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COMPUTATIONAL ANALYSIS AND DESIGN OF SINGLE SCREW EXTRUDERS HAVING SCREWS OF COMPLEX GEOMETRY WITH MIXING ELEMENTS

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Abstract

The methodology is based on some conventional models for flow in the hopper, solids bed and melting zone. In the melt pumping zone the Hele – Shaw approximation is applied, which describes spreading flow in two dimensions. The momentum and energy equations are solved layer – by – layer starting from the barrel wall. This methodology enables significant reduction of computer time required for simulation of extruders with complex screw geometry, over the fully 3D approach. Good agreement was obtained with some available experimental data and further evaluations of predictive capabilities are currently underway.

Introduction

Mathematical modeling of single screw extruders has received considerable attention in the literature, starting with the DuPont team of Carley et al [1] in USA and Maillefer [2] in Europe. Numerous references can be found in the textbooks by Tadmor and Gogos [3], Chung [4] and Rauwendaal [5]. There are still several challenges relating to solids transport, melting and melt flow in complicated geometries involving various designs of barrier screws and mixing elements. For design purposes a computational model must be able to predict flow of the pellets or powders from the hopper to the solids conveying zone, the rate of melting, the solids bed profile, pressure and temperature development, torque, power and other quantities such as velocities, strain rates, stresses and residence time.

In the present integrated model, the methodology described by one of the authors [6] in a previous publication is followed for the solids conveying and melting zone. In the melt pumping zone the Hele – Shaw flow approximation is applied layer – by – layer, similar to the methodologies in injection molding cavity filling, known as 2.5D flow analysis. The screw geometry description is fully 3D allowing any configuration to be easily inputted and subsequently modified for “what if” design purposes.

Mathematical Model

The integrated model involves five interdependent sections as shown in Figure 1: the feed hopper, the solids – conveying, the melting, melt – conveying zones and the die.

For the feed hopper and solids conveying zone, there has been a recent innovative approach based on the Discrete Element Method by Moysey and Thompson [7], but the present authors decided to use the more traditional approach described by Agur and Vlachopoulos [6]. The pressure at the base is determined by using Walker’s model [8] assuming both a straight and convergent section.

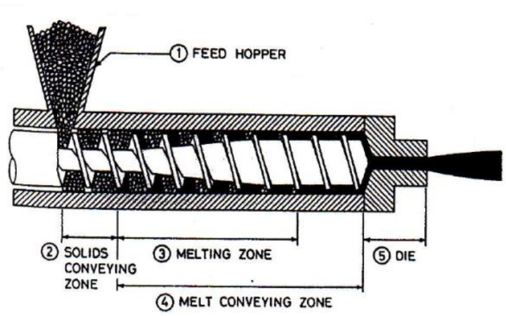

Figure 1. Schematic diagram of a plasticating extruder showing the components of the present computer model.

In the solids conveying zone the pressure build – up is determined on the basis of the Darnell and Mol [9] model and is described as

$$P = P_o \cdot e^{-\lambda z_b} \tag{1}$$

where z_b is the down – channel distance on the barell wall and λ is a function of the friction coefficients between solid polymer particles and barrel and screw surfaces and the screw geometry.

In the melting zone, Tadmor’s model [10] for the rate of melting and a heat balance at the interface of solid and molten polymer film is used, to determine the solid bed profile. Of course, there are more recent developments in modeling of this region, notably the work of Alimkaynak et al [11]. These will be taken into consideration in future modifications of the present integrated model for the whole extruder.

In the melt – conveying zone the following equations of conservation of mass, momentum and energy represent a reasonable approximation of melt flow (x is the circumferential direction, y the thickness direction and z the screw axis direction):

Mass:

$$\frac{\partial \upsilon_x}{\partial x} + \frac{\partial \upsilon_z}{\partial z} = 0 \tag{2}$$

Momentum:

$$-\frac{\partial p}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} = 0 \tag{3}$$

$$-\frac{\partial p}{\partial z} + \frac{\partial \tau_{yz}}{\partial y} = 0 \tag{4}$$

Energy:

$$\rho_m C_{p_m}\left(\upsilon_x \frac{\partial T}{\partial x} + \upsilon_z \frac{\partial T}{\partial z}\right) = k_m \frac{\partial^2 T}{\partial y^2} + \tau_{yx}\frac{\partial \upsilon_x}{\partial y} + \tau_{yz}\frac{\partial \upsilon_z}{\partial y} \tag{5}$$

where p is the pressure, υ_x and υ_z the velocity components, T is the temperature, τ_{yx} and τ_{yz} the stress components, ρ_m the density, C_{Pm} the heat capacity of the melt and k_m the thermal conductivity of the melt.

Boundary Conditions:

$$p = p_o, T = T_o \;\; on \;\; z = 0(inlet) \tag{6}$$

$$q = q_o, \frac{\partial T}{\partial n} = 0 \;\; on \;\; z = L(outlet) \tag{7}$$

$$\upsilon_x = \upsilon_z = 0, \frac{\partial T}{\partial n} = 0 \;\; on \;\; y = 0(screw \;\; surface) \tag{8}$$

$$\upsilon_x = V_{barrel}, \upsilon_z = 0, T = T_{barrel} \;\; on \;\; y = H(barrel \;\; surface) \tag{9}$$

The two components of the momentum equation represent the Hele – Shaw flow approximation and are expressed in the form

$$q_x = \int_0^H \upsilon_x dy = -S\frac{\partial p}{\partial x} + \Psi \tag{10}$$

$$q_z = \int_0^H \upsilon_z dy = -S\frac{\partial p}{\partial z} \tag{11}$$

where

$$S = \gamma - \frac{\beta^2}{a}$$
$$\Psi = \left(H - \frac{\beta}{\alpha}\right)V_{barrel}$$
$$a = \int_0^H \frac{1}{\eta}dz, \beta = \int_0^H \frac{z}{\eta}dz \tag{12}$$
$$\gamma = \int_0^H \frac{z^2}{\eta}dz$$

where η is the viscosity expressed by a purely viscous shear thinning model (Carreau).

The above equations are solved layer – by – layer using the finite element method, simultaneously with the energy equation, starting from the barrel wall to the screw root. This solution methodology is similar to that applied in injection molding cavity filling and it is referred to as 2.5D flow analysis.

The decision to apply the above simplification, rather than fully 3D flow analysis, was made for the purpose of

Table 1. Measured and simulated mass flow rates and peak pressures (D=38 mm, L/D=24).

HDPE		**40 rpm**	**60 rpm**	**80 rpm**
Measured	Flow rate	6.32 kg/h	9.75 kg/h	13.34 kg/h
	Pressure	21.10 MPa	25.60 MPa	29.75 MPa
Present Simulation	Flow rate	6.97 kg/h	10.11 kg/h	13.67 kg/h
	Pressure	19.90 MPa	23.57 MPa	27.21 MPa
LDPE		**40 rpm**	**60 rpm**	**80 rpm**
Measured	Flow rate	6.88 kg/h	10.61 kg/h	14.28 kg/h
	Pressure	13.75 Mpa	16.75 MPa	18.75 MPa
Present Simulation	Flow rate	7.14 kg/h	10.79 kg/h	14.40 kg/h
	Pressure	13.37 MPa	16.08 MPa	18.21 MPa

reducing computer time. Practical experience has shown that even minor modifications of the shape or size of the barrier flight or mixing element geometry may have enormous influence on the extrusion process. The present calculation procedure requires less than a minute to be completed in most personal computers. "What if" scenarios can easily be tried for design purposes.

After the end of the melt – conveying zone the pressure drop for flow through the screens, adaptor and die is assumed to be equivalent to the flow through a single tubular die. The length and the diameter can be chosen such as to produce a desired level of pressure drop.

Results and Comparisons to Experiments

The first test of the present integrated model was against the experimental data of Agur and Vlachopoulos [6]. The predicted and simulated mass flow rates and peak pressures, shown in Table 1, are in excellent agreement. The extruder had a standard single – flighted screw without any mixing sections. Consequently, this test can be considered as not very demanding.

A more severe testing procedure is currently underway using the experimental data of Castillo et al [12]. The screws were of 88.9 mm in diameter, with barrier flights running parallel to the main flight and mixing elements. The screw dimensions and screw configurations are given by Castillo et al [12]. Figure 2 shows a relatively good agreement between measured and predicted pressure along the axis, for LDPE at 32.3 rpm and 98 kg/h. The predicted temperature distribution and solid bed profile are shown in Figure 3. At a higher screw speed, 93.3 rpm and 253 kg/h, shown in Figure 4, the agreement between experiment and simulation, is not as good. These differences are currently being examined and may lead to some modifications of the model used.

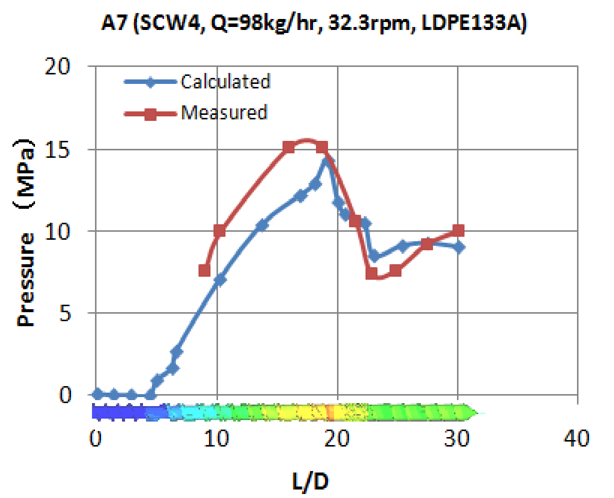

Figure 2. Pressure along axis. Measured data from ref. [12].

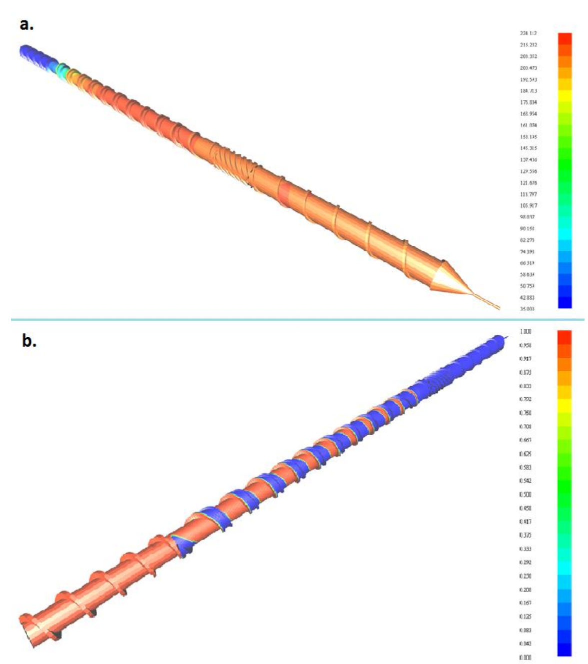

Figure 3. a) Temperature distribution, b) Solid bed distribution.

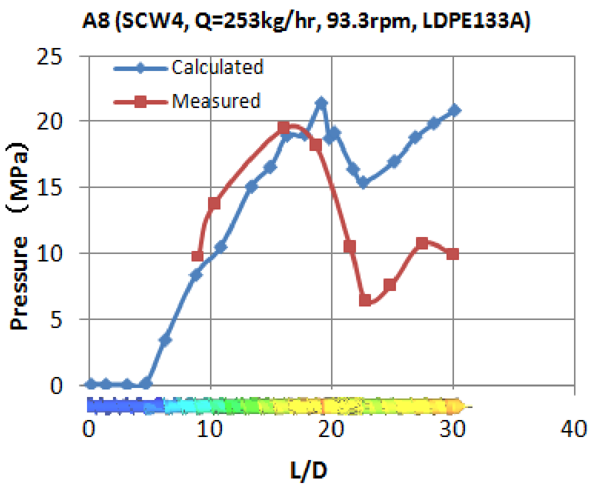

Figure 4. Pressure along axis. Measured data from ref. [12].

Concluding Remarks

The present integrated model gives some very encouraging results when compared to experimental data for both single – flighted screws and barrier screws having mixing elements. The Hele – Shaw flow approximation in the melt pumping zone enables complete simulation to be carried out in very short computer times and it can easily be used for "what if" scenarios associated with screw design. Of course, the usefulness of this methodology depends on its ability to make predictions in good agreement with experimental data. For this reason, further testing is currently underway and will be reported during the conference.

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