Chung Model

A melting model of an extruder has been developed based on experimental results by a unique simulative apparatus called “screw simulator” and theoretical studies on them, by Mount, Chung et al. There were discussions about the adequacy of applying the knowledge from the screw simulator to real single screw extruders. Chung and coworkers persevered in their research, and published their achievements in book form [1].

A computer program, which simulates the melting process of a plasticating extruder using the model, is made. The simulation program seems to give reasonable results judging from some trial calculations.

Hereinafter, the model developed by Mount, Chung et al. is referred to as “Chung model” for the sake of simplicity.

1. Theory [1]

When analyzing the melting process by Chung model, the screw channel in Fig. 1 is unwrapped as shown in Fig. 2. This is the common treatment used in other models too.
In Fig.1 and Fig.2, \( H \) is the channel depth, \( W \) is the width of the screw channel perpendicular to the flights, \( D_0 \) is the barrel inside diameter (= the screw outer diameter), \( t \) is the screw pitch, \( e_s \) is the screw flight width along the screw axis, \( \phi \) is the helix angle of the screw flight, \( \theta \) is the solid conveying angle, \( x \) is rectangular coordinate (cross channel direction), \( y \) is rectangular coordinate (channel depth direction), \( z \) is rectangular coordinate (down channel direction) and \( \Delta z \) is the small distance of the solid bed in \( z \) direction.

When the solid bed is melted by viscous dissipation in a melt film, which exists between the barrel and the solid bed, the melting rate \( \Omega \) is

\[
\Omega = M \cdot \rho_m \cdot U_{sb} \quad \text{(1) [P.356, Nomenclature]}
\]

where \( M \) is the melting efficiency, \( \rho_m \) is the melt density and \( U_{sb} \) is the relative velocity of the solid bed to the barrel.
The solid bed width $X_0$ is the solid bed width measured along the direction of the solid bed movement relative to the barrel and $\sigma$ is the reduced pressure. $G(a)$, $H(a)$ and $A$ are given in Eq. (11), (13), (14) below.

When neglecting the effect of pressure, $M$ becomes

$$M = \left( \frac{\delta_0}{X_0} \right) \cdot \left\{ \frac{A}{G(a)} + \sigma \cdot H(a) \cdot A^3 \right\} \quad \text{(3) [P. 231, (4.142)]}$$

The solid bed velocity on the barrel $U_{sb}$ is given

$$U_{sb} = \frac{\pi ND_0}{\sin \theta} \cdot \frac{\sin \phi}{\sin(\theta + \phi)} \quad \text{(4) [P. 201, (4.3)]}$$

where $N$ is the rotational speed of the screw.

The volumetric solid conveying rate $Q_s$ is expressed in terms of the solid conveying angle $\theta$, the screw geometry and the screw speed $N$.

$$\frac{Q_s}{N} = \pi \cdot W \cdot H \cdot (D_0 - H) \cdot \frac{\sin \theta}{\sin(\theta + \phi)} \quad \text{(5) [P. 175, (4.5)]}$$

The solid conveying angle $\theta$ is found by iteration using the above Eq. (5).

The solid bed width $W_s$ becomes smaller than $W$ as melting proceeds, then the following Eq. (5a) shall be applied.

$$\frac{Q_{ss}}{N} = \pi \cdot W_s \cdot H \cdot (D_0 - H) \cdot \frac{\sin \theta}{\sin(\theta + \phi)} \quad \text{(5a)}$$

where $Q_{ss}$ is the mass flow rate of the solid bed, and not equal to the total solid conveying rate $Q_s$.

From Eq. (5a),
The characteristic melt film thickness $\delta_0$ is given as follows:

$$ W_s = \frac{Q_{ss}}{\pi \cdot N \cdot H \cdot (D_0 - H) \cdot \frac{\sin \theta}{\sin(\theta + \varphi)}} $$  \hspace{1cm} (5b)

$$ \delta_0 = \sqrt{\frac{k_m \cdot (T_b - T_f) \cdot X_0}{\rho_m \cdot \Delta H \cdot U_{sb}}} $$  \hspace{1cm} (6) \hspace{1cm} [P. 226, (4.102b)]

where $k_m$ is the thermal conductivity of the melt, $T_b$ is the barrel temperature, $T_f$ is the melting point of the polymer and $\Delta H$ is the enthalpy necessary to convert the solid to the melt at $T_f$. The solid bed width $X_0$ at the start is

$$ X_{0,\text{start}} = \frac{W}{\sin(\theta + \varphi)} $$  \hspace{1cm} (7) \hspace{1cm} [P. 201, (4.44)]

When the solid bed width $W_s$ becomes smaller than $W$, then the following Eq. (7a) shall be applied.

$$ X_0 = \frac{W_s}{\sin(\theta + \varphi)} $$  \hspace{1cm} (7a)

The reduced pressure $\sigma$ is

$$ \sigma = \frac{\delta_0^2 \cdot P_0}{\eta_0 \cdot U_{sb} \cdot X_0} $$  \hspace{1cm} (8) \hspace{1cm} [P. 357, Nomenclature]

where $P_0$ is the local pressure. The characteristic viscosity $\eta_0$ is given by making the reference temperature $T_0 = T_b$ and $T = T_b$ in the following power-law equation.

$$ \eta = m_0 \cdot \exp[-b(T - T_0)] \cdot \dot{\gamma}^{(n-1)} $$  \hspace{1cm} (9) \hspace{1cm} [P. 223, (4.89b)]

$$ \eta_0 = m_0 \Big|_{T_b} \left( \frac{U_{sb}}{\delta_0} \right)^{n-1} $$  \hspace{1cm} (10) \hspace{1cm} [P. 356, Nomenclature]

where $m_0$, $n$, $b$ are the power-law constants and $\dot{\gamma}$ is the shear rate. It will be appropriate to fit the above power-law equation over the range of about 10 to 1000 1/s.
When calculating $\eta_0$, the following Eq. (10a) can be used too.

$$\eta_0 = m_0 \cdot \exp[-b(T_b - T_0)] \left( \frac{U_{sb}}{\delta_0} \right)^{(n-1)} \quad (10a)$$

$H(a)$, $G(a)$ and $A$ are given by the following equations.

$$G(a) = \frac{a \cdot (1 - e^a)}{a + 1 - e^a} \quad (11) \quad [P. 231, (4.139)]$$

$$a = \frac{b \cdot (T_b - T_f)}{n} \quad (12) \quad [P. 357, Nomenclature]$$

where $b$ is the power-law constant in Eq. (9).

$$H(a) = \frac{(1 - e^{-a})^2 - a^2 \cdot e^{-a}}{a^3 \cdot (1 - e^{-a})} \quad (13) \quad [P. 233, (4.149)]$$

$$A = \sqrt{\frac{2G(a)}{5/6 \cdot Gr} \ln \left[ \frac{5}{6} \cdot G_r \cdot \left( 1 + \frac{B_r}{2} \right) \right]} \quad (14) \quad [P. 232, (4.144)]$$

Graetz number and Brinkman number are

$$G_r = \frac{\delta_0^2 \cdot U_{sb} \cdot \rho_m \cdot C_{pm}}{k_m \cdot X_0} \quad (15) \quad [P. 357, Nomenclature]$$

$$B_r = \frac{\eta_0 \cdot U_{sb}^2}{k_m \cdot (T_b - T_f)} \quad (16) \quad [P. 357, Nomenclature]$$

In Eq. (16), when the unit of $\eta_0$ is Pa·s and the unit of $k_m$ is cal/cm·s·°C, the following equation should be used.

$$B_r = 2.389 \times 10^{-7} \frac{\eta_0 \cdot U_{sb}^2}{k_m \cdot (T_b - T_f)} \quad (16a)$$

When the unit of $\eta_0$ is g-force·s/cm² and the unit of $k_m$ is cal/cm·s·°C, the
The following equation should be used.

\[
B_r = \frac{2.343 \times 10^{-5}}{k_m \cdot (T_b - T_f)} \eta_0 \cdot U_{sb}^2
\]  (16b)

The enthalpy necessary to convert the solid to the melt \( \Delta H \) is

\[
\Delta H = C_{ps} \cdot (T_f - T_s) + \lambda
\]  (17)  [P. 215, (4.79)]

where \( C_{ps} \) is the specific heat of the solid, \( \lambda \) is the heat of fusion and \( T_s \) is the solid temperature.

Chung model assumes that the melting starts at the point where the solid bed is fully compacted. Before that point, the melt of \( T_f \) that comes from the melt film developed between the barrel and the solid bed, penetrates into the solid bed and fills the void between polymer pellets. At the point where the melting starts, the compaction factor \( C = 1 \), and the solid bed temperature is raised from the initial solid temperature \( T_{s0} \) to \( T_{ss} \). After the start point of melting, the solid bed temperature is kept constant. \( T_{ss} \) may be calculated as follows:

\[
T_{ss} = C_0 \cdot T_{s0} + (1 - C_0) \cdot T_f + \frac{(1 - C_0)}{C_{ps}} \cdot \lambda
\]  (18)

where \( C_0 \) is the compaction factor at the inlet of the extruder. The general expression of the compaction factor \( C \) is

\[
C = \frac{\rho_{sb}}{\rho_s}
\]  (19)  [P. 355, Nomenclature]

where \( \rho_s \) is the solid density and \( \rho_{sb} \) is the apparent density of the solid bed.

Volumetric melting rate of the solid bed during a small increment \( \Delta z \) is

\[
\Delta Q_s = \Omega \cdot W_s \cdot \Delta z / \rho_s
\]  (20)

It is known that the profile of the barrel temperature \( T_b \) can be described by the
following equation [2, 3].

\[ T_b = B_0 \cdot (1 - B_1 \cdot e^{-B_2 \cdot l}) \]  \hspace{1cm} (21)

where \( B_0, B_1, B_2 \) are constants and \( l \) is the axial distance of the screw from the beginning of melting starts.

Using the above-described equations, the changing process of the solid bed width etc. during melting can be simulated.

The motor power for the melting zone is calculated as follows. Not considering the shear stress between the barrel surface and screw flight, and the shear stress on the barrel surface over the melt pool, only the shear force \( F_s \) on the barrel by the shear stress over the solid bed is considered here.

\[ F_s = \tau_s \cdot A_s \]  \hspace{1cm} (22) \hspace{1cm} [P.277, (4.227a)]

where \( \tau_s \) is the shear stress on the barrel surface over the solid bed and \( A_s \) is the area of the solid bed in contact with barrel surface.

The shear stress \( \tau \) along the solid bed velocity \( U_{sb} \) is

\[ \tau = S \cdot \tau_0 \]  \hspace{1cm} (23) \hspace{1cm} [P.214, (4.76)]

where \( \tau_0 \) is the reference shear stress of the polymer melt measured at \( T_b \) and shear rate \( \dot{\gamma} = 1 \). From Eq. (10) and (10a) \( \tau_0 \) is expressed by

\[ \tau_0 = m_0 \exp[-b(T_b - T_0)] \]  \hspace{1cm} (24)

The stress efficiency \( S \) is

\[ S = \left( \frac{U_{sb}}{\delta_1} \right)^n \cdot \left( \frac{a}{A \cdot (1 - e^{-a})} \right)^n \cdot \left( \frac{2}{2 - n} \right) \]  \hspace{1cm} (25) \hspace{1cm} [P.232, (4.148)]

\[ \delta_1 = \delta_0 \cdot \left[ \frac{(1 + 4\sigma)^{1/2} - 1}{2\sigma} \right] \]  \hspace{1cm} (26) \hspace{1cm} [P.233, (4.150)]

When not considering the effect of pressure, \( S \) becomes
\[ S = \left( \frac{U_{sh}}{\delta_0} \right)^n \cdot \left( \frac{a}{A \cdot (1 - e^{-a})} \right)^n \cdot \left( \frac{2}{2 - n} \right) \]  

(27)  

[P.232, (4.143)]

Form Eq. (22) and (23), the shear force \( \Delta F_s \) for a small increment \( \Delta z \), along the direction of the screw rotation, can be expressed

\[ \Delta F_s = S \cdot \tau_0 \cdot \cos \theta \cdot W_s \cdot \Delta z \]  

(28)

The motor power \( \Delta M_p \) for the same increment is

\[ \Delta M_p = \Delta F_s \cdot U_s \]  

(29)

where \( U_s \) is the screw velocity.

When calculating the motor power by Eq. (29), adjustment of units shall be considered. When the unit of \( \tau_0 \) in Eq. (28) is Pa and that of \( \Delta M_p \) is W, Eq. (29) becomes

\[ \Delta M_p = 1.0 \times 10^{-6} \Delta F_s \cdot U_s \]  

(29a)

when the unit of \( \tau_0 \) is G/cm² and that of \( \Delta M_p \) is W, Eq. (29) becomes

\[ \Delta M_p = 9.8 \times 10^{-5} \Delta F_s \cdot U_s \]  

(29b)

The screw velocity \( U_s \) is

\[ U_s = \pi N D_0 \]  

(30)

Using the above equations the motor power for melting the solid bed can be calculated.
2. Computer program

Simulation program itself is not so complicated, and a brief flow chart is shown in Fig. 3.

![Fig.3 Program flow chart](image)

- Start
  - Calculate solid bed temperature, solid conveying angle, solid conveying rate etc., where melting starts
  - Start calculation for a small increment of z-direction: \(X_0, \delta_0, M, \Omega\) etc. at inlet of the increment
  - Calculate values at the outlet of the increment: \(Q_s, W_s\) etc.
  - End of screw or solid bed width becomes very small?
    - No
    - Yes
      - Write results
  - End
3. Example

The Chung model simulation is carried out for extruding PET under the following conditions.

Screw diameter \( D_0 \) (cm) = 15.0
Turns of feed zone = 10.0
Turns of compression zone = 6.0
Turns of metering zone = 8.7
Turns of delay in melting = 5.0
Depth of feed zone channel \( H_f \) (cm) = 1.40
Depth of metering zone channel \( H_m \) (cm) = 0.40
Screw pitch \( t \) (cm) = 15.0
Flight width \( e_s \) (cm) = 1.50
Number of revolution \( N \) (rpm) = 38.0
Output \( G \) (kg/hr) = 300.0
Barrel temperature parameter \( B_0 \) (°C) = 290.0
Barrel temperature parameter \( B_1 \) = 0.0
Barrel temperature parameter \( B_2 \) = 0.0
Viscosity equation meter \( m_0 \) = 2.052
Viscosity equation parameter \( b \) = 3.600E-02
Viscosity equation parameter \( n \) = 0.835
Viscosity equation parameter \( T_0 \) (°C) = 290.0
Density of solid \( \rho_s \) (g/cm\(^3\)) = 1.34
Density of melt \( \rho_m \) (g/cm\(^3\)) = 1.20
Specific heat of solid \( C_{ps} \) (cal/g·°C) = 0.40
Heat of fusion \( \lambda \) (cal/g) = 17.7
Specific heat of melt \( C_{pm} \) (cal/g·°C) = 0.48
Thermal conductivity of melt \( k_m \) (cal/s·cm·°C) = 0.000520
Melting point \( T_f \) (°C) = 265.0
Solid temperature at inlet \( T_{s0} \) (°C) = 30.0
Solid bed compaction factor at inlet \( C_0 \) = 0.60
Solid width ratio at start melting \( W_s / W \) = 1.0
(Note: viscosity unit is [G·s/cm\(^2\)])
Fig. 4 shows the calculation result.

Another example of simulation for extruding N66 is shown in Fig. 5.

4. Summary

To develop a simulation program based on Chung model is much easier than other models, such as Tadmor [2, 3] and Donovan model [4], and the simulation seems to give reasonable results. Both Chung and Donovan model give considerably different results from Tadmor model, but the reasons are not same.

The characteristic melt film thickness $\delta_0$, the melting efficiency $M$ etc. of Chung model are derived from experiments by the screw simulator, and mathematically
expressed. Using these values, the melting capacity of a screw extruder is obtained.

On the other hand, Donovan model is based on Tadmor model, but allows the solid bed to accelerate during melting by introducing SBAP (solid bed acceleration parameter), and takes into account the heat transfer from the screw by dealing the solid bed with finite thickness. These two points are the essential differences with Tadmor model. By some preliminary calculations, the present writer found that the effect of the latter point is rather bigger than that of the former.

It is interesting to note that Chung model gives similar results to Donovan model as shown in Fig. 4 and Fig. 5 in spite of the extremely different standpoints of these two models.

References