Developments in the analysis of steady screw extrusion of polymers

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A review is undertaken of theoretical and experimental work which has advanced the understanding of the single screw extrusion process for polymers. Detailed consideration is given to the many published theoretical models of solids conveying, melting and melt flow in the channel of a plasticating extruder. Development of such models is traced in terms of the gradual relaxation of simplifying assumptions to provide methods of analysis which give realistic predictions of machine performance. Comparisons between the results of such analyses and observed machine behaviour are also discussed.

INTRODUCTION

Nearly all polymeric materials are processed at least once by a single screw extruder, if not to form the final product then during earlier homogenizing or compounding operations. Many injection moulding machines also rely on the screw principle for melting and mixing prior to injection. Increasing demands for higher output of better quality extrudate from a machine of a given size or cost have stimulated many theoretical and experimental analyses of extruder performance. The objectives of much of this research have been to advance the understanding of the extrusion process with a view to improving both the performance of existing machines and the design of new ones.

The purpose of this review is to trace the main developments in screw extrusion research and to compare and contrast the methods employed and results obtained. The list of references cited is by no means exhaustive, but contains many of the books and papers which in the author's view have made significant contributions to the subject, or which themselves contain more detailed surveys of particular topics. The preponderance of theoretical contributions reflects the scarcity of well-documented experimental data. While it is a comparatively simple matter to measure overall performance parameters such as output rate, power consumption and possibly the screw delivery pressure, reliable figures for polymer temperatures, pressures and velocities within an extruder are much more difficult and costly to obtain.

Attention is concentrated on the performance of single screw extruders. Neither machine control nor mechanical design are discussed in detail. For the most part attention is also confined to conventional screw designs having simple feed, compression and metering sections. Vented two-stage screws are not considered, although these can be regarded as two single stage screws in series.

MATHEMATICAL MODELS OF EXTRUSION

Most mathematical treatments of the screw extrusion process recognize three distinct regions where the polymer is either conveyed in the solid state, melted under the action of conducted heat and shear, or the resulting melt is mixed and pumped. *Figure 1* shows a cross-section of a typical machine. The three sections of the screw, namely the constant channel depth feed section, tapering compression or transition section, and the constant depth metering section, are normally associated with these three functions although there is often considerable overlap. For example, melting often starts in the feed section of the screw and continues into the metering section. Early attempts to analyse extruder performance were concentrated on melt flow towards the delivery end of the machine. It is therefore convenient to review melt flow analyses before considering solids conveying and melting, particularly as melting models involve such analyses. In some processes, such as homogenization immediately after polymerization, extruders may be supplied with melt rather than solid granules or powder, and a melt flow analysis alone is sufficient.

Models of the extrusion process are usually based on the principles of continuum mechanics which ignore the molecular nature of the materials concerned. Except in relatively trivial cases the resulting mathematical equations can only be solved numerically, normally with the aid of a digital computer. As increasingly sophisticated models are evolved the cost of obtaining solutions rises and may become excessive, and compromises must be sought between cost and accuracy.

Not all mathematical treatments of extrusion have been based on continuum mechanics. For example, Marshall *et al.*[1–3] used a regression analysis to fit a system of empirical equations to experimental data obtained from a highly instrumented extruder. These equations were then used to describe the performance of other machines of a similar

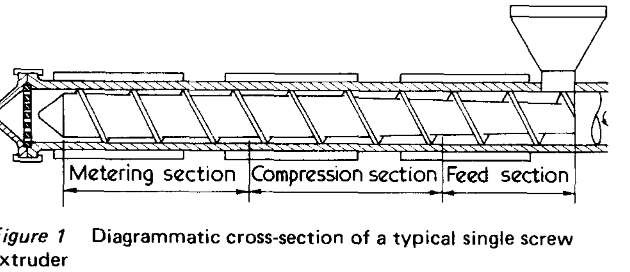

Figure 1 Diagrammatic cross-section of a typical single screw extruder

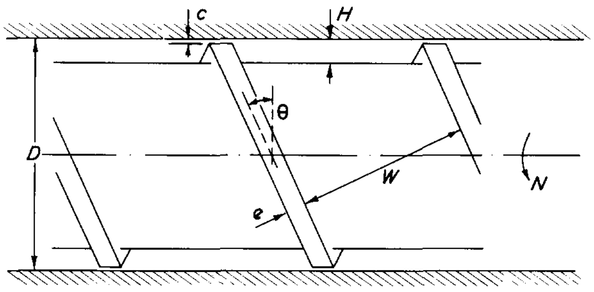

Figure 2 Geometry of an extruder screw

size. Such an approach relies on appropriate experimental data being available and the range of applicability, particularly in terms of machine size, is likely to be very limited. Also, it adds very little to the fundamental understanding of the extrusion process.

ANALYSIS OF MELT FLOW IN EXTRUDERS

Before attempting to review published solutions for melt flow it is convenient to outline the mathematical derivations which are common to most contributions. The principal assumptions involved are numbered consecutively as they occur in the analysis.

Extruder geometry

Figure 2 shows an enlarged view of part of the screw and barrel shown in *Figure 1,* and serves to define the geometry. D is the internal barrel diameter, H the screw channel depth, W and e the channel and flight widths, respectively (measured along a cylindrical surface, often that generated by the flight tip), c the radial clearance between flight and barrel, and θ is the helix angle (again measured at the flight tip). Although the screw shown has only one flight, multistart screws can also be accommodated[4,5]. The screw rotates as shown at N revolutions per unit time, and the geometric assumptions are as follows.

(A) The sides of the flight are radial to the screw axis.
(B) The depth of the screw channel is constant across its width.
(C) Chamfers or fillets on the flight may be neglected.

A coordinate system fixed relative to the screw is selected as being simple to use. A further simplification is to treat the barrel as rotating about a stationary screw, which is a valid procedure for the following reasons.

(D) Body forces such as those due to gravity are negligible in comparison with viscous and pressure forces.
(E) Centrifugal inertia forces are likewise negligible.

The most natural coordinate system to use is a helical one. Zamodits[6] set up the relevant equations in helical coordinates and obtained some solutions for non-Newtonian melts. Nebrensky *et al.*[7] used a variational analysis and helical coordinates with a view to eventual solution by a finite element method. Griffith[8] derived corrections for Newtonian fluid flows in slightly curved channels and Booy[9] used cylindrical polar coordinates. A geometric simplification sometimes employed is to use cylindrical polar coordinates and to assume axial symmetry (that is, zero helix angle but with the correct barrel velocity components relative to the screw). This method has been used by Tadmor[10] and Dyer[11] to approximate channel curvature effects.

In the melt flow regions of most single screw extruders the screw channel is relatively shallow, that is:

$$H \ll D \tag{1}$$

and it is often reasonable to assume that:

(F) the channel may be unrolled and treated as rectilinear and Cartesian coordinates used.

Figure 3 shows the screw of *Figure 2* unrolled onto a plane. Although this plane is often taken as the one generated by the flight tip, Martin[12] has suggested that the plane at the mean channel depth would be more appropriate. The numerical values of the helix angle and channel and flight widths are affected by the choice of plane for unrolling, and may be obtained from the geometry of *Figure 3*[4,5]. For an axial length, L, of screw the length along the helical channel is:

$$Z = L/\sin\theta \tag{2}$$

The Cartesian coordinate axes x, y, z, may be chosen as shown in *Figures 3* and *4,* the latter being a view along the screw channel in the downstream direction parallel to the flight. *Figure 3* also shows a portion of the barrel surface moving with velocity V relative to the screw, which may be resolved into components V_z and V_x in the downstream and transverse (normal to the flight) directions:

$$V = \pi DN,\ V_z = V\cos\theta,\ V_x = V\sin\theta \tag{3}$$

Conservation equations

The continuum mechanics equations governing melt flow are those of conservation of mass, momentum and energy. These can be concisely expressed in tensor notation[5,13]. The viscous stress and rate of deformation tensors may be represented by τ_{ij} and e_{ij}, where:

$$e_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) \tag{4}$$

v_i being the local velocity component in the x_i coordinate direction. Assuming that:

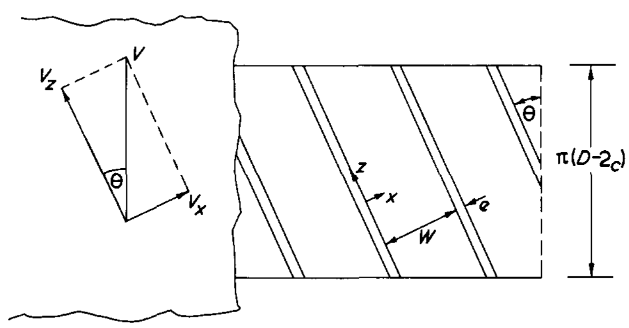

Figure 3 Screw and barrel unrolled onto a plane

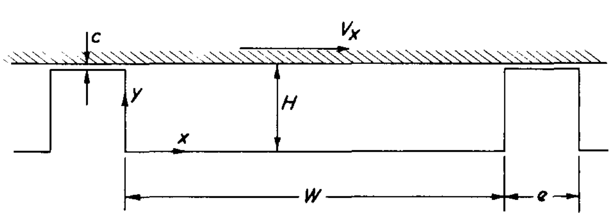

Figure 4 View down screw channel in the positive z direction

(G) the density of the melt is locally constant,
the continuity equation for conservation of mass reduces to:

$$e_{ii} = 0 \tag{5}$$

While melt densities depend on both temperature and pressure, local variations are negligible. Overall variations in density along the screw channel can be accommodated[5].

The conservation of momentum involves a balance between inertia, viscous, pressure and body forces, the last of which have already been eliminated by assumption (D). Because the Reynolds numbers associated with melt flows are extremely small[13,14] it may be assumed that such flows are laminar and that:

(H) inertia effects are negligible in comparison with viscous and pressure forces.

The equations for conservation of momentum therefore reduce to:

$$\frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} \tag{6}$$

where p is the local hydrostatic pressure.

Turning to the conservation of energy, the following assumptions are usually made.

(I) The flow is steady.

(J) Thermal conductivity, k, is locally constant.

(K) The specific heat at constant pressure, C_p, is locally constant.

The resulting energy equation is:

$$\rho C_p v_i \frac{\partial T}{\partial x_i} = k \frac{\partial^2 T}{\partial x_i^2} + \tau_{ij} e_{ij} \tag{7}$$

where T is temperature and ρ is density. Of the three assumptions only the first is likely to cause significant errors: unsteady flow is discussed under the heading of surging.

Constitutive equation

The relationships between stresses and rates of deformation depend on the nature of the melt. Because melts are subjected to large rates of deformation for relatively long times while flowing in extruder channels it is reasonable to assume that:

(L) melts may be treated as inelastic viscous fluids[13].

Even with this simplification the most general constitutive equation for a non-Newtonian material is impractical to use[5,13]. For the purposes of treating screw channel flow, however, it is reasonable to assume that:

(M) an empirical power-law constitutive equation may be employed.

One way of expressing such an equation is:

$$\tau_{ij} = 2\mu e_{ij} \tag{8}$$

where the shear viscosity, μ, is given by[5]:

$$\mu = \mu_0 \left(\frac{(4I_2)^{1/2}}{\gamma_0} \right)^{n-1} \exp[-b(T - T_0)] \tag{9}$$

The constant μ_0 is the effective viscosity at some convenient reference shear rate, γ_0, and temperature, T_0, and I_2 is the second invariant of the rate of deformation tensor:

$$I_2 = \tfrac{1}{2} e_{ij} e_{ij} \tag{10}$$

The value of μ_0 for a particular material, together with the values of the power-law index, n, and temperature coefficient of viscosity, b, are obtained by fitting equation (9) to data covering suitable ranges of deformation rate and temperature. The value of n is generally in the range 0.3–0.6, shear stress being proportional to the nth power of the shear rate in simple shear, and b is of the order of 10^{-2} °C^{-1}. An advantage of equation (9) is that it allows viscous properties to be expressed in terms of only three parameters. In using this form of constitutive equation it is assumed that:

(N) viscosity is independent of pressure,

a necessary assumption in view of the shortage of relevant data.

Boundary conditions

In order to solve the conservation equations the appropriate boundary conditions must be specified. For the velocity components (u, v, w in the coordinate directions x, y, z shown in *Figures 3* and *4*) these are:

$$\begin{aligned} &u = v = w = 0 \text{ on } x = 0, x = W, y = 0 \\ &u = V_x,\ v = 0,\ w = V_z \text{ on } y = H \end{aligned} \tag{11}$$

assuming no flow into the channel boundaries and that:

(O) there is no slip at the boundaries.

Kennaway[15] reported maximum bond shear stressed at interfaces between melts and metals, above which slip occurred. Except in the case of an unplasticized poly(vinyl chloride) these stresses were above the normal range for extruder channel flow. Slip may occur, however, in regions of high shear stress such as in the clearance between the screw flight and barrel. At least for the purposes of solving the channel flow equations it is reasonable to assume that:

(P) there is negligible leakage of melt over the flight tip.

and within the channel:

$$\int_0^H u \times \mathrm{d}y = 0 \tag{12}$$

Thermal boundary conditions may involve both temperatures and first derivatives of temperature with respect to the coordinate normal to the boundary. At the barrel surface it is reasonable to assume that:

(Q) there is a good thermal contact between the melt and metal surfaces,

$$T = T_b(z) \text{ on } y = H \tag{13}$$

where T_b is the temperature of the inner surface of the barrel. Similarly, at the screw surface:

$$T = T_s(z) \text{ on } y = 0, x = 0, x = W \tag{14}$$

where T_s is the screw temperature, which in most cases is not known. Alternative conditions sometimes used are:

$$\frac{\partial T}{\partial y} = 0 \text{ on } y = 0, \qquad \frac{\partial T}{\partial x} = 0 \text{ on } x = 0, x = W \tag{15}$$

which assume that a negligible amount of heat is conducted between the melt and uncooled screw. Martin[16] in a detailed study of heat transfer between melt flow and a metal boundary confirmed that the screw surface behaves as though almost thermally insulated. The best choice of screw temperature boundary condition is, however, intimately linked with the choice of mathematical model for melt flow and is discussed in connection with particular solutions. In practice, extruder screws are sometimes cooled, thereby affecting the thermal boundary condition. Heat transfer rates due to screw cooling have been studied by Fenner[5]. Since the convection terms in equation (7) allow for development of temperatures in the directions of flow, it is necessary in general to specify some initial temperature profile at the beginning of the region where melt flow is to be analysed.

Lubrication approximation

Further simplifications to the channel flow equations are usually introduced with the aid of the lubrication approximation. In essence, this involves the local replacement of the actual flow in the parallel or nearly parallel gap between smooth surfaces by uniform flow between plane parallel surfaces[13,17,18]. As the screw channel depth is either constant or varies slowly in the downstream direction, it is reasonable to apply the lubrication approximation in the z direction to velocities and assume that:

(R) velocities are fully developed in the downstream direction,

$$u = u(x,y),\ v = v(x,y),\ w = w(x,y) \tag{16}$$

Continuity equation (5) becomes:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{17}$$

and equilibrium equations (6) become:

$$\frac{\partial p}{\partial x} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} \tag{18}$$

$$\frac{\partial p}{\partial y} = \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \tag{19}$$

$$\frac{\partial p}{\partial z} = P_z = \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} \tag{20}$$

where the pressure gradient P_z is independent of x and y.

Owing to the presence of significant convection terms in equation (7) it is much less reasonable to apply the lubrication approximation in the z direction to temperatures. Pearson[13] showed that this procedure is only marginally justified in small extruders (and is much less so in large machines[14,19]), a view which was reinforced by Yates[20]. If, however, it is assumed that:

(S) temperatures are fully developed in the downstream direction,

then $T = T(x,y)$ and the energy equation reduces to:

$$\rho C_p \left(u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} \right) = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \tau_{xx}\frac{\partial u}{\partial x} + \tau_{yy}\frac{\partial v}{\partial y} +$$

$$\tau_{xy}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \tau_{yz}\frac{\partial w}{\partial y} + \tau_{zx}\frac{\partial w}{\partial x} \tag{21}$$

The next stage of simplification frequently employed is to apply the lubrication approximation in the x direction. Assumption (B) ensures that the channel depth is constant in this direction, except at the flight. Therefore, for the approximation to be valid it must be assumed that:

(T) the influence of the flight is negligible, and the flow may be treated as though the channel were infinitely wide. Symbolically:

$$H \ll W \tag{22}$$

and equations (16), and (18) to (21) reduce to:

$$u = u(y),\ v = 0,\ w = w(y) \tag{23}$$

$$\frac{\partial p}{\partial x} = P_x = \frac{\mathrm{d}\tau_{xy}}{\mathrm{d}y} \tag{24}$$

$$\frac{\partial p}{\partial y} = 0 \tag{25}$$

$$P_z = \frac{\mathrm{d}\tau_{zy}}{\mathrm{d}y} \tag{26}$$

$$k\frac{\mathrm{d}^2 T}{\mathrm{d}y^2} = -\tau_{xy}\frac{\mathrm{d}u}{\mathrm{d}y} - \tau_{yz}\frac{\mathrm{d}w}{\mathrm{d}y} \tag{27}$$

where the pressure gradient P_x is independent of x and y. Equation (17) is automatically satisfied although continuity must still be satisfied in terms of overall channel flow rate. From equations (8) and (10):

$$\tau_{xy} = \mu\frac{\mathrm{d}u}{\mathrm{d}y},\ \tau_{yz} = \mu\frac{\mathrm{d}w}{\mathrm{d}y} \tag{28}$$

$$I_2 = \frac{1}{4}\left[\left(\frac{\mathrm{d}w}{\mathrm{d}y}\right)^2 + \left(\frac{\mathrm{d}u}{\mathrm{d}y}\right)^2 \right] \tag{29}$$

The flow is now two-dimensional in the sense that there are only two non-zero velocity components, u and w, which are functions of the third coordinate y.

Another very useful combination of assumptions, first employed by Yates[20], is provided by taking velocity profiles to be locally fully developed in both the downstream and transverse directions and retaining thermal convection in the downstream direction only. The energy equation becomes:

$$\rho C_p w\frac{\partial T}{\partial z} = k\frac{\partial^2 T}{\partial y^2} + 4\mu I_2 \tag{30}$$

where I_2 is given by equation (29).

One-dimensional, isothermal and Newtonian flow assumptions

Further simplification of equations (24) to (29) involves the assumption that:

(U) the contribution of the transverse flow to viscosity determination and viscous heating is negligible.

Equation (24) is no longer required and equations (27) and (29) reduce to:

$$k\frac{d^2T}{dy^2} = -\tau_{yz}\frac{dw}{dy} \tag{31}$$

$$I_2 = \frac{1}{4}\left(\frac{dw}{dy}\right)^2 \tag{32}$$

and the flow is now one-dimensional.

A simplification which is applicable to either one-dimensional, two-dimensional or more sophisticated models is often somewhat misleadingly called the isothermal assumption. It implies that:

(V) velocity profiles are independent of temperature profiles,

a situation which is obtained when variations of the product $b(T - T_0)$ in the viscosity equation (9) are negligible.

A final assumption which is sometimes introduced is that of Newtonian melt flow behaviour, that is:

(W) the viscosity is constant.

A reasonable value for this viscosity is that at some suitable temperature and shear rate, such as the barrel temperature and the mean downstream shear rate V_z/H.

Dimensionless parameters for melt flow

It is often convenient to express the results of a screw channel melt flow analysis in terms of dimensionless parameters. Two of the most important performance characteristics are flow rate and downstream pressure gradient, which may be expressed in dimensionless form as:

$$\pi_Q = \frac{Q}{WHV_z} \tag{33}$$

$$\pi_P = \frac{P_z H}{\bar{\tau}} \tag{34}$$

Q is the volumetric flow rate along the channel:

$$Q = \int_0^W \int_0^H w \times dy \times dx \tag{35}$$

which, provided the flow is steady and incompressible, must be independent of z in order to conserve mass. The mean shear stress, $\bar{\tau}$, is evaluated at some mean shear rate and temperature (for example, the mean downstream shear rate, V_z/H, and the barrel temperature). Other slightly different definitions of these dimensionless parameters have been used. For example, there is a good case for using V in place of V_z[13].

Two further important parameters arise when the energy equation, for example equation (30), is expressed in dimensionless form:

$$Pe w^* \frac{\partial T^*}{\partial z^*} = \frac{\partial^2 T^*}{\partial y^{*2}} + 4GI_2^* \tag{36}$$

where:

$$w^* = w/V_z,\ T^* = b(T - T_0),\ z^* = z/H$$
$$y^* = y/H,\ I_2^* = I_2(H/V_z)^2 \tag{37}$$

Pe is a Peclet number:

$$Pe = \rho C_p H V_z/k \tag{38}$$

and expresses the ratio between convective and conductive heat transfer. The parameter G has been given the name Griffith number[21] after R. M. Griffith who was the first to use it in the present context. It has also been called a Brinkman number[5,13], and is defined as:

$$G = b\bar{\mu}V_z^2/k \tag{39}$$

$\bar{\mu}$ being the mean viscosity defined at the same conditions as $\bar{\tau}$. The value of G expresses the importance of heat generation in terms of its effect on melt viscosity and hence on local velocity profiles. In most extruders Pe is of the order of 10^3–10^5 and G is 10 or more[14]. These figures serve to emphasize the importance of thermal convection and show why the isothermal assumption (V) is usually unsafisfactory. Pearson[22] has provided a more detailed analysis of heat transfer in polymer melt flow.

Newtonian solutions

Most of the early attempts to analyse melt flow in screw extruders assumed Newtonian melt flow behaviour (assumption W) and isothermal flow (assumption V). Consequently, downstream and transverse channel flows are independent, as are the effects of drag flows due to the relative motion of the channel boundaries and pressure flows due to the pressure gradients generated. Equation (20) is the governing one for downstream flow, and for a Newtonian melt becomes:

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = \frac{P_z}{\mu} \tag{40}$$

with boundary conditions (11). Transverse flow can be treated as either two-dimensional governed by equations (17) to (19), or one-dimensional governed by equations (12) and (24), again with boundary conditions (11). Series solutions to equation (40) may be obtained, which when integrated to give flow rate according to equation (35) can be expressed in the following dimensionless form[4,5]:

$$\pi_Q = \frac{F_D}{2} - \frac{\pi_P F_P}{12} \tag{41}$$

The drag and pressure flow shape factors, F_D and F_P, involve convergent infinite series and are functions of the channel shape parameter H/W. For $H \ll W$ both factors tend to unity and for typical screw channels are within a few per cent of this figure.

The first isothermal analysis of screw viscosity pumps handling Newtonian fluids was published anonymously[23] in a paper which is often attributed to Rowell and Finlayson who later extended the work[24]. These early contributions were developed and applied to the extrusion of polymers by the team of Carley, Strub, Mallouk, McKelvey and

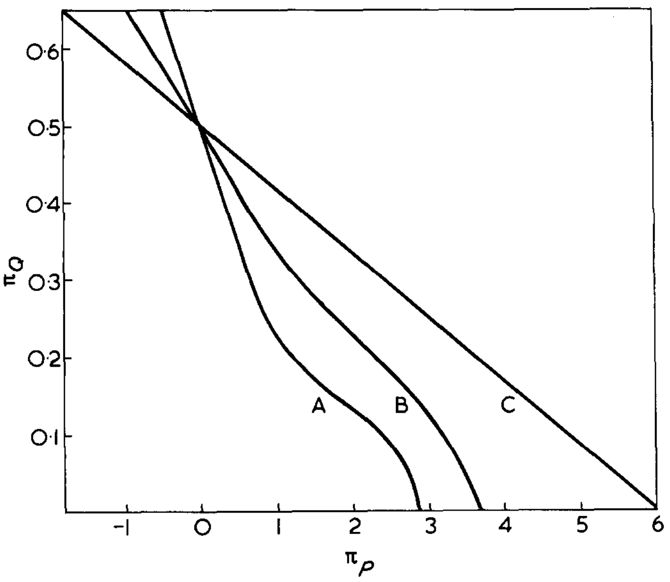

Figure 5 Dimensionless flow rate plotted against dimensionless pressure gradient for one-dimensional isothermal flow and several values of power-law index: A, n = 0.25; B, n = 0.5; C, n = 1.0

Jepson[25–31]. Numerous other papers have since appeared which use the same basic assumptions but apply various corrections and refinements. Details may be found in, for example, Bernhardt[32] and McKelvey[4]. Many further examples of Newtonian solutions may be found in the works of Schenkel[33] and Pawlowski[34]. Some attempts were made to introduce thermal effects, for example by McKelvey[35] who used a simple energy balance and assumed adiabatic running conditions.

Early experimental work supporting the theoretical analyses was generally carried out under essentially isothermal Newtonian conditions. Examples include McKelvey[28], Squires[36] who obtained confirmation of the drag flow shape factor, and Werner[37]. Velocity profiles were measured in detail by Eccher and Valentinotti[38], also by Holmes and Vermeulen[39].

Although isothermal Newtonian solutions provide in relatively simple analytical form useful qualitative descriptions of some aspects of screw extruder performance, they cannot provide accurate quantitative descriptions of practical processing operations. Both shear and temperature dependence of melt viscosity and the influence of thermal convection must be included if flow behaviour is to be predicted realistically.

Non-Newtonian isothermal solutions

The constant viscosity assumption was the first of the simplifications inherent in isothermal Newtonian solutions to be rejected. Initially solutions were obtained for isothermal one-dimensional downstream flow governed by equations (26), (28) and (9) [with b = 0 and I_2 given by equation (32)] with boundary conditions (11). Examples include Kennaway and Weeks[40], Weeks and Allen[41] and Mori and Matsumoto[42]. Jacobi[43] incorrectly assumed that drag and pressure flows could be treated separately and superimposed. Rotem and Shinnar[44] obtained solutions for more general forms of constitutive equation.

Published solutions for one-dimensional power-law flow result in a pair of simultaneous non-linear algebraic equations from which the relationship between flow rate and downstream pressure gradient is obtained. These equations cannot in general be solved analytically and the results of even this simplest form of non-Newtonian solution must be obtained numerically. *Figure 5* shows the resulting dimensionless flow rate *versus* pressure gradient extrusion characteristics for several values of power-law index. The straight line shown for n = 1 represents equation (41) (with $F_D = F_P = 1$ for one-dimensional flow). All the curves pass through π_Q = ½ under pure drag flow conditions. In the presence of significant pressure gradients it is clear that the use of a Newtonian analysis seriously over-estimates the magnitudes of such gradients.

In the case of non-Newtonian flow, the inclusion of transverse flow to make the solutions two-dimensional increases considerably the complexity of the analysis. Equations (24) and (26) must now be solved simultaneously with the aid of equations (28), (29) and (9) (again with b = 0), subject to boundary conditions (11) and (12). Such solutions were obtained by Griffith[8] and Zamodits[6,45] as parts of more general studies of two-dimensional melt flow. Results may be expressed in the form of *Figure 5*, the effect of the inclusion of transverse flow being to displace the characteristics by relatively small amounts[5]. The curves no longer pass through a common point for drag flow, and have screw helix angle as an additional independent variable.

Still retaining the isothermal assumption, the effect of the screw flight in forming a channel of finite width can be examined. For downstream flow alone equation (20) can be solved for power-law material behaviour. This has been done by Middleman[46] and Fenner[5] using finite difference techniques, and Palit and Fenner[47] using a finite element technique. One of the advantages of the latter method lies in its geometric flexibility which, for example, makes it very suitable for analysing channel flows in which assumption (C) concerning fillets at the flight root is no longer valid. The effect of finite channel width on the extrusion characteristics is relatively small for typical channel proportions in the metering sections of extruder screws. The recirculating transverse flow in a finite channel governed by equations (17) to (19) has also been analysed under isothermal conditions by finite difference[48] and finite element[49] methods, both independently of and coupled with the downstream flow[50].

Fully developed non-Newtonian flow solutions

Initial attempts to allow for the effects of temperature variations on velocity profiles treated temperature profiles as being fully developed in both the downstream and transverse directions. Colwell and Nickolls[51] obtained solutions for fully developed one-dimensional downstream flow, that is, to equations (26) and (31) for velocity and temperature, respectively, with constitutive equation (9) and boundary conditions defined in equations (11), (13) and (14).

Solutions for fully developed two-dimensional flow, that is, to equations (24) to (29) and (9) subject to boundary conditions (11) to (14), were first obtained by Griffith[8]. Further results, including some for temperature boundary condition (15) at the screw root were presented by Zamodits[6,45]. It is interesting to note that Griffith assumed the screw surface temperature to be equal to the barrel surface temperature on the grounds that the very large Peclet number associated with melt flow in a screw channel implies that temperature is constant along a streamline. If there is no leakage over the flight tip (assumption P) the screw and barrel boundaries form a single continuous streamline. A number of other workers[6,20], including the present writer[5], initially failed to appreciate the significance of this assumption and continued to use mainly the insulated screw condition (15). More recent work by Martin *et al.*[21] and Pearson[22] showed that Griffith's assumption provides a realistic and useful way of allowing for the thermal convection associated with recirculating transverse flow in two-dimensional solutions which effectively exclude such recirculation. For given thermal boundary conditions, the inclusion of non-isothermal flow effects in fully developed flow solutions introduces the Griffith number as a further independent variable for the extrusion characteristics, such as those shown in *Figure 5*. Detailed comparisons of one and two-dimensional solutions, both isothermal and non-isothermal, were made by Fenner[5].

The most complete form of solution for flow which is fully developed in the downstream direction allows for the finite width of the channel. The governing equations are (17) to (21) and (8) to (10) subject to boundary conditions (11), (13) and (14) or (15). The usual approach is to seek numerical solutions to a set of four simultaneous coupled second order non-linear partial differential equations, two governing transverse flow (derived from equations 17 to 19), and the other two governing downstream flow and heat transfer. This problem has been studied extensively by Martin[52] using finite difference techniques. Dyer[11] attempted essentially the same problem and presented a limited number of results, but his computer program contained a number of faults[5]. Finite element methods are also applicable to this problem[50].

Martin's work[52,21] provided a number of important results. It showed the dominant effect of thermal convection, at least in transverse flow, confirming that for the high values of Peclet number encountered in practice the isotherms tend to take up shapes which lie along streamlines. For typical screw channels having relatively small depth-to-width ratios it appears to be reasonable to apply the lubrication approximation in the transverse direction (assumption T), provided a screw temperature boundary condition is employed which accounts for thermal convection in the recirculating transverse flow as already discussed. This is fortunate in view of the high cost of obtaining even fully developed flow solutions for channels of finite width. Martin also demonstrated the potentially important effects of leakage flow over the screw flight, assuming that such flow occurs, on melt temperatures in the channel. While the no leakage condition imposed by equation (12) appears to be reasonable for the purposes of computing velocity profiles in the channel, owing the intense shear in the clearance between screw and barrel a significant amount of heat may be convected into the channel rather than be conducted into the barrel or flight tip surfaces[12].

Developing flow solutions

Few attempts have been made to include the development of temperature profiles in the downstream direction. Yates[20] worked with equations (24), (26), (28) to (30) and (9) subject to conditions (11) to (13) and (15) together with an assumed temperature profile at the beginning of melt flow, and obtained solutions for relatively small values of Griffith number. Martin[12,53] subsequently reported that the limitation on the degree of coupling between temperatures and velocities had been overcome. As already discussed, a better choice of screw temperature boundary condition is equation (14) with $T_s = T_b$. Fenner[19] used the same mathematical model to study the design of large melt extruders and demonstrated the importance of developing flow effects in such machines. Kaiser and Smith[54] presented a much less rigorous analysis which allowed for downstream thermal convection.

The usual method for solving the equations associated with the Yates model may be outlined as follows. Starting from a channel cross-section at which both velocity and temperature profiles are known, a small step downstream is made with the aid of equation (30) expressed in finite difference form to determine the temperature profile at the new cross-section, assuming the velocity profiles remain unchanged. Then, using equations (24), (26), (28), (29), (9) and the new temperature profile, the corresponding new velocity profiles are computed which satisfy not only the velocity boundary conditions but also the requirements of constant downstream and zero transverse flow rates. Although velocities are treated as being locally fully developed they do develop slowly by virtue of the developing temperature profile. The results of a developing flow analysis are difficult to present in a concise form. For example, flow characteristics of the form shown in *Figure 5* are no longer relevant. The most useful result is the computer program itself, which can be made efficient enough in terms of computing time and cost for use in routine design calculations. One of the most important features of the Yates model is its ability to make realistic predictions of temperature rise along the channel of an extruder. While detailed temperature profiles over the depth of the channel are of interest[19], they may be summarized in terms of a bulk mean temperature:

$$\bar{T} = \int_0^H wT\mathrm{d}y \Big/ \int_0^H w\mathrm{d}y \tag{42}$$

at any cross-section.

Various refinements to the Yates model have been proposed. Martin[12] suggested that the axial velocity component should be employed both in the convection term of the energy equation (30) and in the above definition of bulk mean temperature in preference to the downstream component. So far there appear to have been no attempts to solve the fully three-dimensional problem of developing flow in a channel of finite width.

Melt flow experiments

Some of the early experimental work on flow in extruders was reviewed in connection with Newtonian solutions to the flow equations. Such experiments were generally conducted on small model extruders under essentially isothermal Newtonian flow conditions. Griffith[8] and Fenner[5,55] carried out similar model experiments under mildly non-isothermal non-Newtonian and nearly fully developed conditions and demonstrated satisfactory agreement with solutions for fully developed flow.

Although model experiments using materials which are liquid at ambient temperature are of interest in the study of melt flow they are of only limited relevance to the practical extrusion of polymers. the other main class of experimental work has been concerned with measurements made on actual extruders, usually of the plasticating rather than melt-fed type. Unfortunately, most production machines lack sufficient instrumentation for temperature and pressure to permit melt flow analyses to be adequately tested. On the other hand, well-instrumented laboratory extruders for reasons of cost are often too small to exhibit marked non-isothermal flow effects. Both Peclet number and Griffith number are significantly dependent on extruder size, and a laboratory extruder of even 60 mm diameter operates under very different thermal conditions from production machines of 200 mm diameter or more. Practical difficulties are encountered in making reliable measurements of temperature, particularly of melt temperature. Owing to the low thermal conductivities of polymers compared to those of metals, measurements of melt temperatures tend to be influenced by the temperature of the metal supporting the thermocouple used. Considerable care has to be taken with the design and positioning of thermocouple probes[56,57].

On the topic of screw temperature measurements, Janeschitz-Kriegl[58] presented results which showed the temperature of the screw surface to be slightly higher than that of the barrel in the metering section of a model extruder processing an unspecified high viscosity material. Both Marshall *et al.*[1] and Palit[59] reported more detailed results obtained from 63.5 mm (2.5 inch) extruders processing materials such as low density polyethylene, polypropylene and poly(vinyl chloride) which showed screw surface temperatures rising rapidly along the feed and compression sections to steady values slightly higher than the barrel temperature along most of the metering sections. These results support the suggestion discussed earlier that the melt flow thermal boundary condition at the screw should be for the screw temperature to be equal to the barrel temperature.

Although many workers have presented experimental results obtained from instrumented extruders in support of particular solutions to the melt flow equations, these data are rarely measured or published in sufficient detail to allow adequate comparisons to be made with other solutions. Among the more detailed sets of data are those published by Weeks and Allen[41] and Marshall *et al.*[1].

The shortage of good experimental data and comparisons with existing melt flow analyses was recognized by the European Federation of Chemical Engineering's working party on Non-Newtonian Liquid Processing. Extensive data provided by Van Leeuwen[60] derived from experiments on a 45 mm diameter extruder were studied in detail by Martin[12]. Some of his more important conclusions may be summarized as follows. A developing flow solution of the Yates type generally gives good predictions of mean melt temperatures. The greatest discrepancies are probably caused by the difficulty of estimating a mean melt temperature from a limited number of thermocouple readings, and by the relatively poor accuracy with which material properties such as thermal conductivity can be measured. It proved to be more difficult to obtain satisfactory agreement between measured and predicted pressure profiles. This was mainly due to the predicted pressure gradients being very sensitive to the nature of the channel unrolling assumption (F). Helix angle, channel length and width, also the barrel relative velocity components all change with the radial position of the plane onto which the channel is unrolled. The values of dimensionless parameters such as flow rate defined in equation (33) are therefore affected and in terms of extrusion characteristics of the type shown in *Figure 5* if the operating point is close to drag flow small changes in π_Q can have large effects on both the dimensionless and dimensional pressure gradients. Indeed, Martin demonstrated at least one case where a change of plane for unrolling converted positive predicted pressure gradients into negative ones. He concluded that in order to predict melt pressures reliably more detailed account should be taken of channel curvature. At a later meeting of the working party, Smit[61] provided further experimental data from a 90 mm extruder processing high density polyethylene. While these showed satisfactory agreement with the Yates developing flow model, minor discrepanies in the pressure gradients close to drag flow were again demonstrated. The ability to accurately predict pressure gradients in melt flow is not, however, as important as was once thought by workers who analysed only the melt flow. If the metering section is operating under nearly drag flow conditions with correspondingly small pressure gradients in the melt much of the delivery pressure required at the end of the screw is provided by the feeding and melting processes.

ANALYSIS OF SOLIDS CONVEYING IN EXTRUDERS

In comparison with the large amount of published work on melt flow in screw extruders, relatively little attention has been given to the conveying of solid granules or powder from the feed hopper of a plasticating extruder to the position at which a significant amount of melting has occurred. There are several reasons for this. Solids conveying is usually a relatively minor part of the overall extrusion process and occurs only over the first few turns of the screw channel. It rarely controls directly the output from the machine, which is normally determined by the later melting and melt pumping processes. An analysis of the solids conveying process can therefore only provide estimates of the upper limit on the output capacity of the machine and the pressures that can be generated in the feed section.

A set of continuum mechanics equations can be established for solids conveying in screw channels similar to those governing melt flow. Even though such a continuum approach ignores the particulate nature of polymer feedstocks it is still difficult to obtain useful solutions. Most published analyses therefore make the further simplification of treating material movement as plug flow in the channel, ignoring the effects of stresses and deformations within the bulk of the solid.

One-dimensional plug flow solutions

Observations of velocity profiles in flows of polymer granules in a model extruder with a transparent barrel[62] serve to support the validity of the plug flow assumption, under which the downstream velocity component is independent of position in the channel cross-section. The main restriction is that the channel must be full of material, a condition which is normally satisfied very early in a plasticating extruder due to the conveying rate being limited by the later melting and metering processes.

Some of the assumptions made in melt flow analyses are also relevant to solid plug flow. Assumptions (A) to (C) concerned with screw geometry, (G) for locally constant bulk density, (H) for negligible inertia forces, (I) for steady flow and (P) for no leakage over the flight tip are normally all applied. Of the remaining assumptions which might be relevant to solid flow only (F) for unrolling the screw channel and (O) for no slip at the flow boundaries are definitely not applicable. The relatively deep channels in screw feed sections cannot be unrolled for analytical purposes without due allowance being made for channel curvature. Conditions at the boundaries of the solid plug are assumed to be determined by a Coulomb friction mechanism between the material and the screw and barrel surfaces. Assumptions (D) and (E) concerning negligible gravity and centrifugal forces are also frequently employed, and are valid once significant stresses have been generated in the solid plug.

Darnell and Mol[63] were the first to obtain useful plug flow solutions. They presented their analytical results in terms of the feed angle at which the solid plug moves relative to planes perpendicular to the screw axis. *Figure 6* shows a portion of solid plug in a screw channel, α being the feed angle measured at the barrel surface and the arrow showing the direction of motion of the plug (relative to the stationary barrel). Assuming the flight width is negligible compared to the channel width ($e \ll W$), Darnell and Mol derived the following relationship between volumetric flow rate per screw revolution and the feed angle by means of a simple kinematic argument:

$$\frac{Q}{N} = \frac{\pi^2 DH(D - H) \tan \alpha \tan \theta_b}{(\tan \alpha + \tan \theta_b)} \tag{43}$$

where θ_b is the flight helix angle at the barrel surface. Schneider[64] later applied a simple correction factor to this result to allow for the effect of finite width. The magnitude of the feed angle is determined with the aid of the equations of equilibrium for the forces acting on the plug.

It is convenient to define a pressure in the solid plug, p, as the direct compressive stress acting in the downstream direction. In one-dimensional plug flow solutions this pressure is assumed to be constant both across the width of the channel and through its depth. The compressive stresses at the screw and barrel surfaces are in general not equal to p, but may be expressed as $k_1 p$ acting on the barrel surface, $k_2 p$ on the sides of the channel and $k_3 p$ on the screw root. The equilibrium of pressure and frictional forces acting on the solid plug should be examined for the downstream, transverse and radial directions[62]. Both Darnell and Mol[63] and Schneider[64], while retaining the most significant effects of channel curvature, simplified the problem and avoided the need to consider radial equilibrium. After a considerable amount of manipulation Schneider arrived at an equation of the following form for determining the feed angle:

$$\cos \alpha = K \sin \alpha + \frac{\mu_f}{\mu_b} \times \frac{k_2}{k_1} \frac{2HE}{A} (K \tan \bar{\theta} + E) + \frac{\mu_s}{\mu_b} \times \frac{k_3}{k_1} \times C \cos \theta_s (K \tan \theta_s + C) + \frac{HE \cos \bar{\theta}}{\mu_b k_1} (K \tan \bar{\theta} + E) \frac{1}{p} \frac{\mathrm{d}p}{\mathrm{d}z} \tag{44}$$

$$\text{where } K = \frac{E(\tan \bar{\theta} + \mu_f)}{(1 - \mu_f \tan \bar{\theta})}, E = \frac{D - H}{D}, C = \frac{D - 2H}{D}$$

and A is the axial channel width ($W \sec \theta$ in *Figures 2* and *3*). θ_s and $\bar{\theta}$ are the flight helix angles at the screw surface and mean channel depth, respectively, while μ_s, μ_f and μ_b are the coefficients of friction at the screw root, flight sides and barrel surfaces, respectively, and are independent of pressure and rubbing speed. The downstream coordinate, z, is measured at the mean channel depth, and is therefore related to axial position by equation (2) with $\theta = \bar{\theta}$. Equation (44) is a slight generalization of Schneider's result as he assumed $\mu_f = \mu_s$.

The result obtained by Darnell and Mol is equivalent to equation (44) when their assumption of isotropic pressure ($k_1 = k_2 = k_3 = 1$) is taken into account. In addition to assuming $\mu_f = \mu_s$, they also assumed that $\mu_b = \mu_s$ in the main part of their analysis. The main theoretical contribution of Schneider's work[64,65] was the introduction of pressure ratios k_1, k_2 and k_3 based on the observation that when a granular material is compressed in a tube the radial stress generated is substantially less than the applied axial stress. Schneider performed tests of this type and found that for typical polymeric materials the ratio between radial and axial stress was essentially independent of the magnitudes of the stresses and lay in the range 0.4 to 0.6. There is considerable doubt, however, over the applicability of such data measured under relatively simple states of stress to the much more complex situation existing in plug flow in an extruder screw channel.

Irrespective of the particular simplifications made, equation (44) may be expressed in the form:

$$\cos \alpha = K \sin \alpha + M \tag{45}$$

from which α can be found provided the pressure and its gradient are known. Equation (44) can also be expressed as a differential equation for pressure in the form:

$$\frac{1}{p} \frac{\mathrm{d}p}{\mathrm{d}z} = \lambda \tag{46}$$

where λ is independent of p and z. Hence:

$$p = p_0 e^{\lambda z} \tag{47}$$

where p_0 is the initial pressure at $z = 0$. The need to specify an initial pressure is a difficulty not readily overcome in simple plug flow analyses whose assumptions imply a zero value for p_0.

Some general conclusions may be drawn from equations (43) and (44). The conveying rate is proportional to screw speed provided the back pressure and friction coefficients are independent of speed. In order to increase the solids conveying capacity of an extruder the ratios μ_s/μ_b and μ_f/μ_b should be decreased; that is, the screw should be smooth and the barrel rough. If equation (44) is applied to a typical screw feed section with an axial length several times its diameter then for realistic values of back pressure at the end of the section the predicted effect of back pressure on feed angle and hence conveying rate is small[64]. Reduction of the distance over

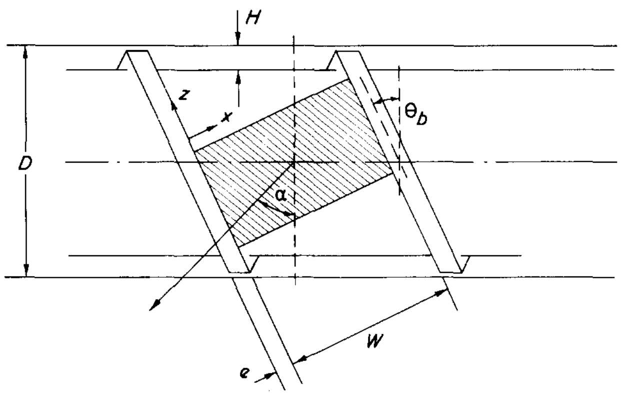

Figure 6 Direction of motion of the solid plug in the screw channel

which the Coulomb friction mechanism applies, for example by melting of material in contact with the hot barrel, increases the sensitivity of this rate to changes in back pressure.

One of the main difficulties in applying any analysis of solids conveying in an extruder lies in assigning appropriate numerical values to the coefficients of friction. Schneider[64], for example, showed that for a given combination of polymer and metal surface the coefficient of friction was significantly dependent on both temperature and the time for which relative motion occurred. The coefficient for a clean metal surface was generally very much lower than the steady value obtained when the surface had become thoroughly coated with polymer. The time required for this transition increased with the hardness of the polymer and in some cases was of the order of several hours.

There have been various refinements applied to the one-dimensional plug flow analysis. Martin *et al.*[21] and Chung [66] discussed the introduction of viscous drag in thin melt films in place of Coulomb friction at the interfaces between the solid plug and hot metal boundaries. The creation and development of such films is reviewed later in connection with the melting process. In practice, there is often a significant length of channel over which a viscous drag mechanism exists at the barrel surface while the screw is still cool enough for Coulomb friction to be the dominant mechanism. Broyer and Tadmor[67] allowed for both varying channel depth in the downstream direction and for the bulk density of the solid plug to be a function of pressure. Tadmor and Broyer[68] described a method for calculating the temperature rises within the plug during the conveying process, both as a means of providing better estimates of the temperature dependent friction coefficients and for predicting the formation of melt films. Kacir and Tadmor[69] have suggested that the region where surface melt films exist but before the later melting mechanism is established be called the delay zone of the extruder.

Lovegrove[62,70,71] demonstrated the importance of gravity forces in initiating the plug flow mechanism. He rejected the idea previously proposed[72] that the initial pressure p_0 appearing in equation (47) is solely due to the pressure developed by material in the hopper, on the grounds that the height of material there has no significant effect on feeding performance and that the screw channel may run only partly full of material until compaction into a solid plug occurs. Although gravity forces are negligible compared to pressure and frictional forces once the plug flow mechanism has been established, they appear to provide a means of initiating pressures between the solid particles and channel boundaries thus generating frictional forces. The cyclic nature of the supply of material from the hopper to the screw channel, due to the screw flight passing the hopper throat, causes a corresponding cyclic variation of the initial pressure build-up. Lovegrove and Williams[71] also included the effects of centrifugal forces on pressure initiation which become more important as extruder size is increased.

Two-dimensional plug flow solutions

In one-dimensional plug flow solutions the pressure or direct compressive stress in the downstream direction is assumed to vary only in this direction. The relative motions of the screw, solid plug and channel are such, however, that frictional forces generate not only a pressure gradient in the downstream direction but also one in the transverse direction. Since in a typical extruder the length of screw channel over which Coulomb friction conditions exist is of the order of at most ten times the channel width, the pressure difference across this width is likely to be significant compared to the pressure built up in the downstream direction.

If pressure is assumed to be a two-dimensional function of both channel coordinates z and x (*Figure 6*) then Lovegrove[62,70] showed that a pair of differential equations of the following form govern the plug flow:

$$k_2\frac{\partial p}{\partial x} + \frac{\partial \tau}{\partial z} = G_1 p + H_1(x,z) \tag{48}$$

$$\frac{\partial p}{\partial z} + \frac{\partial \tau}{\partial x} = G_2 p + H_2(x,z) \tag{49}$$

The positive constant k_2 is still the ratio between local direct compressive stresses in the x and z directions. This result is obtained after considerable manipulation, including averaging over the depth of the plug and taking into account channel curvature. Thus pressure, $p(x,z)$, and shear stress, $\tau = \tau_{xz} = \tau_{zx} = \tau(x,z)$, are both averaged in the radial direction. The parameters G_1, G_2, H_1 and H_2 are determined by the screw geometry, coefficients of friction, stress ratios k_1 and k_3 and the feed angle. H_1 and H_2 only appear when gravity or centrifugal forces are included in the analysis. If such forces are neglected and the one-dimensional assumption of insignificant variations in the x direction is introduced then equation (49) reduces to the form displayed by equation (46).

Still neglecting body forces, τ may be eliminated from equations (48) and (49) to give:

$$k_2\frac{\partial^2 p}{\partial x^2} - \frac{\partial^2 p}{\partial z^2} = G_1\frac{\partial p}{\partial x} - G_2\frac{\partial p}{\partial z} \tag{50}$$

which yields solutions of the form:

$$p = p_0 e^{\lambda_1 z} e^{\lambda_2 x} \tag{51}$$

The pressure profiles in both the downstream and transverse directions tend to be of the exponential form. If body force terms are retained, solutions to the full governing equations (48) and (40) for two-dimensional plug flow can generally only be obtained numerically[62,70] and are necessary for studying in detail both pressure initiation and the cyclic pressure variations already discussed in connection with one-dimensional solutions.

More sophisticated solutions

One of the main limitations in most existing analyses of solids conveying is the assumption of plug flow in which the plug of compacted particles does not deform under local variations in the state of stress. Also, the possibility of internal slipping between layers of particles leading to loose granular flow is ignored. Lovegrove[73] has made a preliminary study of the stresses and deformations in elastic solids being conveyed and has examined the validity of the plug flow assumption.

Solids conveying experiments

Darnell and Mol[63] performed some relatively simple solids conveying experiments in extruders at ambient temperature using various combinations of screw and barrel surface roughnesses, and obtained at least qualitative agreement with their theoretical work. Some experiments reported by Schenkel[74] demonstrated the very considerable pressures that can be generated by the feed section of an extruder. The work described by Miller[75] was concerned not only with the conveying action of screws but also with flow from hoppers into extruders.

The experiments performed by Schneider[64] to measure coefficients of friction have already been mentioned. He also carried out a series of conveying experiments on a relatively short extruder equipped with temperature control of both screw and barrel to allow friction coefficients to be varied. Several uniform screws of the same length but with different channel depths were tested, and a means of varying and measuring the back pressure at the delivery of the machine was provided. Results confirmed the direct proportionality between flow rate and screw speed and also showed that flow rate is largely independent of back pressure. This latter effect would appear to be due to the use of a length of screw considerably greater than that normally associated with Coulomb friction boundary conditions.

Lovegrove[62,76] in a similar series of experiments varied the effective length of screw used for conveying. He confirmed the insensitivity of flow rate to back pressure for screws with length-to-diameter ratios of about 8, but showed that back pressure can significantly reduce flow rate for screws of about half this length, in accordance with plug flow theories. Data were obtained for different materials and screw channel depths and in attempting to compare with theoretical predictions the difficulties of selecting material properties for use in the calculations were highlighted. Also, the cyclic nature of the flow rate against a nominally constant back pressure, due to the pressure initiation mechanism[70], was demonstrated.

Following the work of Schneider, further experimental studies at IKV Aachen[77] led to the development of special feed sections for extruders. These take the form of efficiently cooled barrel liners with internal axial grooves of various shapes. The grooves serve to increase the effective coefficient of friction between feedstock and barrel surface, while the cooling delays the transition from Coulomb friction to viscous drag. Using such an arrangement very high pressures can be generated at the end of the feed section, thereby increasing the flow rate through the machine.

ANALYSIS OF MELTING IN EXTRUDERS

Mention has already been made of the onset of melting in an extruder when a thin film of melt is formed between the hot barrel surface and the compacted plug of material in the screw channel. The first traces of melt presumably flow into the gaps between the particles forming the solid plug[69] before a continuous film is created. The thickness of this film increases as the plug moves along the screw channel and similar films are in due course formed at the screw root and flight surfaces. Kacir and Tadmor[69] suggested that the film at the barrel surface increases in thickness to several times the size of the clearance between the screw flight and barrel before there is any observable change in the mechanism of melting. As already mentioned, analysis of this delay zone can be accomplished with the aid of viscous drag boundary conditions in the analysis for solids conveying[21,66,69], together with a non-isothermal treatment of the solid plug[68]. A much more thorough theoretical analysis of flow and heat transfer in the film formed between a moving hot surface and a melting solid has been published by Pearson[78].

Observed melting mechanisms

Whereas analyses of solids conveying and melt flow in extruders can be developed from fundamental mechanical principles with little or no reference to observed behaviour, attempts to treat the intervening melting process are usually based on observed mechanisms. The essence of the experimental method used by many different workers is to first achieve the required steady operating conditions and then to stop the screw and cool the barrel as rapidly as possible. After extracting the screw from the barrel the helical strip of solidified polymer is removed from the screw channel and sectioned. Various visual aids have been employed to help distinguish between material melted in the presence of shear before the screw was stopped and that which has melted subsequently by thermal conduction alone. These aids include the use of granules of mixed colours, the addition of dry colouring to coat individual granules, and changing feedstock colour just prior to stopping the machine. Among the first to report experiments of this type were Maddock[79] and Street[80].

Once past the delay zone typical sections through the contents of the screw channel are as shown schematically in *Figures 7a* and *7b*, views from a stationary screw equivalent to *Figure 4*. In *Figure 7a* the screw surface temperature, T_s, is below the melting temperature, T_m, of the polymer and no melt film is present at the screw. Such a situation normally exists for a relatively short distance before T_s exceeds T_m and a film is formed at the screw as shown in *Figure 7b*. Both sectional views are somewhat idealized in that the channel is actually curved and the corners of the solid bed become rounded. The term solid bed customarily used in work on melting is equivalent to the solid plug of conveying analyses.

There are up to four distinct regions in the screw channel cross-section, namely the upper and lower melt films at the barrel and screw surfaces, respectively, the solid bed and the melt pool. The lower melt film could be regarded as two regions, the film along the screw root and the one on the trailing edge of the flight. The melting mechanism described by most observers[72,79-84] may be summarized as follows. Owing to the proximity of the heated barrel and the intense shear, much of the melting occurs in the upper melt film. The motion of the barrel relative to the solid bed sweeps the melt so formed into the melt pool region between the bed and leading edge of the flight. Clearly this pool is only

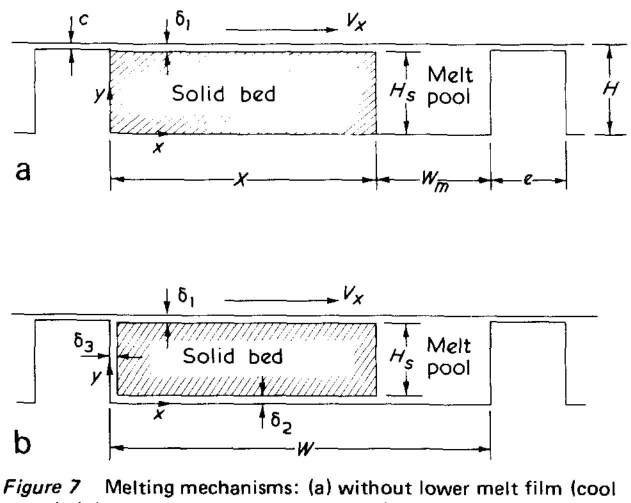

Figure 7 Melting mechanisms: (a) without lower melt film (cool screw); (b) with lower melt film formed (hot screw)

likely to be formed when the thickness of the upper melt film, δ_1 in *Figure 7*, exceeds the clearance between the flight and barrel, and the flight can act as a scraper. While it is to be expected that δ_1 varies with both the transverse coordinate x and downstream coordinate z, such variations are difficult to measure. δ_1 remains small as newly melted material is transferred to the pool. The flow in this pool is a combination of clockwise circulation and downstream motion due to the dragging actions of both the barrel and bed moving relative to the screw, together with the effect of the downstream pressure gradient which normally exists.

If melt films are formed at the screw surfaces their thicknesses, δ_2 at the screw root and δ_3 at the flight, are observed to be independent of x and y, respectively. As the motion of the solid bed relative to the screw is in the downstream direction the lower films grow in thickness in this direction. This growth can be considerable due to the retention of all melted material. Usually the main change exhibited by successive cross-sections along the screw is a reduction in the width of the solid bed, with a corresponding increase in the melt pool width. With screws having rapidly reducing channel depths in their compression sections, however, it is possible to observe a temporary increase in solid bed width as the bed is forced into the resulting wedge.

Completion of melting, which is often not achieved until well into the metering section, can occur in various ways. If the process is stable and the bed remains continuous in the downstream direction, the corners of the bed become rounded and either its width or depth diminish to negligible proportions. The final disappearance of the bed can be quite rapid once the temperature of the bulk of the solid has risen close to the melting temperature. Very often the melting process becomes unstable in the sense that the bed suffers breaks along planes normal to the downsteam direction. This phenomenon has become known as solid bed break-up and is discussed in more detail below. The resulting pieces of compacted solid then decrease in size, often as much by thermal conduction as by shearing in thin melt films.

Although most published experimental findings serve to confirm the above mechanism of melting, there are some significant exceptions. Menges and Klenk[85] reported quite different behaviour of rigid poly(vinyl chloride) (PVC) powder. Fusion appeared to occur mainly in the clearance between screw flight and barrel, and a form of melt pool developed against the trailing face of the flight. The overall rate of melting was slow, with a proportion of solid material always remaining at the end of the screw. This difference of mechanism was attributed to the non-wetting nature of PVC. Assumption (O) concerning slip at solid flow boundaries discussed earlier in connection with melt flow analyses is not necessarily applicable to PVC materials under extruder channel flow conditions. Gale[86] has since shown that the melting mechanism of PVC powder is highly dependent on the lubricant used and its concentration. Another variant of the usual melting mechanism has been reported by Lindt[87] for polypropylene processed in a 90 mm diameter extruder, somewhat larger than other machines normally used for this type of experimental work. He showed that melt remained in relatively thick films surrounding the solid bed, and outlined an appropriate theoretical model.

Theoretical models for melting

Returning to the melting mechanism of the type shown in *Figure 7*, it is convenient to review the development of theoretical models and the supporting experimental work together. In addition to machine dimensions and melt film thicknesses previously defined, further dimensions shown in *Figure 7* are melt pool width, W_m, solid bed width, X, and depth, H_s. While the solid bed may be treated as being freely deformable, in all models published to date it is assumed to melt and deform so slowly that its downstream velocity relative to the screw, V_{sz}, is the dominant component and is independent of x and y. Many of the assumptions outlined earlier for melt flow analyses are also employed in deriving melting models. Assumptions (A) to (O), also (Q) are generally used, particularly for melt flow regions, assumption (P) is applicable to at least the flow in the melt pool. Appropriate versions of some of the later assumptions are also introduced according to the level of sophistication of the particular model. Following assumption (K) for melt specific heat, C_{pm}, it is also customary to assume a constant specific heat, C_{ps}, for the polymer in the solid state, also that there is a sharp melting point, T_m, and an associated latent heat of fusion, λ.

Tadmor[88] was the first to propose a theoretical model for melting based on the mechanism shown in *Figure 7a*. He assumed that downstream bed velocity, V_{sz}, is independent of z and calculated its value as that necessary for the solid plug prior to melting to give the prescribed total mass flow rate along the channel. As a consequence of this considerable simplification the motion of the bed is prescribed and conditions for its equilibrium need not be examined. A further simplification was the omission of the lower melt film. Given the constant V_{sz} assumption, however this merely implies that the rate of melting is determined by the upper melt film alone.

Tadmor assumed that the thickness of the upper melt film, δ_1, is independent of x and that the flow there can be treated as fully-developed isothermal Newtonian drag flow. Having argued a case for neglecting the effects of pressure gradients in the film on the grounds that δ_1 is small and the shear stresses large it was perhaps natural to assume constant viscosity associated with constant shear stress. Both this and the isothermal assumption failed to take account of the variation of viscosity with the considerable change of temperature through the thickness of the film. The analysis of heat transfer in the film was for fully-developed temperature profiles, heat generated in the flow being conducted to either the solid bed or barrel surface. Temperature boundary conditions were prescribed termperatures T_b and T_m at the barrel and bed surfaces, respectively. The direction of flow in the film was that of the barrel relative to the bed.

Tadmor's analysis of heat transfer in the solid bed treated the bed as a semi-infinite solid with temperature variations in the y direction only. In addition to avoiding the need to specify temperature boundary conditions at the screw this also rendered the bed temperature profile independent of downstream position. Due to the simplicity of the model there is no need to analyse flow in the melt pool in detail, the downstream mass flow rate there implicitly balancing with the flow rates in the bed and upper film to give the required overall rate. No mention was made of pressure gradients in the screw channel.

Two mass balances are involved in the Tadmor model. Because δ_1 remains locally independent of z all material melted into the upper film is dragged into the melt pool. Neglecting flow over the flight:

$$\omega_1 X = \tfrac{1}{2} V_x \delta_1 \rho_m \tag{52}$$

where ω_1 is the rate of melting per unit area from the top of the bed and ρ_m is the melt density. Also, the downstream mass flow rate in the bed decreases due to the loss of material by melting:

$$\frac{d}{dz}(\rho_s V_{sz} X H_s) = -\omega_1 X \tag{53}$$

where ρ_s is the density of the compacted solid bed. Both ρ_s and V_{sz} are constant and Tadmor assumed $H_s = H$ (that is, $\delta_1 \ll H$), a known function of z. The melting rate ω_1 was obtained from a heat balance at the solid–melt interface as:

$$\omega_1\lambda = k_m\left(\frac{dT}{dy}\right)_m - k_s\left(\frac{dT}{dy}\right)_s \tag{54}$$

where k_m and k_s are the thermal conductivities of the melt and solid, respectively, and the corresponding temperature gradient subscripts refer to gradients at the interface in the melt and solid. Expressions for these gradients were obtained from the temperature profiles already derived. Tadmor in fact expressed parts of his analysis in terms of a solid bed velocity into the interface, V_{sy}, where $V_{sy} \ll V_{sz}$.

Equations (52) and (54) may be solved for δ_1 and ω_1, which are respectively proportional and inversely proportional to the square root of the bed width, with the constants of proportionality being given in terms of known quantities. Hence, equation (53) may be solved to give analytical expressions for bed width as a function of z, and the overall melting length, for both parallel and tapering screw channels.

In addition to the limited experimental verification provided by Tadmor[88], further experiments on melting were reported in a companion paper by Marshall and Klein[89]. Klein and Marshall[90] discussed the development of a computer program which incorporated the Tadmor model. They also compared measured and calculated pressure profiles, the latter apparently derived from an analysis of flow in the melt pool. Detailed comparisons between the Tadmor model and experimental data were reported by Tadmor *et al.*[81]. These comparisons were made in terms of the easily measured reduced solid bed widths, X/W, plotted as functions of axial position along the 63.5 mm (2.5 inch) diameter extruder processing various polyethylenes, polypropylene, PVC and nylon. While the agreement shown was generally satisfactory, discrepancies were noted when the barrel temperature was much higher than the melting temperature of the polymer. These were attributed to both the isothermal Newtonian assumptions for the flow in the upper melt film, and the failure to allow for the thermal convection associated with newly melted material entering the film from the bed. The model was modified by adopting an analysis of fully-developed drag flow in the film with viscosity being determined by equation (9). Instead of treating the energy and momentum conservation equations (equivalent to equations 31 and 26 with zero pressure gradient) as coupled equations to be solved simultaneously, the authors assumed a particular mathematical form for the temperature profile based on the result for isothermal Newtonian flow. While this modification produced a marked improvement in the model, further improvement was obtained by allowing for the heat necessary to raise the temperature of the newly melted material to the bulk mean temperature of the film, $\bar{T}_1$, by defining an effective latent heat of fusion as:

$$\lambda_1 = \lambda + C_{pm}(\bar{T}_1 - T_m) \tag{55}$$

to be used in equation (54). The introduction of these modifications made the mathematics of the melting model considerably more sohpisticated such that only numerical solutions were obtainable, with the aid of a digital computer. It is worth noting that in virtually all the experiments reported by Tadmor *et al.*[81] the flow rates in the screw metering sections probably exceeded the drag flow rates there[5] and therefore represent a relatively limited range of operating conditions.

Various refinements have been added to the Tadmor model. For example, Chung[91,92] treated the solid bed as being of finite thickness and the screw surface as being thermally insulated for the purpose of analysing the temperature profile in the bed. Tadmor and Klein[72] made more significant modifications when they introduced correction factors for channel curvature and allowed for flow in the flight clearance which altered the mass balance expressed in equation (52). Assuming pure drag flow and a linear velocity profile in the clearance:

$$\omega_1 X = \tfrac{1}{2}V_x\delta_1\rho_m - \tfrac{1}{2}V_x c\rho_m \tag{56}$$

although with the non-Newtonian non-isothermal analysis for flow in the upper melt film the expression for flow rate there is more complex. Tadmor and Klein[72] also commented that despite experimental evidence that δ_1 usually appears to be constant across the width of the bed it can be expected to increase towards the melt pool as newly melted material is entrained. The new version of the melting model was used to examine the effects of changing various design and operating parameters[72,93], including flow rate, screw speed, barrel temperature, channel dimensions, helix angle and flight clearance. A much more recent paper[94] also discussed the last of these in connection with screw wear.

Hinrichs and Lilleleht[95] also derived correction factors for screw channel curvature, allowed for flow in the flight clearance, and used a somewhat more sophisticated method for calculating solid bed velocity. Vermeulen *et al.*[96] developed a model in which δ_1 was allowed to vary with x. In other respects the model was based on Tadmor's and suffered from the limitation that the heat generation term was omitted from the energy equation used to analyse heat transfer in the upper melt film.

Donovan[97,98] described some much more significant modifications to the Tadmor model. Working from experimental observations he questioned the assumption of constant solid bed velocity, V_{sz}, and proposed the use of a 'solid bed acceleration parameter' to allow the velocity to increase in a prescribed manner. The results demonstrated that V_{sz} does vary, but not in a way that can be readily prescribed. Donovan also refined the analysis of the solid bed by including the downstream thermal convection which is responsible for the gradual heating of the bulk of the bed. The boundary condition used at the screw surface was $T = T_m$, which implicitly acknowledged the existence of a melt film there. Donovan's analysis of the drag flow in the upper film treated the correctly coupled energy and momentum equations with the aid of the analytical solution developed by Martin[99]. He also assumed that the thickness of this film varies linearly across the width of the bed, starting from a value equal to the flight clearance at the trailing edge of the flight, to allow for the entrainment of melt. A method was also described[98] for calculating the downstream pressure gradient from an analysis of flow in the melt pool. This analysis was for isothermal fully-developed melt flow but introduced corrections for non-Newtonian material behaviour.

In all the melting models so far reviewed, the solid bed velocity is a prescribed function of z, and in most cases is assumed to be constant. Although this simplification often allows satisfactory predictions to be made concerning overall melting performance it does not provide a realistic description of solid bed motion, particularly in the later stages of melting. Clearly, the bed suffers substantial deformation in order that its width may decrease while most of the melting is taking place at its upper surface. This deformation need not be confined to the x,y plane: elongation of the bed in the z direction may contribute to its reduction in width. The bed velocity should be regarded as a slowly varying function of z. Consequently, equilibrium of the bed must be considered, and the lower melt films at the screw surface become important in terms of the shear stresses exerted on the bed in addition to the melting caused.

The first melting model to treat V_{sz} as an unknown function of z was described by Shapiro[100] and has since been developed by Pearson and Halmos[101–103]. A somewhat simplified version of this model was used by Edmondson[83,84], the principal differences lying in the treatment of the upper melt film. In all cases lower melt films were included once the screw temperature is high enough for these to be formed.

The mass balance in the upper melt film can be generalized as:

$$\begin{pmatrix}\text{Rate of change}\\ \text{of downstream}\\ \text{mass flow rate}\\ \text{in upper film}\end{pmatrix} = \begin{pmatrix}\text{Rate of}\\ \text{melting}\\ \text{from}\\ \text{solid bed}\end{pmatrix} - \begin{pmatrix}\text{Rate of change}\\ \text{of downstream}\\ \text{mass flow rate}\\ \text{in melt pool}\end{pmatrix} \quad (57)$$

If the film thickness δ_1 is assumed to be independent[102], of z, the left hand side of equation (57) is zero. In the case of the lower films, which are each assumed to be of uniform thickness at a particular channel cross-section, all the melt is retained:

$$\frac{\mathrm{d}}{\mathrm{d}z}(m_{2z}X) = \omega_2 X, \qquad \frac{\mathrm{d}}{\mathrm{d}z}(m_{3z}H_s) = \omega_3 H_s \quad (58)$$

m_{2z} and m_{3z} are the downstream mass flow rates per unit width of film in the screw root and flight films, respectively, ω_2 and ω_3 being the corresponding melting rates per unit area. Neglecting melting at the interface between the bed and melt pool, equation (53) for the rate of loss of solid material by melting is now:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho_s V_{sz} X H_s) = -\int_{\delta_3}^{\delta_3 + X} \omega_1 \mathrm{d}x - \omega_2 X - \omega_3 H_s \quad (59)$$

where the melting rate ω_1 may now vary with x. The mass flow rate in the melt pool depends on its size, the velocities of the barrel and solid bed relative to the screw, and the downstream pressure gradient, P_z. An overall mass balance is used to equate the total flow rate along the screw channel, which is assumed to be both a known quantity and for steady flow to be independent of z, to the sum of the flow rates in the melt films, solid bed and melt pool.

In addition to mass balances, a force balance in the downstream direction for the solid bed gives:

$$P_z H_s X = \int_{\delta_3}^{\delta_3 + X} \tau_1 \mathrm{d}x - \tau_2 X - \tau_3 H_s \quad (60)$$

where τ_1, τ_2 and τ_3 are the shear stresses in the z direction at the bed surfaces in the melt films. The much smaller stresses on the bed due to the melt pool are neglected. In order to determine many of the parameters in equations (57) to (60), detailed flow and heat transfer analyses must be performed for the five distinct regions. In the case of the solid bed no attempt has so far been made to analyse internal deformations in detail. The temperature profile within the bed may be obtained with the aid of the energy equation. For example, Edmondson and Fenner[84] assumed temperature to be independent of x and retained only radial conduction and downstream convection terms from equation (7) to give:

$$\rho_s C_{ps} V_{sz} \frac{\partial T}{\partial z} = k_s \frac{\partial^2 T}{\partial y^2} \quad (61)$$

with $T = T_m$ at the upper and lower faces of the bed and ambient temperature throughout at the beginning of melting. Radial convection due to solid material moving into the melting interfaces was accounted for in the equations for melting rates at these interfaces. The solid bed temperature profile was obtained numerically at each successive channel cross-section. Shapiro *et al.*[102] argued that most of the bed remains at the initial temperature and used a much simpler analytical approach. As a result of neglecting bed temperature variations in the x direction it is not possible to analyse realistically the melting into the film at the screw flight. It is therefore convenient to assume $\delta_3 = \delta_2$ and treat this side film as an extension of the one at the screw root.

A thorough analysis of flow and heat transfer in the melt pool presents problems at least as great as those already discussed for flow in a melt-filled channel. In addition to a new influx of melt and two moving boundaries instead of one, the assumption of an infinitely wide channel (assumption T) is much less justifiable. Both the Shapiro and Edmondson melting models treated flow in this region as isothermal and Newtonian to obtain a relationship between downstream mass flow rate and pressure gradient. While this approach may be reasonable in the early stages of melting it is clearly much less so as the fully molten state is approached. The objection to using a more sophisticated form of analysis is that it would absorb a disproportionate amount of computing time in the context of the overall melting analysis.

Analyses of the lower melt films assume the downstream flow there to be locally fully-developed. Pearson[78] in a detailed study of melting films justified this assumption under certain conditions which normally apply in practice. Edmondson and Fenner[84] assumed the lower films to be sufficiently thin for the pressure gradient to have negligible effect on the flow and adapted the largely analytical method developed by Martin[99] to treat the resulting non-Newtonian non-isothermal drag flow (governed by equations (26) with $P_z = 0$, (31), (32), (28) and (9) with appropriate velocity and temperature boundary conditions). Shapiro *et al.*[102] retained the downstream pressure gradient with a view to treating more realistically the later stages of melting when the lower films may become relatively thick. Both models rely on the temperature at the screw surface being a known function of z, and Edmondson[83] described an empirical method for prescribing such a profile in the absence of measured data.

The thickness of the upper melt film normally remains

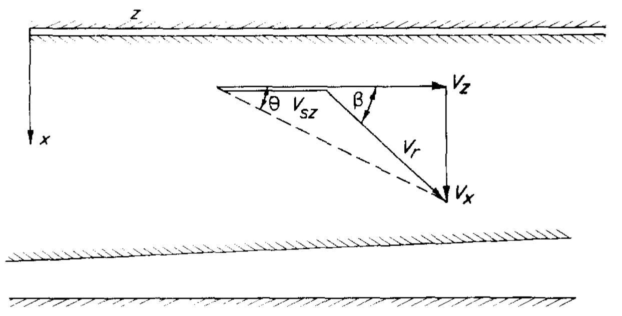

Figure 8 Relative velocity diagram for the solid bed

sufficiently small for drag flow conditions to be assumed. Pearson[78] examined this assumption and concluded that the presence of pressure gradients sufficiently large to affect the flow would imply pressure variations over the width of the solid bed which it could not sustain (and which are not observed in practice[84]). Also, the melt film thickness δ_1 cannot remain constant. Entrainment of melted material must result in growth of the film in the direction of relative motion between the barrel and bed. This direction is that of the relative velocity, V_r, shown in *Figure 8*. As the magnitude of V_{sz} rarely exceeds half that of V_z[83,84], V_r is not predominantly in either the downstream or transverse directions. While δ_1 should be treated as a function of both x and z, this is likely to prove very costly[102]. Shapiro *et al.* chose to assume $\delta_1 = \delta_1(x)$ and Edmondson and Fenner took the other extreme $\delta_1 = \delta_1(z)$: it is at this point that the models differ significantly. It is not yet clear which provides the better representation of actual melting behaviour, or indeed whether a compromise must be sought.

The initial conditions at $x = 0$ in *Figure 7* for flow in the upper melt film are strongly influenced by the leakage flow through the flight clearance. The melting rates appearing in equations (58) and (59) may be determined by expressions equivalent to equation (54) but with effective latent heats of fusion in the form of equation (55) which allow for thermal convection normal to the melting interface. While Shapiro[100] and Edmondson and Fenner[84] used the bulk mean melt temperature in equation (55) for this purpose, Pearson[78] has shown more recently that the resulting modification to λ should be reduced on the grounds that the heat necessary to raise the temperature of the newly melted material to that of the bulk of the melt comes not only from the melting interface but also from the other flow boundary.

Whichever model is adopted, a set of simultaneous first order ordinary differential equations is obtained for variables such as film thicknesses, solid bed width and pressure, with z as the independent variable. Given suitable initial conditions at the start of melting derived from analyses of solids conveying and melt film formation, these equations may be solved numerically using iterative step-by-step procedures to follow the course of melting.

While comparisons with experimental data have yet to be reported for the Shapiro model, Edmondson[83] based his work on an extensive series of experiments on a 38 mm (1.5 inch) diameter extruder. Correlations with the theoretical model were generally satisfactory. For most polymers and screws the predicted solid bed velocity remained nearly constant over much of the melting process, while with plasticised PVC it increased significantly. Rapid increases of bed velocity towards the end of melting were associated with bed break-up.

Solid bed break-up

Many workers have reported the periodic occurrence of breaks in the solid bed in the plane of the channel cross-section towards the end of melting[72,81–84,97,98]. This phenomenon is presumably due to the state of stress within the bed departing too far from one of isotropic compression[78], although in the absence of a detailed stress analysis for the bed no formal criterion has been established. As indicated by equation (60), the equilibrium of the bed involves a balance between forces associated with the downstream pressure gradient and shear forces acting on its sides. As melting proceeds the upper melt film remains relatively thin while the lower films increase in thickness, and unless the pressure gradient increases significantly the bed velocity must increase to help balance the shear forces in the films. An increase in the pressure gradient, particularly towards the end of melting where the melt pool is relatively wide, would reduce the mass flow rate in the pool and require an increase in the bed velocity to maintain the overall mass balance.

Edmondson[83,84] demonstrated a close correlation between the observed start of bed break-up and the predicted onset of rapid bed acceleration. Once a break has occurred the gap is completely filled with melt and the new end of the continuous part of the bed moves downstream until the accelerating forces applied to it are sufficient to cause another break. Bed break-up is therefore a periodic instability occurring at frequencies of the order of five to ten times lower than that of screw rotation[84]. The lengths of the broken pieces of bed are of the order of several times their widths. Existing melting models are not satisfactory for analysing melting after the bed has broken.

One practical way to prevent bed break-up is to apply screw cooling which delays the formation of a melt film at the screw surface[84], thereby maintaining a more stable balance between the shear forces on the bed but reducing the output from the extruder. While bed break-up can occur in both parallel and tapering screw channels, Martin[82] and Klein[104] described a similar phenomenon associated with periodic wedging of the solid bed in a rapidly tapering channel.

POWER CONSUMPTION IN EXTRUDERS

An important result of any analysis of extruder performance is an estimate of the machine's total power requirement. This power includes both the mechanical power supplied through the screw drive and the thermal power supplied by the barrel heaters. The drive power is normally the greater of the two and must be matched to both the capacity of the motor and the torsional strength of the screw. Heater capacities are normally determined more by the need for rapid heating of the barrel before the machine can be used rather than the heat required in normal running. Indeed, a net cooling of the barrel may be necessary, particularly on large machines.

The mechanical power consumption is normally calculated as the rate of working at the interface between material in the screw channel and the barrel. This rate is:

$$\dot{E} = V_z \tau'_{yz} + V_x \tau'_{xy} \tag{62}$$

per unit area, where the shear stresses are evaluated at the barrel. The total power is found by integrating this expression over the entire barrel surface, not only for the solids conveying, melting and melt flow regions but also over the leakage flow in the flight clearance. The values of the shear stresses used for this purpose clearly depend on the particular theoretical model used.

Many, though by no means all, published analyses of solids conveying, melting and melt flow have included results for power consumption. For melt flow, Mallouk and McKelvey[29] were the first to consider power requirements in detail, using an isothermal Newtonian model. Results obtained from both one and two-dimensional fully-developed flow analyses were compared and contrasted by Fenner[5]. While transverse flow in the screw channel has a relatively small influence over the relationship between flow rate and downstream pressure gradient, it has a much greater effect on power. Fenner[5] also gave results for power consumption in screw channels of finite width for both Newtonian and non-Newtonian isothermal downstream flows, highlighting the difficulties of treating the regions of flow close to the flight clearance. Published details of more sophisticated analyses of melt flow have tended to omit results for power consumption although these are readily obtainable. For example, Fenner[19] showed the effect of barrel temperature on drive power for large melt fed extruders with the aid of a developing flow analysis.

Schneider[64] was the first to calculate and measure mechanical power consumed in the screw conveying of solid polymeric materials. Further attention was given to this problem by Broyer and Tadmor[67]. In the case of the melting process, Tadmor *et al.*[81] proposed a different but equivalent approach for calculating power consumptions associated with the Tadmor model of melting. More recently, Klein[94] has discussed changes in power consumption due to screw wear predicted by such a model. Chung *et al.*[105] studied the dependence of power consumption on both screw speed and size.

Power consumption in the flight clearance

Irrespective of the method used to analyse leakage flow over the screw flight, the results suggest that a substantial proportion of the total drive power is dissipated in the clearance. There is a limited amount of evidence to suggest that this is not necessarily so in practice. Fenner[5,55] performed metering screw experiments using silicone polymers and showed that the measured drive power was often closer to the calculated power for the screw channel alone than to the predictions which included power consumed in the clearance. The fact that the measured powers, which included some transmission losses, never exceeded the theoretical powers for channel and clearance suggested that there was little or no leakage flow. A recent paper by Worth and Helmy[106] which describes essentially identical work serves to confirm these findings. Barr and Chung[107] examined the effects of varying clearance on extruder performance and also concluded that at least for small clearance there may be no flow over the flight.

The postulated absence of leakage flow would appear to be caused by slip between melt and metal surfaces at the high shear stresses associated with flow in and near the flight clearance. Such slip has already been discussed in connection with assumption O for melt flow analyses. Recent as yet unpublished work[108] shows that above a critical shear stress in leakage flow the lubricating effect of the melt film in the flight clearance breaks down, and metal-to-metal contact occurs even in the absence of significant lateral loads on the screw.

MIXING IN EXTRUDERS

An important function of a screw extruder is to produce a homogenous extrude. As perfect uniformity is impossible to achieve, the degree of homogeneity is a major factor affecting product quality[109–111]. Homogeneity is achieved by mixing of the melt in the extruder and is particularly important when colourants, fillers or other additives are to be incorporated.

A precise quantitative definition of mixing and mixedness is difficult, and must in general be statistical owing to the random nature of the mixing process. Danckwerts[112] proposed two quantities that are useful for describing mixedness, namely scale of segregation and intensity of segregation. The scale of segregation is a measure of the mean size of regions of the same component in the mixture, while the intensity of segregation is a measure of the difference in concentration of the relevant property, such as colour, between the components. This difference in concentration is affected by diffusion at a molecular level. As such diffusion is negligible in extrusion processes the intensity of segregation is constant. An extrudate can be said to be well-mixed when the scale of segregation is less than the scale of examination[4].

The scale of segregation is affected by both dispersive and distributive mixing. Dispersive mixing involves rupturing the lumps of the various components of the mixture, and therefore depends primarily on the stresses in the material[4,113]. On the other hand, distributive mixing depends on the total deformation which spreads the lumps into thin layers. In an extruder screw channel distributive mixing is the more important, although various special mixing devices are sometimes added to the screw which promote dispersive mixing.

Analysis of distributive mixing in an extruder

The degree of distributive mixing imparted by a process such as screw extrusion can be defined as the ratio between the initial and final thicknesses of striations of a component of the mixture[114]. In a simple shear flow the rate of mixing (rate of reduction of striation thickness) is equal to the shear rate. Mohr *et al.*[115] analysed mixing in two-dimensional isothermal Newtonian channel flow, as did McKelvey[4], by treating the downstream and transverse flows separately and then adding the associated degrees of mixing. Separation of the two flows avoided the need to evaluate mixing in a complex state of deformation.

Fenner[5] suggested that the natural extension of the result for simple shear to more complex flows is to take the local rate of mixing as:

$$M = (4I_2)^{1/2} \tag{63}$$

where M is the degree of distributive mixing and I_2 is the second invariant of the rate of deformation tensor, defined in general by equation (10). One approach to the analysis of mixing is to integrate equation (63) along the paths taken by particular elements of material. This type of method has been used by, for example, Mohr *et al.*[115], McKelvey[4] and Pinto and Tadmor[116] to plot both the degree of mixing and residence time as functions of the initial position of the element in the channel. While such plots emphasise variations of the degree of mixing over the channel, a single parameter for describing the mixing performance of a machine is often more useful. Such a parameter is provided by an alternative approach which determines the bulk mean mixing as[5]:

$$\bar{M} = \frac{1}{Q}\iiint (4I_2)^{1/2}\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \qquad (64)$$

where Q is the volumetric flow rate and the integration is carried out over the entire melt filled region of the screw channel. An equivalent expression for two-dimensional flow was proposed by Pearson[13] and used by Yates[20]. Fenner[5] compared and contrasted the mixing performances predicted by various one and two-dimensional fully-developed melt flow analyses and used equation (64) as a basis for assessing the performance of large hot melt homogenizers[19].

If transverse flow is ignored an estimate of the bulk mean mixing in the metering section can be obtained from equation (64) as:

$$\bar{M} = \frac{1}{\pi_Q} \times \frac{Z}{H} \qquad (65)$$

where π_Q, Z and H are respectively the dimensionless flow rate (equation 33), helical length and depth of the channel in the metering section. This simple result is equivalent to the form first proposed by Maddock[109], namely the product of the mean shear rate, V_z/H, and average residence time in the molten state WHZ/Q. Clearly, mixing is improved when the flow rate is reduced. The magnitude of the ratio Z/H, which is generally of the order of 10^3, helps to explain why single screw extruders are efficient mixers.

Special mixing devices

In order to further improve the mixing performance of single screw extruders numerous special mixing devices have been added to conventional screws. These include smear heads, blisters, turbine mixing heads, reverse flighted sections and channel dams[32,117–119]. The functions of such devices appear to be threefold. Namely, to apply some distributive mixing, to apply dispersive mixing, and to disturb established flow and temperature profiles.

OVERALL MACHINE PERFORMANCE

If analyses of solid conveying, melting and melt flow in extruders are to be useful in studying machine design and performance they must be combined in order to predict overall behaviour. The two transitions between successive processes cause some difficulties, particularly the one between melting and melt flow. Even in the absence of breaks in the solid bed, existing melting models become increasingly unrealistic towards the end of melting, particularly in the way they treat flow in the melt pool which eventually increases in size to fill the entire screw channel. At some point well before the end of melting a more sophisticated melt pool analysis, presumably of the developing flow type, needs to be introduced to effect the transition to fully molten flow.

Although it is not always made clear in analyses of extruder performance, the mass flow rate along the screw must normally be prescribed. It is this parameter which provides the link between solids conveying, melting and melt flow, and between successive channel cross-sections within the regions associated with these processes. Provided the machine is operating steadily the mass flow rate is independent of both time and position along the screw. In practice the flow rate is often determined by a balance between the performance of the screw and the flow characteristics of the breaker plate, screen pack, die and any other restriction at the delivery end of the extruder. These characteristics provide relationships between flow rates and delivery pressures which must be generated by the screw. Given a flow rate, an analysis of overall machine performance can in principle predict the pressure profile along the screw and hence the delivery pressure. With the aid of an iterative procedure the flow rate can be adjusted until the pressures balance. This need for repeated analyses of the entire extrusion process is one of the main reasons why accurate predictions of flow rate are still difficult to make.

The above mode of operation is often described as melt-controlled[13], although this term has also been used in the more restricted sense of a balance being achieved between the melt flows in the die and metering section alone. As the melting process is capable of generating large pressure rises its contribution to the overall pressure balance cannot be neglected. The contribution of the solids conveying process is generally less important in melt-controlled operation. The other main mode is that of feed-controlled operation[13] where the flow rate is determined by the capacity of either the hopper supplying the extruder or the feed section of the screw. An accurate analysis of solids conveying is clearly much more important in such a situation.

In the case of melt-fed machines, feed-controlled operation appears to be much more common. Such a mode of operation is readily observed in laboratory extruders[5]. With large hot melt extruders flow rates tend to be determined by feed section capacity[19], or possibly at high speeds by hopper flow capacity.

Design criteria

With the aid of existing methods of analysis it is possible to estimate the performance of a given extruder processing a particular polymer under known operating conditions. The next step towards improving the design or performance of this machine is to investigate the effects of changing, for example, the screw dimensions or the operating conditions. In order to do this effectively appropriate design criteria must be prescribed. Although the relative importance of these vary according to the application they are likely to include at least some of the following: (1) maximum output; (2) adequate mixing; (3) delivery temperature as uniform as possible and within prescribed limits; (4) minimum machine size and cost; (5) minimum power consumption; (6) maximum machine life. Such requirements are of course very interdependent and the last is concerned with mechanical design problems which are not considered here. Given the design constraints it is possible in principle to determine an optimum design and set of operating conditions. The few attempts that have been made to carry out such optimizations are based on relatively simple models of the extrusion process[120–122].

Extruder scale-up

One of the main uses for an analysis of overall machine performance is in predicting the behaviour of an extruder larger than those previously employed for a particular application. Even if performance cannot be reliably predicted from purely theoretical considerations it should at least be possible to scale-up the design of an existing machine. The earliest attempts to do this were based on simple isothermal Newtonian melt flow analyses[30,123]. When non-isothermal melt flow effects are included it is much more difficult to maintain similar conditions[14]. Recently, Yi and Fenner[124] have discussed the scale-up of plasticating extruders on the basis of melting performance using the Edmondson melting model. Pearson[125] has outlined a rational method for scaling-up which takes account of solids conveying, melting and melt flow.

SURGING IN EXTRUDERS

So far in this review only steady extrusion has been considered. In practice, however, surging (periodic fluctuation of flow rate and pressures) is sometimes a serious problem. Variations in melt temperatures associated with the pressure fluctuations have also been measured[1,126]. Attention is confined here to some of the apparent causes of such instabilities.

A thorough analysis of surging requires the retention of the time-dependent terms in the equations governing flow. Also, the viscoelastic nature of polymers is more important in unsteady flow. A simple analysis of transient viscoelastic melt flow in an extruder was presented by Chan *et al.*[127]. As in the case of steady flow, the early attempts to treat unsteady behaviour were confined to melt flow. For example, Kirby[128] examined the response of the melt flow in the metering section to small disturbances in the rate of melt supply. Both the analysis and laboratory experiments were concerned with essentially isothermal Newtonian flow. In an associated paper, Krueger[129] extended the experimental investigations to a more practical form of extruder. The main limitation of the approach is that only the tendency of the melt flow to amplify or damp out disturbances can be examined[53]. The cause of the disturbance is not elucidated.

Turning to the feed end of extruders, Lovegrove[62,70,71] showed that pressure fluctuations are unavoidably associated with the solids conveying process. These fluctuations occur at the same frequency as the screw rotation but may not be significant in magnitude compared to the overall pressures generated. Various types of mathematical model have been proposed for simulating the dynamic response of the melting process in a plasticating extruder[130,131]. Again, only the response rather than the cause is studied.

Many experimental investigations of the melting process have demonstrated a link between surging and the occurrence of solid bed break-up, which has already been discussed. The frequencies of pressure fluctuations and bed break-up are very similar[83,84]. Klein[104] reported another form of surging associated with wedging of the solid bed in the taper of the screw channel.

There appear to be at least three different types of surging occurring at different frequencies[72,84,104]: (1) variations associated with the rotation of the screw, particularly due to the solids conveying process, and occurring at the same frequency; (2) fluctuations due to instabilities in the melting process and occurring at rather lower frequencies; (3) very slow fluctuations over periods of minutes or even hours caused by instabilities in the temperature control systems or changes in the environment. The second of these is probably the most commonly encountered, and is often difficult to eliminate. Maddock[126] demonstrated experimentally the advantages of screw cooling for this purpose, but was not able to explain why. As already discussed, more recent work has shown that screw cooling inhibits solid bed break-up by delaying the formation of a melt film between the bed and the screw.

CONCLUSIONS

Considerable advances have been made over the last two decades towards a thorough understanding of the single screw extrusion process for polymeric materials. Analyses have been developed for the three main regions within an extruder which are both realistic in their treatment of flow behaviour and sufficiently economical to be used routinely in studying machine design and performance. For the melt flow region a two-dimensional analysis of developing non-isothermal non-Newtonian flow appears to be satisfactory for most practical purposes. The solids conveying region is generally less important and is usually adequately treated by an analysis which assumes plug flow of the compacted polymer. A one-dimensional solution of this type is often satisfactory, while a two-dimensional solution provides a more realistic treatment of the initiation of pressure in the plug. In the special case of melt-fed extruders there is a lack of information on flow in the hopper and feed section which often determine the flow rate through the machine.

Melting in an extruder is best represented by a theoretical model which allows deformation of the solid bed both in the plane of the screw channel cross-section and in the downstream direction. The best choices of some of the detailed assumptions in models of this type have yet to be determined. Probably the main deficiency of existing melting models is their inability to cope adequately with the later stages of melting, both in the treatment of the melt pool which gradually widens to fill the channel, and in the analysis of melting after solid bed break-up has occurred. There would appear to be a need for a fundamental analysis of melting which does not assume a particular melting mechanism. This need is emphasised by reports of a different mechanism in extruders larger than those normally used in experimental investigations.

There is a severe shortage of published experimental data obtained from large extruders. For reasons of cost most serious experimental work is carried out on laboratory machines whose sizes are at the lower end of the range normally used by processors and polymer manufacturers. Most production machines are not sufficiently well instrumented and it is often not practical to employ screw extraction procedures developed for small machines.

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