# Improved Approximations in Thermal Properties for Single Screw Extrusion

Modified on Friday, 01 May 2015 11:49 PM by mpieler — Categorized as: Paper of the Month

## Improved Approximations in Thermal Properties for Single Screw Extrusion

*Eberhard Grünschloss* and María del Pilar Noriega*
*ICIPC – Plastics and Rubber Institute*
*Carrera 49 No. 5 Sur-190, Medellin, Colombia, South America*
**Schweitzerstrasse 36, D-70619 Stuttgart, Germany*

## Abstract

Actual screw design software is capable to simulate the performance of a single screw extruder based on elaborated program codes. The aim of this work is to present improved approximations in relevant thermal properties for simulation and design of single extrusion screws in combination with analytical calculations appropriate for the industrial practice. The developed approximation functions for thermal properties, such as, specific heat capacity, enthalpy, thermal conductivity and density, were obtained looking for small number of parameters. A comparison between the improved approximation functions, existing known functions and measured data for some common polymer families is shown.

## Background

The thermal properties of polymers affect the single screw extrusion process from the feeding zone to the metering and mixing zone. These properties have an effect on solids conveying, melting rate and melt conveying of an extruder screw. The melting rate of the polymer material has an important effect on extrusion melting efficiency and it is strongly affected by such properties as specific heat, thermal conductivity and density obtained from a p-v-T diagram.

Specific heat capacity describes the amount of energy that it takes to raise the temperature of a polymer. LDPE requires an average of 2.596 J/(g.K) in the molten state, while PS requires 1.95 J/(g.K), [1]. Therefore, it takes almost 33 % more energy to raise the temperature of 1 g of LDPE than 1 g of PS. Additionally, it means that more power is necessary to process LDPE than PS at the same extrusion processing conditions like output in kg/h and melt temperature. It is well known that the specific heat capacity is the derivative of enthalpy with respect to temperature.

Thermal conductivity is the ability of the polymer to conduct heat. In general, the polymers exhibit a low thermal conductivity. LDPE has an average thermal conductivity of 0.25 W/(m.K) in the molten state, while PS is 0.14 W/(m.K), [1]. Because LDPE has a higher thermal conductivity than PS, the heat flux for LDPE from barrel to polymer is higher.

Solid and melt density can be obtained from p-v-T diagram, for example, Tait´s equation of state. The density is found from reciprocal of specific volume. Nevertheless, other authors have shown in the literature that Tait´s equation does not work well for semicrystalline polymers [2]. The research work of Sanchez-Cho on equation of state for polymers seems to be until now the most accurate equation of state [2, 3].

**Improved Approximations:** The developed approximation functions for thermal properties were obtained looking for small number of parameters, and they are: specific heat capacity for solid state and molten state, enthalpy for solid state and molten state, thermal conductivity from the solid state to the molten state and density from the solid state to the molten state.

The solid state enthalpy ($H_S$) is proposed as a fourparameter function as follows:

$$Hs = A \cdot \left\{ 1 - \frac{T}{B} - \exp\left(\frac{T-C}{D}\right) \right\}$$

Where,
A: Parameter in J/g
B: Parameter in K
C Parameter in K
D: Parameter in K
T: Temperature in K
The enthalpy for molten state ($H_m$) is proposed as a two-parameter function as follows:

$$Hm = F + E \cdot T^2$$

Where,
F: Parameter in J/(g.K)
E: Parameter in J/(g.K$^2$)
T: Temperature in K

The specific heat capacity for solid state ($Cp_S$) is suggested as a four-parameter function:

$$Cp_s = -\frac{A}{B} - \frac{A}{D}.\exp\left(\frac{T-C}{D}\right)$$

Where the parameters A, B, C and D are taken from the enthalpy function,

A: Parameter in J/g
B: Parameter in K
C: Parameter in K
D: Parameter in K
T: Temperature in K

The specific heat capacity for molten state ($Cp_m$) is suggested as a two-parameter function:

$$Cp_m = 2 \cdot E \cdot T$$

Where the parameter E is taken from the enthalpy function,

E: Parameter in J/(g.K)
T: Temperature in K

The heat of fusion for semicrystalline polymers can be obtained graphically from the enthalpy function as shown in Fig. 1 for a HDPE. The heat of fusion is the amount of heat energy that is required to convert a polymer from a solid to a liquid or melt.

The thermal conductivity (k) from the solid state to the molten state is proposed as one function with six parameters:

$$k = A \cdot \left(\frac{T}{B} + 1\right) \cdot \frac{\frac{\pi}{2} - ATN\left[\left(\frac{T}{C}\right)^E - D\right]}{\frac{\pi}{2} - ATN(-D)} + F$$

Where,
A: Parameter in W/(m.K)
B: Parameter in K
C: Parameter in K
D: Dimensionless parameter
E: Dimensionless parameter
F: Parameter in W/(m.K)
T: Temperature in K

This function is suitable for the range from room temperature up to typical melt temperatures in the single screw extrusion process.

The solid state density ($\rho_S$) is obtained from reciprocal of specific volume ($\upsilon_S$) and it is proposed as a six-parameter model, as follows:

$$v_s = A + \frac{T}{B} \cdot \exp\left(-\frac{p}{C}\right) + exp\left[\frac{T-D}{E} - \frac{p}{F}\right]$$

Where,
A: Parameter in cm$^3$/g
B: Parameter in K

C: Parameter in bar
D: Parameter in K
E: Parameter in K
F: Parameter in bar
T: Temperature in K
p: Pressure in bar

The density for molten state ($\rho_m$) is obtained from reciprocal of specific volume ($\upsilon_m$) and it is proposed as a three-parameter model after Spencer and Gilmore, as follows [4]:

$$v_m = A + \frac{C \cdot T}{(p + B)}$$

Where,
A: Parameter in $cm^3/g$
B: Parameter in bar
C: Parameter in (bar.cm3) / (g.K)
T: Temperature in K
p: Pressure in bar

The thermal diffusivity ($\alpha$) can be calculated from previous functions, such as, specific heat, thermal conductivity and density.

$$\propto = \frac{k}{\rho \cdot Cp}$$

Other Authors have investigated extensions of some of the above mentioned equations or functions, [5, 6, 7]. The functions described in this work have been found more suitable for simulation and design of screws in single screw extrusion, and they were obtained looking for small number of parameters, what it is appropriate for the industrial practice.

There is no fundamental theory behind the equations presented in this paper. This is reasonable because in practice the polymers are normally not pure but mixed with additives and reinforcing agents, blended with other polymers to combine their properties, etc. This will alter the polymer physics and complicate an appropriate fundamental theory.

The previous approximation functions contribute to an easier single screw calculation to simulate the performance of a single screw extruder with regard to output, pressure build-up, melting rate, heat transfer and melt temperature. These thermal functions can be used for the calculations in the screw melting zone, screw metering zone and extrusion die, Fig. 2, specially, for the prediction of pressure build-up and melt temperature profile.

## Experimental

*Polypropylene:* a polypropylene homopolymer reference 505P produced by SABIC with a Melt Index Flow, MFI, of 2.0 g/10 min at 230ºC/2.16 kg according to ISO 1133. This is a multipurpose grade for extrusion and injection molding applications.

*Modulated DSC:* A Q200 Differential Scanning Calorimeter from TA Instruments was used for measuring total heat flow, enthalpy and heat capacity. Test conditions were carried out following the standard ASTM E 1269.

A 10 mg of sample was heated from an initial temperature up to a final temperature under high purity nitrogen, using a heating rate of 20°C/min. An isotherm at final temperature is required during 5 minutes.

## Results

The solid state enthalpy (Hs) and for molten state (Hm) for PP Ref. 505P proposed as two functions in previous numeral have converged to the following parameters:

A: -971.49 J/g
B: 350.44 K
C: 475.11 K
D: 15.18 K
E: 0.0034 $J/(g.K^2)$

F: -303.155 J/g

The Fig. 3 shows the measured data and the obtained approximation functions. From the figure it is possible to observe that the approximation functions match the data very well.

The specific heat capacity for solid state ($Cp_s$) and for molten state ($Cp_m$) for PP Ref. 505P proposed as two functions in previous numeral have the same parameter values for A, B, C, D and E than the enthalpy functions, since specific heat capacity is the derivative of enthalpy with respect to temperature.

The Fig. 4 shows the obtained approximation functions from measured enthalpy data. This figure illustrates that the approximation functions match the data properly.

The thermal conductivity (k) from the solid state to the molten state for a HDPE reported by VDMA [8] has met the following parameters:

A: 0.19886 W/(m.K)
B: -0.00538 1/K
C: 0.00873 1/K
D: -4.76
E: 16.81785
F: 0.25451 W/(m.K)

The Fig. 5 shows the measured data and the obtained approximation function. From the figure it is possible to observe that the approximation function fits the data satisfactorily.

The solid state density ($\rho_s$) for a PP measured by Borealis is obtained from reciprocal of specific volume and it has converged to the following parameters:

A: 1.042 $cm^3/g$
B: 3540 K
C: 2166 bar
D: 422.1 K
E: 8.364 K
F: 353.3 bar

The density for molten state ($\rho_m$) for a PP measured by Borealis is obtained from reciprocal of specific volume and it has met the following parameters:

A: 0.9537 $cm^3/g$
B: 2435 bar
C: 1.8542 (bar.cm3)/(g.K)

The Fig. 6 shows the measured data and the obtained approximation functions for the solid and the molten state. From the figure it is clear that the approximation functions fit the data very well.

The Fig. 7 is demonstrating the use of the above described thermal functions in combination with analytical calculations, [9], for the prediction of pressure build-up in a single screw of D = 20 mm and L/D = 20 for PE processing. The left ordinate axis shows the screw pitch, the right ordinate axis shows the screw channel depth and the abscissa or X-axis is the axial screw length.

Solids bed profiles (SBP) could be obtained for several polymers and single screws using the experimental values of X/W versus L/D from a patented device compared to analytical melting models using the mentioned thermal functions, [10].

## Conclusions

This work presented improved approximations with reduced number of parameters in thermal properties that are relevant for simulation and design of single extrusion screws. These approximations in combination with analytical calculations are appropriate for the industrial practice, since they deliver accurate enough predictions of output and pressure build-up of extruder screws, among others.

There is no fundamental theory behind the equations shown in this paper. This is reasonable because in practice the polymers are normally not pure but mixed with additives and reinforcing agents, blended with other polymers to combine their properties, etc. This will alter the polymer physics and complicate an appropriate fundamental theory.

The developed approximation functions for thermal properties, such as, specific heat capacity, enthalpy, thermal conductivity and density, fitted the measured data very well. The authors gave an adequate mathematical representation of the measured data, suitable for inclusion in future analytical models and papers.

## References

/1/ Kühnle, H. and Grünschloss, E., "Berechnung der Austragszone von Einschneckenextrudern", Rheologie in der Kunststofftechnik, Technische Akademie Esslingen, Ostfildern, Germany, 1999
/2/ Zoller Paul, "PVT Reltionship and Equations of State of Polymers,
/3/ Cho, J. and Sanchez, I., "PVT Relationship and Equations of State of Polymers"
/4/ Spencer, R.S. and Gilmore, G.D., "Equation of state for high polymers", Journal of Applied Physics, 21, pp. 523-526, (1950).
/5/ Sanchez, I. and Cho, J., "A universal equation state for polymer liquids", Polymer, Vol. 36, No. 15, pp. 2929 – 2939, 2005
/6/ Naranjo, Alberto, "Measurement of the Thermal Diffusivity of Thermoplastics under Processing Conditions", IKV-Berichte aus der Kunststoffverarbeitung, Mainz, G., Germany, 2004
/7/ Sedlacek, T., et.al. "On relationship between PVT and rheological measurements of polymer melts", Annual transactions of the Nordic Rheology Society, Vol. 13, 2005.
/8/ VDMA, "Thermodynamik", Carl Hanser Verlag, Munich, Germany, 1979
/9/ Grünschloss, E., "Polymer Single Screw Extrusion: Modeling", Encyclopedia of Materials: Science and Technology, Elsevier Science Ltd., 2001
/10/ Noriega, María del Pilar, et. al., "Method and device to visualize in-line and quantify the polymer melting in plasticating screw machines without significantly affecting its thermal regime", U.S Patent No. 7314363, January 1, 2008.

## Acknowledgments

Thanks are also due to the Instituto de Capacitación e Investigación del Plástico y del Caucho (ICIPC) in Medellín, Colombia, Institute for Plastics Technology (IKT) in Stuttgart, Germany, German Academic Exchange Service (DAAD) and ICETEX in Colombia for their valuable support to develop this research project.

## Nomenclature

D Extruder diameter
L/D Dimensionless Extruder length
X/W Dimensionless screw channel width
$H_s$: Solid state enthalpy
Hm: Enthalpy of the melt
$Cp_s$: Specific heat capacity of the solids
$Cp_m$: Specific heat capacity of the melt
k: Thermal conductivity
$\rho_s$: Solid state density
$\rho_m$: Density of the melt
$\upsilon_s$: Specific volume of the solids
$\upsilon_m$: Specific volume of the melt
α: Thermal diffusivity
R: Gas constant, 8.3144 J/(mol.K)
p: Pressure
T: Temperature
LDPE: Low density polyethylene
HDPE: High density polyethylene
PP: Polypropylene
PS: Polystyrene

**Key Words:** Single screw extruder, thermal properties, specific heat capacity, enthalpy, density, thermal diffusivity, LDPE, HDPE, PP, PS

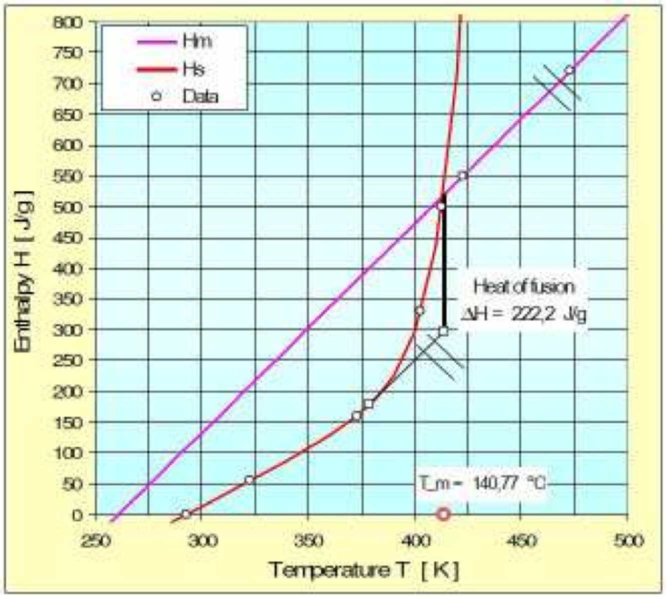

Figure 1: Graphically obtained heat of fusion for HDPE

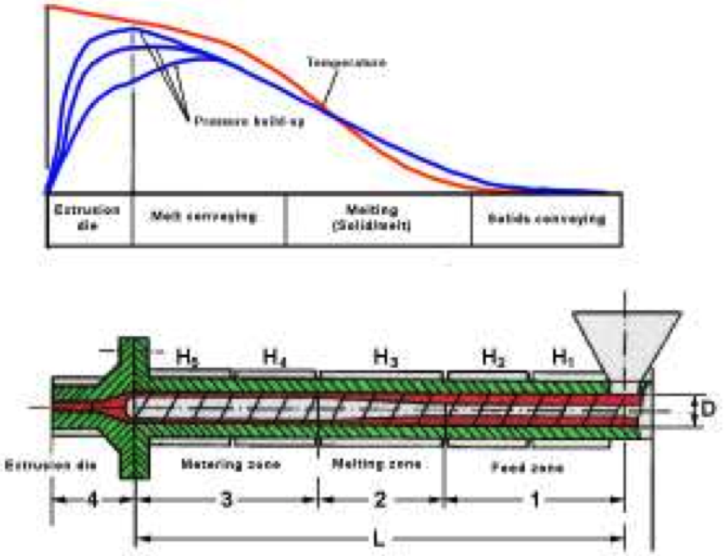

Figure 2: Zones in a single screw extruder

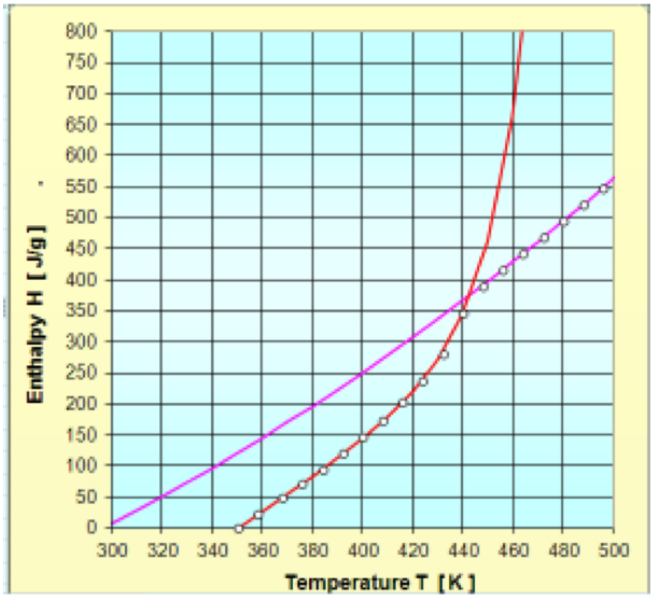

Figure 3: Enthalpy of PP- SABIC 505P: Measured data and approximations

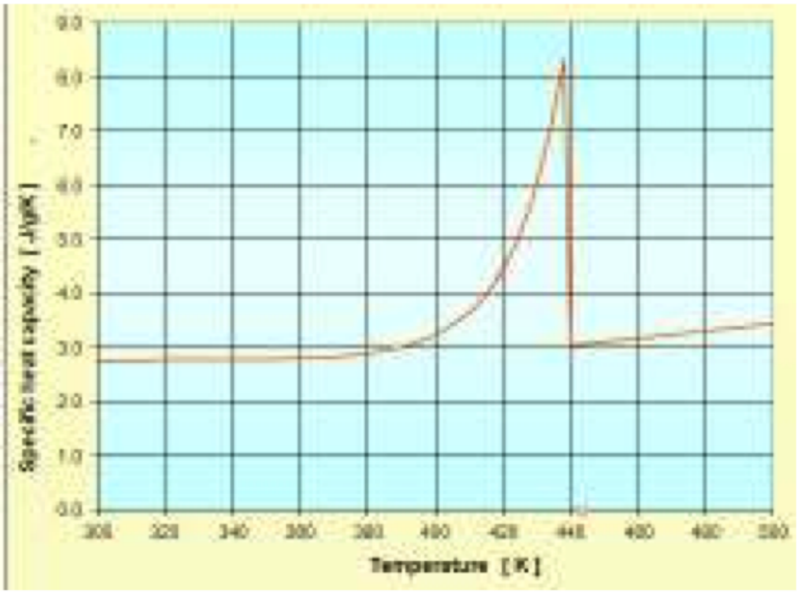

Figure 4: Specific heat capacity of PP- SABIC 505P: Approximations

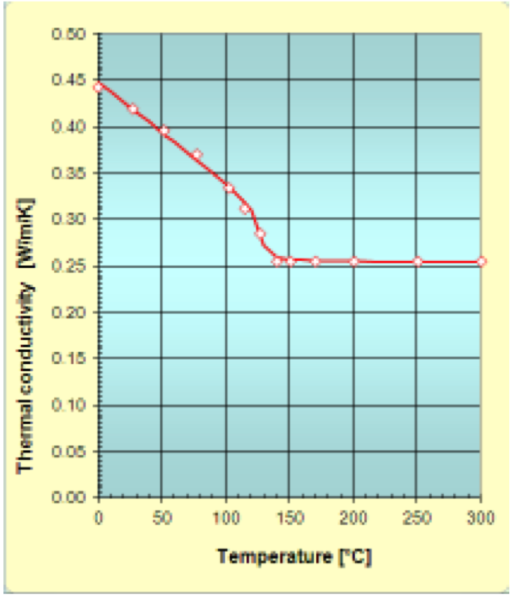

Figure 5: Thermal conductivity of HDPE: Measured data and approximation

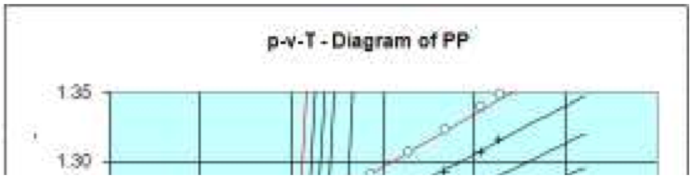

Figure 6: p-v-T diagram of PP (Borealis): Measured data and approximations

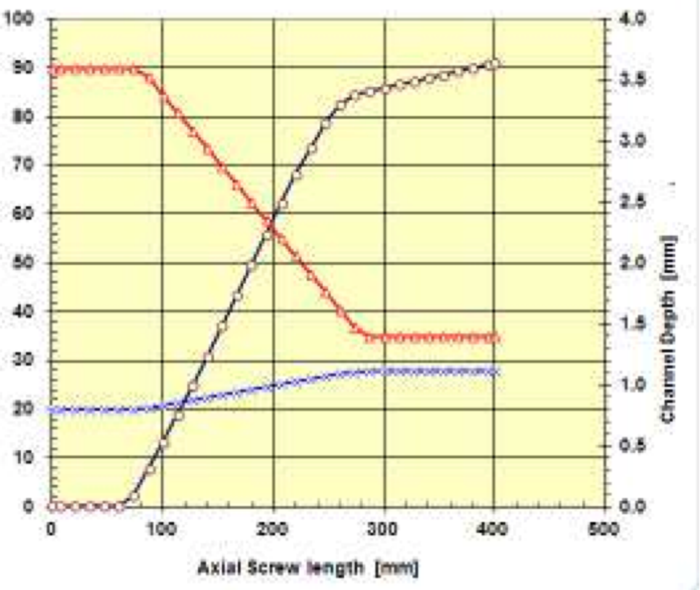

Figure 7: Pressure build-up (o) of a Ø20 mm screw for PE, channel depth (Δ) and screw pitch (x) versus axial screw length

Return to Paper of the Month.