Prediction of Nonlinear Viscoelastic Recovery of Thermoplastic Polymers using Abaqus Parallel Rheological Framework (PRF) Model

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Abstract: *Thermoplastic polymers show significant nonlinear viscoelastic behavior due to which, after removing the applied load, these materials have some viscoelastic recovery over time before permanent deformation or set occurs. In this work, Abaqus PRF model is used to predict this time dependent viscoelastic recovery. Unlike linear viscoelastic model in Abaqus, PRF model can predict the typical nonlinear viscoelastic behavior of thermoplastic materials. Two types of testing, stress relaxation and cyclic loading at three different strain levels, are used to calibrate the coefficients of PRF model. SIMULIA's optimization tool Isight is used to optimize these coefficients. Using the optimized coefficients, the PRF model is able to predict the time dependent nonlinear viscoelastic recovery of thermoplastic polymers.*

Keywords*: Thermoplastic, nonlinear Viscoelasticity, PRF, Recovery, Relaxation, Calibration, Isight.*

1. Introduction

In many applications, thermoplastic polymers are increasingly replacing metal due to its high strength-to-weight ratio, low cost and manufacturing feasibility of complex parts. Unlike metals, however, mechanical properties of plastics depend on different environmental and loading conditions. Due to this complex behavior, optimum and accurate design of parts with plastic materials are challenging and requires many test data at different conditions. One of the unique properties of plastics is its viscoelastic behavior where, under loading, materials show both elastic and viscous behaviors. Due to this viscoelastic nature, during unloading, plastic has both instant elastic recovery and nonlinear rate dependent viscous recovery which occurs over a certain period of time depending on the loading strain as shown in Figure 1. This viscoelastic constitutive behavior has been successfully explained and modeled by using different combinations of spring-dashpot system [1, 2]. In addition, due to hysteresis nature, the unloading of plastics does not follow the loading path. Cyclic load testing at different strain levels can be used to measure this hysteresis loading-unloading behavior. In this work, testing is done on a DuPont thermoplastic material to measure this elastic and viscous recovery during unloading and an Abaqus PRF material model [3] is used to model this behavior. Unlike traditional linear viscoelastic model in Abaqus, PRF can predict the nonlinear viscoelastic behavior of material. However, this advantage of PRF model requires more complex methods for calibrating the model coefficients. In this work, Isight optimization tool is used to accurately calibrate and optimize these coefficients.

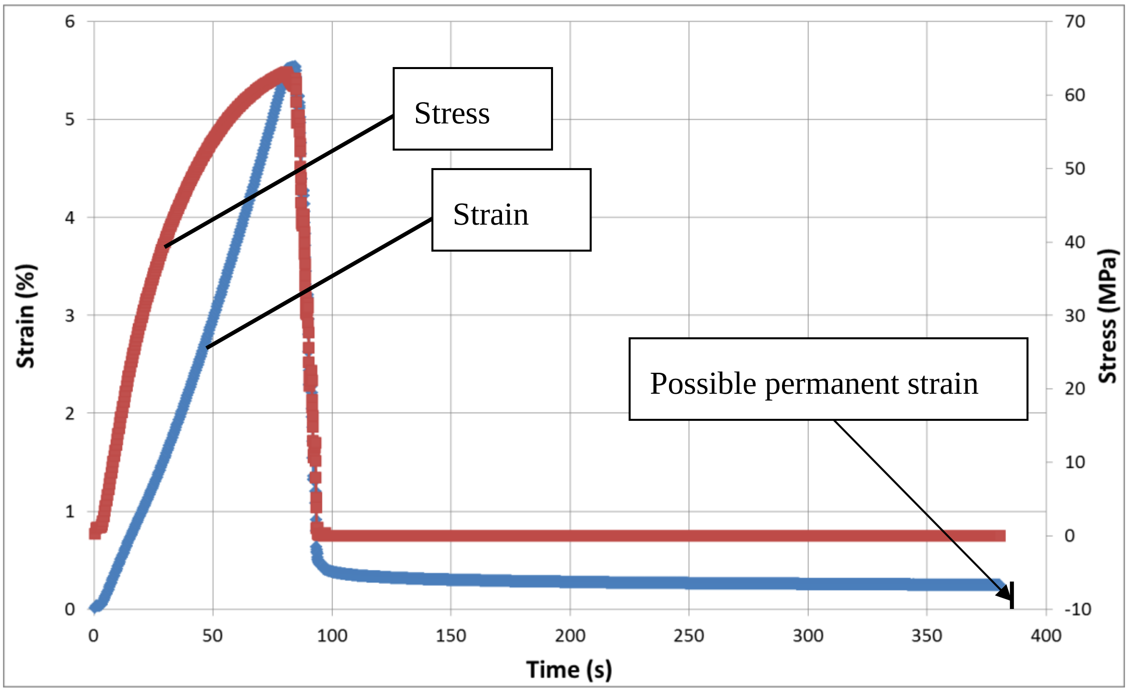


Figure 1: Time dependent viscoelastic recovery of a thermoplastic material

2. Testing to Measure Viscoelastic Recovery

In a viscoelastic recovery testing, also known as yield strength prediction testing, a thermoplastic tensile specimen is pulled to a certain strain level before load is removed instantly. As a result of rapid unloading, the specimen shows an instant elastic unloading followed by time dependent viscous recovery strain. If the specimen is given enough time, it could go back to zero strain or could show some residual strain depending on the loading strain and material type. Details of the testing are explained in references [7, 8]. For all of the testing done in this work, the specimens are given five minutes to recover after unloading. The stress associated with the lowest loading strain that result in a residual strain in the specimen five minutes after unloading is considered as yield strength of the material. An extensometer is used throughout the testing period to record the strain recovery.

The material tested is DuPont's Delrin™500P. Three ISO 527-2 Type1 injection molded dumb-bell-shaped tensile specimens at four different strain levels (1.5%, 3.5%, 4.5%, and 5.5%) are tested at room temperature and at 50 mm/min speed in an Instron setup. Figures 2 & 3 show the strain-time and stress-time plot at different loading strains, respectively and Figure 4 shows the stress-strain plot from the same testing. The figures show that as specimen unloaded instantaneously after the prescribed loading strain, stress reaches to zero immediately and strain has some instant elastic recovery followed by slow viscous recovery. As mentioned earlier, in this testing, recovery of the specimens are measured for five minutes and the residual strain after five minutes can be considered as permanent deformation or plastic strain. By observing closely in Figures 3 & 4, one can see that both 1.5% and 3.5% loading strains, the specimen returned to zero strain almost instantly. For 4.5% and 5.5% strains, however, the material shows some residual strain. Therefore, stress corresponding to 3.5% strain can be considered as initial yield strength of this material.

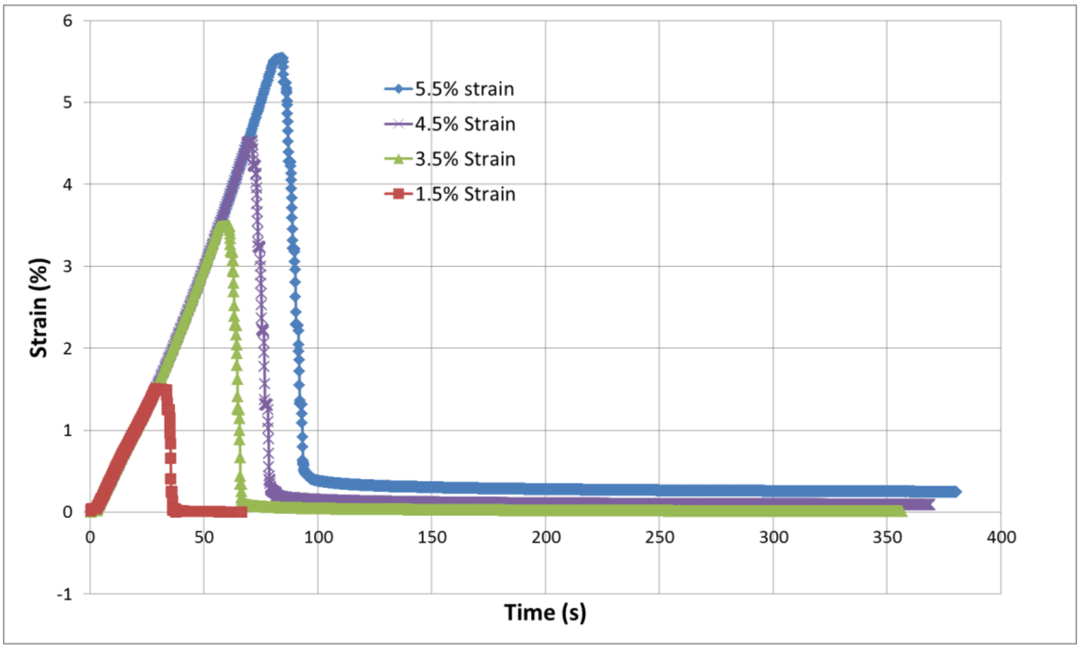


Figure 2: Strain vs Time at different loading strains from viscoelastic recovery testing

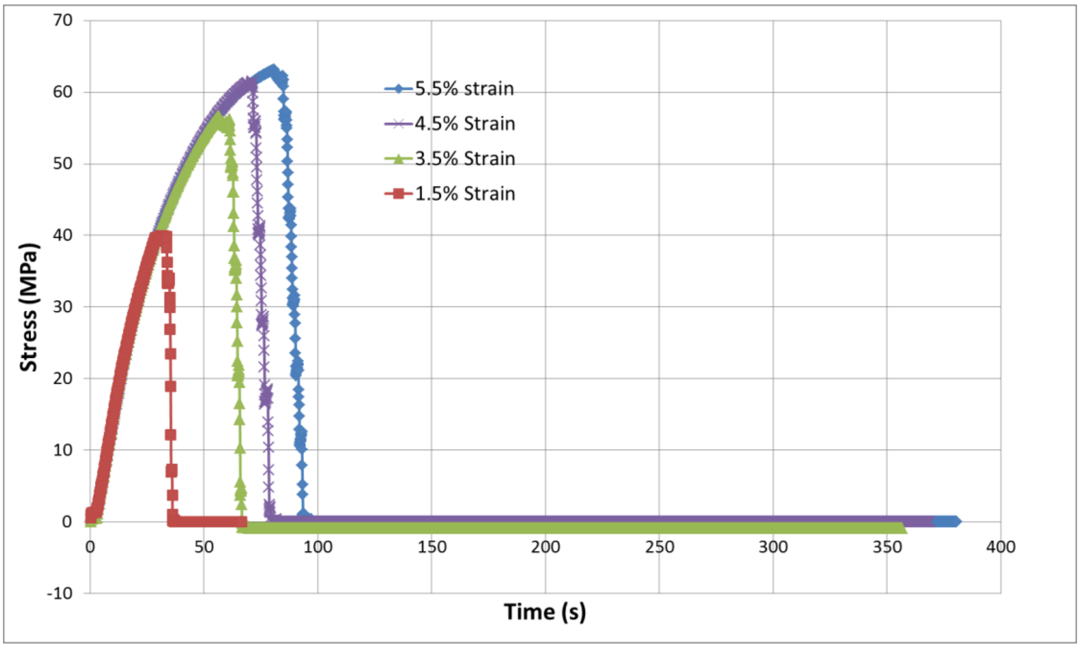


Figure 3: Stress vs Time at different loading strains from viscoelastic recovery testing

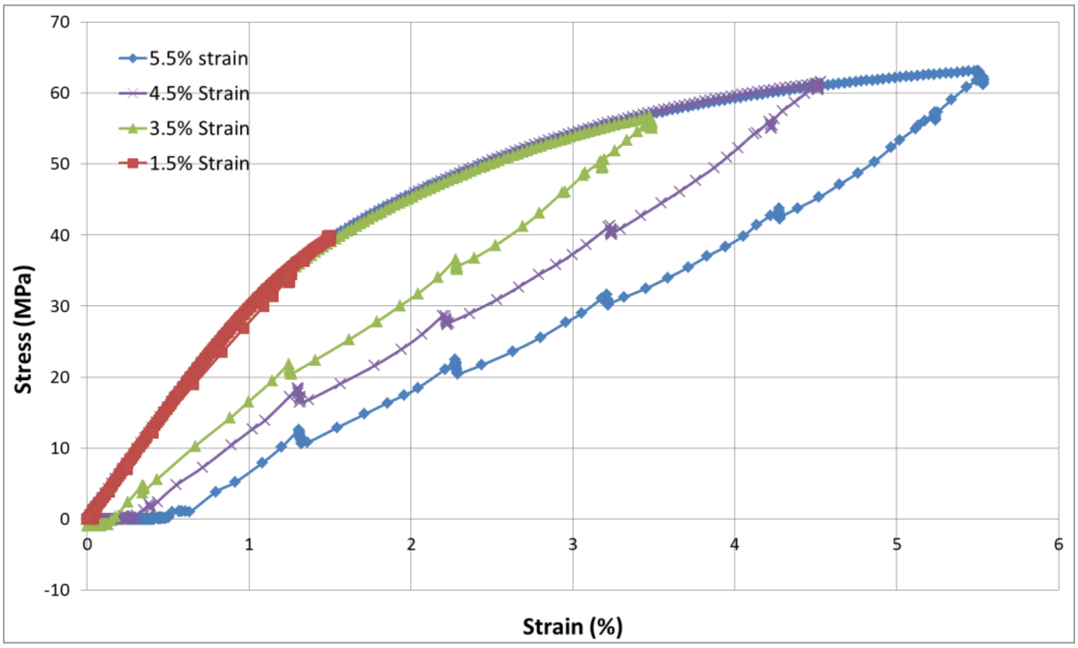


Figure 4: Stress vs strain at different loading strains from viscoelastic recovery testing

3. Calibration of PRF Model

Unlike linear viscoelastic model in Abaqus, PRF model can capture the nonlinear viscoelastic behavior of thermoplastic polymers. To learn more about PRF model, the author refers to Abaqus documentation [3].

The goal of this work is to predict nonlinear viscoelastic recovery through Finite Element Analysis (FEA) during unloading where material experiences both loading-unloading and slow time-dependent viscous recovery. To capture these complex behaviors in FEA, both cycling loading-unloading testing at three different strain levels and long term stress relaxation testing at different strain levels are performed on tensile specimens. Using these two sets of test data, coefficients of PRF model are optimized in the Isight optimization tool. In the next two sections, the testing and the Isight optimization process are explained.

3.1 Testing to Calibrate PRF Model

Both cyclic and stress relaxation testing are done on DuPont’s Delrin™500P injection molded dumb-bell-shaped tensile specimen. Specimen sizes are based on ISO 527-2 Type1 [4] and the test is done at room temperature and at 50 mm/min speed in an Instron setup.

During cyclic testing, three loading strains (3.5%, 5.5% and 7%) are applied in a single test on a particular specimen, where in each cycle the specimen is loaded to the specified strain level followed by unloading to zero stress (not zero strain) and followed by reloading to the next strain level. Figure 5 shows the stress-strain curve from the cyclic loading test where one can see that unloading and reloading to the next strain levels does not follow the same path which is typical behavior for thermoplastic materials.

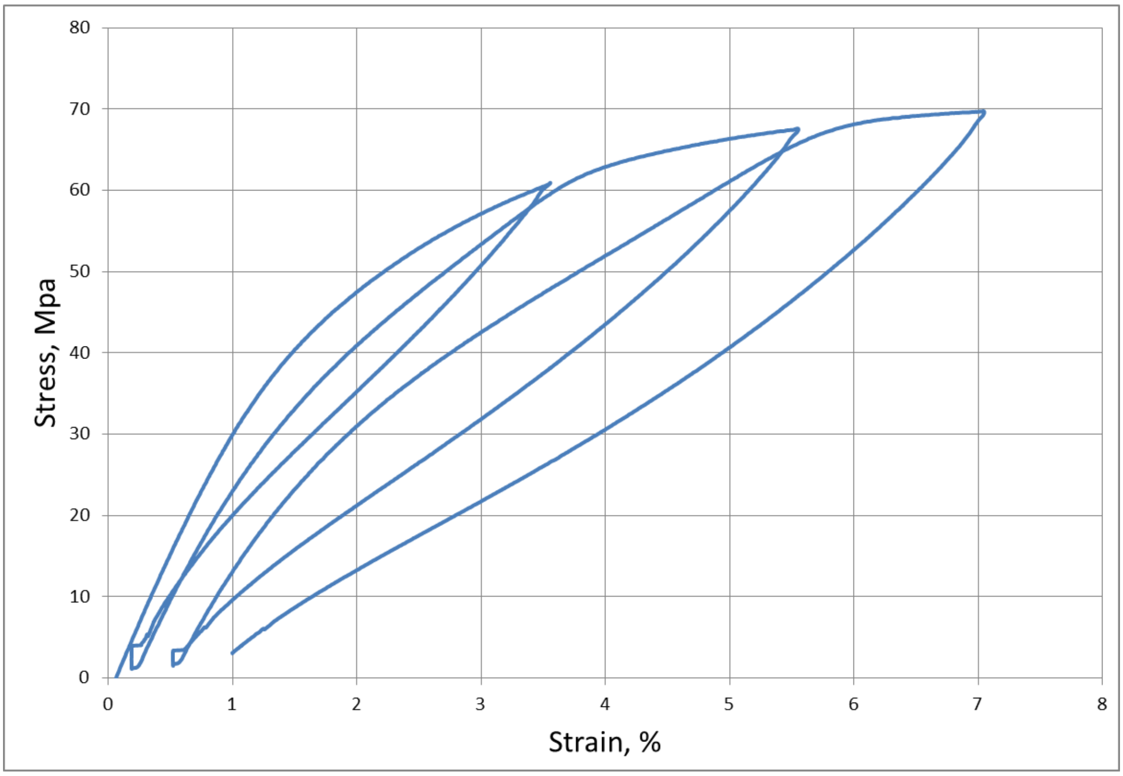


Figure 5: Stress vs strain plot from cyclic loading at three different loading strains

Stress relaxation test is also done using the same type of tensile specimen as cyclic testing and at room temperature. In relaxation test, the specimen is pulled to a certain strain level at 50 mm/min speed and holds that strain for 10 minutes to observe the relaxation of the material. Four virgin specimens are tested at four different holding strains (1.5%, 3%, 5% and 7%). Figure 6 shows the material relaxes over time at different constant strains along with the initial loading portion of the curves. It is clearly seen from the figure that relaxation rates are dependent on holding strain showing nonlinear nature of material. Therefore PRF model should be used to fully capture this nonlinear behavior.

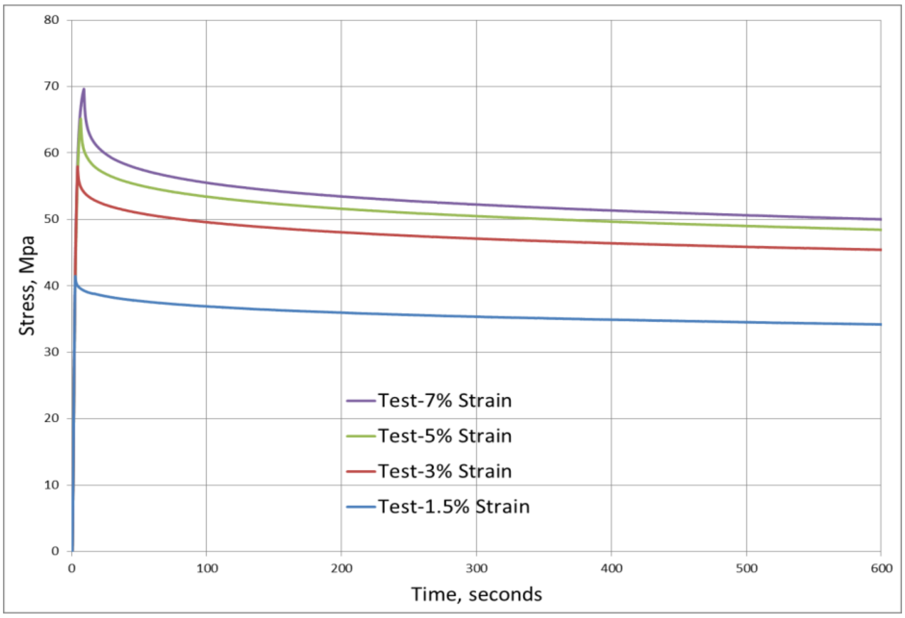


Figure 6: Stress vs time plot from stress relaxation testing at different holding strains

3.2 Optimization of PRF Coefficients in Isight

Isight optimization workflow set up is shown in the Figure 7. Hooke-Jeeves is selected as optimization technique. In order to facilitate the optimization process, the PRF coefficients along with hyperelastic Yeoh coefficients are first calibrated by MCalibration® tool from Veryst Engineering to learn the approximate range of the coefficient values that are used as the initial values for Isight optimization. There are four Abaqus simulations of relaxation test at four different strain levels and one Abaqus simulation of cyclic test. In Abaqus, single element model is used instead of full dogbone model for computational time saving. The corresponding Data Exchanger components are programmed to prepare input files for Abaqus components. Predicted stress history curves of four relaxation tests are compared with test data in the Data Matching component. Considering the model doesn't include any damage or plasticity, only the loading part of cyclic test and simulation is compared in Data Matching component.

The optimized values are obtained after hundreds of cycles and the optimized model predictions are compared with test data as shown in Figure 8. The PRF model predicts the relaxation behavior very well, especially for the high strain level. In addition, there is good agreement between the model and the test for the loading part of the cyclic test. The discrepancy of the unloading part indicates that Mullins effect and/or plasticity features need to be considered for further model improvement. In Appendix section, the Isight optimized coefficients values are given in Abaqus input deck format.

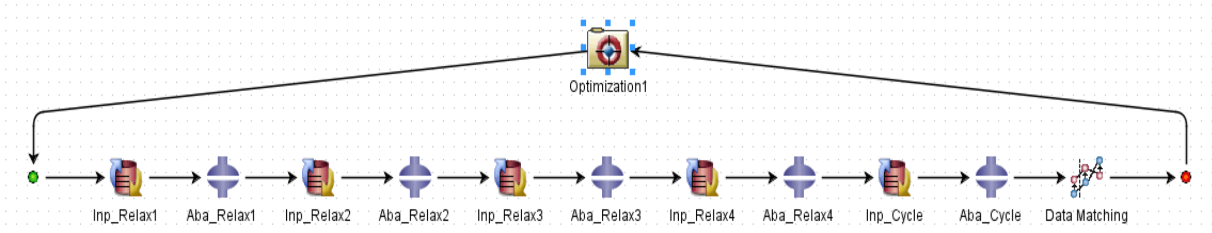
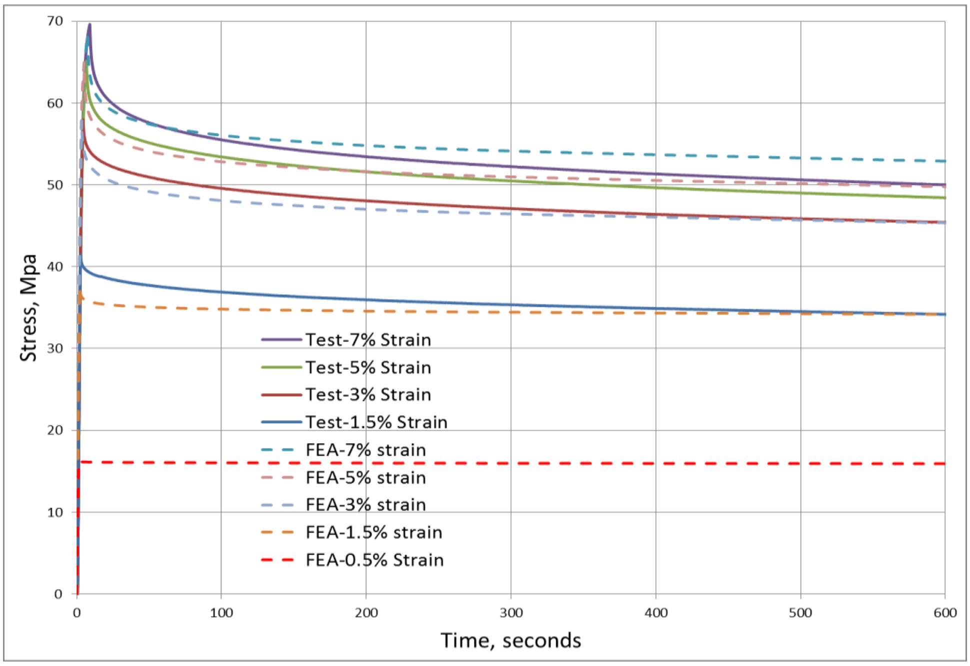
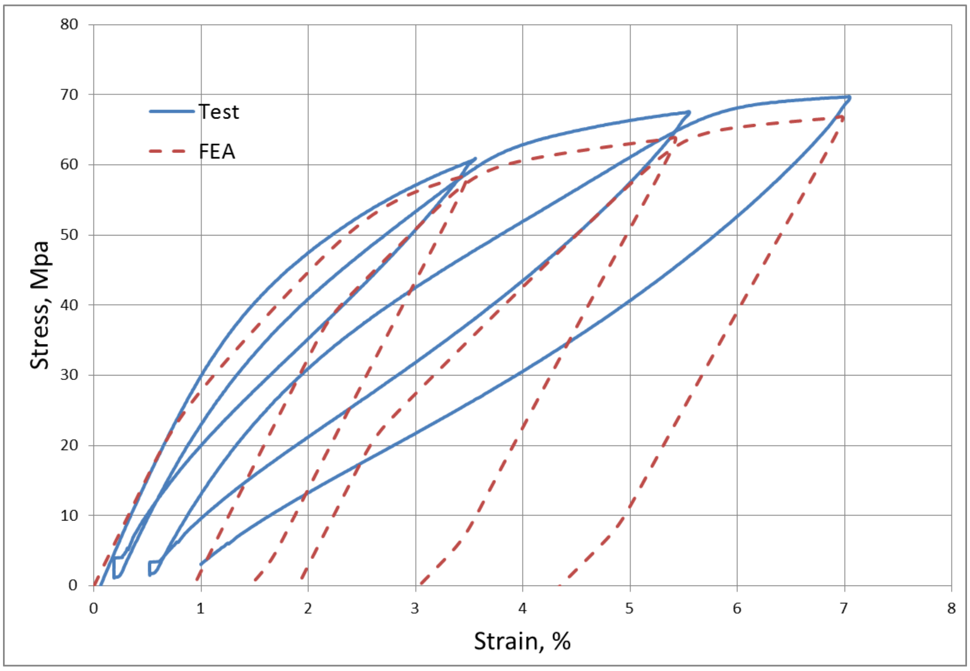


Figure 7: Isight workflow

Figure 8a also included the FEA prediction of stress relaxation at 0.5% strain using the same Isight optimized coefficients showing very little relaxation compare to high strain levels which further proves the nonlinear prediction of the PRF model.



(a) Relaxation test



(b) Cycle test

Figure 8: Comparison of single element model FEA prediction through Isight and measured data

4. FEA Model to Predict Viscoelastic Recovery

To predict viscoelastic recovery shown in Figures 2 – 4, an FEA model is developed in Abaqus. To be consistent with testing, same ISO 527-2 Type1 specimen is modeled and meshed with hex element in Abaqus/CAE with appropriate boundary conditions as shown in Figure 9. Abaqus/Standard is used as solver.

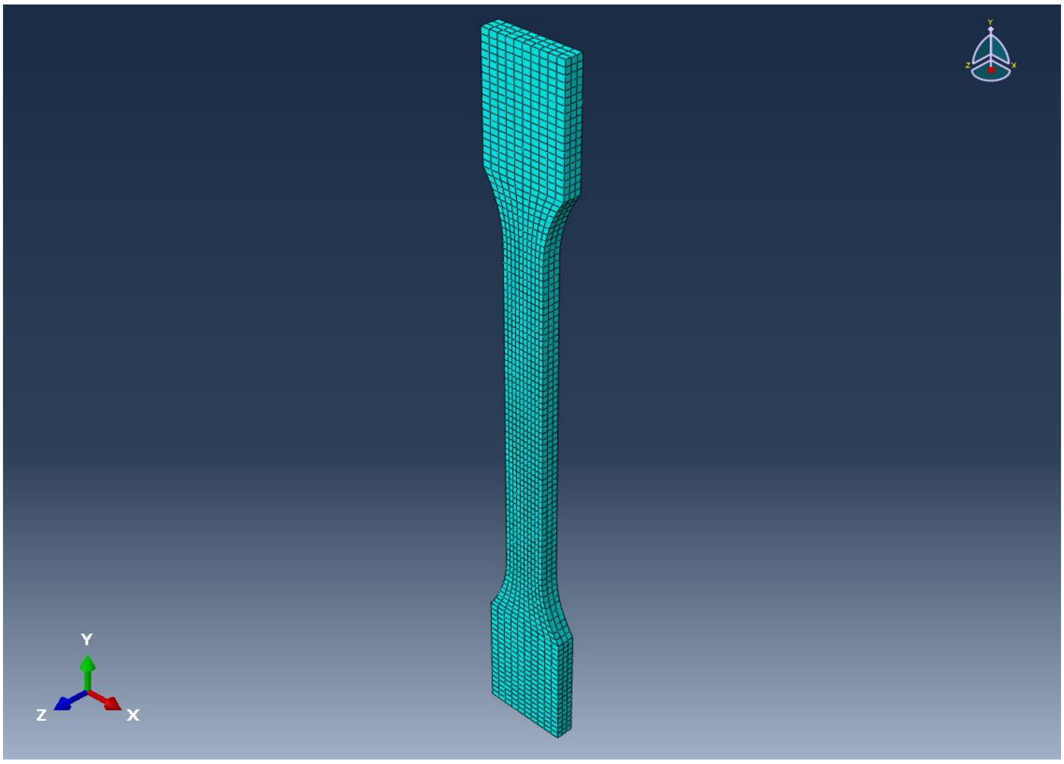


Figure 9: Abaqus/CAE mesh used to predict viscoelastic recovery

The same PRF coefficients along with hyperelastic Yeoh model determined via Isight optimization as described in previous section is used in this FEA model. Figures 10-12 show the prediction of strain recovery through FEA as compare to testing at different loading strains. It can be seen from Figure 10 in stress-strain plot that FEA is able to predict the slow viscous recovery of the material as shown in the horizontal portion of the curve at zero stress. Also notice the dependence of the amount of strain recovery on the loading strain showing the prediction of nonlinear nature of the recovery. Figures 11 & 12 show the same comparison between FEA and test using strain-time and stress-time plots, respectively. The difference in unloading curves between test and FEA in Figures 10 & 11 are related to the difference shown in Isight optimization in Figure 8b in the unloading portion of the cyclic test data.

Therefore, it can be concluded that using PRF model, viscoelastic recovery and subsequent permanent set can be modeled in Abaqus as long as both loading-unloading cyclic testing data and long term stress relaxation or creep data are available.

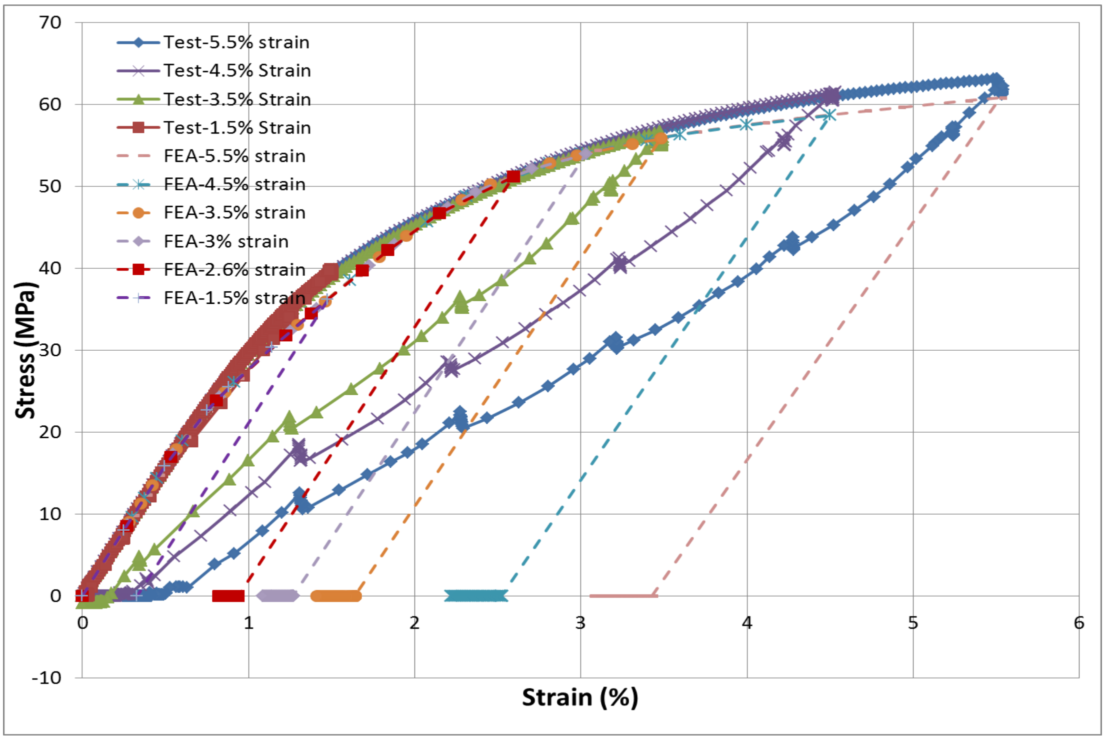


Figure 10: Stress-strain plot of viscoelastic recovery between FEA and experiment

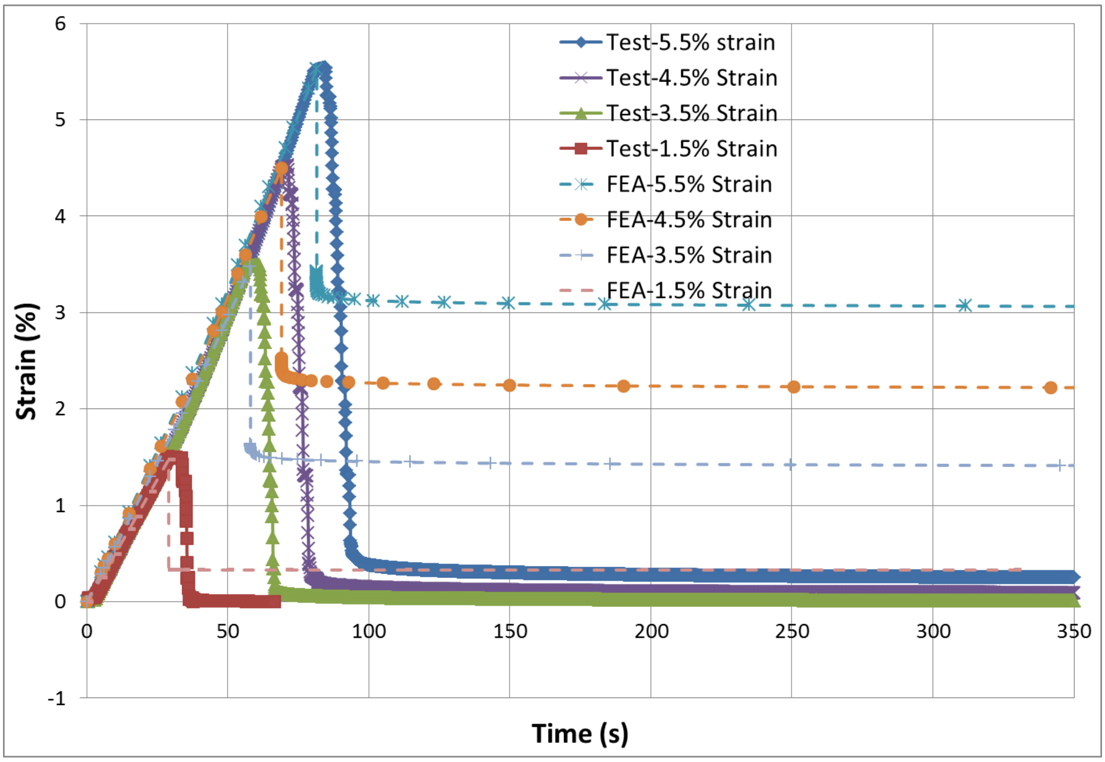


Figure 11: Strain-time plot of viscoelastic recovery between FEA and experiment

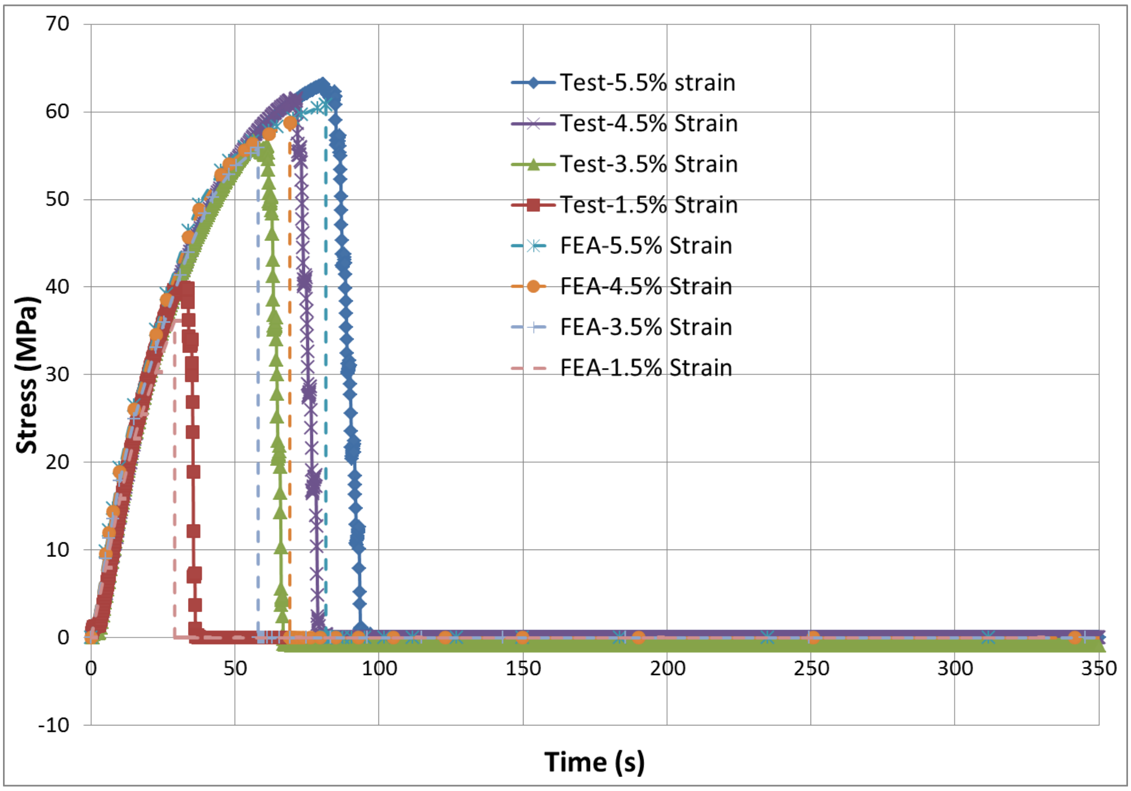


Figure 12: Stress-time plot of viscoelastic recovery between FEA and experiment

5. Summary and Conclusions

This paper describes the procedure to predict viscoelastic recovery of thermoplastic materials in Abaqus using Parallel Rheological Framework (PRF) material model. Two types of material test data, instantaneous loading-unloading cyclic test and long term stress relaxation or creep test data are required to calibrate the PRF coefficients. Simulia's optimization tool Isight is used to optimize those coefficients. Following important conclusions can be made from this work:

- Same values of PRF coefficients can be used to predict both cyclic and stress relaxation test data. However, more work needs to be done to better predict the unloading portion of cyclic test data.
- Overall, PRF model can be used to predict both instant elastic recovery and slow time dependent viscous recovery
- Based on this work, it can be concluded that PRF model can also be used to predict compression set which is very crucial properties of elastomeric materials

6. References

1. Gibson, R., Principles of Composite Material Mechanics, Chapter 8.
2. Karim, M. R.. and Hoo Fatt, M. S., "Rate-dependent constitutive equations of carbon-fiber reinforced epoxy," Polymer Composites, 2006, vol. 27, number 5, pp. 513–528.
3. Abaqus Analysis User's Guide, Version 6.14, Dassault Systèmes Simulia Corp., Providence, RI.

4. ISO 527-2, Plastics-Determination of tensile properties, 2012
5. Bergstrom, J. S., “Constitutive modelling of Elastomers-Accuracy of predictions and numerical efficiency,”.
6. Dalrymple, T., and Choi, J., “Elastomer rate-dependence: A testing and material modelling methodology,”172nd Technical Meeting of the Rubber Division of the American Chemical Society, 2007.
7. N. Brusselle-Dupend, et al., “Experimental Characterization and Modeling of the Uniaxial Mechanical Behavior of Polypropylene before Necking,” Oil and Gas Science and Technology-Rev. IFP, Vol. 57 (2002), No. 2, pp. 155–168.
8. R. Quinson, J. Perez and M. Rink, A. Pavan, “Yield criteria for amorphous glassy polymers,” Journal of Materials Science 32 (1997), pp. 1371–1379.

7. Appendix

Isight optimized PRF and Yeoh model coefficient values in Abaqus input deck format are given below

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** Units: [length]=millimeter, [force] = Newton, [time] = seconds, [temperature] = Kelvin
** Calibration file name: Delrin500_simulation17.mcal
*Density
1e-09
*Hyperelastic, Yeoh, Moduli=instantaneous
 633.952,-2364.4450000000015,-2252.045800000001, 0.001,0,0
**
*Viscoelastic, Nonlinear, NetworkId=1, SRatio=0.00345838, Law=strain
1.07023E-22, 8.67071,-0.535679
**
*Viscoelastic, Nonlinear, NetworkId=2, SRatio=0.5195, Law=strain
3.9037999999999985E-16, 11.367135000000003,-0.6343880000000004
**
*Viscoelastic, Nonlinear, NetworkId=3, SRatio=0.424629, Law=strain

2.73916E-22, 12.039979999999998,-0.49440799999999896
```

8. Acknowledgment

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