SOLVING THE TWIN SCREW EXTRUSION CONFIGURATION PROBLEM - A PLASTICATING MODELING PROGRAM

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Abstract

Co-rotating twin-screw extruders are widely used by polymer materials producers and compounders due to a number of interesting constructive and functional features. In fact, a broad range of polymer systems can be prepared / processed by adjusting adequately the operating conditions (output, screw speed and barrel temperature profile) and the screws geometry/configuration.

This work presents a model for plasticating co-rotating intermeshing twin-screw extrusion, covering sequentially solids conveying, melting of a moving solid plug followed by melting of solid particles surrounded by melted polymer, and melt conveying, which are the typical process stages that materials are subjected to in these machines. The model is then used to investigate the influence of the operating conditions and screw configuration on relevant process responses such as melt exit temperature, mechanical and thermal energy consumption, degree of mixing and average residence time.

Keywords: polymer extrusion, compounding, process modelling, twin-screw extruders

1 Introduction

Co-rotating twin-screw extruders are widely used by polymer materials producers and compounders due to a number of interesting constructive and functional features. The modular construction of screws and barrel provides great flexibility and adaptability to the particular requirements of each polymer system. Both are built by elements of various available types, thus allowing a good control of dispersive and distributive mixing, residence times, feeding sequence, etc. Therefore, in industrial practice the performance of twin screw extruders is dictated by the proper choice of the operating conditions (screw speed and output, which are controlled independently, and barrel temperature profile) and screw configuration.

The optimization of such a system is a complex task, which is usually accomplished by experimental trial-and-error procedures (thus, not really ensuring that a true optimum has indeed been obtained). Nevertheless, many studies have contributed to a better understanding of the physical, thermal and rheological phenomena occurring in these machines [1-11]. Some attempts have also been made to develop optimization methodologies, able to define the best screw configuration and/or operating conditions for a given application, which are based on couplings
between process modelling and optimization algorithms [12]. Unfortunately, most of these efforts have been compromised by the fact that the available modelling programmes are either too basic to provide precise/complete predictions, or are only capable of covering part of the process (usually melt conveying) [1, 3, 9].

This paper reports an effort to develop a global modelling program for co-rotating twin-screw extruders accounting for the entire process, i.e., from hopper to die (this is usually denoted as plasticating extrusion). It is organized as follows: initially, the relevant physical phenomena are identified and their mathematical description is presented briefly. Computer implementation is then presented. Finally, cases studies are used to discuss the influence of process parameters on performance measures.

2 Process Modelling

2.1 Physical phenomena

As the name implies, in co-rotating intermeshing twin-screw extruders two parallel screws interlocked as much as possible rotate in the same direction and at the same circumferential speed. The screws are built by connecting sequentially individual elements, the most representative types being represented in Figure 1. We can distinguish between: i) transport (or right handed) elements, that have a positive helix angle and, consequently, conveying capacity, ii) kneading blocks, built from various staggered disks forming various possible angles, i.e., with different degrees of conveying/kneading action, and iii) left-handed elements, with a negative helix, inducing intensive mechanical action upon the material.

These extruders work under starve feed conditions (a dosing screw is used), which has three main consequences:

- the screw’s filling ratio changes along the screw axis, depending on the conveying capacity of each element;

- the pressure profile can be very complex, with significant values along restrictive elements and zero in most conveying zones;

- melting takes place when the material reaches the first restrictive element.
Figure 2 identifies schematically the physical phenomena developing along a representative co-rotating twin-screw extruder, as well as the corresponding typical pressure profile. The solid polymer pellets or powder enter the screw channel via a gravimetric or volumetric feeder. Initially, the solids remain relatively cold and are conveyed in partially filled channels in a figure-of-8 pattern, caused by the rotation of right-handed elements. Eventually, the presence of restrictive kneading blocks and/or left-handed elements downstream induces progressive channel filling and pressure develops. Soon after, efficient heat conduction due to solids compaction and heat dissipation due to friction and mechanical compressive and shearing actions upon the solids yields their melting, which is usually more intense near to the inner barrel wall. Very often, melting is completed before the polymer starts flowing along the first restrictive element upstream. Therefore, during the remaining screw length, we must deal with melt conveying, which is either purely drag-based in partially filled channels, or has a pressure component in fully filled zones.

2.2 Mathematical models

In order to describe mathematically the above sequence of events, it is convenient to approach each step separately and then describe the global behaviour by linking adjacent steps through the appropriate boundary conditions. Adequate modelling of the conveying of loose solids in the initial screw turns is quite complex and involves the application of computationally demanding numerical techniques, such as the discrete element method [13]. Since this step does not contribute significantly to the
 thermo-mechanical experience of the material inside the extruder, it will be disregarded.

Figure 2: Physical phenomena and pressure developing along a typical co-rotating twin-screw extruder

Figure 3 schematizes the physical models assumed for each process step. Calculations start when pressure begins to develop and a solid plug moves in the down-channel direction (Figure 3-I). An equivalent situation for single screw extruders was studied by Broyer and Tadmor [14], who considered heat dissipation at all surfaces. The increase in temperature is calculated by solving the energy equation (using finite differences), taking into account heat conduction from the barrel and heat dissipation due to friction at all surfaces [14, 15]. This step ends when the material in the vicinity of the barrel reaches its melting temperature. Then, a melt film appears, giving rise to the delay zone - Figure 3-II (eventually, a second melt film close to the screw surface may also form) [15]. Thus, friction at metallic walls is replaced by viscous drag and viscous dissipation must be also accounted for, given the high average values of shear rate.

We assume that when the thickness of this melt film grows beyond the value of the screw flight clearance melt accumulates near to the active flank, and a specific melting mechanism develops [14]. Although the nature of the latter is still a matter of debate in the literature, here we propose the following chain of events (based on
the reports of previous visualization studies [16, 17]): i) initially, the solid plug becomes surrounded by a melt pool (near to the active flank) and melt films at the remaining surfaces (Figure 3-III); ii) the decrease in solids content can be described by the 5-zone melting model proposed by Lindt et al [18] for single screw extrusion; iii) when the solids content is lower than 50%, the local mechanical forces induce rupture of the plug and dispersion of individual solid particles within the molten phase (Figure 3-IV); iv) from now onwards, the diameter of the pellets suspended in melt decreases due to heat conduction from the melt [9-11]. The change in radius during an increment of time $\Delta t$ is given by:

$$\frac{\Delta R}{\Delta t} = \frac{h_s(T_s - T_i)}{\rho_s(C_{ps}(T_m - T_s) + \Delta H)}$$

(1)

where $\rho_s$ is density, $C_{ps}$ is the heat capacity of the solids, $h_s$ is the heat transfer coefficient towards the solids pellets, $T_s$ and $T_i$ are the temperature of the solids and melt, respectively, and $\Delta H$ is the melting enthalpy. Details of these calculations can be found elsewhere [9].

3 Computer implementation
Figure 6 presents the flowchart of the program developed for plasticating extrusion. One starts by defining the geometry, operating conditions and relevant material properties. Calculations progress from hopper to die, checking whether each individual screw element is restrictive. When the first of this type of elements is detected, flow calculations are set to begin at a given location upstream of this point \(L_0\) and encompass solids conveying, delay, melting and melt conveying along small down-channel increments. If at the end of each restrictive zone pressure is higher than a prescribed value \(E\), a new \(L_0\) value is defined and the calculations repeated.

The procedure is repeated for the remaining restrictive zones, but now only melt conveying occurs, yielding the profiles of velocity, temperature, pressure, power consumption and degree of fill along the screw and die.

4 Results and discussion

4.1 Material and equipment

Table 1 presents the configuration selected for a modular Leistritz LSM 30-34 laboratory twin screw extruder that will process a polypropylene homopolymer PP (HB121J, from Borealis). This material has a melt density of 0.902, a heat capacity of 2000 J/kg.K, a thermal conductivity of 0.2 W/m.K and melts at 163°C. The viscosity follows the Carreau-Yasuda law:

\[
\eta(\dot{\gamma}) = \eta_0 \left[ 1 + (\lambda \dot{\gamma} a_T)^n \right]^{\frac{n-1}{n}}
\]

where

\[
a_T = \exp \left[ \frac{E}{RT} - \frac{1}{T_0} \right]
\]

with the following parameters: \(n = 0.35\), \(a = 0.733\), \(\lambda = 1.726\) s, \(\eta_0 = 22200\) Pa.s, \(E/R = 5564\) K and \(T_0 = 473\) K.

Table 1- Screw layout from hopper to die.

<table>
<thead>
<tr>
<th>Element</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (mm)</td>
<td>97.5</td>
<td>150</td>
<td>60</td>
<td>120</td>
<td>60</td>
<td>30</td>
<td>60</td>
<td>30</td>
<td>30</td>
<td>45</td>
<td>60</td>
<td>30</td>
<td>90</td>
<td>30</td>
</tr>
<tr>
<td>Pitch (mm)</td>
<td>45</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>45</td>
<td>30</td>
<td>20</td>
<td>30</td>
<td>30</td>
<td>45</td>
<td>KB</td>
<td>KB</td>
<td>-60</td>
<td>-30</td>
</tr>
</tbody>
</table>

KB –30 denotes a kneading block with a staggering angle of –30°. Each kneading element is 7.5 mm thick.

The effects of operating conditions and screw geometry on the extruder response will be studied (see Table 1). Changes in screw speed, output and barrel temperature
will be followed in case studies 1 to 3, respectively. Case study 4 will illustrate the role of the screw configuration (see Figure 5 for the corresponding screw profiles).

Table 2: Case studies.
4.2 Influence of operating conditions

Figures 6 to 8 display the influence of screw speed, output and barrel temperature on the pressure and melt temperature profiles along screw and die, respectively. As screw speed increases (at constant throughput) the average degree of fill decreases and heat conduction becomes less efficient (Figure 6). Thus melting is delayed and so is temperature development. The peak pressure increases with increasing screw speed, since the flow is determined by the balance between drag and pressure flows, and thus, the pressure gradient is directly proportional to the velocity. When the output is increased (Figure 7) melting speed is delayed because the presence of a higher quantity of material, which difficult the heat conduction from the barrel. The pressure peak increases in this case due to the fact that higher outputs increase the degree of fill. The melt temperature subsists practically unaltered since there are not effects of the viscous dissipation due to the fact that the increase in pressure is very small. As would be anticipated, an increase in barrel temperature (Figure 8) favours heat transfer, hence viscosity decreases and so does pressure.

4.2 Influence of screw configuration

As shown in Figure 9, the model proposed here is sensitive to the location and geometrical features of the restrictive elements (left handed and kneading blocks), which dictate the location, amplitude and breath of the pressure peaks. Comparisons were performed for constant operating conditions. Hence the peak on the right, corresponding to die flow, remains unaltered.
Figure 6: Pressure and melt temperature profiles for different screw speeds.

Figure 7: Pressure and melt temperature profiles for different outputs.
Figure 8: Pressure and melt temperature profiles for different barrel temperatures.

Figure 9: Pressure and melt temperature profiles for different screw configurations.

5 Conclusions
A computer program able to take into account the main phenomena from hopper to die and process parameters of co-rotating twin screw extrusion was developed. In general, the predictions are in accordance with theoretical and experimental evidence, although direct confrontation with experiments should be carried out in the next stage of the work.

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References


