TMG News
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The Madison Group
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The Importance of Material Characterization for Simulation Applications

John R. Nebbia

Problem: A PC/PBT resin was the selected material for an injection molding application. The material was not characterized for Moldflow. Therefore, a "Drop-in" substitute was recommended by the material supplier to move forward with the analysis. This "Drop-in" substitute resin was also listed as an equivalent resin on the material supplier's line card. Initially, the analysis was intended to establish a proper gating configuration, and establish a prediction of the part's warpage mode. Later, the customer expressed an interest in finding linear shrinkage values to aide in cutting of the tool. The analysis was to be performed using injection molding simulation. A comparison of the materials that the analysis used are shown below in **Table 1.** This highlights that while the resin supplier lists these materials as a "Drop-in" substitute, there is a distinct difference in the materials. Specifically, it appears that the substitute material is a higher molecular weight material.

Table 1: *The table shown below highlights the material differences between the Characterized and Drop-in substitute materials.*

	Material	
	Characterized	"Drop-In" Substitute
Melt Flow Volume @ 250°C/5.0 kg (cm^3/10min)	24	8
Specific Gravity	1.27	1.34
Flexural Modulus (MPa)	1,972	2,060
Tensile Strength at Yield (MPa)	57.9	48
Tensile Strain at Break (%)	60	110
Notched Izod @ 23C (J/m)	614	534

Evaluation: During the evaluation of the part and process, the simulation with the substitute resin showed reasonable filling parameters. The substitute resin was able to capture the filling pattern and balance of fill. Additionally, the pressures did not raise any concern during the preliminary analysis with only the substitute resin. The predicted filling pattern was similar to the Characterized resin, as well as similar to short-shots taken at the press. However, during the warpage analysis, excessive amounts of warpage and shrinkage were predicted. These values were far greater than expected based on the geometry and previous experience with PC/PBT resins. Therefore, there was little confidence in the predicted data in regards to dimensional stability by both The Madison Group and the customer.

With this lack in confidence regarding the data, the resin supplier ultimately decided to have the material characterized for Moldflow. The Madison Group coordinated the characterization and fit the material data to generate the newly characterized material file. The Characterized resin was then used in simulation with the process settings that were established for the substitute resin (Case 2).

Inside This Issue:

The Importance of Material Characterization for Simulation Applications (cont.)

John R. Nebbia

The Drop-in substitute material (Case 1) and the newly Characterized resin (Case 2) used the same process settings, but simply changed the materials, **Table 2.**

Table 2—*Overview of the processing parameters used for Cases 1 and 2.*

Simulation Summary		
Case	1	2
Material	"Drop-In" Substitute	Characterized
Fill Time (sec.)	1.86	1.84
Pack Profile (psi/ sec.)	9,394/ 2.50	9,394/ 2.50
Total Cycle Time (sec.)	31.36	31.34

This comparative analysis highlighted a few major findings. The predicted pressures to fill the cavity were much higher than with the Drop-in substitute resin, **Figure 2.** This may seem counterintuitive based on the melt flow volume data. However, after looking into the rheological data, the shear thinning behavior seemed to support the findings corresponding to the increase in pressure with the Characterized resin. This further supported the fact that these materials are inherently different. Additionally, it is important to note that while spending time at the press with the customer, the observed pressures tended to range between 22,000—25,000 psi. This helped create greater confidence in the Characterized resin.

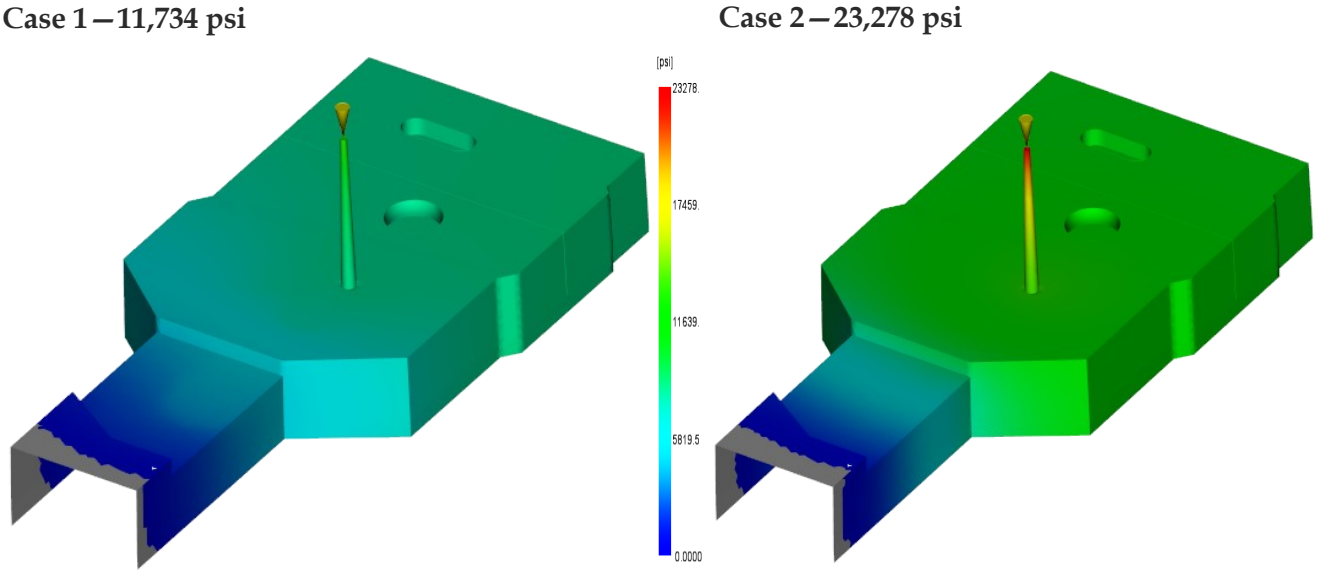

Figure 2—*Plot showing the pressure distribution at switchover for Cases 1 and 2.*

The Importance of Material Characterization for Simulation Applications (cont.)

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Along with the difference in pressures observed during filling, the difference in predicted warpage was drastic. The only change made between Cases 1 and 2, was the resin. The drastic change in warpage showed that the newly Characterized resin was predicted to deflect significantly less with respect to the length and width of the part, but showed an increase in the out-of-plane deflection, **Figure 3.**

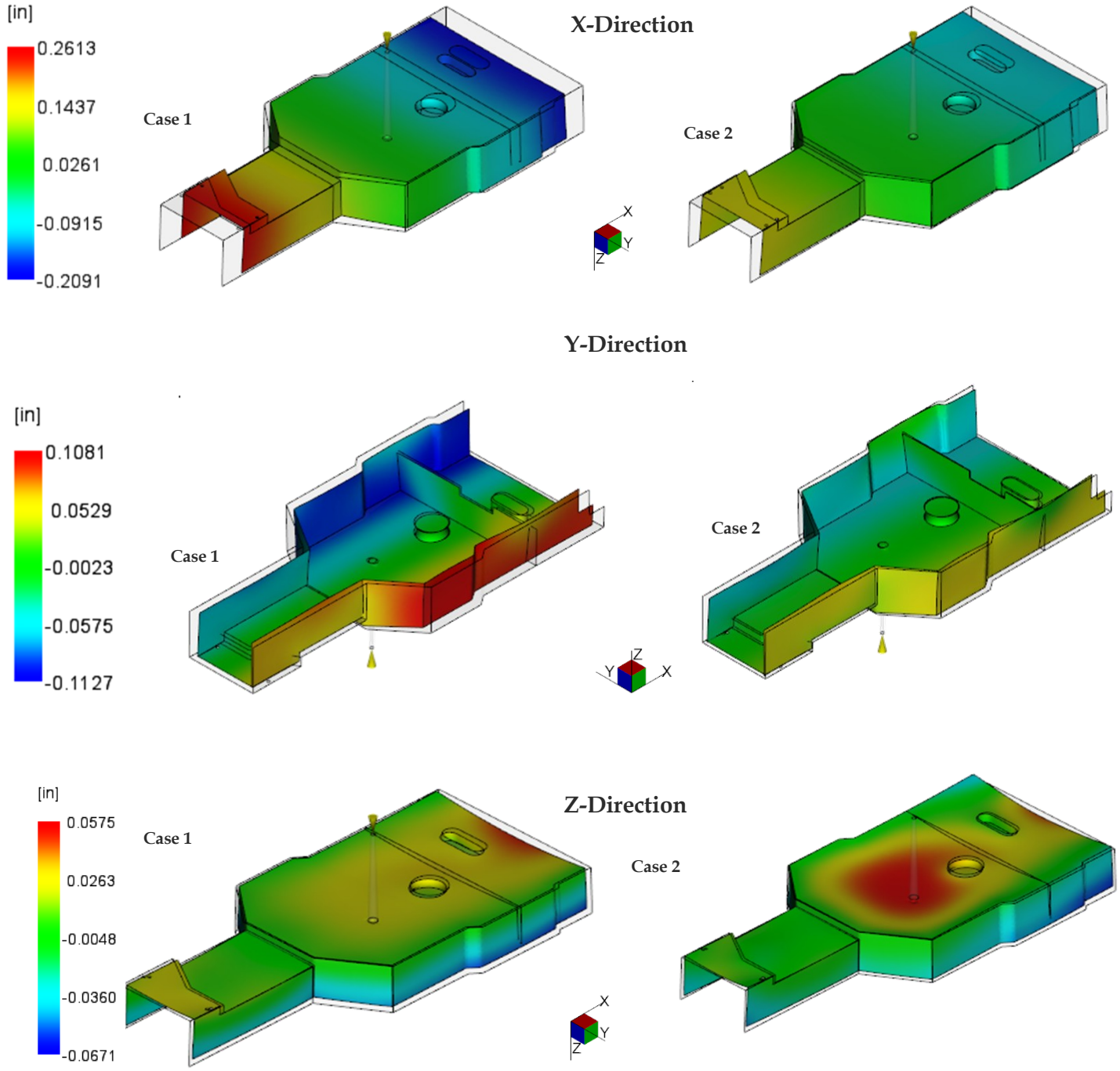

Figure 3 — *Comparison of the warpage modes and magnitudes for Cases 1 and 2 in the X, Y, and Z directions.*

The Importance of Material Characterization for Simulation Applications (cont.)

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The increase in volumetric shrinkage under the sprue and the increase in the out-of-plane deflection on the same face suggested that the newly Characterized material had the ability to be packed for a significantly longer time than the Drop-in substitute resin. With this newly found information regarding the Characterized resin's packing behavior, the process settings were re-designed around the newly Characterized resin. (Case 3). This resulted in a packing time that increased from 2.5 seconds to 10 seconds. That is a 4x increase in the packing time, which has the potential to greatly impact the dimensional stability of the part. The warpage for Case 3 is shown below in **Figure 4.**

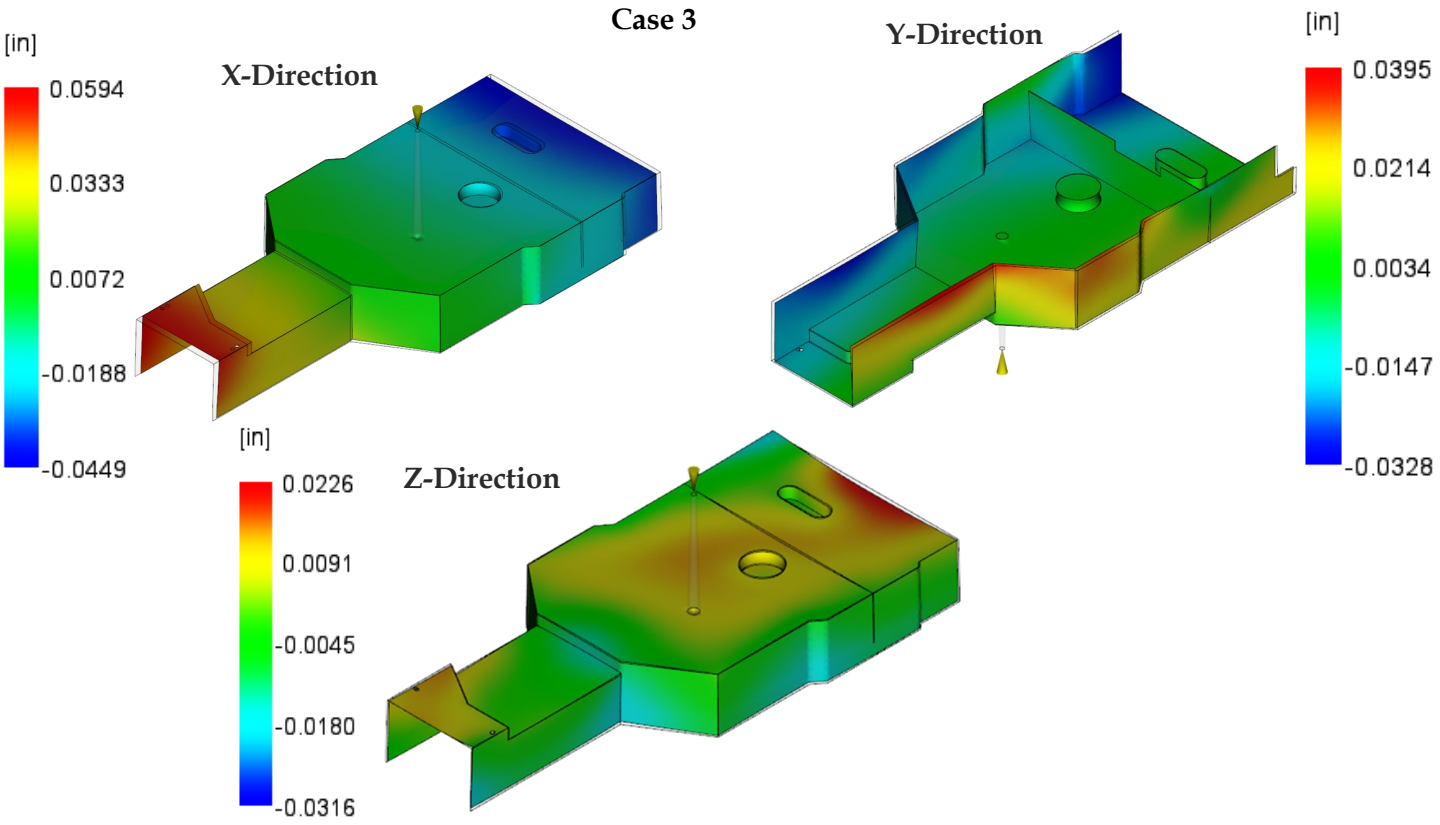

Figure 4 — *Comparison of the warpage modes and magnitudes for Case 3 in the X, Y, and Z directions.*

Simulation Summary			
Case	1	2	3
Material	Drop-in Substitute	Characterized	Characterized
Pack Profile (psi/ sec.)	9,394/ 2.50	9,394/ 2.50	18,500/10.00
Δ in X-Direction Warpage (%)	-	- 40	- 77
Δ in Y-Direction Warpage (%)	-	- 35	- 60
Δ in Z-Direction Warpage (%)	-	+ 11	- 48

Table 3 — *Table showing the magnitude of improvement that can be made by changing both of the materials and adjusting the process for the new material.*

The Importance of Material Characterization for Simulation Applications

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The customer had also expressed an interest in linear shrinkage, as they would like to use the simulation as an aide while cutting their tool. See below for a comparison of the theoretical linear shrinkage values in **Table 4:**

Linear Shrinkage (in/in)			
	Case 1	**Case 2**	**Case 3**
Resin	**Drop-in Substitute**	**Characterized**	**Characterized**
Packing (psi/sec)	9,394/ 2.50	9,394/ 2.50	18,500/10.00
Location 1	0.026	**0.016**	**0.007**
Location 2	0.024	**0.014**	**0.003**
Location 3	0.026	**0.015**	**0.005**
Location 4	0.025	**0.015**	**0.005**
Location 5	0.024	**0.014**	**0.003**
Average Linear Shrinkage	0.025	**0.015**	**0.005**

Table 4 — *A table showing the linear shrinkage rates for the cases in this study.*

The corresponding locations that the measurements were taken from are shown in **Figure 5.** The listed shrinkage on the data sheet for the resin was 0.006-0.010 in/in. The theoretical values obtained from the Characterized resin are much more representative of the resin than the Drop-in substitute.

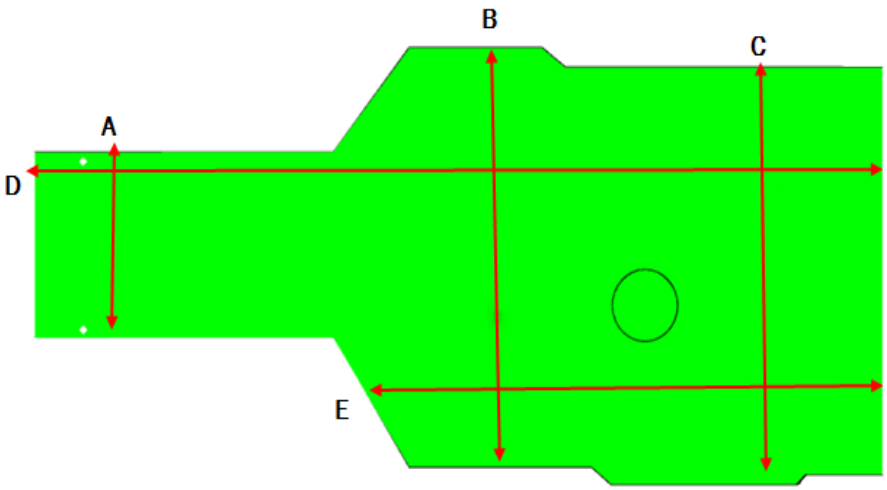


Figure 5 — *An image showing the locations of the linear shrinkage measurements taken on the models in Moldflow.*

Information regarding additional case studies can also be found at:
https://www.madisongroup.com/case-studies.html

Conclusion: When running an analysis and choosing a substitute resin, one must look beyond the typical figures given on a data sheet. While sometimes these values may look similar for short-term performance they may not tell the whole story in terms of long-term material properties. Additionally, even if the values are similar, they can obscure the variations in material composition. This is especially important for material blends such as PC/PBT or PC/ABS. Therefore, when looking to get the most accurate simulation results out of these materials up front, The Madison Group strongly encourages material characterization. This will ultimately help to save time, money, and headaches in the long run for tool design and manufacturing.

Upcoming Educational Webinars

Webinars provide a cost-effective way to expand your knowledge of plastics.

Below is a list of the upcoming webinars presented by TMG Engineers:

Wednesday, Dec 5, 2018 – *Jeffrey A. Jansen* – SpecialChem
Best Combination of DMA, DSC, FTIR... for Optimal Material Analysis
9:00 AM (CST)

You often have to **mix multiple tools (DSC, DMA, FTIR, TMA...) to either characterize** your materials or solve complex formulation or processing issues.

It is important to understand which tool to use, and how to complement data from these multiple techniques for better analyses.

The following sections will be covered during this session:

1. **Plastics Development & Role of Multiple Characterization Techniques**

2. **Characterization Methods Commonly Employed with Plastics Materials**
   (In the scope of discussion of this course)

- FTIR: Fourier transform infrared spectroscopy
- DSC: differential scanning calorimetry
- TGA: thermogravimetric analysis
- GC-MS: gas chromatography/mass spectroscopy
- GPC: gel permeation chromatography
- DMA: dynamic mechanical analysis

3. **When to Best use Which Characterization Tool**

4. **Correlation of Material Properties & Plastics Performance**

- Crystallinity, Molecular Weight, Thermal History, Specific Heat Capacity, Viscoelasticity, Reaction Kinetics and Degree of Cure

5. **Application of Analytical Techniques to Plastics Developments**

- Polymers/Additives Identification (Minimize unwanted interactions)
- Purity / Contamination
- Oxidative Stability

6. **Combination of Data Generated by Different Methods**

7. **Optimization of Plastics Formulations using data from different methods**

- Polymer Blends Compatibility
- Addition of Additives/Fillers
- Use of Data to Optimize Formulations

8. **Real Life Cases of Plastics Performance Optimization**
   (On use of different methods, data extraction and combining information in an optimal way)

Click here to register.

If you are interested in having The Madison Group come and speak or providing training to your team, please feel free to contact us at info@madisongroup.com.

Information regarding upcoming educational opportunities can also be found at:
http://www.madisongroup.com/events.html

Upcoming Educational Webinars (cont.)

Below is a list of the upcoming webinars presented by TMG Engineers:

Thursday, December 6, 2018 – *Jeffrey A. Jansen* – **SPE**
Thermal Analysis in Failure and Compositional Analysis
10:00 AM (CST)

Thermal analysis is an important group of tests used in the analysis of plastics and other polymeric materials. It consists of a family of well-established techniques that evaluate material properties as they change with temperature, time, and ambient environment under conditions of thermal programming. The results of thermal analysis tests provide qualitative and quantitative information about the material being evaluated. In particular, this information is important to address plastic failures or in characterization of the material composition and physical properties.

The upcoming webinar on thermal analysis will introduce the four primary techniques:

- Differential Scanning Calorimetry (DSC)
- Thermogravimetric Analysis (TGA)
- Thermomechancial Analysis (TMA)
- Dynamic Mechanical Analysis (DMA)

The webinar is designed to introduce the techniques to the attendees so that they may get a better understanding of how the techniques can be used to evaluate plastic materials and solve problems. No single thermal analysis technique is best suited universally, but together, they provide essential data for the characterization of plastics materials. This presentation will review thermal analysis techniques and their application to plastic problem solving through case studies. The webinar will be a practical treatment of the techniques, and the focus will be on how the techniques can be utilized to better understand polymeric materials.

Click here to register.

Thursday, February 14, 2019 – *Jeffrey A. Jansen* – **SPE**
Creep Failure of Plastics
10:00 AM (CST)

Creep is the tendency of a polymeric material to deform permanently under the influence of constant stress, as applied through tensile, compressive, shear, or flexural loading. It occurs as a function of time through extended exposure to levels of stress that are below the yield strength of the material. Given sufficient time, this can lead to creep rupture; the failure within a material as a result of continuously applied stress at a level below the short-term tensile strength. Plastic materials are particularly prone to creep rupture through exposure to static stresses, and a recent study indicates that 22% of plastic failures are associated with creep failure.

The relatively high frequency of creep failure is linked to the widespread lack of awareness and understanding of the effects of time on polymeric materials, particularly at the design stage; the unique difference in time dependence between polymeric materials and metals, and the increasing use of plastic materials in diverse applications with longer time demands.

The concept of creep is extremely important to manufacturers and designers of plastic components.

The upcoming webinar will cover:

- Introduction to Creep
- Plastics Failure Mechanism
- Creep Failure Mechanism
- Proactive Creep Testing and Lifetime Projection Methods
- Case Studies

Click here to register.

Information regarding upcoming educational opportunities can also be found at:
http://www.madisongroup.com/events.html

Upcoming Educational Webinars

Webinars provide a cost-effective way to expand your knowledge of plastics.

Below is a list of the upcoming webinars presented by TMG Engineers:

Thursday, April 11, 2019 – *Jeffrey A. Jansen* – ***SPE***
Basic Rubber Technology
10:00 AM (CST)

This webinar will introduce the attendees to the basics and most important topics related to thermoset rubber compounds. About 15 billion kilograms of rubber are produced ever year. Rubber finds its way into a wide range of applications in the automotive, medical, appliance, electrical, and chemical industries. As a class of materials, rubber has many useful properties because of its unique molecular structure. These properties include being soft and relatively flexible, high ultimate elongation coupled with good elastic recovery, useful over a wide temperature range, and good chemical resistance.

As part of the presentation, the following topics will be covered:

- Introduction to Polymers — Rubber vs. Plastics
- Overview of Rubber Properties
- How Rubber Compound Recipes are Created
- The Essentials of Rubber Mixing and Molding
- Specify Rubber Compounds

Click here to register.

Thursday, June 13, 2019 – *Jeffrey A. Jansen* – ***SPE***
An Introduction to Dynamic Mechanical Analysis (DMA)
10:00 AM (CST)

Dynamic Mechanical Analysis (DMA) is a thermoanalytical technique that measures the stiffness (modulus) and damping (tan delta) of polymeric materials to assess the viscoelastic properties as a function of time, temperature, and frequency. Polymeric materials display both elastic and viscous behaviors simultaneously, and DMA can separate these responses. Polymers, composed of long molecular chains, have unique viscoelastic properties, which combine the characteristics of elastic solids and Newtonian fluids.

As part of the DMA evaluation, a small deformation is applied to a sample in a cyclic manner. This allows the material's response to stress, temperature, and frequency to be studied. The analysis can be in several modes, including tension, shear, compression, torsion, and flexure.

DMA is a very powerful tool for the analysis of plastics and can provide information regarding:

- Modulus
- Damping
- Glass Transition
- Softening Temperature
- Creep Behavior
- Stress Relaxation
- Degree of Cure

This webinar will provide an introductory look into DMA and how it can be applied to better understand plastic behavior, both long-term and short-term.

Click here to register.

For more educational opportunities, please go to our website: www.madisongroup.com/events.html

The Power of Modulated® DSC (MDSC) - Part 1

Dayton Ramirez, M.S., and Jack DeSousa

Differential scanning calorimetry (DSC) is a thermoanalytical technique that measures temperatures and heat flows associated with thermal transitions in a material. The results are used to understand physical and chemical changes involving endothermic or exothermic reactions or changes in heat capacity. In thermoplastic and thermoset materials, these transitions could include the glass transition temperature (T_g), melting temperature (T_m), cold crystallization, crystallization during cooling, enthalpic relaxation, curing, and more.

Using this transition data, information can be obtained regarding the following:

- What annealing temperatures to utilize
- What the approximate melt temperature should be during processing
- How cooling will affect the material (mold coolant)
- If there are any adverse effects from processing (e.g., crystallization and degradation)
- What degree of crystallinity was obtained in a molded component
- Information regarding crystallization behavior
- What curing temperatures and times should be utilized

It is also important to understand these thermal transitions because the material will undergo significant changes in properties as it gets closer to and moves through the transition temperatures. This is due to the mobility of the molecules, which is commonly referred to as viscoelasticity. A viscous material, such as honey, will displace when a stress is applied. This viscous material will not recover its strain and return to its original position when the stress is relieved. The material will become permanently deformed. In contrast, elastic materials, such as steel that undergoes displacement from a stress application, will return to its original position when the stress is relieved. Polymers exhibit both the elastic response, like steel, and viscous response, like honey. The amount of viscous and elastic responses are highly dependent on the application temperature in relation to the thermal transitions. The closer to the thermal transitions that a material is used, the more mobility the molecules will have to undergo a viscous response. In other words, they will respond more like honey and less like steel the closer they are to the thermal transitions.

During a typical DSC experiment of a polymeric material, the material starts to be heated below the thermal transitions being studied during the experiment. The exact starting temperature is dependent on the material undergoing analysis, as well as the DSC's ability to develop a baseline and equipment restrictions. As polymers undergo thermal transitions over a range of temperatures, starting and ending points are chosen to ensure the thermal transition will not be affected by the temperatures. Furthermore, the material is maintained below temperatures that will degrade or adversely affect the polymeric material.

As previously noted, the DSC is a powerful tool that can provide a lot of information by analyzing thermal transitions exhibited by the material. When analyzing materials, they will often exhibit multiple transitions (exothermic and/or endothermic) during testing. In some cases, these transitions can occur within the same temperature range, making interpretation of the thermal transitions and information more difficult. Some examples of this are enthalpic relaxation due to aging and molecular re-orientation, glass transition or crystallization and melting, which typically occur at the same temperature range. One solution to separate these overlapping transitions is to apply both a sinusoidal and linear heating/cooling rate to the sample through the use of Modulated ® DSC (MDSC).

The Power of Modulated® DSC (MDSC) - Part 1 (cont.)

Dayton Ramirez, M.S., and Jack DeSousa

Figures 1 and 2 show an example of the sinusoidal heating rate for an MDSC experiment. In this experiment, a sinusoidal heating rate that fluctuated from 6.0 °C/min to 0 °C/min, was applied to the sample. This was done so that an average heating rate of 3.0 °C/min would also be maintained.

With both the average and modulated heat flows being observed, essentially two sample experiments were being conducted at once. The samples behavior could then be used to separate the irreversible transitions (cold crystallization and enthalpic relaxation) from the reversible transitions (T_g and T_m). This would allow for more accurate quantitative measurements from the data.

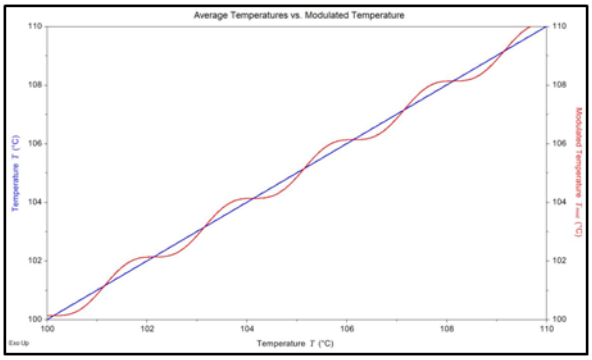


Figure 1 — *Comparison view of a sinusoidal and average temperature for MDSC.*

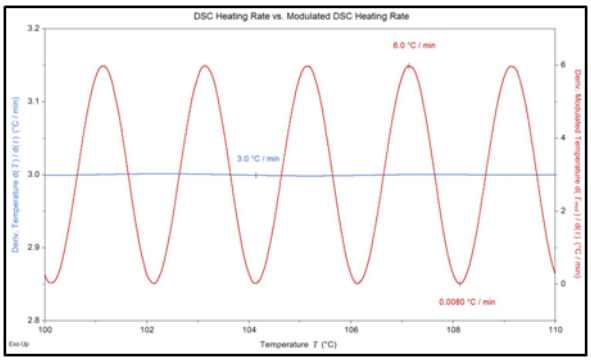
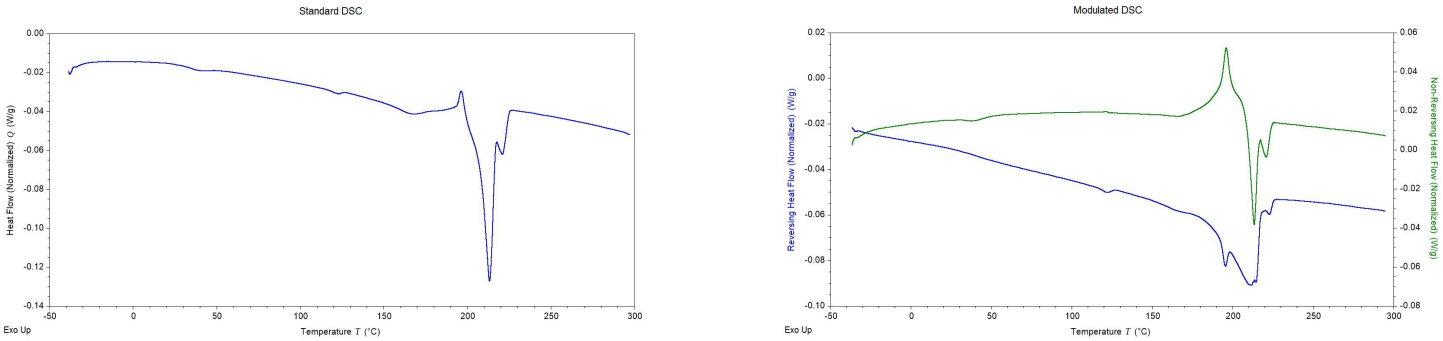


Figure 2 — *Comparison view of the sinusoidal and average heating rates for MDSC.*



These figures show the difference between running a Standard DSC and MDSC.

Please stay tuned for Part 2 in the next TMG newsletter, where we will explore further into the topic of MDSC.

Information regarding additional case studies can also be found at:
https://www.madisongroup.com/case-studies.html