Computer Aided Design of Plasticating Screws

Programs in FORTRAN and BASIC

by Natti S. Rao

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Preface

Plasticating extrusion is one of the most widely used processes for processing polymers. However, the design of the plasticating screw, the most important part of the extruder is still carried out largely on a trial and error basis. This empirical method not only involves high costs, particularly when the machine size is large, but also does not allow any optimisation of the screw geometry on a scientific basis.

Based on proven mathematical models developed in industry and universities this book presents programs in FORTRAN and BASIC for designing and optimising screws of any geometry as applied to today's high output single screw extrusion and injection molding.

Starting from programs for fitting the thermodynamic data of polymers detailed programs are given for storing rheological properties of polymer melts obtained from measurements of melt viscosity. The melt flow behaviour is described by different relationships currently used in practice.

A general equation for calculating the output of an extruder as a function of resin and screw geometry is proposed and its application demonstrated through an example.

The solids content of the extrudate according to the melting model of Tadmor is used to characterize the quality of melt at the end of extrusion. Programs for calculating the melting profiles of single screw extruders and those of reciprocating screws employed in injection molding machines are presented with detailed worked-out examples.

The possibility of predicting the output of an extruder and characterising the melt by means of the solid bed profile provides the basis for optimising the screw geometry for different operating conditions. To illustrate this approach to solve practical problems detailed simulations of screw geometries with input and output are presented for a couple of problems, so that the user will have no difficulty in using the programs for his requirements.

This work arose during the author's tenure as visiting professor at the Indian Institute of Technology, Madras, India. Particular thanks are due to Miss Anuradha for her assistance in performing the programming work. The author is also pleased to thank Dr. Helmut Muenstedt of BASF AG for fruitful discussions.

Natti S. Rao

Contents

1. Conventional Methods of Designing Plasticating Screws

The processing of thermoplastic resins involves creating a melt from a resin which is initially in the solid state. The quality of the part made from the melt depends on the homogenity of the melt which in turn is closely related to the geometry of the screw. Thus it is essential to use a screw which is best suited to the given properties of the resin and operating conditions of the extruder.

The usual method of designing a screw is empirical and based on trial and error. The screw is designed on the basis of data gathered over years and tested. If the experiment does not give the expected result, certain geometrical changes are made on the screw and the experiment repeated. In this way the screw is more or less, so to say, fitted to the resin concerned. Although this method can lead to positive results, the experimental effort involved can be considerable. The cost of experimentation can be indeed very high when the screw diameter is large, for example in the range of 200 mm or 250 mm. Furthermore this method has no scientific background and can neither be scaled up or down with certainity.

Quality products can be made from resins by structuring them through controlled processing which requires a homogeneous melt at a uniform temperature. This can be accomplished only by an accurately designed screw. Here again the trial and error method has serious limitations.

2. Computer Aided Design of Plasticating Screws

The general steps involved in designing any machine element used for polymer processing with computers can be outlined as follows:

1 Forming a physical picture of the process
2 Mathematical formulation of the physical process (model)
3 Putting the model into the computer language (program)
4 Testing the program with various input variables on a computer (process simulation)
5 Evaluation of output data and comparison with physical picture
6 Checking the computer predictions with experiment
7 Feedback of experimental results into the model (improvement of model)

The development of physically meaningful mathematical models [3] has put the design of plasticating screws on a scientific basis. Employing the above procedure outlined the successful application of these models using high speed digital computers to practical screw design problems has been reported in the work [2]. As explained therein the Tadmor model [3] traces the history of the melt from its origin to the end of screw, enabling one to calculate the melting process all along the screw. The calculation of solid bed profile or melting profile gives a picture of how solids are being converted into melt in the extruder. Knowledge of the necessary changes in the screw geometry to be made in order to attain complete and uniform melting can be therefore gained from the melting profile according to Tadmor model [2], [3].

2.1 Extrusion Screws

Plascticating screws used in modern high output extrusion are in most cases multistage screws with shearing and mixing devices with diameters in the range of 150 mm to 250 mm (Fig. 2.1) [1]. The positioning of a shearing device requires the knowledge of the melting profile which can be obtained only by simulating the melting process on a computer, as will be shown in Chapter 4. It is also necessary to know the solids content of the extrudate at the inlet of the mixer. If this value is too high, the mixer may not be able to plasticate the resin completely and the melt would be inhomogeneous. This information can again be had only through computer aided screw design which also gives melt temperature and pressure along the screw [2].

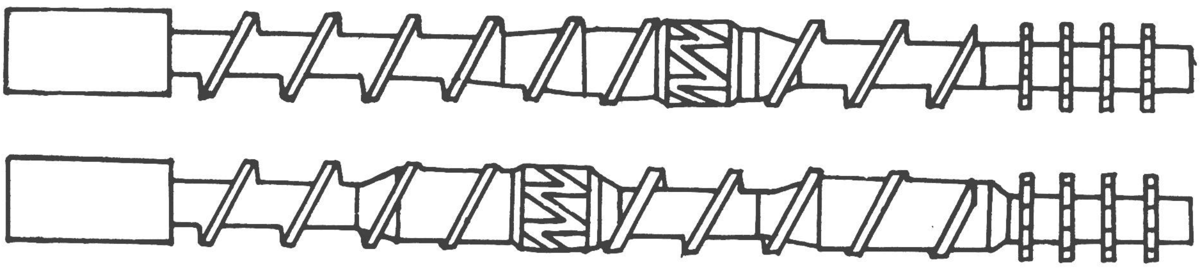

Fig. 2.1 Multistage screws with shearing and mixing devices [1]

2.2 Injection Molding Screws

The reciprocating screws used in injection molding machines are usually of the three zone type having feed, compression and melting zones, the aim of which is to convey the solids, melt the resin and supply a homogeneous melt to the mold. The plasticating process during the screw rotation is a time dependent extrusion process and can be described by a modified melting model developed by Donovan [4]. A brief description of the melting process in an injection molding screw according to Donovan [4] is given in Chapter 5.

3. Polymer Properties Required for Designing Screws

Designing screws by computer modelling requires the knowledge of the properties of polymers, particularly those of polymer melts. These can be classified mainly as thermodynamic and rheological properties.

3.1 Thermodynamic Properties

Important thermodynamic properties necessary for design calculations are:

specific heat c_p
enthalpy h
thermal conductivity k
and
specific volume v

of the polymer as functions of termperature and in the case of specific volume of pressure as well.

The thermodynamic properties do not vary much within a particular class of thermoplastic resins. Taking for example LDPE the thermal properties are approximately the same, whether it is LDPE of low or high melt flow index.

3.1.1 Fitting Thermodynamic Properties of Polymers by Polynomials

Designing with computers makes it necessary that the data of polymer properties are readily available in the computer when design calculations are in progress.

For sufficiently accurate dimensioning of machine elements these data are required as functions of at least one variable like temperature. This means that the whole functions have to be stored in the computer. This is done by curve fitting the measured data by means of regression analysis. The regression coefficients occurring in the equation for a measured curve characterize the polymer with respect to the measured property concerned. These coefficients can be stored in the computer for any polymer and retrieved for use in design problems. By incorporating the equations for the properties concerned in a program the dependence of any property on a variable like temperature can then be taken into account in the calculation on the basis of these coefficients. The following procedure illustrates this method:

The thermodynamic properties mentioned above can be described for the melt state of the resin by the following equations [5] with sufficient accuracy:

$$c_p(T) = A(0)c_p + A(1)c_p \cdot T + A(2)c_p \cdot T^2 \quad (3.1.1)$$
$$h(T) = A(0)_h + A(1)_h \cdot T + A(2)_h \cdot T^2 \quad (3.1.2)$$
$$k(T) = A(0)_k + A(1)_k \cdot T + A(2)_k \cdot T^2 \quad (3.1.3)$$

where T is temperature in °C, $A(0)c_p$, $A(1)c_p$ and so one are empirical coefficients. An equation of the form [13]

$$v = A(0)_v + A(1)_v \cdot p + A(2)_v \cdot T + A(3)_v \cdot T \cdot p \quad (3.1.4)$$

is found to be useful to express the relationship between specific volume v in cm^3/g, pressure p in bar and temperature T in °C. The coefficients occurring in the equations above can be found by multiple linear regression from the measured data.

The program in its general form will fit an equation of the type

$$y = a_0 + a_1x_1 + a_2x_2 + \dots a_mx_m \quad (3.1.5)$$

and prints the coefficients a_0, a_1 and so on for the best fit.

3.1.2 Program for Fitting Thermodynamic Data by Regression with Examples

The listing given in Fig. 3.1 finds the above mentioned coefficients in the Eqns. (3.1.1) to (3.1.4). The data fields for input are shown in Fig. 3.2 and Fig. 3.3. Examples of input data and printout of the computer are given in Chapter 6 on BASIC programs.

Fig. 3.1 Program for fitting thermodynamic data by regression polynomials (continued on page 12)

```
C
C       POLYNOMIALS FOR
C       SPECIFIC VOLUME
C       SPECIFIC HEAT
C       ENTHALPY
C       THERMAL CONDUCTIVITY
C
        DIMENSION X(100),D(7),E(6),A(6,7)
     10 READ(1,1000,END=999) M,N,KENN
        M1=M+1
        M2=M+2
        DO 20 I=1,M2
        D(I)=0.
        DO 20 J=1,M1
     20 A(J,I)=0.
        MEIN=M1
        IF(KENN.NE.0) MEIN=2
        DO 40 K=1,N
        READ(1,1100)(X(I),I=1,MEIN)
        X(M1)=FUNKY(X(MEIN))
        IF(KENN.EQ.0) GOTO 30
        X(1)=FUNKX(X(1))
        DO 25 I=2,M
     25 X(I)=X(I-1)*X(1)
     30 D(M2)=D(M2)+X(M1)**2
        D(1)=A(1,M2)+X(M1)
        A(1,M2)=D(1)
        DO 40 I=1,M
        I1=I+1
        A(I1,1)=A(1,I1)+X(I)
        A(1,I1)=A(I1,1)
        D(I1)=A(I1,M2)+X(I)*X(M1)
        A(I1,M2)=D(I1)
        DO 40 J=I,M
        J1=J+1
        A(I1,J1)=A(I1,J1)+X(I)*X(J)
     40 A(J1,I1)=A(I1,J1)
        A(1,1)=N
        DO 50 I=2,M1
     50 E(I)=A(1,I)
        DO 110 IS=1,M1
        DO 60 IT=IS,M1
        IF(A(IT,IS).NE.0.) GOTO 70
     60 CONTINUE
        WRITE(3,3000)
        STOP
     70 DO 80 J=1,M2
        B=A(IS,J)
        A(IS,J)=A(IT,J)
     80 A(IT,J)=B
        C=1./A(IS,IS)
        DO 90 J=1,M2
     90 A(IS,J)=C*A(IS,J)
        DO 110 IT=1,M1
        IF(IT.EQ.IS) GOTO 110
        C=-A(IT,IS)
        DO 100 J=1,M2
    100 A(IT,J)=A(IT,J)+C*A(IS,J)
    110 CONTINUE
        WRITE(3,3100)
        DO 120 IT=1,M1
        I1=IT-1
    120 WRITE(3,3200) I1,A(IT,M2)
```

```
      GOTO 10
  999 STOP
C
C     FORMATE
C
 1000 FORMAT(3I5)
 1100 FORMAT(6E13.0)
 3000 FORMAT('1END   OF   ITERATION      ')
 3100 FORMAT('1')
 3200 FORMAT('0A(',I2,') =',E16.8)
      END
```

```
                    FUNKX

 FUNCTION FUNKX(X)
 FUNKX=X
 RETURN
 END
```

```
                    FUNKY

 FUNCTION FUNKY(Y)
 FUNKY=Y
 RETURN
 END
```

Fig. 3.1

Degree of the Polynomial	m	columns 1 - 5
Number of data points	n	columns 6 - 10
Program selection number		columns 11 - 15

m = 2, if the data points are to be fit by a second degree polynomial. The program selection number is 1 for m = 2. Only for a fit with a straight line (m = 1) it is zero. The number of data points is limited to 100 and the number of variables or degree of the polynomial to 5.

Right-justified data entry without decimal point

First card

Temperature	T (°C)	columns 1 - 13
Specific heat	c_p (KJ/kg·K)	columns 14 - 26
or		
Enthalpy	i (KJ/kg)	columns 14 - 26
or		
Thermal conductivity	k (W/m·k)	columns 14 - 26

Right-justified data entry in exponential format

Second and following cards

Fig. 3.2 Input data fields for thermal properties as functions of temperature according to the program in Fig. 3.1

Number of variables	m	columns 1 - 5
Number of data points	n	columns 6 - 10
Program selection number		columns 11 - 15

The values to be input for m and the program selection number are 3 and 0 respectively. The number of data points is limited to 100.

Right-justified data entry without decimal point

First card

Pressure	p (bar)	columns 1 - 13
Temperature	T (^{o}C)	columns 14 - 26
Product	T·p (^{o}C·bar)	columns 27 - 39
Specific volume	v (cm^3/g)	columns 40 - 52

Right-justified data entry in exponential format

Second and following cards

Fig. 3.3 Input data fields for the program specific volume as a function of temperature and pressure in Fig. 3.1

3.2 Rheological Properties

Analysis for the flow behaviour of melt in the screw provides the basis for designing plasticating screws. This analysis necessitates the knowledge of the rheological properties of the melt, above all the shear viscosity, which is defined as

$$\eta = \frac{\tau}{\gamma} \qquad (3.1.6)$$

where η is shear viscosity, τ is shear stress and γ is the shear rate. The viscosity η as a function of apparent shear rate instead of true shear rate is sufficiently accurate to characterize the flowability of melt for design purposes.

3.2.1 Relationships for Melt Viscosity

The theories developed for modelling viscosity [6] have led to different relationships for calculating viscosity. Of these the following are recommended for use in design work owing to their accuracy in reproducing the melt flow curves: The Muenstedt polynomial [7] is given by

$$\log \eta = \log a_T + A_0 + A_1 \log (a_T \gamma) + A_2 (\log (a_T \gamma))^2 + A_3 (\log (a_T \gamma))^3 + A_4 (\log (a_T \gamma))^4 \qquad (3.2.1)$$

with η in (Pa. s) and γ in (sec^{-1}). The shift factor a_T for polyolefines is

$$a_T = b_1 (T_0) \exp (b_2/T) \qquad (3.2.2)$$

where b, and b_2 are constants, T and T_0 are melt and reference temperature (K) respectively. The shift factor a_T for styrene polymers is derived from the WLF – equation and can be written as

$$\log a_T = \frac{-c_1 (T-T_0)}{c_2 + (T-T_0)} \qquad (3.2.3)$$

where c_1 and c_2 are constants, T and T_0 are melt and reference temperatures (°C) respectively.

The Klein viscosity function [8], which is a regression fit for the measured data is given by

$$\ln \eta = a_0 + a_1 \ln \gamma + a_{11} (\ln \gamma)^2 + a_2 T + a_{22} T^2 + a_{12} (\ln \gamma) \cdot T \qquad (3.2.4)$$

with η in $lb_f \cdot sec/in^2$, γ in sec^{-1} and T in °F.

The Carreau equation [9] can be represented as

$$\eta = \frac{A\, a_T}{(1 + B\, a_T \gamma)^C} \qquad (3.2.5)$$

with η in (Pa. s) and γ in (sec^{-1}). The shift factor a_T is calculated from Eqns. (3.2.2) and (3.2.3).

3.2.2 Determining the Coefficients in Muenstedt Polynomial for Melt Viscosity with an Example

The coefficients in the Muenstedt polynomial, Eq. (3.2.1) can be obtained from the regression program given in Fig. 3.1. In the program listing shown in Fig. 3.4 the necessary transformations to find A_0 to A_4 in Eq. (3.2.1) directly have already been made, so that the measured data can be input according to the instructions shown in Fig. 3.5. The numerical example in Fig. 6.5 given for the corresponding BASIC program for determining the coefficients in Muenstedt polynomial in Chapter 6 shows sample input and output data.

```
C
C     DETERMINATION OF THE COEFFICIENTS OF VISCOSITY
C
      DIMENSION X(100),D(7),E(6),A(6,7)
   10 READ(1,1000,END=999) M,N,KENN
      M1=M+1
      M2=M+2
      DO 20 I=1,M2
      D(I)=0.
      DO 20 J=1,M1
   20 A(J,I)=0.
      MEIN=M1
      IF(KENN.NE.0) MEIN=2
      DO 40 K=1,N
      READ(1,1100)(X(I),I=1,MEIN)
      X(M1)=FUNKY(X(MEIN))
      IF(KENN.EQ.0) GOTO 30
      X(1)=FUNKX(X(1))
      DO 25 I=2,M
   25 X(I)=X(I-1)*X(1)
   30 D(M2)=D(M2)+X(M1)**2
      D(1)=A(1,M2)+X(M1)
      A(1,M2)=D(1)
      DO 40 I=1,M
      I1=I+1
      A(I1,1)=A(1,I1)+X(I)
      A(1,I1)=A(I1,1)
      D(I1)=A(I1,M2)+X(I)*X(M1)
      A(I1,M2)=D(I1)
      DO 40 J=I,M
      J1=J+1
      A(I1,J1)=A(I1,J1)+X(I)*X(J)
   40 A(J1,I1)=A(I1,J1)
      A(1,1)=N
      DO 50 I=2,M1
   50 E(I)=A(1,I)
      DO 110 IS=1,M1
      DO 60 IT=IS,M1
      IF(A(IT,IS).NE.0.) GOTO 70
   60 CONTINUE
      WRITE(3,3000)
      STOP
   70 DO 80 J=1,M2
      B=A(IS,J)
      A(IS,J)=A(IT,J)
   80 A(IT,J)=B
      C=1./A(IS,IS)
      DO 90 J=1,M2
   90 A(IS,J)=C*A(IS,J)
      DO 110 IT=1,M1
      IF(IT.EQ.IS) GOTO 110
      C=-A(IT,IS)
      DO 100 J=1,M2
  100 A(IT,J)=A(IT,J)+C*A(IS,J)
  110 CONTINUE
      WRITE(3,3100)
      DO 120 IT=1,M1
      I1=IT-1
  120 WRITE(3,3200) I1,A(IT,M2)
      GOTO 10
  999 STOP
C
C     FORMATE
```