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4.4.1 New Developments in Thermal Diffusivity Measurement

In related research activities at ICIPC in Colombia and under collaboration with the IKV in Germany [2, 3], a new quenching method to directly obtain the thermal diffusivity from temperature measurements under real processing conditions for injection molding has been developed.¹

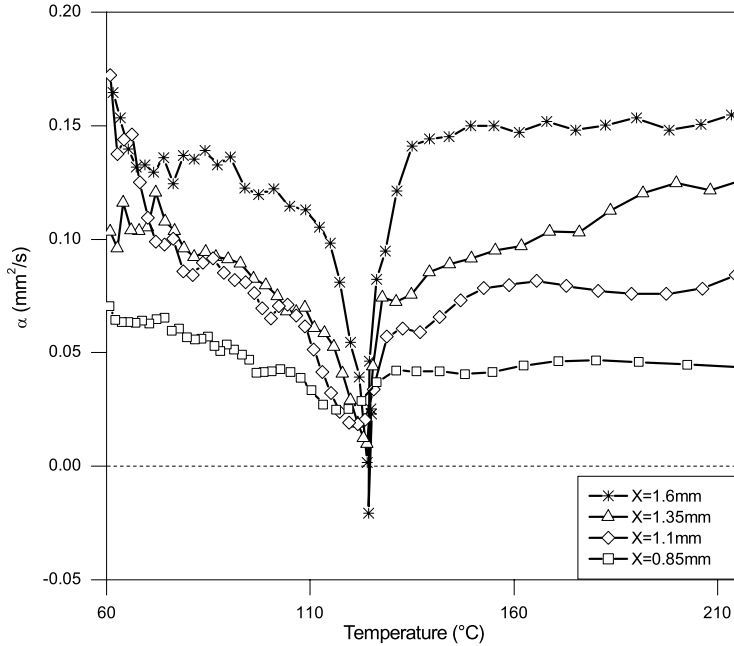


Figure 4.19: Thermal diffusivity of HDPE measured with the new method

¹The method uses the approximated expression of the numerical solution of Fourier's equation for the case of a one-dimensional heat flow which simplifies to

$$\frac{\partial T}{\partial t} = \alpha(T, x) \frac{\partial^2 T}{\partial x^2}.$$

To determine the thermal diffusivity α , this equation is written in a finite difference expression, which defines α as the quotient between a forward difference approximation for the time derivative and a central difference approximation for the space derivative, built from temperature values $T_{i-1,j}$, $T_{i,j}$, $T_{i+1,j}$ and $T_{i,j+1}$ that are the values for three positions $x_{i-1} = x_i - \Delta x$, $x_{i+1} = x_i + \Delta x$ for the time $t = j$ and the temperature in position x_i for the time $t + \Delta t$.

$$\alpha(T_{i,t}, x_i) = \frac{\Delta x^2}{\Delta t} \frac{T_{i,j+1} - T_{i,j}}{T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}$$

According to this equation, it is necessary to know the temperature history for three points uniformly distributed over the thickness of the domain and separated by distances Δx . The calculated diffusivity is valid for position x_i and a corresponding temperature $T_{i,j}$.

This method demands very precise measurements of temperature profiles $T(x, t)$ during the process for different points (x_i) equally distributed over the thickness of the mold cavity. From these temperature profiles, it is then possible to obtain the thermal diffusivity by solving a very simple inverse heat conduction problem [1].

Figure 4.19 presents the thermal diffusivity of a HDPE as a function of temperature and of the distance from the cavity wall (X) obtained with this new technique using a 4 mm thick plate, with a 230 °C melt temperature, a 40 °C mold temperature, and a cavity pressure of 120 bar [2]. These measurements show a minimum in the thermal diffusivity curves at the crystallization temperature, $T_c \approx 124.6$ °C.

■ INDUSTRIAL APPLICATION 4.1

Measuring Thermal Diffusivity of a Polypropylene

A complete set of injection molding experiments was carried out with a polypropylene to study the dependency of thermal diffusivity on processing conditions [3]. As expected, the resulting thermal diffusivity values show a remarkable dependence of temperature and consequently, because of different local cooling rates, the thickness of the part. The peak of thermal diffusivity is closely related to the crystallization temperature and shows a dependence of cavity pressure and cooling rate.

A mathematical model to describe the thermal diffusivity was developed, due to the fact that simulation programs require material data in the form of a model, or as table values when the property can be expressed using single values. The model takes into account melt temperature, internal cavity pressure during packing, mold wall temperature, and thickness of the injected part.

The model describes thermal diffusivity as a function of temperature for a particular location over the thickness and uses a dimensionless temperature θ^* and position x^* defined by $\theta^* = \frac{T-T_w}{T_c-T_w}$ for the melt region $\theta^* \geq 1$ and for the solid region $\theta^* \leq 1$. Here T_w is the wall temperature and T_c is a temperature value related to the crystallization temperature of the material under local pressure and local cooling rates. The thermal diffusivity for the melt ($\alpha = \alpha_{melt}$) is described by

$$\alpha_{melt} = \frac{A_1 - A_2}{1 + \exp\left(\frac{(1-\theta^*)}{A_3}\right)} + A_2; \quad \theta^* \geq 1 \quad (4.3)$$

The crystallization and solid region are described separately by Eqs. 4.4 and 4.5:

$$\alpha_{cryst} = A_1 + A_4 \cdot A_5 \cdot (1-\theta^*) \cdot \exp(A_5 \cdot (1-\theta^*)); \quad \theta^* \leq 1 \quad (4.4)$$

$$\alpha_{solid} = A_6 \cdot \exp\left(\frac{-A_7}{(1-\theta^*)}\right); \quad \theta^* \leq 1 \quad (4.5)$$

The parameters A_i are a function of the dimensionless coordinate for position x^* where s is the part thickness.

$$A_i = a_{0,i} + a_{1,i} \cdot x^* + a_{2,i} \cdot x^{*2} \quad \text{where } x^* = x/\left(\frac{s}{2}\right) \quad (4.6)$$

These A_i parameters have a very noticeable dependency on processing conditions and can be described expressing the b_j ($j=1,2,3$) coefficients by Eq. 4.7. In order to simplify the description of all these parameters, only the parameter A_4 , which describes the effect of crystallization, was considered as a linear function of x^* ($b_2 = 0$ for all A -parameters, and $b_1 = 0$ for all but not for A_4).

$$b_i = c_{0,i} + c_{d,i} \cdot d + c_{p,i} \cdot p + c_{T_M,i} \cdot T_M + c_{T_W,i} \cdot T_W \quad (4.7)$$

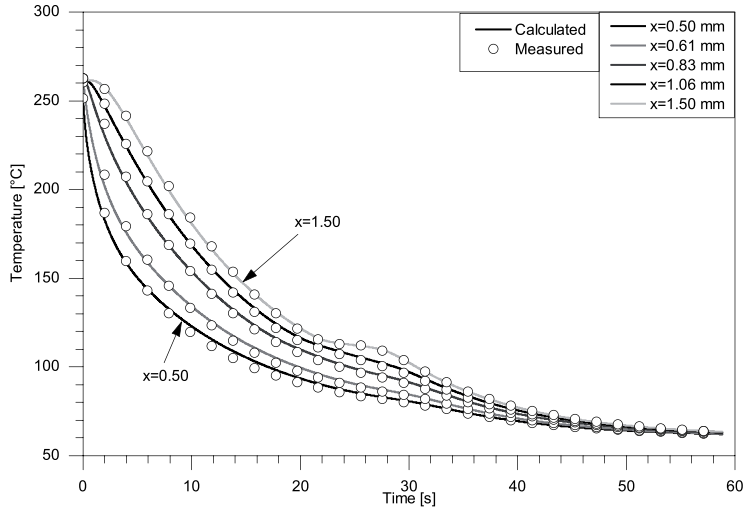


Figure 4.20: Measured and calculated temperature evolution in the PP part

Table 4.2: Coefficients c for the calculation of the PP thermal diffusivity

	A1 (b0)	A2 (b0)	A3 (b0)	A4 (b1)	A5 (b0)	A6 (b0)	A7 (b0)	Tc (b0)
c_0	7.03E-02	5.00E-03	5.50E-03	1.45E-01	1.39E+01	-2.30E-04	3.46E-01	1.07E+02
c_d	2.88E-03	0	0	6.48E-03	3.87E-01	2.42E-03	-2.03E-02	3.11E+00
c_p	-2.63E-05	0	0	-6.44E-05	6.98E-03	5.38E-05	-2.17E-04	2.17E-02
c_{T_m}	-2.96E-05	0	0	-3.51E-05	2.48E-02	1.44E-04	2.82E-04	-5.32E-02
c_{T_w}	-4.50E-05	0	0	2.55E-04	-1.11E-01	-9.43E-05	2.26E-03	1.09E-01

The coefficients c are shown in Table 4.2. They are only valid for specific processing conditions and they were validated with experiments using the following conditions:

- Pressure – from 150 to 300 bar
- Melt temperature – from 230 to 270 °C

- Mold wall temperature – from 20 to 60 °C, and
- Part thickness – from 3 to 5 mm

Figures 4.20 and 4.21 show the measured evolution of thermal diffusivity and temperature over the thickness and is compared to the predicted values.

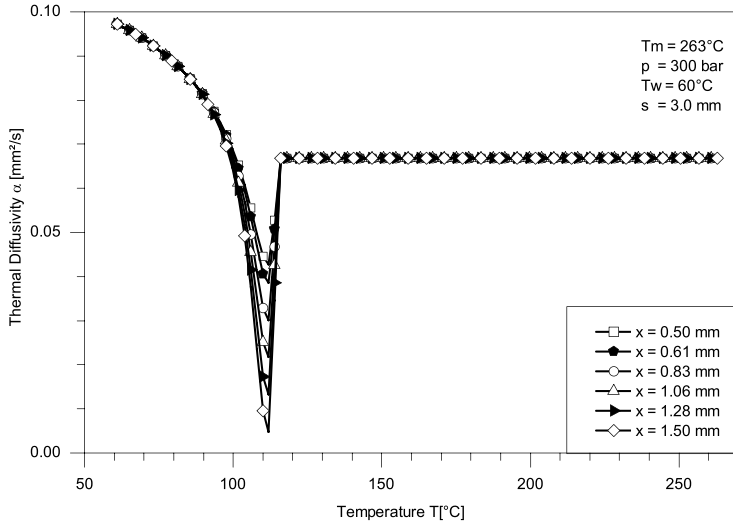


Figure 4.21: Calculated thermal diffusivity of PP with the new method

4.5 LINEAR COEFFICIENT OF THERMAL EXPANSION

The linear coefficient of thermal expansion is related to volume changes that occur in a polymer because of temperature variations and is well represented in the pVT diagram. For many materials, thermal expansion is related to the melting temperature of that material, shown for some important polymers in Fig. 4.22. Similarly, there is also a relation between the thermal expansion coefficient of polymers and their elastic modulus, as depicted in Fig 4.23.

Although the linear coefficient of thermal expansion varies with temperature, it is often considered constant within typical design and processing conditions. It is especially high for polyolefins, where it ranges from $1.5 \times 10^{-4} \text{K}^{-1}$ to $2 \times 10^{-4} \text{K}^{-1}$; however, fibers and other fillers significantly reduce thermal expansion. The linear coefficient of thermal expansion is a function of temperature. Figure 4.24 presents the thermal expansion coefficient for a selected number of thermoplastic polymers. The figure also presents thermal expansion perpendicular and parallel to the fiber orientation for a fiber-filled POM.

A rule of mixtures is sufficient to calculate the thermal expansion coefficient of polymers that are filled with powdery or small particles as well as with short fibers. In case of continuous

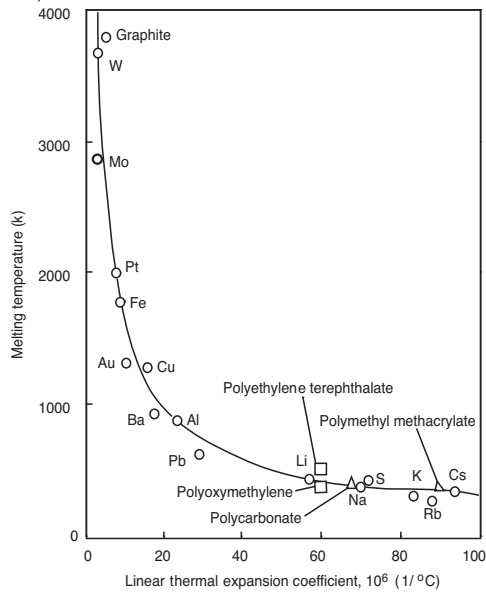


Figure 4.22: Relation between thermal expansion of some metals and plastics at 20 °C and their melting temperature

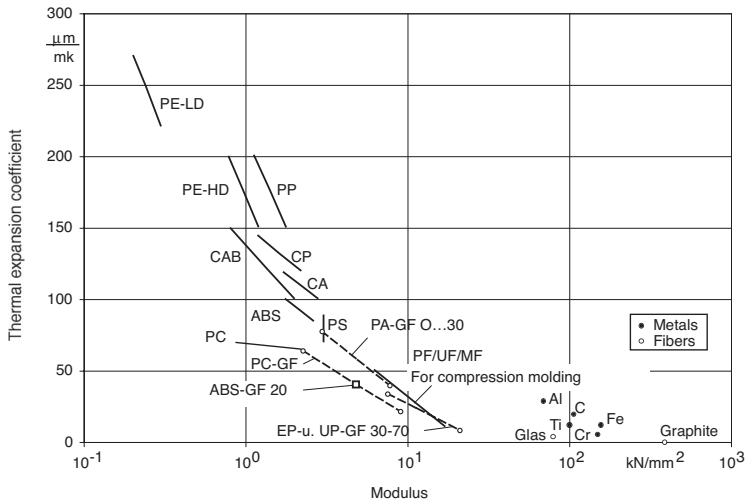


Figure 4.23: Relation between thermal expansion of some metals and plastics and their elastic modulus

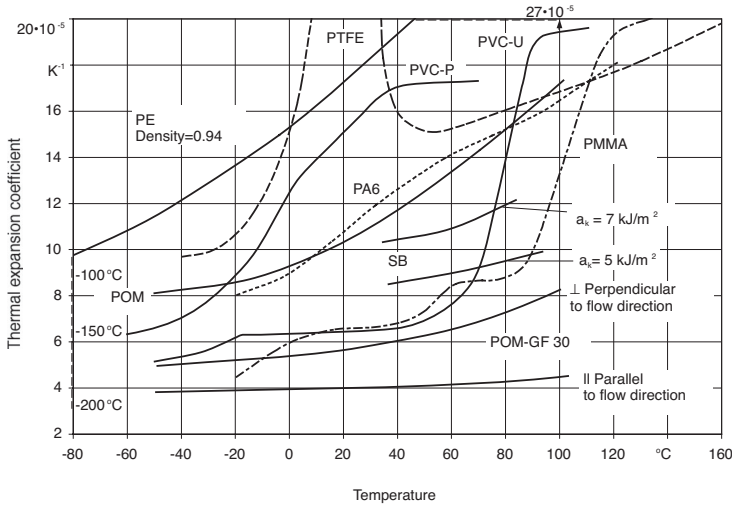


Figure 4.24: Coefficient of thermal expansion of various plastics as a function of temperature

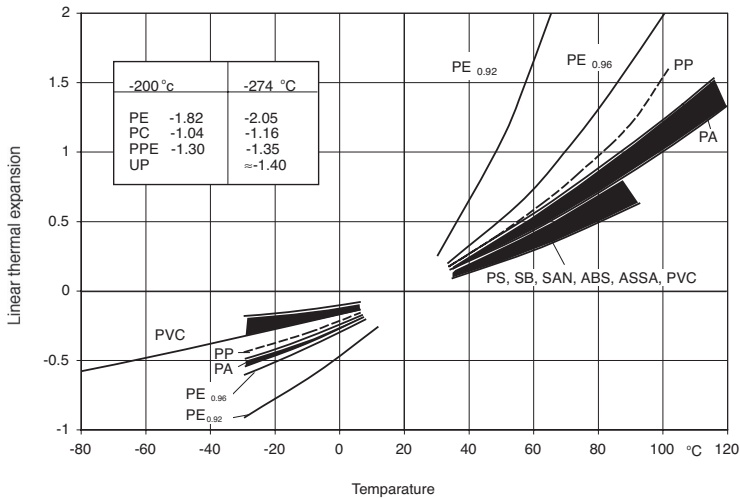


Figure 4.25: Length change as a function of temperature for various thermoplastics; index for PE denotes specific gravity

fiber-reinforcement, the rule of mixtures applies for the coefficient perpendicular to the reinforcing fibers. In fiber direction, however, the thermal expansion of the fibers determines the linear coefficient of thermal expansion of the composite. Extensive calculations are necessary to determine coefficients in layered laminated composites and in fiber-reinforced polymers with varying fiber orientation distribution.

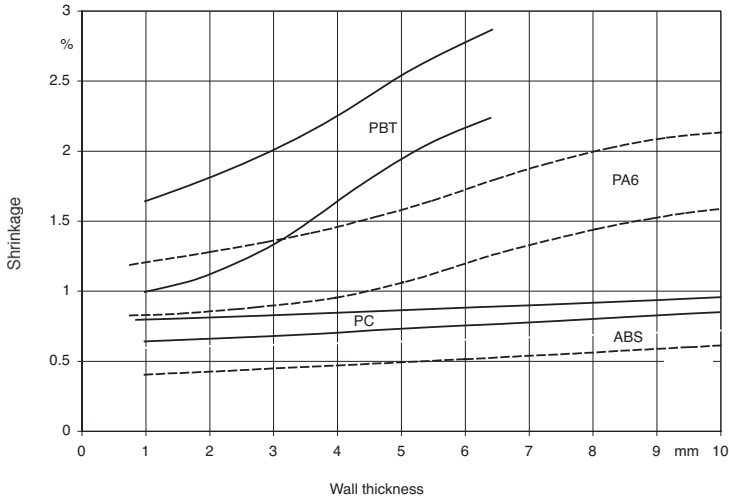


Figure 4.26: Wall shrinkage as a function of wall thickness for a selected number of thermoplastics

The temperature variation of the thermal expansion coefficients can be seen by the shape of the curves in Fig. 4.25, which present % length change as a function of temperature for several thermoplastics.

Molecular orientation also affects the thermal expansion of plastics. The thermal expansion is often affected by the cooling time during processing. This is especially true with semicrystalline polymers whose crystallization process requires time. For example, a thin part that cools fast will have a lower degree of crystallinity and will therefore shrink less. This is illustrated in Fig. 4.26 in which the range of wall shrinkage as a function of wall thickness for two semicrystalline polymers (PA6 and PBT) and two amorphous polymers (PC and ABS) is presented. The figures show how the semicrystalline plastics are more affected by the increase in wall thickness. The coefficient of linear thermal expansion is measured using the standard tests ISO 11359 and ASTM E831, see Table 4.3.

Thermal expansion data are often used to predict shrinkage in injection molded parts. Injection molding shrinkage data are measured using ASTM D955 and ISO 294-4 tests, see Table 4.4.