Distribution of Specific Energy in Twin-Screw Corotating Extruders Using One-Dimensional Process Simulation

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Distribution of Specific Energy in Twin-Screw Corotating Extruders Using One-Dimensional Process Simulation

Adam Dreiblatt, Century Extrusion, Traverse City, MI
Eduardo Canedo, PolyTech, Campina Grande, Brazil

Abstract

Specific mechanical energy (SME) is a single parameter that represents the energy transfer from the main drive motor through frictional heating for melting, mixing and die pressurization in the compounding process. The calculation of SME is performed using the extruder motor load (e.g. shaft torque), screw speed and total throughput to provide energy input on a unit mass basis. Use of one-dimensional computer simulation to analyze the axial distribution of specific energy reveals strategically where this energy is applied in fullyintermeshing, co-rotating twin-screw extruders as a function of screw design.

Introduction

Co-rotating intermeshing twin-screw compounding extruders are the predominant machine in use today for compounding polymers with additives, fillers, etc. The compounding process is a complicated sequence of events whereby polymer(s), impact modifiers and additives are first melted to create a specific morphology. Particulate fillers, pigments, etc. are typically introduced into a downstream feeding port for dispersion into the melt, followed by a second downstream feeding port for addition of reinforcing fillers (e.g. glass fiber) or additional particulate filler with subsequent homogenization. Finally, volatiles are removed through vacuum degassing port(s) and the compound is pressurized through a die or melt filtration device.

For a given formulation, the resulting properties (e.g. rheological, physical, etc.) are determined largely by the mechanical energy input to the materials within the residence time of the compounding extruder. If too much mechanical energy is applied in homogenizing glass fibers, for example, the mechanical properties will suffer. Conversely, insufficient mechanical energy input can also result in incomplete melting of polymer which will also produce inferior properties. The interactions between raw materials (and feeding position), screw design and operating variables are captured within the single parameter SME and can therefore be used to correlate directly with compound quality.

The value of SME is derived from the extruder motor load (using percent torque instrumentation or direct measurement of power from the main drive) and represents the cumulative effect of energy input along the entire screw axis.

This is a similar situation with measurement of residence time. There are many citations correlating mixing with residence time distribution (RTD). We can measure the distribution of residence time using a tracer, however, this information does not provide insight as to the distribution of residence time in each element of the extruder. The only means to obtain such information would be to measure RTD for each segment of the extruder. It is physically possible to assemble and operate an extruder consisting only of the solids conveying section and measure RTD. Then increase the length of the extruder by adding a melting section and repeat the RTD measurements. While a tedious and time-consuming exercise, the information could be obtained using this technique.

Similarly, the distribution of specific energy can provide valuable insight as to where the energy is applied within the compounding process. As mentioned above, it would be possible (although time-consuming) to physically measure the energy contribution of each part of the screw design by assembling extruders with incremental lengths.

An alternative to this method uses one-dimensional (1D) simulation to analyze the mechanical energy contribution for each part of the screw design. Such 1D computer modeling programs have been commercially available and have been validated to provide close approximations to the actual compounding process[2,3,4]. Simulation provides the capability to measure differential values along the screw axis for power, temperature, residence time, etc. and is the basis for this investigation. The overall energy balance in the processing chamber of the extruder may be approximately formulated as:

$$W = Q_{HT} + G\left(\Delta H + \overline{v}\Delta p\right) \qquad (1)$$

where W is the power delivered to the material, QHT is the rate of heat transfer between the polymer and the processing chamber wall (usually the barrel internal wall, as the screws are assumed adiabatic), ΔH and Δp are specific enthalpy and pressure difference between output and input, G is mass throughput and v is the mean specific volume.

For simple systems, ΔH can be easily estimated from the thermodynamic properties (heat capacities of solid and molten polymers and fillers, effective latent heat of fusion of polymers, etc.) in terms of the feed and discharge temperature and Δp is associated to the head pressure. The power delivered by the motor may be computed from measured motor torque and screw speed. Thus, Eq. (1) may be used to estimate the heat transferred between the extruder and the material.

Simulation by general purpose software using simplified one-dimensional models allows the computation of the power dissipated during compaction and melting of polymer solids (by friction between the particulate solids and the barrel wall and screw and between solid particles themselves, by plastic deformation of the softened solid particles, etc.) and during the transport and mixing and pressurization of the molten material (essentially by viscous dissipation). The heat transport between the processing chamber and the barrel wall for a given barrel temperature profile may also be computed (albeit with greater uncertainty). All these calculations are performed element by element along the extruder. Likewise, simulation software computes the internal pressure profile. Thus, simulation software allows the prediction of the axial temperature profile, prediction that may be verified against process data and the models adjusted accordingly.

Once the simulation software has been validated, the computation of the power profile along the extruder, or the mechanical energy input profile (power per unit throughput), is a powerful tool to investigate where power is dissipated within the extruder, and how the specific energy profile depends on screw design and operating conditions (screw speed, feed rate, barrel temperature profile, etc.)

With this approach, the individual contribution to specific energy for each screw element type can be quantified and optimized for melting and mixing efficiency as well as for scale-up to larger screw diameters.

Methodology

The one-dimensional computer simulation program WinTXS™ from PolyTech was used for this analysis. The simulations were performed using a polypropylene (PP) resin with melt index = 5, 10 and 20 dg/min (230 ^{o}C, 2.16kg) and a 70 millimeter twin-screw extruder with diameter ratio = 1.55, length/diameter ratio = 32. The screw configuration used for simulation is shown in Figure 1. Die pressure was maintained constant at 30 bar, feed rate was held constant at 1200 kg/hr and screw speed varied between 400 rpm and 800 rpm.

The energy required to raise the temperature of a unit mass of a polymeric material from the feed temperature T_1 to the discharge temperature T_2 may be computed, approximately as:

$$\Delta H = c_S (T_m - T_1) + \Delta H_m + c_L (T_2 - T_m) \qquad (2)$$

where c_S and c_L are the average specific heats of the solid and molten polymer, respectively, ΔH_m is the effective heat of fusion of the polymer (which depends on the material; for amorphous polymers ΔH_m, = 0), and T_m is the melting or softening temperature.

The melting temperature for PP was 170 ^{o}C and heat capacity 2.34 kJ/kg ^{o}C (solid state) and 1.61 kJ/kg ^{o}C (melt at 200^{o}C). Shear viscosity data for the MF=5 resin is shown by Figure 2 using Carreau-Yasuda viscosity model.

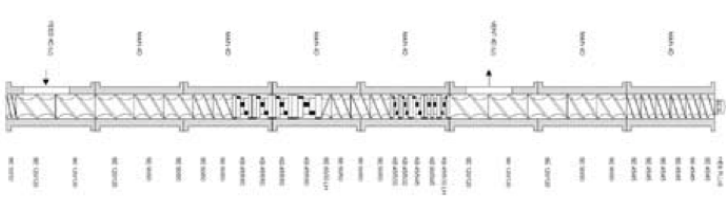

Figure 1. Screw configuration used for 70mm simulation

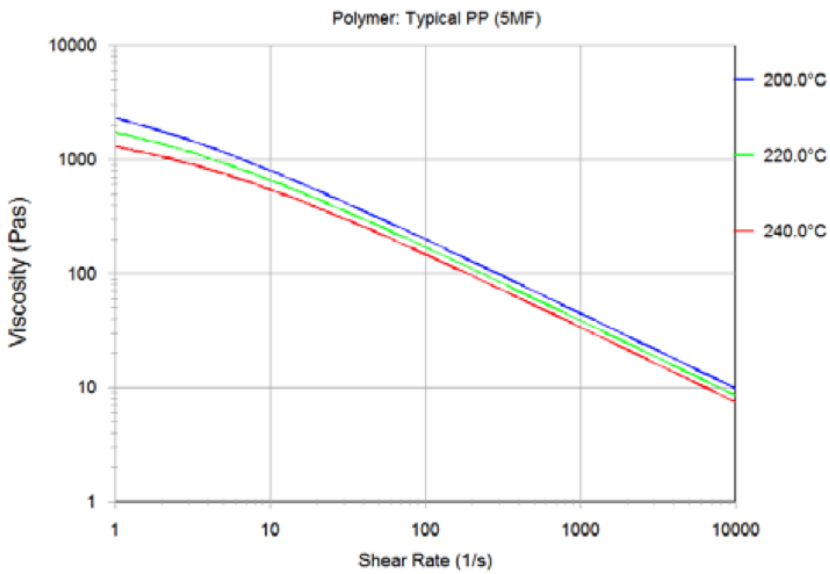

Figure 2. Shear viscosity data for PP resin

Discussion

The net distribution of power along the screw axis is shown in Figure 3. This curve represents the mechanical energy input to the extruder and does not account for energy removed through barrel cooling or the 'no-load' power required to turn the motor, gearbox and empty screws. The contribution of power for each section of the extruder reveals most of the energy is consumed in resin melting; an energy balance for this section of the extruder can be used to corroborate the predicted melt temperatures.

The theoretical energy requirement to raise the solid polymer from ambient to melting temperature (170^{O}C) at 1200 kg/hr is 77.75 kW and the theoretical energy requirement to melt the polymer at 1200 kg/hr is 20.0 kW. Combining these two, the theoretical energy requirement for polymer melting is 0.081 kWh/kg. Predicted SME results for resin melting range from 0.092 kWh/kg at 400 rpm to 0.097 kWh/kg at 800 rpm.

The theoretical energy requirement to raise the temperature of the melt to predicted discharge temperature is 40.17 kW (221.5^{O}C @ 400 rpm), 42.9 kW (225^{O}C @ 600 rpm) and 47.6 kW (231^{O}C @ 800 rpm). The theoretical SME for the compounding process ranges from 0.115 at 400 rpm to 0.121 kWh/kg at 800 rpm. These values are compared to the simulation predictions in Table 1.

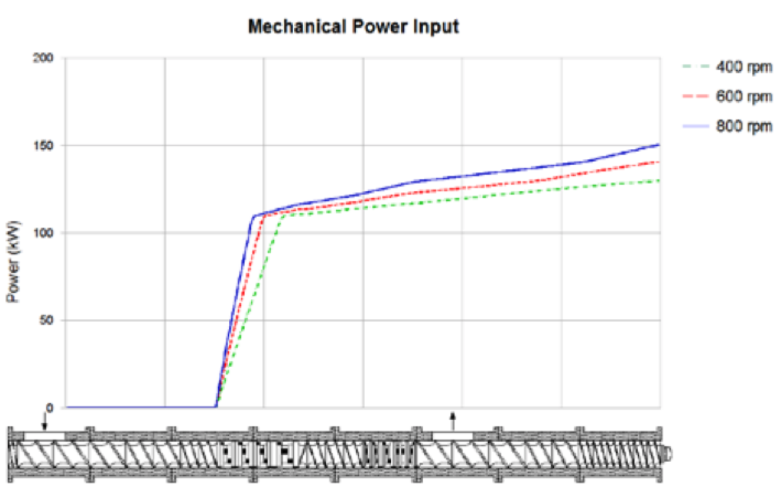

Figure 3. Power consumption versus screw speed

The objective of this investigation is to determine where this energy is applied along the screw axis.

Screw speed, rpm	400	600	800
Predicted melt temp, °C	221.5	225	231
Theoretical SME, kWh/kg	0.115	0.117	0.121
Predicted SME, kWh/kg	0.108	0.117	0.125

Table 1. Predicted SME (kWh/kg) and melt temperature (°C) versus screw speed.

Solids Conveying

Simulation results indicate zero power consumption for the initial solids conveying. In reality, given the available power for a given diameter extruder and the ‘no load’ power to rotate the drive motor, gearbox and screw shafts, it is not an unreasonable estimate. Typical industrial extruders do not have the resolution required to measure this small amount of energy. We do not expect the energy requirement to be more than negligible for most powders, pellets, flakes, etc. within the range of most compounds. This situation changes, however, when melt feeding a twin-screw extruder directly from a reactor where the power required is for melt conveying (versus solids conveying).

The process length (in terms of L/D) required for initial solids conveying is usually in the range of 6D to 8D; increasing the length of the solids conveying section would not increase the energy requirement. As there is virtually no mechanical energy expended in this section, any increase in material temperature is via thermal heat transfer from barrel heating. Given the low degree-of-fill of the screws in the solids conveying area and relatively short residence time (less than 1.5 seconds for the material to move from the feed barrel to the first kneading element), the temperature of the solid polymer pellets is far from its melting temperature.

Polymer Melting

The distribution of mechanical energy within the melting configuration is a function of screw speed and feed rate. At high screw speed (i.e. high shear stress), the plastic deformation of solids occurs within the first kneading elements. This energy transfer is extended to the following kneading elements at lower screw speed (i.e. lower shear stress).

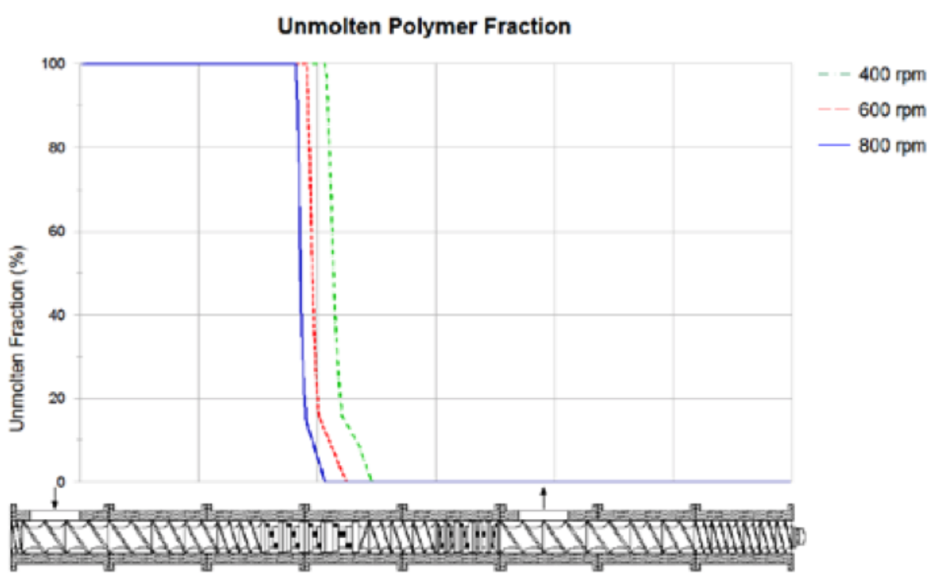

Figure 4. Position of resin melting versus screw speed

Note that the polymer is not yet melted, although most of the mechanical energy is transferred to the polymer. This energy is expended to deform and compress the (solid) polymer resin and results in a rapid temperature rise as illustrated in Figure 5. Melting (phase change) occurs in the kneading elements that follow; the specific kneading elements responsible for melting are determined by screw speed and feed rate. At high screw speed, polymer phase change occurs in the third kneading element while the remaining kneading elements are required to accomplish this same task at lower screw speed.

Once the polymer is molten, mechanical energy input deteriorates rapidly in the following kneading elements as viscous dissipation – this axial change in the rate of energy transfer is shown as a rapid change in slope (i.e. flattening) of the power distribution curve in Figure 3. In this case, polymer melting is completed at the third kneading element with high screw speed and the remaining kneading elements are transferring mechanical energy to the melt increasing the melt temperature. At the lowest screw speed, there is no mechanical energy input as viscous dissipation in this first kneading section.

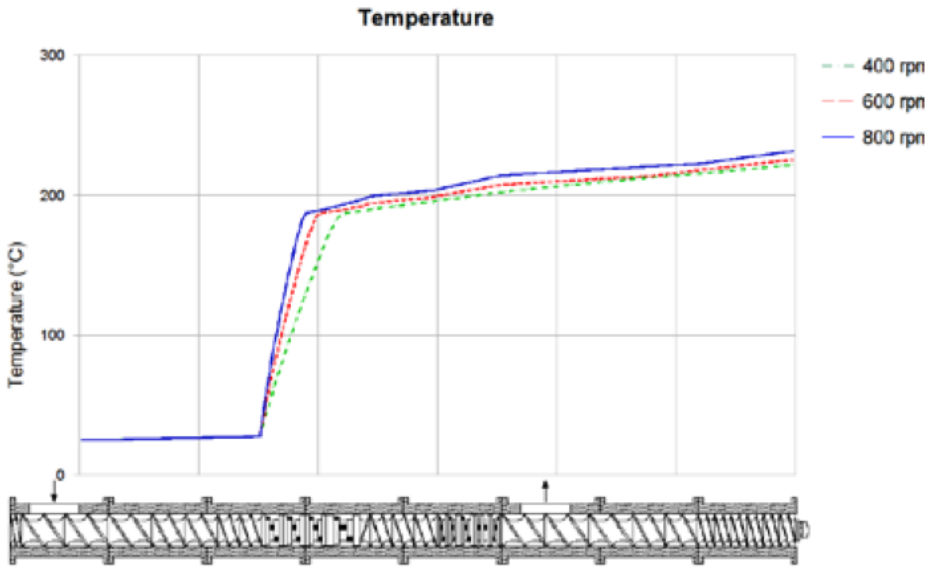

Figure 5. Axial temperature versus screw speed

Most of the energy contribution occurs prior to actual melting where the temperature increases rapidly (less than two seconds) as a result of plastic deformation of solids.

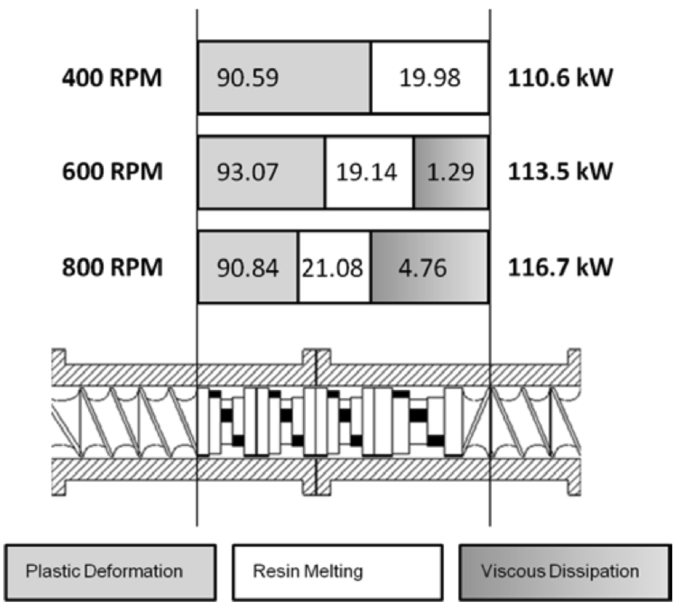

Figure 6. Energy input (in kilowatts) by type and position within the melting section as a function of screw speed

The distribution of mechanical energy within the melting configuration is shown in Figure 6 where the simulation predicts the exact position of solids melting as a function of screw speed. The power distribution curve was used to quantify the mechanical energy input within the melting part of the screw configuration by energy type.

Intermediate Melt Conveying

Mechanical energy is applied to the molten polymer in subsequent conveying sections of the extruder increasing the melt temperature. Since the polymer melting represents a substantial percentage of the total energy requirement, the viscous dissipation of energy in downstream conveying elements represents only a small fraction of the total SME and is shown in Table 2. At increasing values of SME (whether achieved by increased screw speed, lower throughput or by screw design changes) the additional mechanical energy is expended in viscous dissipation since the energy required for polymer melting is constant.

Function	Percentage of SME		
Screw speed, rpm	400	600	800
Solids conveying	0	0	0
Resin melting	85.2	80.6	77.5
Intermediate melt conveying	2.7	3.3	3.7
Melt mixing	2.2	3.5	4.7
Melt conveying and pumping	9.9	12.6	14.1

Table 2. Percentage contribution of SME by function versus screw speed (Melt Flow = 5.0).

The rate of energy input in the downstream melt conveying section is more depending on the melt viscosity as shown in Figure 7. In this case, simulations were performed using PP with different melt flow rates (MF = 5, 10, 20) at the same extruder conditions (1200 kg/hr, 600 rpm) to see the difference in the power distribution in the downstream melt conveying section.

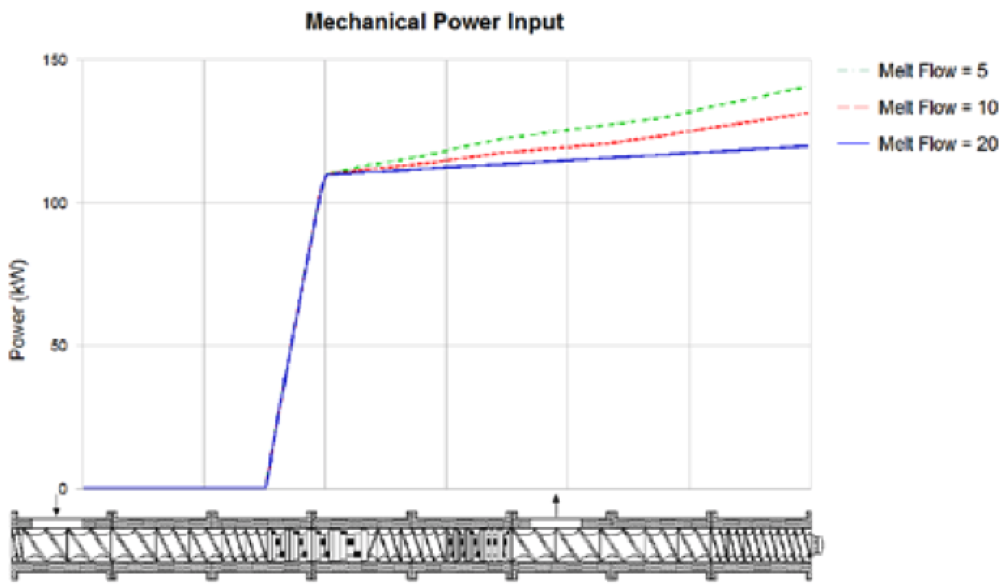

Figure 7. Power consumption (in kilowatts) versus polymer viscosity at 1200 kg/hr and 600 rpm screw speed.

Figure 7 also illustrates the mechanical energy requirement to melt the PP polymer does not change with melt flow, however, the resulting viscous dissipation is strongly affected by polymer viscosity. The flattening of the power distribution curves (in Figure 7) with decreased polymer melt viscosity confirms reduced viscous heating.

Melt Mixing

Kneading elements are installed downstream of polymer melting for dispersive and distributive mixing of impact modifiers, pigments, additives. fillers, etc. which may be introduced with the polymer in the main feed opening or added through downstream feeding. In the case of downstream feeding, the thermal cooling of the melt from ambient solids entering the process is not considered in this investigation (all solids are entering via the main feed opening, downstream feeding is foreseen in future work). The mechanical energy input from downstream kneading elements, as a percentage of total SME, is not much different than for melt conveying elements as shown in Table 2.

A second screw design with additional downstream mixing elements (Figure 8) does not contribute significant SME as shown in Figure 9. Comparing the slope of the power distribution curve in this region, there is little change in viscous dissipation from the additional kneading elements. The total SME does not change with this alternate screw design.

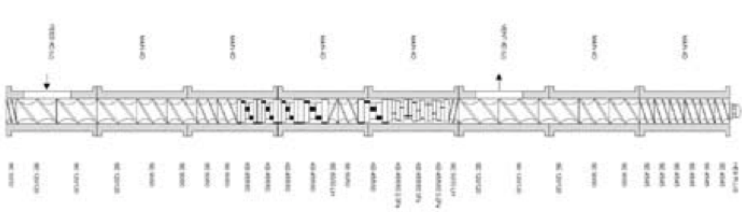

Figure 8. Alternate screw design with additional downstream kneading elements.

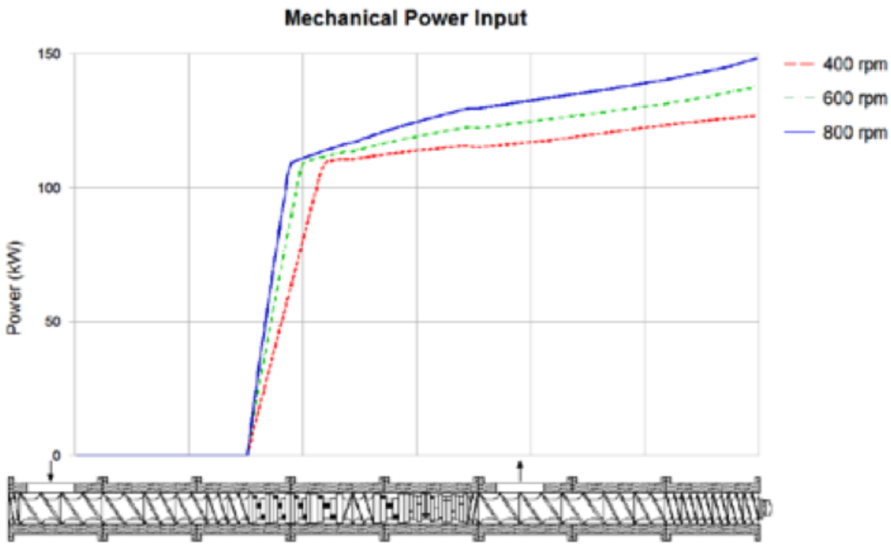

Figure 9. Power consumption (in kilowatts) for alternate screw design with additional downstream kneading elements (PP melt flow = 5, 1200 kg/hr and 600 rpm).

The small increase in viscous energy input in this downstream mixing section (thereby decreasing melt viscosity) results in decreased viscous energy input in the following melt conveying and die pressurization sections.

Die Pressurization

As shown in Table 2, the final melt conveying (e.g. in vacuum degassing) and die pressurization sections add between 10 and 15 percent of the total SME. Increasing conveying length, melt viscosity and SME increases this percentage. There is little difference, as seen in the slope of the power distribution curve, in SME input for conveying with and without pressure (all simulations were conducted at 30 bar die pressure). The incremental energy added via viscous heating translates to increased melt temperature.

Conclusions

One-dimensional computer modeling of the compounding process provides insight as to where and how mechanical energy is transformed within the screw design and enables twin-screw extruder screw designs to be optimized for melting efficiency and minimizing melt temperature.

The distribution of specific energy is concentrated in the first kneading elements where mechanical energy is applied to the solid polymer prior to actual melting. The exact position and extent of this energy is dependent on extruder operating conditions.

SME does not reflect how the energy is applied in terms of mixing and/or homogenization. What is not included within SME is the residence time over which the energy is applied and the resulting shear stress within the polymer.

Future work will validate some of these predicted results and investigate SME distribution for downstream feeding and different screw diameters to confirm scale-up behavior.

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