Developing an ANSYS Creep Model for Polypropylene from Experimental Data

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Abstract

This paper describes a procedure for modeling the primary creep behavior for one of the most widely used commodity resins, polypropylene. The procedure involves using ANSYS to verify an assumed mathematical creep model and calculated creep behavior material properties. ANSYS results are compared to both creep and stress relaxation experimental data and then calibrated to give a good correlation to the response of this particular grade of polypropylene.

Introduction

Creep behavior is an important design consideration for polymers. Creep is responsible for time-dependent changes in the dimensions of a product and for important strength reductions that could affect the ability of products to resist design loads. Polymers are particularly susceptible to creep even at room temperature. They are also susceptible to stress relaxation. Since design applications require that a part be loaded for long-time duration, this loading will lead to creep which may induce unacceptable permanent deformations or loss of assembly preload. Both creep and stress relaxation are key design considerations for products like carbonated beverage bottles, pumps or other pressurized vessels, and parts undergoing continual stress.

It is known that creep phenomena in plastics are extremely complex. Many mathematical models have been generated to represent some of these complex phenomena [Ref 1]. These could include time dependent properties within the plastic including: stress rate, strain rate, temperature variations, time-dependent stiffness variations, and stress-strain levels. This paper limits its scope to a time frame of one hour of loading, to stresses within an elastic range, to one temperature, and to a specific material. It is a study to compare acquired creep data within these specified limits to one of these analytical models. The purpose is to simulate within ANSYS a good correlation using this limited data accompanied by verification by independent experiments that are driven by creep.

This paper limits its discussion to the creep response to a popular commodity resin, polypropylene. This polymer is selected because of its high primary creep response in the first hour of loading. The designer knows that without accurately solving for this early response, any subsequent response will be inaccurate.

Creep data is used to determine the polypropylene's viscoelastic material coefficients. These coefficients are put into one of the many ANSYS mathematical models. [Ref 2] To do this, the creep data and the selected mathematical creep model are used together to calculate the creep coefficients. A solution is then run in ANSYS to model a single creep element. Ironically, since the mathematical model itself is used together with the creep data to calculate the creep coefficients, even coefficients calculated from the wrong mathematical model would give ANSYS results that show a good match with the experimental creep data. Therefore, an independent verification is needed to test the validity of the calculated coefficients and the chosen ANSYS mathematical model. A good independent method was found to be the stress relaxation experimental data of the polypropylene. Since creep phenomenon generates stress relaxation in materials, then the coefficients generated from the creep data and subsequently from the ANSYS solution, should also match the data generated from stress relaxation testing.

Background

Primitive modeling of Polypropylene

Polypropylene owes its popularity to its versatility in the family of commodity resins. It is of fairly low cost, is compatible with many processing techniques, and is therefore found in many commercial applications that employ extrusion, extrusion coating, blown and cast film, blow molding, injection molding and thermoforming. Polypropylene is available in three forms: homopolymer, copolymer, and random copolymer grades. The grade of polypropylene used for this study is the copolymer form.

Figure 1 shows a schematic of the molecular structure that represents polypropylene. Under a tensile load, the amorphous molecular structure is easily susceptible to polymer molecules untangling and slipping by each other due to a low inter-molecular bond. The crystalline molecular structure has a stronger and denser bond. It is susceptible to tilting and reorienting, as well as slight expansion. All these responses of the polypropylene are dependent on time, temperature, and loading.

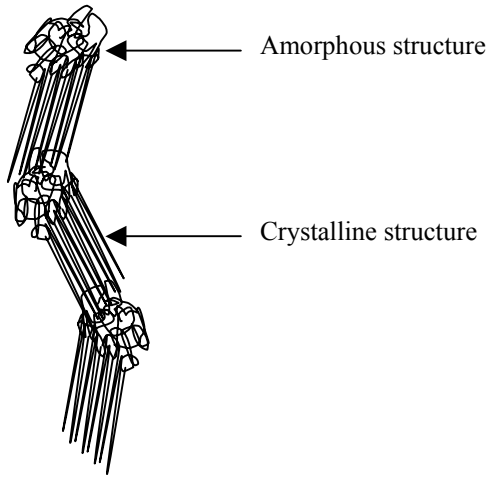

Figure 1 - Schematic of Polypropylene Molecule Structure

Stephen L. Rosen in Fundamental Principals of Polymeric Materials [Ref 3] and others [Ref 4,5] symbolize the response of polymers under load as a combination of linear viscoelastic models. Two models, attached to each other, are shown in Figure 2, the Maxwell model and the Kelvin-Voight model. Together these models represent both the creep and stress relaxation responses of a polymer within its elastic range.

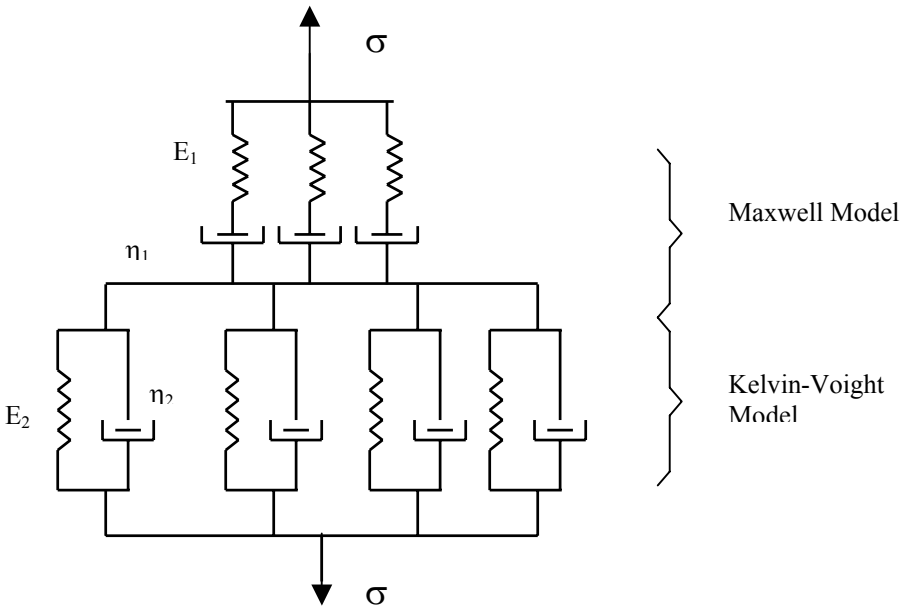

Figure 2 - Maxwell and Kelvin Voight Material Models

The Maxwell model, used for many metals at room temperature, forms a portion of the polymer model. The elastic spring of the Maxwell model represents the elasticity of the material, E, and loads and unloads immediately. The viscoelastic dashpot represents the time dependent strain in the material that is proportional to the stress applied, σ, and inversely proportional to the viscosity of the material, η. This viscoelastic "dashpot" response is represented by σ/η. The Maxwell model shows the elastic spring and viscoelastic dashpot in series; hence, under load equal stresses occur simultaneously. When the load is removed, only the spring reacts and the viscoelastic dashpot remains permanently deformed. This model represents both creep and stress relaxation responses of a material within its elastic range.

The Kelvin-Voight model responds differently than the Maxwell model. Instead of equal stress in the elastic spring and viscous dashpot, this model represents the stress within the material to be a combination of both the elastic spring and dashpot. If the load is applied, the spring only stretches if the time-dependent viscous dashpot has sufficient time to deform. Conversely, when the load is removed, the deformation that has accumulated in the elastic spring will continue to work toward deforming the viscoelastic dashpot. In a polymer, this would be seen in the slight shrinkage movement that occurs after a tensile load is removed.

Rosen explains that within a polymer, the Maxwell dashpot represents molecular slippage that is responsible for material flow. The value of the viscosity, η_1, is the amount of equilibrium slippage within the material. The spring, E_1, represents the elastic straining of bond angles and lengths. All bonds in polymer chains have equilibrium angles and lengths. The value of E_1 is the elasticity of the polymer chains as they pull the atoms within the molecule. The viscoelastic dashpot of the Kelvin-Voight model has a viscosity of η_2. It represents the resistance of the polymer chains to uncoiling and coiling, caused by temporary mechanical entanglements of the chains and molecular friction. Since coiling and uncoiling require cooperative motion of many chain segments, they cannot occur instantaneously and hence account for retarded elasticity. The elasticity of the Kelvin-Voight model represented by E_2 represents the restoring force brought about by the thermal agitation of the chain segments. Imagining the coiling and uncoiling of steel wool strands can portray all of these described phenomenons.

The repeated configuration of Maxwell and Kelvin-Voight as shown in Figure 2 is representative of the complexity of a polymer and its randomness of molecular configuration. If all four values of E_1, η_1, E_2, and η_2 could be isolated by experimentation such that these properties could be directly solved, the response of the polymer would still not be represented accurately. Polymers are susceptible to time hardening and strain hardening. They are also sensitive to thermal conditions and rate of loading. Although the expanded series of Maxwell and Kelvin-Voight models represent the non-linear nature of the true polymer, it still remains primitive compared to the complex nature of the true material.

Creep correlates with stress relaxation.

The time-dependent deformation of creep is the same mechanism that molecularly responds to stress relaxation. [Ref 6] This can also be proven mathematically in a simple fashion. If only the Maxwell model is

used for simplicity, the material's rate of creep is the summation of elastic strain rate, $d\sigma/dt\ (1/E_1)$, and viscoelastic strain, σ / η, and is shown as follows:

$d\varepsilon/dt = d\sigma/dt\ (1/E_1) + \sigma / \eta_1$ since in stress relaxation, $d\varepsilon/dt$ drops out

$d\sigma/dt = -\sigma E_1 / \eta_1$

$d\sigma/\sigma = -[E_1 / \eta_1]\, dt$ separating variables

$\ln \sigma - \ln \sigma_o = -[E_1 / \eta_1]\, t$ integrating and imposing limits

$\ln [\sigma / \sigma_o] = -[E_1 / \eta_1]\, t$

$$\sigma = \sigma_o \exp [-E_1 t / \eta_1] \quad (1)$$

Equation (1), which is derived from a creep response, represents the time dependent change in stress for stress relaxation. From equation (1), it is observed that the slope of the log σ versus time plot is:

$$\text{Slope of log } \sigma \text{ and time} = [-E_1 / \eta_1] \quad (2)$$

This information is helpful since the modulus of elasticity, E_1, can be readily found from a rapidly applied load within the elastic range of the material. The viscosity, η_1, can then be determined using the slope of the log σ versus time graph.

Procedure

Since the purpose of this study is to simulate with ANSYS the primary creep response of a particular grade of polypropylene at room temperature. It is first necessary to gather experimental creep data for a family of varying stresses appropriate to the design. This data is then used to calculate constants used within the chosen ANSYS mathematical model for viscoelastic creep. These constants and the validity of the chosen ANSYS mathematical model will be verified. This is accomplished by solving for both creep and stress relaxation answers within ANSYS, and comparing these answers to the creep and stress relaxation experimental data.

Experimental

Several experiments were performed on ASTM D-638 dog-bone samples of a particular grade of polypropylene to collect data to determine elasticity constant, E_1, and also the creep and stress relaxation responses of the polymer while subjected to a family of stresses. The lowest stress range of 200 psi [1.38 MPa] is chosen to minimize error by excluding a weak response in the material. A high stress range of 2000 psi [13.8 MPa] is chosen because it is slightly beyond the yield limit of the material. All experiments were taken at room temperature, 75°F [23.9°C] since the rigor of varying temperatures is not within the intent of this paper.

It can be seen from Figure 2 that by rapidly loading the polypropylene only the Maxwell elastic spring immediately reacts and not the time-dependent viscoelastic dashpot. By repeating the rapid load of a particular amount, a yield point is defined as the value of stress at which no change occurred from the initial modulus of elasticity. The yield for this grade of polypropylene is determined to be approximately 1600 psi [11MPa] and the initial modulus, E_1, is calculated to be 135,000 psi [0.93GPA].

Successive tests were conducted on polypropylene specimens for stress relaxation data using a Tinius Olsen 1000 tensile tester. Tensile stresses between the 200 psi [1.38 MPa] and 2000 psi [13.8 MPa] were rapidly imposed and then the imposed displacement was held for one hour. A family of curves resulted as shown in Figure 3.

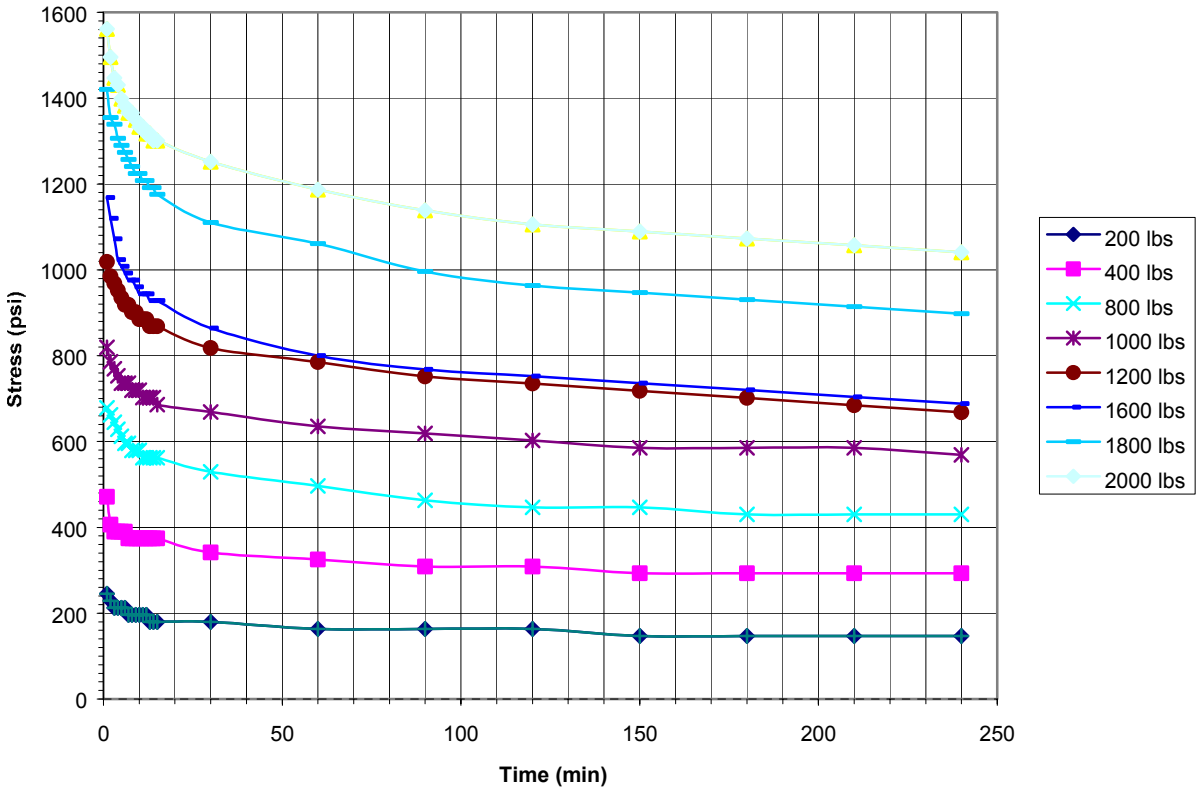

Figure 3 - Stress Relaxation Response of Polypropelyne To Family of Stresses

Figure 4 shows the Brown and Sharp Digit-Hite creep apparatus used for successive creep tests for the polypropylene specimen for a family of stresses. Stresses between 1000 psi [6.9MPa] and 2200 psi[15.2MPa] were used. Lower stress results were showing a large spread in variability because of the small movement and the parallax viewing ambiguity, so this data is not included. The creep test data is shown in Figure 5.

Figure 4 Brown and Sharpe Creep Testing Apparatus

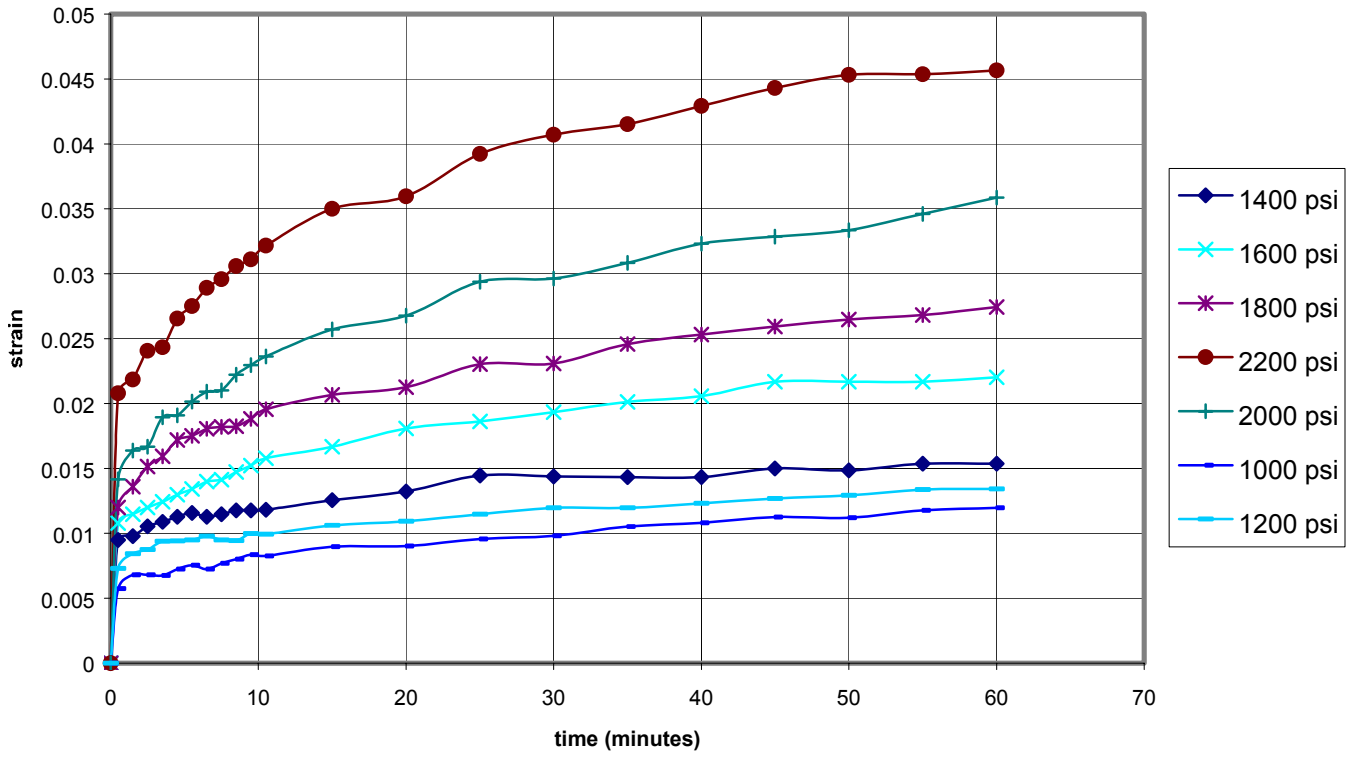

Figure 5 - Polypropylene Creep Experimental Results: Strain versus Time for Family of Stresses

Theoretical FEA Model

Libraries of creep strain rate equations are included under the "Implicit Creep Equations" and "Explicit Creep Equations" sections of ANSYS 6.0 [Ref 2]. There are many explicit and implicit creep models and an added feature of a user defined creep equation. The reference explains that the implicit model is recommended for general use, and is especially applicable to large strains. The designer has the daunting task of either matching the materials performance with one of these empirical formulas or creating ones own equation and subroutine.

Curve fit routines such as the multivariable computer curve fitting routine [Ref 7] are available. Although these methods yield favorable results in matching a particular creep curve at a certain stress level, it is doubtful if the curve fit polynomial would provide a good match to the entire family of stresses. Further, it is questionable if this curve fit polynomial based on creep data would also represent stress relaxation responses. It is felt that a truer mathematical model is based on the material schematic models of Figure 2, in spite of its primitive semblance to the natural material. This model reflects the full range of stresses for both creep and stress relaxation, and can be verified with experimental data.

For the Maxwell and Kelvin-Voight models as shown in Figure 2 to be used for the creep model, material constants for E_1, E_2, η_1 and η_2 need to be determined. The explicit primary creep equation representing the Maxwell model is represented by the following ANSYS equation:

$$d\varepsilon/dt = C1\ \sigma^{C2}\ t^{C3}\ e^{-C4/T} \qquad (3)$$

and the Kelvin-Voight model can be shown to be represented by the following ANSYS equation

$$d\varepsilon/dt = C1\ \sigma^{C2}\ r\ e^{-rT} \qquad \text{where r is } C5\ \sigma^{C3}\ e^{-C4/T} \qquad (4)$$

Although it is correct to merge these two models, it is found to be extremely difficult to isolate material properties from portions of the creep or stress relaxation testing. A good description of isolating the Maxwell and Kelvin-Voight models in creep testing is given in Ref 4. The four material constants E_1, E_2, η_1, and η_2 were being sought to apply to equations (3) and (4). Of further consequence is the realization the stress and time variables are believed nonlinear [Ref 3,4,5].

The authors believed a more viable approach to simulating in ANSYS the creep response of the polypropylene is to use the method described by David J. Dougherty [Ref 7] Dougherty's study described using a practical approach for finding material constants using an ANSYS model. His work showed good correlation between creep data and physical testing.

Dougherty's work focused on a carbon filled PolyPhenylene Sulfide (PPS), which has a elastic modulus of 3.1Msi. This is a much stiffer material than the polypropylene resin used in this study which has a elastic modulus of 0.133 Msi. Although polypropylene is much less viscous than the PPS of Dougherty's study, the authors found Dougherty's method used for the PPS to have three distinct advantages.

1. The ANSYS mathematical model is based on only the Maxwell model and a much simpler mathematical model than the Maxwell and Kelvin-Voight combination.
2. Only three equation constants need to be solved, which is fewer than the five of the of the Maxwell and Kelvin-Voight combination model, which include E_1, E_2, η_1, and η_2 and coefficient constants.
3. It offers a simple procedure to quantify the two nonlinear exponents, each on the stress and time variables.

The ANSYS mathematical model then is chosen to be the primary explicit creep equation taken from Table 5 from ANSYS [Ref 2]. It is in the same form as the implicit equation shown as equation (3). Although implicit solutions are recommended by ANSYS, the explicit solution is used for simplicity. This is because the FEA model used to gather ANSYS solutions for stress relaxation required a prestress on an element, which is easily accomplished with LINK1 element using the explicit solution.

Analysis

Determining Coefficients of ANSYS Creep Law

The ANSYS equation (3), based on the nonlinear version of the Maxwell model, needs C1, C2, C3, and C4 to be provided as input for equation constants. To calculate these constants the integrated form of the equation (3) is used.[Ref 9]

$$\varepsilon_c = \text{creep strain} = (a_o)\, \sigma^{m}\, t^{n}\ \exp(-Q/RT) \qquad (5)$$

This integrated form shows time and stress variables σ^m and t^n, where m and n and are constants representing exponenets of the time and stress variables. The Q represents activation energy, R represents Boltzmann's constant, and T represents absolute temperature. For this study, the temperature term is ignored and –Q/RT is zero, making exp(–0) equal to 1.

Doughtery's procedure [Ref 8] involves taking the log of equation (5) while holding stress constant, as in a creep test. This yields the following:

$$\log(\varepsilon_c) = n \log(t) + \text{constant} \qquad (6)$$

Figure 6 shows the log creep strain, ε_c, plotted versus log time for the several applied stresses. Equation (6) is fitted through each dataset and the slope n is determined. The average n is 0.1736.

In a similar fashion, the log of equation (5) is taken and holding the time constant, as would be the creep at any one time.

$$\log(\varepsilon_c) = m \log(\sigma) + \text{constant} \qquad (7)$$

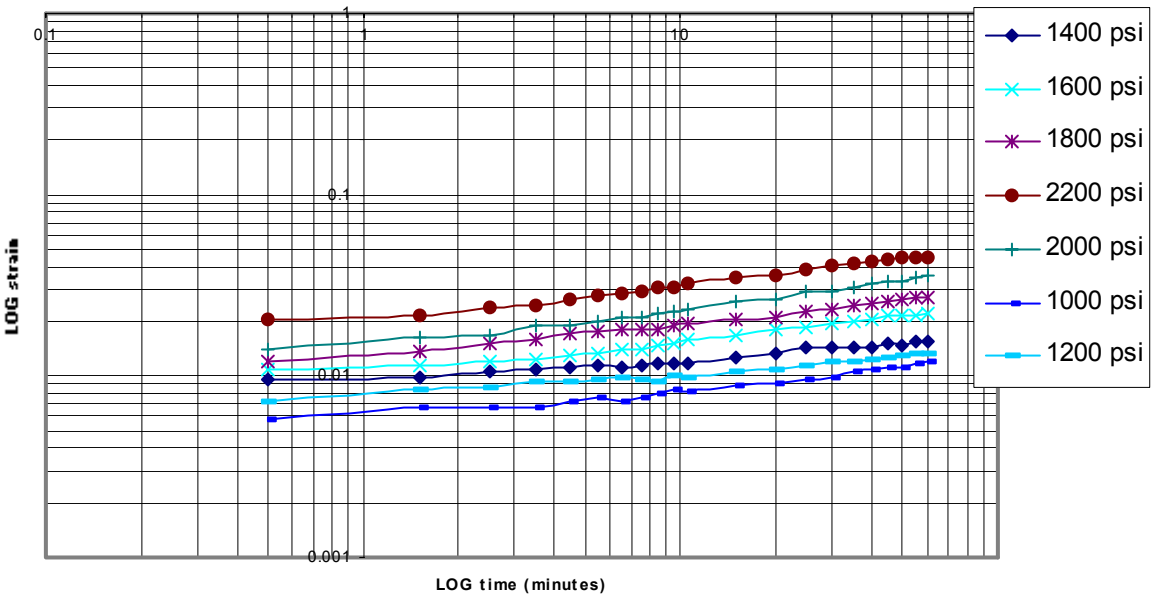

Figure 6 - Polypropylene Creep Experimental Results: log Strain versus log Time

To obtain the stress versus time plots, stresses for selected time values were read from the data. Although the authors did this manually, Dougherty recommends using a registered graphical software called DeltaGraph [Ref 8] Figure 7 shows the log creep strain plotted verses log stress. Slope m was determined and the average m is 1.566.

The a_o coefficient is determined by putting the value of m and n into equation (5) along with strain data from the creep experiments. The average a_o is 1.066 e^{-7}.

The creep strain function based on using these average calculated values can be written as:

$$\varepsilon = 1.066e^{-7}\ \sigma^{1.566}\ t^{0.1736} \quad \text{for time (minutes), stress (psi)} \qquad (8)$$

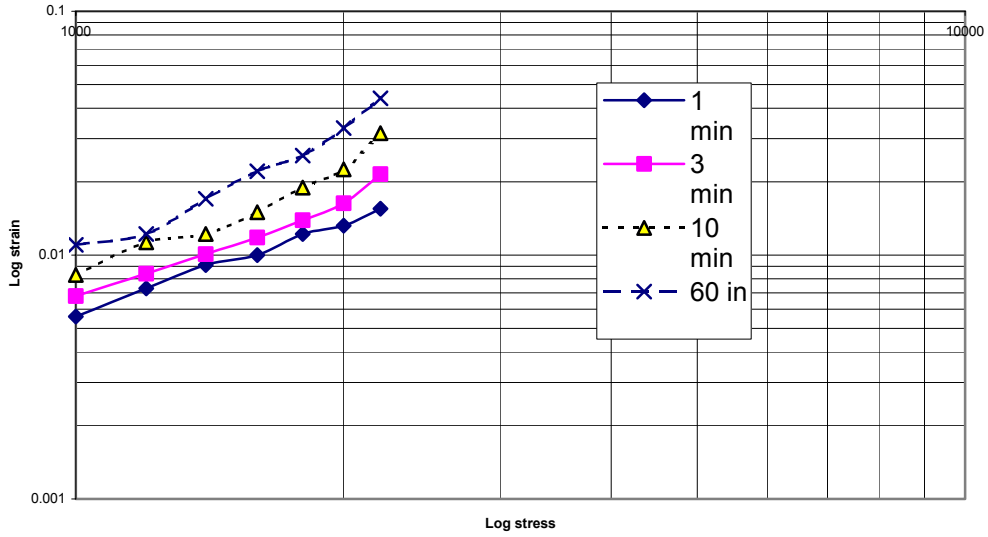

Figure 7 - Polypropylene Creep Experimental Results: log Strain versus log Stress

The final step is to express equation (8) in incremental form so that it can be used directly by ANSYS. ANSYS uses a numerical time stepping procedure based on the incremental rate strain, ε_c. The strain rate is determined by partial differentiating equation (8) with respect to time as:

$$\delta \varepsilon_c / \mathrm{d}\, t = \Delta\varepsilon_c/\Delta t = 1.85e^{-8}\, \sigma^{1.566}\, t^{-0.826} + \zeta \qquad (9)$$

where ζ is the error resulting from the first order incremental approximation.

FEA Model

The incremental strain rate model, equation (9) is applied to evaluate the creep and stress relaxation of a pair of Link 1 elements. Figure 8 shows two elements one located above the other. The lower element represents the stress relaxation model, has fixed displacement constraints at both ends, and has an initial strain, ISTRN, of σ_o/E_1. The upper model represents the creep model and has a constant, applied axial load and is free to stretch horizontally.

The single LINK1 element modeled for each case of creep and of stress relaxation is used to represent two test specimens. If the ANSYS solutions match the experimental data, then there is confidence in the material properties and that a more complicated model could be solved correctly.

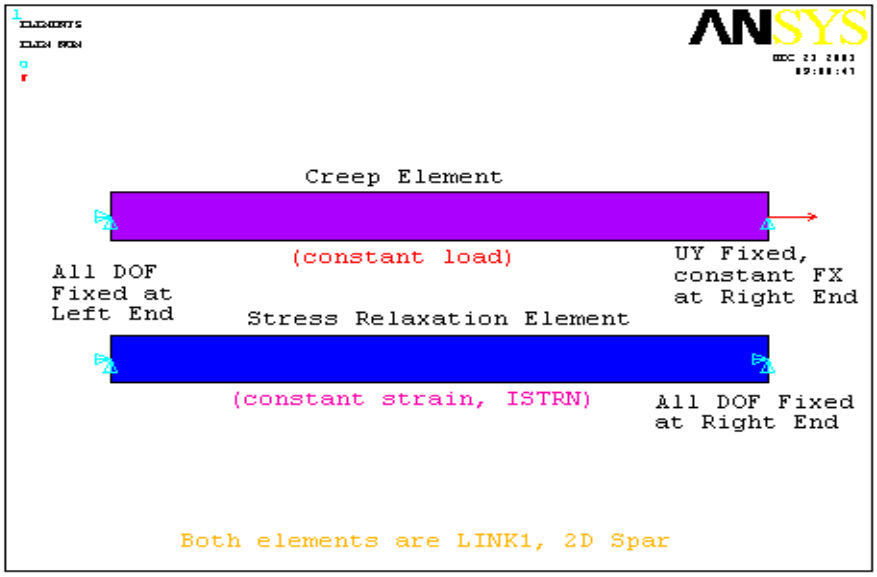

Figure 8 - ANSYS Models for Stress Relaxation and Creep

Analysis Results & Discussion

Figure 9 shows the comparison between *creep experimental* data (designated T on graph legend) with the ANSYS results (designated A on graph legend) using the calculated coefficients and equation (9). A slight adjustment is made to the stress term exponent, m. Instead of m = 1.566 as calculated, it is changed to 1.466 to bring the ANSYS solutions for the lower stresses range closer to the experimental results. This adjustment is expected since equation (9) had a 1st order approximation error, and the stress term is not dealt with in the partial differentiation. Notice there is good correlation in the lower stress ranges, but a high error of 19.4% shows for the 2000psi [13.8 MPa] stress.

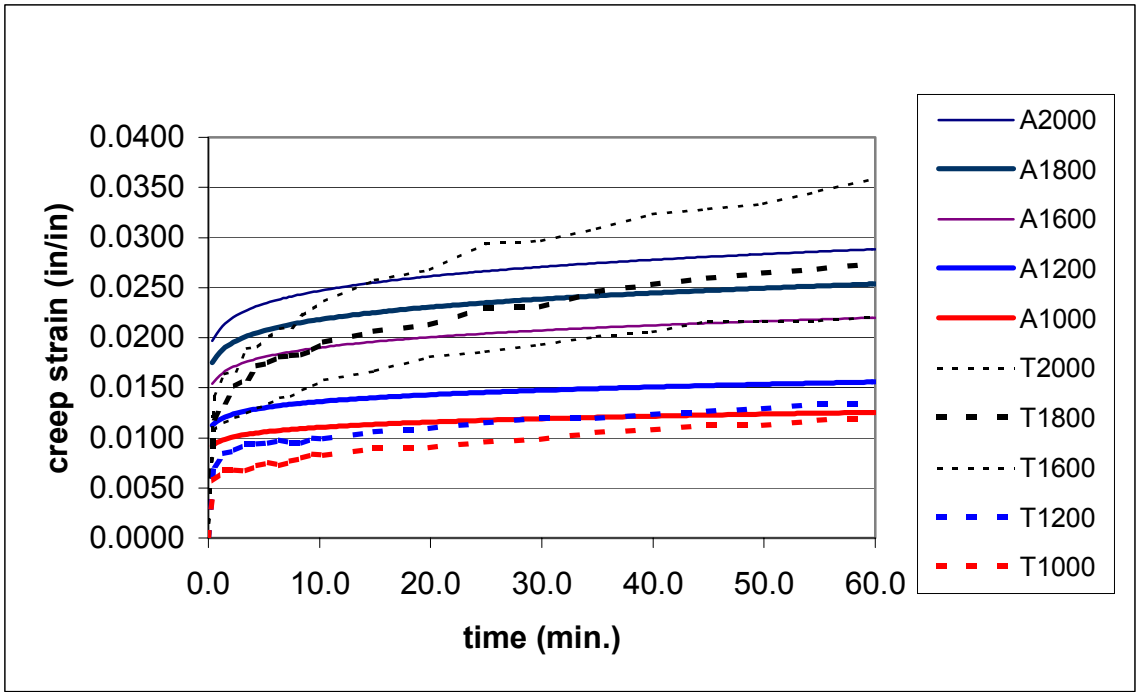

Figure 9 - Creep Experimental Results (T) Compared to ANSYS Creep Solution (A)

It was discovered that better correlation is found between the ANSYS results and the experimental data when a very small initial step size of 0.0001 is initially specified for the time increments, and AUTO stepping is chosen.

By including nonlinear stress-strain material properties, the creep correlation should be closer for the stresses above the 1600 psi [11.0MPa]. When the stress strain curve for the polypropylene is added to the ANSYS solution, the creep values moves up to be closer to the experimental values as shown in Figure 10. There is still good comparisons at the lower stress levels, while the high stress level comparison shows to be 11.1%. The nonlinear material option is not used for the stress relaxation, because most, if not all of the permanent stretch would have occurred at time=0.

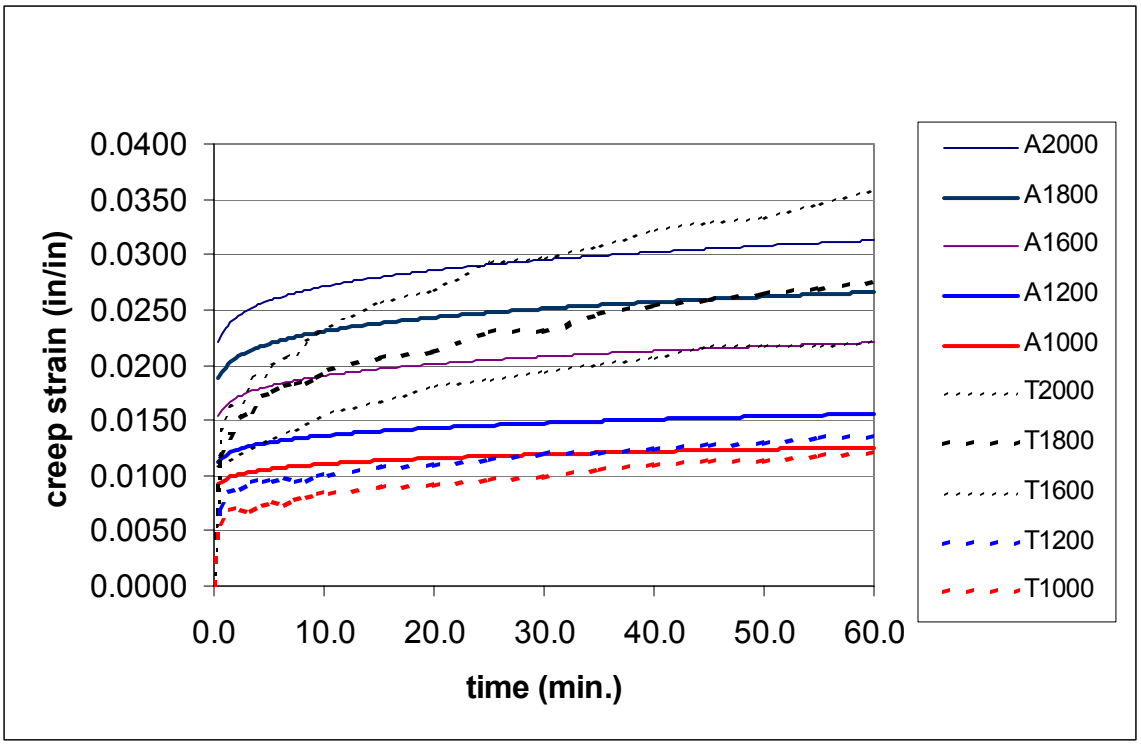

Figure 10 - Creep Experimental Results (T) Compared to ANSYS Adjusted Creep Solutions (A)

Figure 11 show the comparison between *stress relaxation experimental* data (designated as T on the graph) and the ANSYS results. Notice the highest error in comparing the ANSYS solutions to the experimental results is 16.6% at the 2000psi [13.8 MPa] stress.

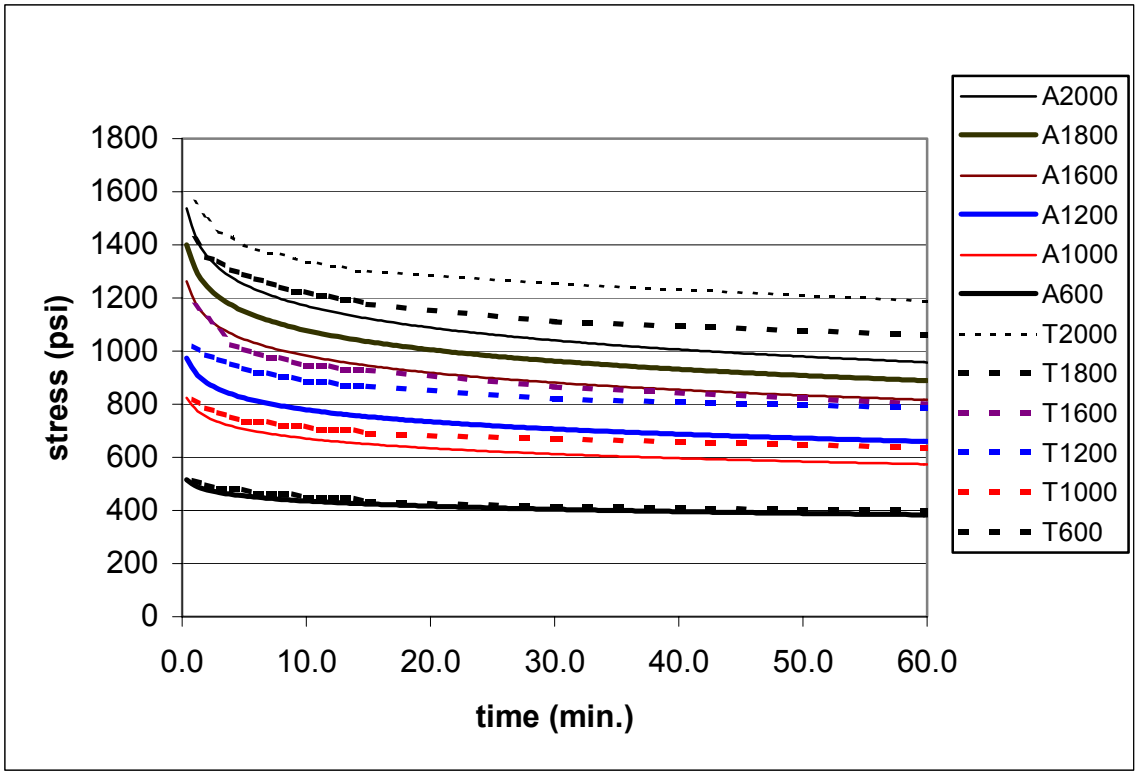

Figure 11 - Stress Experimental Results (T) Compared to ANSYS Stress Relaxation Solutions (A)

It is suggested that the values of m and n, which are the exponent terms of the stress and time, respectively, of equation 8 would be finely adjusted to match the data even further. It is noted that a small change to either exponent m or n results in a significant change in the ANSYS results. Also a stress-strain experimental testing done for the nonlinear material property could have a larger lot size to better represent this to ANSYS.

Conclusion

This paper describes a procedure for modeling the primary creep behavior for one of the most widely used commodity resins, polypropylene. Experimental data showing the responses of polypropylene for creep and stress relaxation are gathered. Based on a procedure described by David Dougherty [Ref 8] creep constants for a non-linear Maxwell model can be found and put into one of ANSYS standard creep formulas [Ref 2]. ANSYS is then used to verify an assumed mathematical creep model and calculated creep behavior material properties

ANSYS results are compared to both creep and stress relaxation experimental data and then calibrated to give a good correlation to the response of this particular grade of polypropylene. Comparisons between ANSYS and the experimental creep data showed good correlation, with the highest error being 11.1%. It is difficult to comprehend the magnitude of this error since the numerical values are so small. The 11.1 % represents 0.016 inch error after one hour in a 4 inch specimen gage length. Comparisons between ANSYS and the experimental stress relaxation data for the polypropylene show the highest error to be 16.6%. This represents a maximum stress error after an hour of 320 psi in a specimen originally stressed to 2000 psi. At some stress levels, both the creep and stress relaxation correlation between ANSYS and the experimental testing after one hour show to be less than 1% variance.

It is known that creep phenomena in plastics are extremely complex. This paper limits its scope to a time frame of one hour of loading, to stresses within an elastic range, to one temperature, and to a specific

material. It is a study to compare acquired creep data within these specified limits to one analytical model. The purpose is to simulate within ANSYS a good correlation using this limited data accompanied by verification by independent experiments that are driven by creep. Further research is needed to investigate expanding these limits including, but not limited to, stress levels approaching or exceeding yield stress, long-term behavior, and other temperature ranges. It is cautioned that the procedure described in this paper is limited to the scope described, and has not been studied to be proven applicable to other polypropylenes grades or commodity resins.

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