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# Thermoforming Simulation of Heat Conductive Plastic Materials Using the K-BKZ Model

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**Abstract.** Generally, Thermoforming is used for the production of simple shaped packaging or housing parts, which do not feature any additional functions. However, by the use of heat conductive plastic materials, a heat loss function can be implemented to the thermoformed parts. Increased filler contents are correlated with higher heat conductivity. Unfortunately, higher filler content also leads to a degraded thermoformability of plastic sheets. As a result, simulation becomes more and more important, when operating the thermoforming process at its limits.

To obtain high predictive accuracy in thermoforming simulation, material models as well as data fitting methods are needed, which match with the real thermoforming material and process. In this investigation the use of the K-BKZ model for thermoforming simulation of heat conductive plastics is evaluated. Two different kinds of parameter fitting algorithms are examined. On the one hand, the K-BKZ model is fitted by a reverse-engineering procedure using the IKT Thermoforming-Material-Characterization-test (TMC-test) as reference test. On the other hand, classic rheological measurements by means of rotational rheometry and Rheotens-test are used for the data fitting of material parameters. As reference material a polystyrene is combined with two graphite fillers (spherical and platelet). The predictive accuracy of the material model and the two parameter fitting procedures are quantified by a comparison of the simulation with real thermoforming experiments.

**Keywords:** Thermoforming, Simulation, Heat Conductive Plastics, Elongational Viscosity

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## THE USE OF HEAT CONDUCTIVE PLASTICS IN THERMOFORMING

Thermoforming is commonly used for the production of simple shaped parts with thin wall thicknesses [1]. Typical products are simple shaped packaging or housing parts, which primarily fulfill the function of holding and protecting a part's inner goods, e.g. food (in packaging) or electronic devices (technical parts). However, by the use of additives, further functionalities can be added to the thermoforming part. Heat conductive fillers for example, allow a heat loss function in thermoforming parts.

Heat conductive plastics are polymeric materials filled with heat conductive fillers [1,2]. Increased filler contents are correlated with higher heat conductivity. Unfortunately, higher filler contents also lead to an altered thermoformability of plastic sheets. [3] shows how heat conductive fillers influence the thermoforming behavior of thermoform sheets. It can be observed that increased filler content leads to a challenging thermoforming behavior. Not only the critical strain is reduced by higher filler content, also the stretching behavior becomes more inhomogeneous by an increased filler/matrix ratio [3]. As a result, simulations become more and more important when using functionalized thermoforming sheets.

## MATERIAL MODELLING

This paper deals with material modelling of heat conductive plastic materials in the thermoforming process. Whereas there are a plenty of possibilities to model the stretching behavior of material during the thermoforming process, a material model often used is the non-linear viscoelastic Kaye, Bernstein, Kearsley, Zapas (K-BKZ) model according to (1) [4]. The model consists of four functional units, which shall be described in the following passage.

$$\bar{\sigma}(t) = \int_{-\infty}^t m^0(t-t') \cdot h(I_1, I_2) \cdot \bar{C}_t^{-1}(t, t') dt' \quad (1)$$

The stress tensor  $\bar{\sigma}(t)$  describes the actual state of stress of a material element at the time  $t$ .  $m^0(t-t')$  is the linear-viscoelastic time-memory-function. It is solved by (2), whereas  $g_i$  are the relaxation modules and  $\tau_i$  the corresponding relaxation times [5].

$$m^0(t-t') = \sum_{i=1}^n \left\{ \frac{g_i}{\tau_i} \cdot e^{-\frac{(t-t')}{\tau_i}} \right\} \quad (2)$$

Since the relaxation-time-spectrum is subject to the time and temperature dependent behavior of polymer materials, a temperature dependency must be included to the model. For amorphous plastics the Williams, Landel and Ferry (WLF) equation (3) can be used.  $\tau_i(T_R)$  is the relaxation time at a reference temperature  $T_R$  of a specific relaxation modulus  $g_i$ .  $\tau_i(T)$  represents the temperature shifted relaxation time at the temperature  $T$ , whereas  $c_1$  and  $c_2$  are the WLF material parameters. [6]

$$\tau_i(T) = \tau_i(T_R) e^{-\frac{c_1(T-T_R)}{c_2+(T-T_R)}} \quad (3)$$

The damping function  $h(I_1, I_2)$  describes the reduced material's memory at high strain. It is used to correct an excessive stress growth at high state of deformation. In this investigation the Wagner-II damping function (4) according to [6] is used since it is supposed to give a satisfactory solution for thermoforming applications (uniaxial and biaxial stretching) [4].

$$h(I_1, I_2) = \frac{1}{\exp(\beta\sqrt{\alpha I_1 + (1-\alpha)I_2 - 3})} \quad (4)$$

The Finger strain tensor  $\bar{\bar{C}}_t^{-1}$  describes the actual state of deformation  $\varepsilon(t)$  in relation to the deformation  $\varepsilon(t')$  at the time of  $t'$ , see (5). [5]

$$\bar{\bar{C}}_t^{-1}(t, t') = \begin{pmatrix} \exp(2\varepsilon(t, t')) & 0 & 0 \\ 0 & \exp(-\varepsilon(t, t')) & 0 \\ 0 & 0 & \exp(-\varepsilon(t, t')) \end{pmatrix} \quad (5)$$

## PARAMETER-FITTING FOR THERMOFORMING SIMULATION

In previous investigations the K-BKZ model was already used for the description of stretching behavior in thermoforming application. According to [4,6,7] the model provides high predictive accuracy for unfilled amorphous and semi-crystalline plastics in thermoforming processes. In addition, the use of K-BKZ model on filled materials was investigated as well, e.g. in [8,9]. The key to a successful modelling lies in a matching characterization method and data fitting procedure. Therefore, in this investigation two parameter fitting methods shall be compared to each other. On the one hand the material fitting by reverse-engineering of the IKT TMC-test in accordance to [4] is used. On the other hand the material fitting is done by combined rheological tests using a rotational rheometer and the Rheotens-test.

The TMC-apparatus is schematically shown in Fig. 1 (a). It is based on the dart penetration test in accordance to EN ISO 6603-02 [10] and derives an integral testing method close to many thermoforming processes. The test specimen is placed on a piston that is coaxially arranged with a circular plug. Once the piston moves up, the specimen is deformed by the plug and the resulting normal force is measured by a piezo-element. Since the whole apparatus is placed inside a temperature chamber, a homogenous tempering of the specimens can be achieved. In the reverse-engineering routine the resulting force/deflection-curves of the experiments are compared to a corresponding simulation. In an iterative process the parameters of the material model are optimized, until the simulated force-deflection curves fit the experimental curves. In this investigation all parameters - the relaxation-time-spectrum  $g_i$  and  $\tau_i$ , the damping parameters  $\alpha$  and  $\beta$  as well as the WLF-constants  $c_1$  and  $c_2$  - are optimized with the TMC-Plugfit procedure by the software T-Sim of the company Accuform, Zlin (Czech Republic), simultaneously. Therefore, TMC-tests were performed at three different piston velocities (20 mm/s, 200 mm/s and 500 mm/s) and three different temperatures (120 °C, 130 °C and 140 °C).

The direct method of determining the relaxation-time-spectrum is described in [11]. Baumgaertel and Winter show, how the modules  $g_i$  and times  $\tau_i$  can be derived according to (6) from Small Amplitude Oscillatory Shear (SAOS) tests using a rotational rheometer [11].

$$G' = \sum_{i=1}^n g_i \frac{\omega^2 \tau_i^2}{1 + \omega^2 \tau_i^2}; \quad G'' = \sum_{i=1}^n g_i \frac{\omega \tau_i}{1 + \omega^2 \tau_i^2} \quad (6)$$

In this investigation SAOS-tests were performed at different temperatures (120 °C, 130 °C and 140 °C) with a maximum strain of 0,1 % and over a frequency range from 0,1 to 100 rad/s. These measurements were also used for the data fitting of the WLF-constants  $c_1$  and  $c_2$ .

After the characterization of the linear-viscoelastic time-memory-function by SAOS-tests, the damping parameters  $\alpha$  and  $\beta$  were derived from Rheotens measurements Fig. 1 (b). The Rheotens-test is described in [12]. It is based on the principle of two rotating wheels, which accelerate a polymer strand. While the polymer strand is continuously extruded to the measuring cell, e.g. by capillary rheometer, the rotating wheels can be accelerated with a predefined acceleration rate  $\dot{v}$ . Due to the strand acceleration; stress is induced to the material. Knowing the cross section of the strand, conversely the strand stress  $\sigma_z$  can be calculated from the bearing force  $F$  of the rotating wheels. In this investigation the measured stress/velocity-curves of the rheotens test were used for the optimization of the damping parameters  $\alpha$  and  $\beta$  using the linear-viscoelastic time-memory-function from the SAOS tests.

According to these material data fitting procedures, reverse-Engineering of the TMC-test on the one hand and rotational- and Rheotens-measurements on the other hand, two material set-ups can be developed. In order to compare these two parameter set-ups, thermoforming simulations were performed, describing the thermoforming experiments of [3]. The reference thermoforming process is a two-step forming process, consisting of mechanical drawing by the positive mold shown in Fig. 1 (c) and following vacuum forming. The comparison of simulation and experiment is performed by sheet thickness measurements.

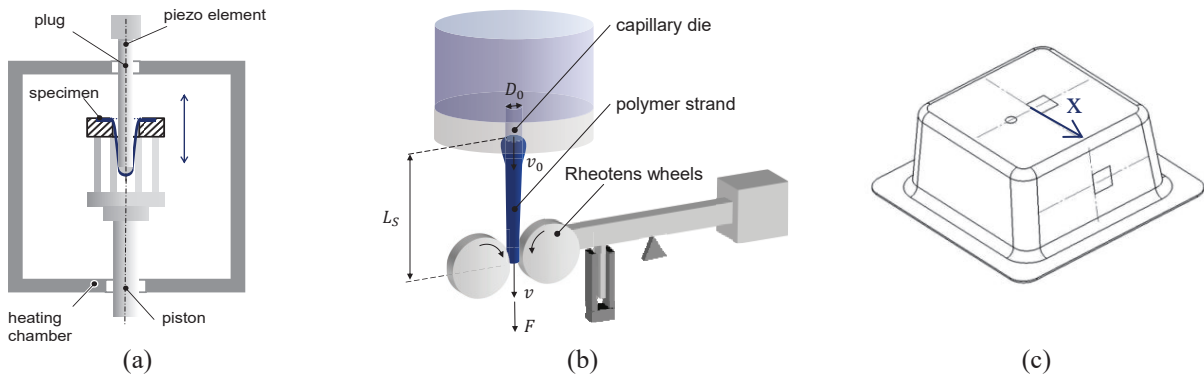


FIGURE 1. IKT TMC-test (a), Rheotens-test (b), Thermoforming mold

The examined materials of this investigation are a polystyrene PSn (PS454N from INEOS Styrolution, Frankfurt) filled with 15 vol.-% spherical graphite fillers Gr (GraphTHERM<sup>®</sup> from LUH, Walluf) and platelet graphite fillers Gp (GraphCOND<sup>®</sup> from LUH, Walluf).

## RESULTS AND DISCUSSION

The TMC-tests can be used for general material characterization as shown in [3] and for material data fitting in reverse-engineering in accordance to [4]. Fig. 2 (a) shows the experimental and simulated force/deflection curves from TMC-tests at a piston velocity of 200 mm/s and a temperature of 130 °C. The simulation is performed with the reverse-engineering material set-up, from T-Sim Plug-Fit procedure. It can be seen, that the simulated force-deflection curves fit quite well with the experimental data. The best fit is achieved for the unfilled material PSn. The spherical filler Gr lead to a better fit than the platelet filler Gp. Fig. 2 (b) shows the corresponding relaxation-time spectrum of the materials. Damping parameters are not needed to reproduce the force-deflection curves.

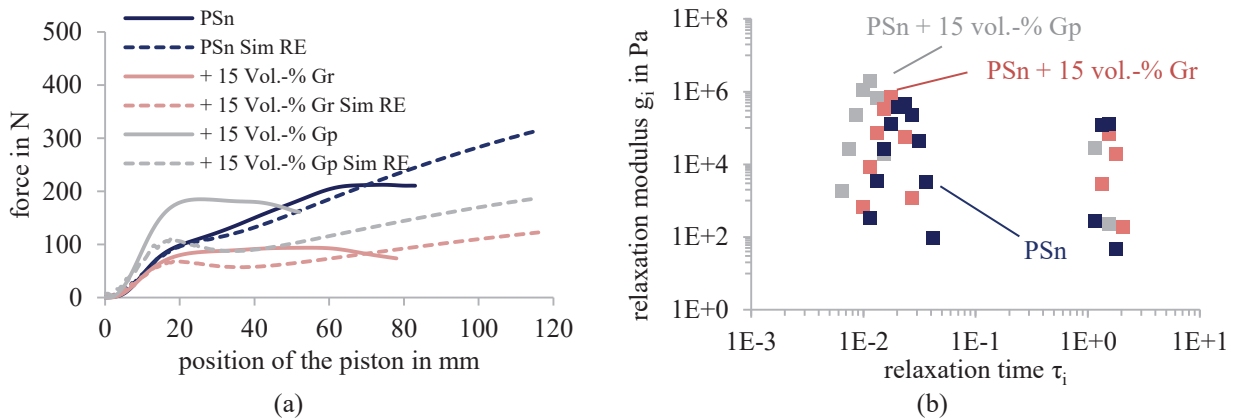


FIGURE 2. Force/deflection-curves from TMC-test (a), relaxation-time-spectrum from reverse-engineering (b)

Fig. 3 (a) shows the Master Curves of the storage-modules  $G'$  of the three materials PSn, PSn + 15 vol.-% Gr and PSn + 15 vol.-% Gp from SAOS-measurements. With increasing filler content  $G'$  is increased as well. The platelet filler Gp leads to a higher increase of viscosity than the spherical fillers Gr. Using  $G'$ -data the relaxation-time-spectrum can be developed according to (6). Fig. 3 (b) shows the resulting relaxation-time-spectrum of the three materials. With the addition of filler the modules  $g_i$  are increased. Furthermore, it can be observed that platelet filler Gp lead to higher modules  $g_i$  than spherical filler Gr, especially at high relaxation times  $\tau_i$ .

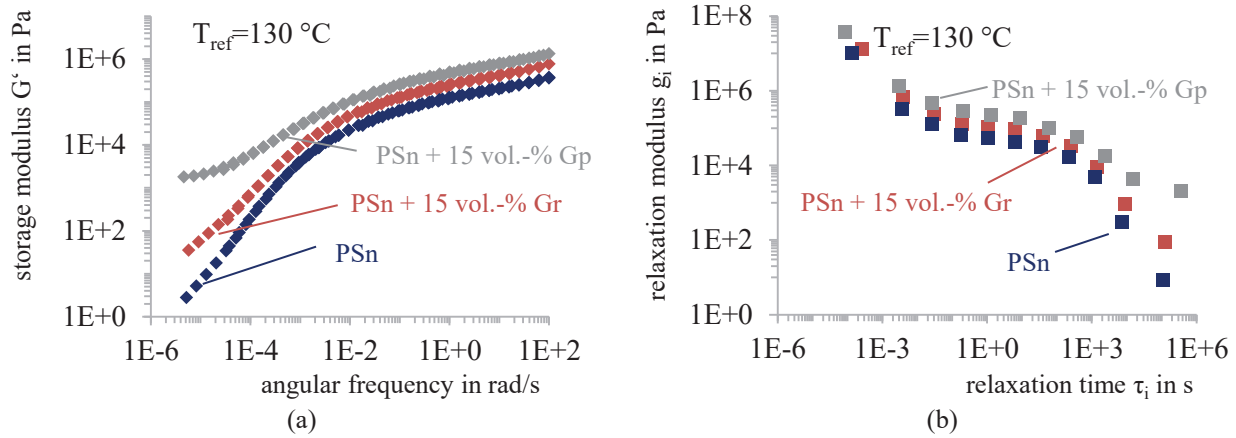


FIGURE 3. Storage- and loss-modulus from SAOS-tests (a), Relaxation-time-spectrum from SAOS-tests (b)

The relaxation-time-spectrum in Fig. 3 (b) is used for the characterization of the damping parameters by Rheotens-test. Fig. 4 (a) shows the stress/velocity-curves of the three materials including the material data fit by K-BKZ model using the linear-viscoelastic time-memory-function from Fig. 3 (b) in combination with the optimized damping parameters. The K-BKZ model is able to describe the Rheotens-curves very well. However, the addition of filler leads to an early strand breakage. As a result the number of data points for the development of damping parameters is reduced, if filler is added. Fig. 4 (b) shows the resulting damping functions for the three materials. The addition of filler leads to higher damping. Platelet Fillers show higher damping than spherical fillers.

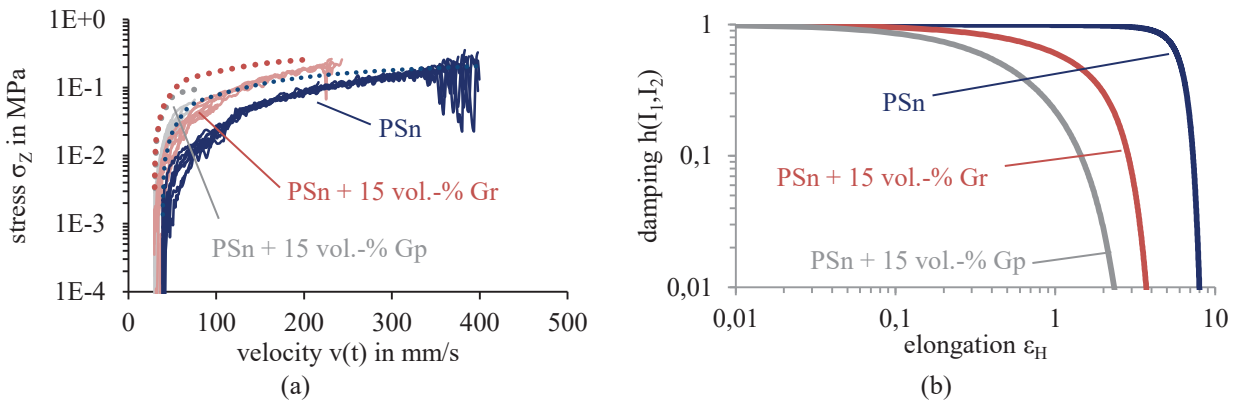


FIGURE 4. Rheotens-curves (a), Damping function (b)

The two fitting procedures lead to differing material data sets. While the reverse-engineering leads to a chaotic relaxation-time-spectrum in combination with a suppressed damping function, the SAOS-test leads to a continuous relaxation-time-spectrum and the Rheotens-tests give a significant damping (comparable to [8,9]). Nonetheless, both data set-ups reproduce their characterization method very well.

Since the resulting material data set-ups are so different to each other, an evaluation of the predictive accuracy in thermoforming is necessary. The thermoforming experiments in [3] are used to compare the simulated and experimental sheet thickness distribution of the thermoformed parts. Fig. 5 therefore shows a comparison of the experimental and simulated sheet thickness distribution. While all boundary conditions in the two simulations are the same, the material data set-up from reverse-engineering procedure “Sim RE” and classical rheological characterization “Sim Rheotens-fit” differ from each other according to the aforementioned characteristics. Both material data set-ups lead to a good fit of the experimental sheet thickness distribution, see Fig. 5. However, the combined characterization by SAOS-test and Rheotens-test show a slightly more accurate prediction than the data

set-up from the reverse-engineering routine. Nevertheless, it is quite interesting, that the data setup from reverse-engineering gives comparable thickness distribution to the direct determination of material parameters by SAOS-test and Rheotens-test. The high predictive accuracy is probably due to the characterization method close to the actual thermoforming process (TMC-test).

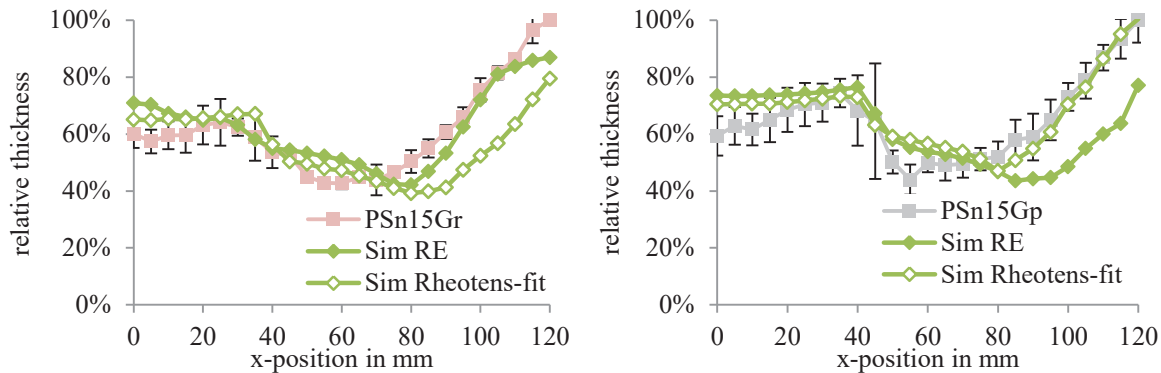


FIGURE 5. Experimental and simulated sheet thickness distribution

## OUTLINE

The investigation shows that K-BKZ Model can be used for material modelling in thermoforming simulation of heat conductive plastic materials. Two parameter fitting methods were discussed. On the one hand the parameter fitting was done by reverse-engineering using the TMC-test as reference test. On the other hand a direct procedure was used, to determine relaxation-time spectrum and damping parameters. Both methods show high predictive accuracy in thermoforming simulation. The direct method leads to a slightly higher accuracy, but also represents the more time and cost consuming characterization method.

## ACKNOWLEDGMENTS

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