasticity model is not suitable since it predicts the same yield stress in tension and compression, which is not in agreement with the experimental data for PTFE.

The Drucker-Prager model (Figure 7) reasonably well captures the experimental data with the exception of the unloading response in compression, and the predicted small punch response. For these loading conditions the model predictions are quite inaccurate.

The predictions from the Dual Network Fluoropolymer (DNF) model and the Three Network (TN) model are in significantly better agreement with the complete set of the experimentally observed behaviors. The DNF model captures the volumetric flow response better than any of the other models, but the TN model is in slightly better overall agreement with the experimental data.
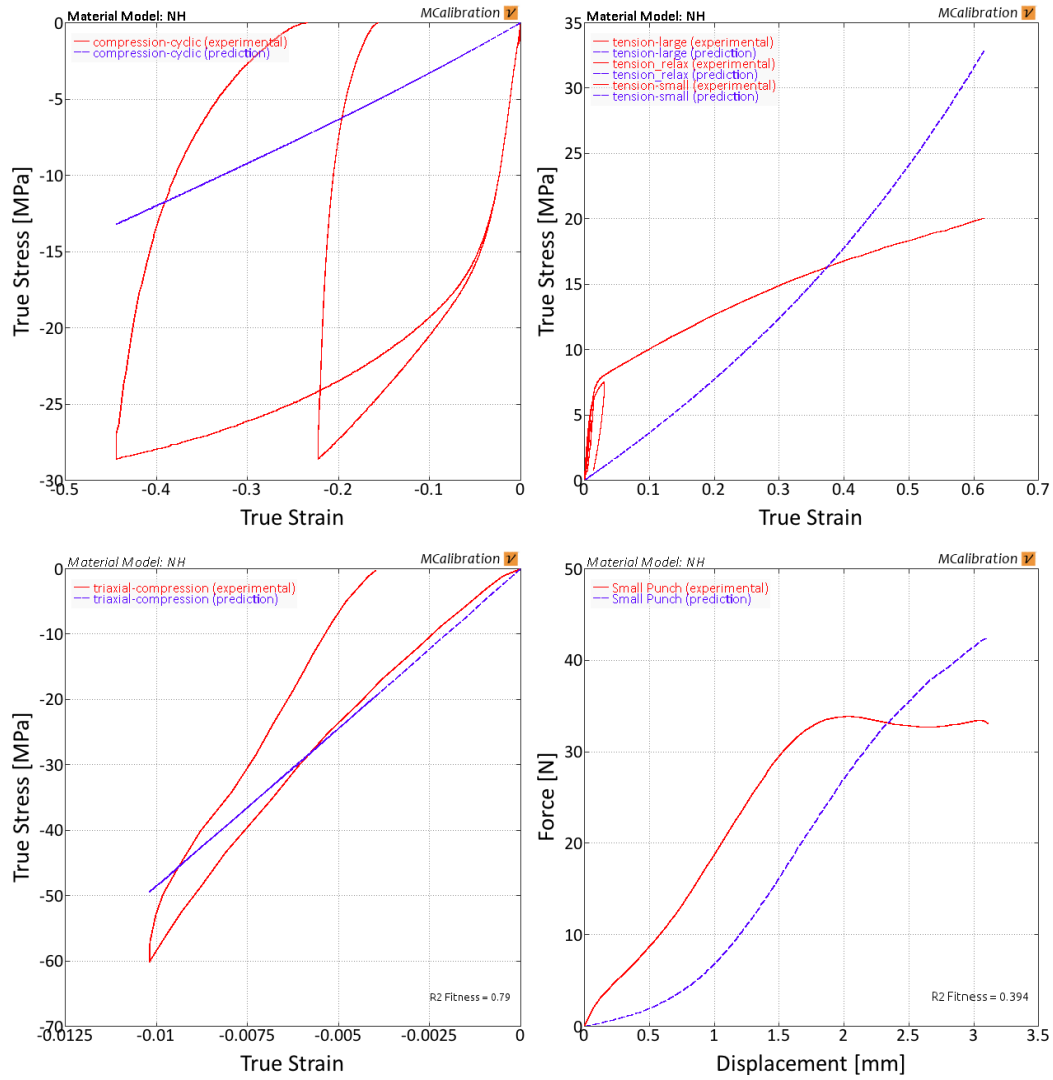
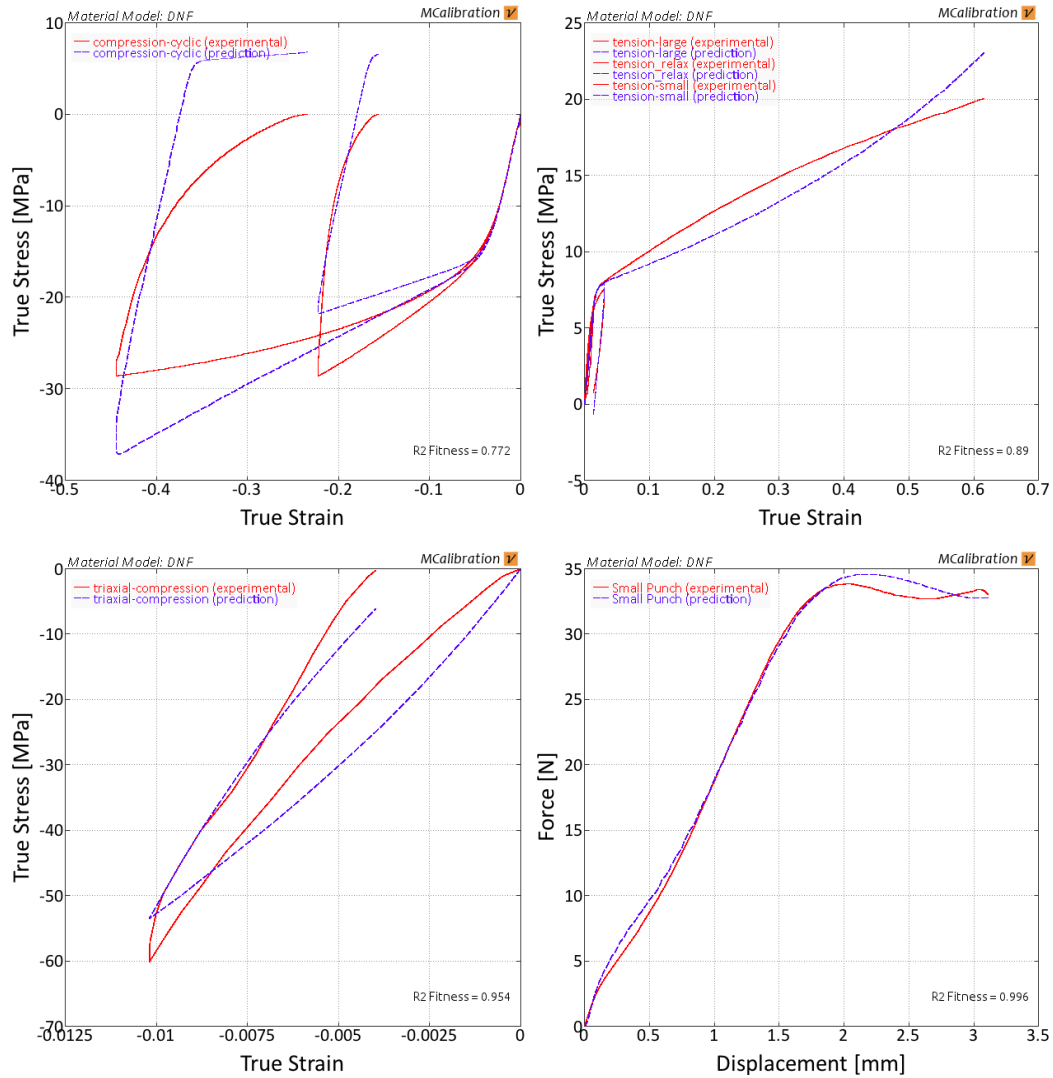**Figure 5. Comparison between the experimental data and predictions from the Neo-Hookean model. Average R^2=0.13.**

Figure 6. Comparison between the experimental data and predictions from the isotropic hardening plasticity model. Average R²=0.40.
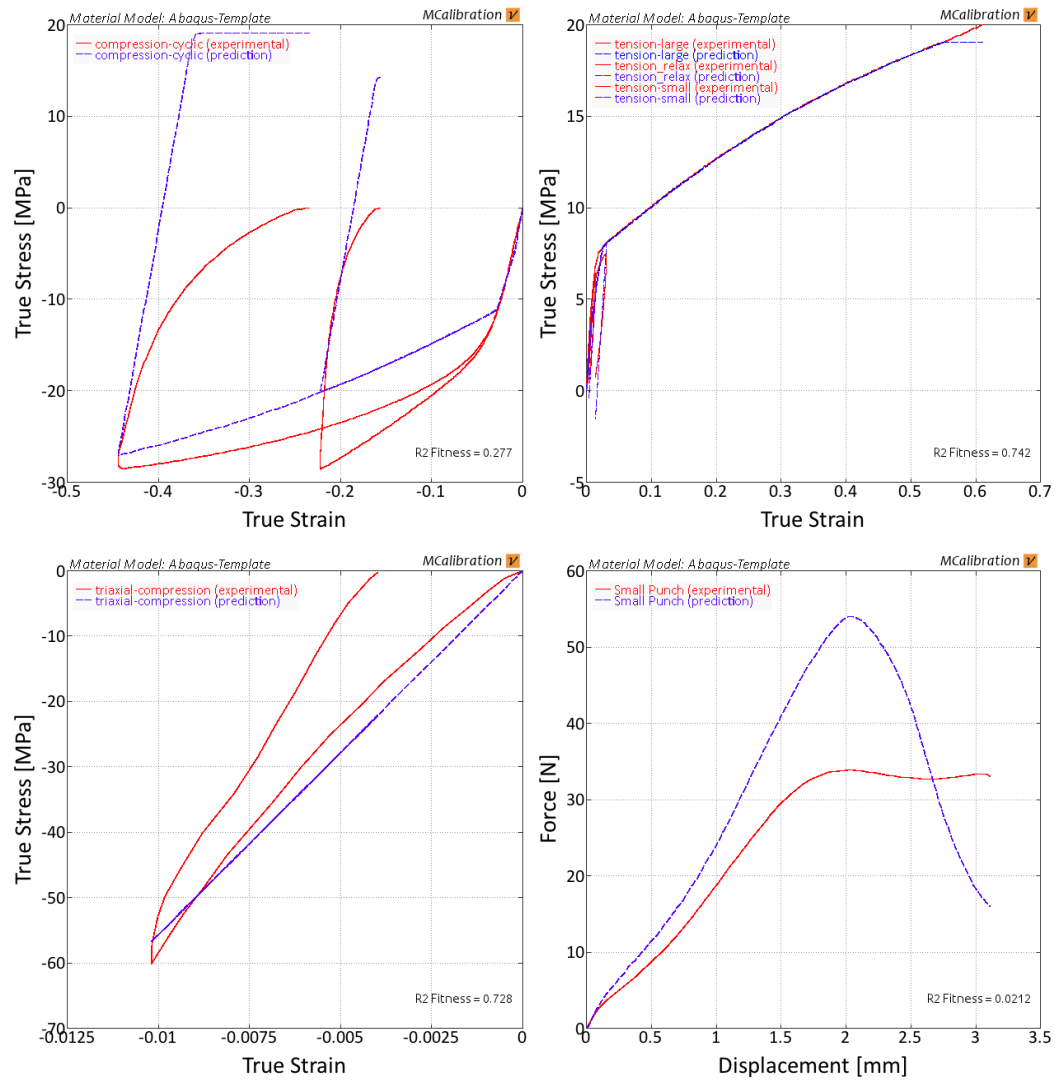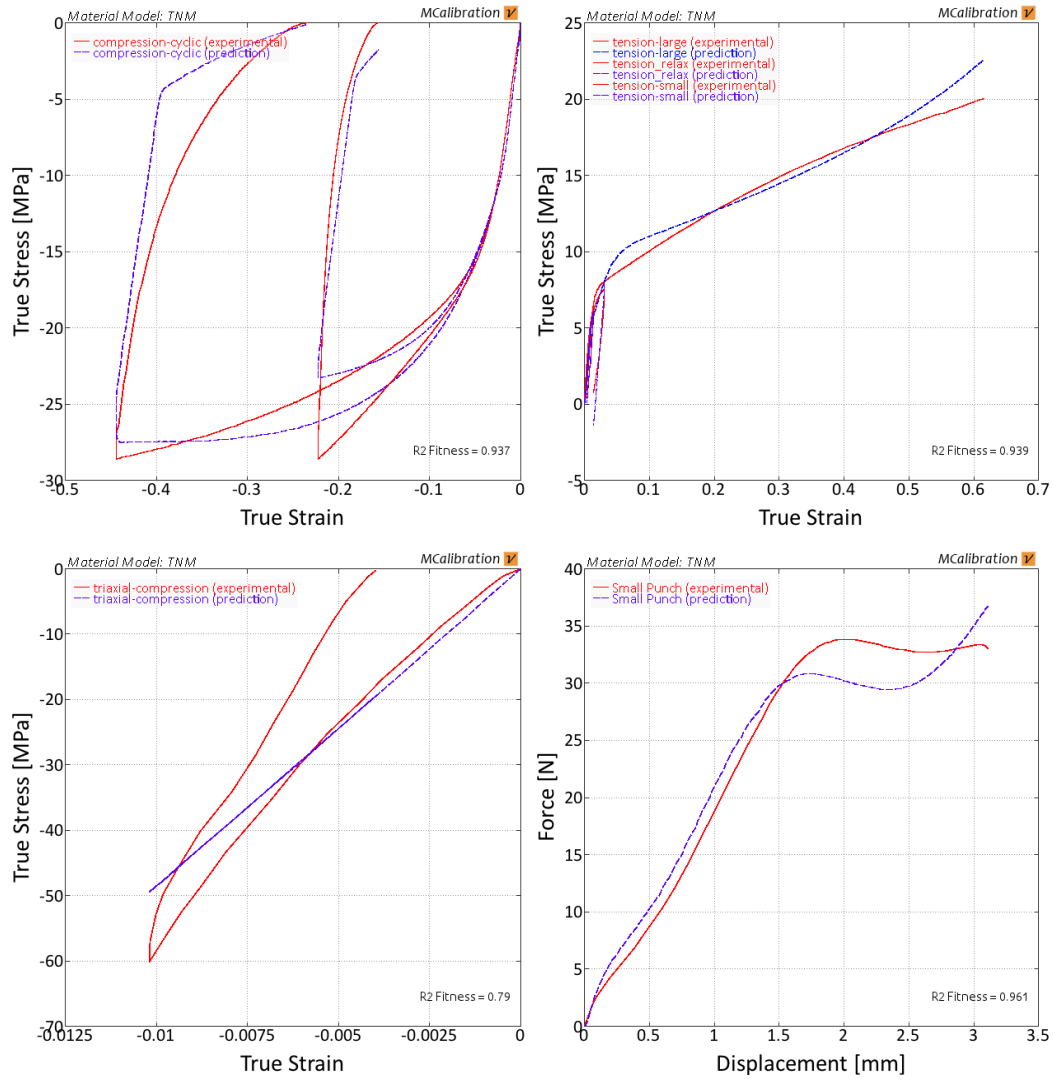
Figure 7. Comparison between the experimental data and predictions from the Drucker-Prager model. Average R^2=0.56.

**Figure 8. Comparison between the experimental data and predictions from the DNF model. Average R²=0.82.**

Figure 9. Comparison between the experimental data and predictions from the Three Network model. Average R²=0.86.

Another important aspect of material model selection is the computational efficiency. Figure 10 plots the R^2-value as a function of normalized run time for each of the selected material models. In this graph a good model should have a small normalized runtime and a large R^2 value.

As expected, the more accurate material models (TNM and DNF) are more numerically expensive than the traditional plasticity models. The difference in run time is caused by the internal differential equations that are used in the DNF and TN models to evolve the internal material state. The plasticity models are algebraic and can be solved quicker.

Also note that the DNF model only runs about 13% slower than the Drucker-Prager model, but provides significantly more accurate results.
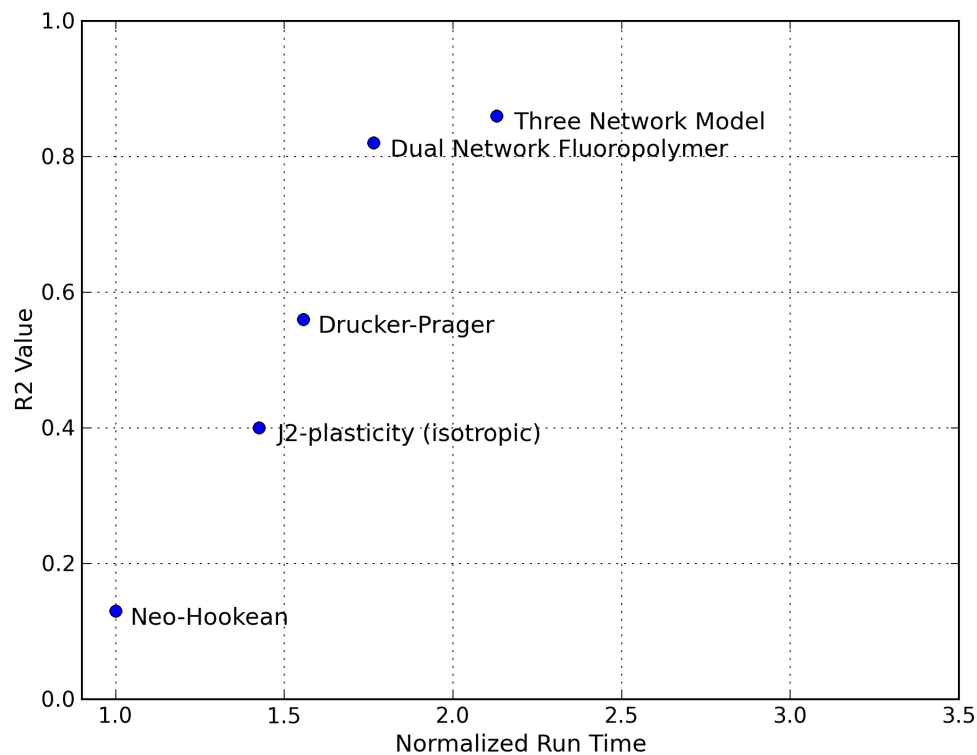
Figure 10. Comparison between simulation accuracy (R^2-value) and run time for Abaqus/Standard simulations. The run time was determined from the one 3D simulation (using 1024 C3D8R elements) and one 2D simulation (using 1024 CPE4R elements) of a dog bone shaped specimen pulled in tension.

6. Discussion

The behavior of thermoplastics can be challenging to predict in a finite element simulation due to the strong non-linearities in the stress-strain response, and dependence on the applied strain-rate. It was shown in this study that the Drucker-Prager material model is the most accurate of the built-in material models for predicting the response of a PTFE fluropolymer thermoplastic material. This material model, however, does not accurately predict the unloading response or the experimentally observed biaxial punch behavior. More accurate simulation results can be obtained by using either the Dual Network Fluoropolymer (DNF) model or the Three Network (TN) model from the PolyUMod library [1]. These two models accurately predicts all of the experimental behaviors of this important thermoplastic material.

7. References

[1] The PolyUMod library of user-material models and the MCalibration software are commercially available from Veryst Engineering (http://www.veryst.com/PolyUModLibrary.html).

[2] ASTM Standard F2183-02. "Standard Test Method for Small Punch Testing of Ultra-High Molecular Weight Polyethylene Used in Surgical Implants".

[3] J.S. Bergstrom, L.B. Hilbert, "A Constitutive Model for Predicting the Large Deformation Thermomechanical Behavior of Fluoropolymers," Mechanics and Materials, 2005, Vol. 37, pp. 899-913.

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

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