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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.

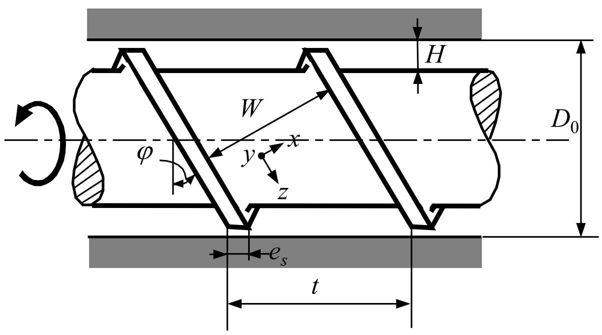

Fig.1 Screw channel geometry

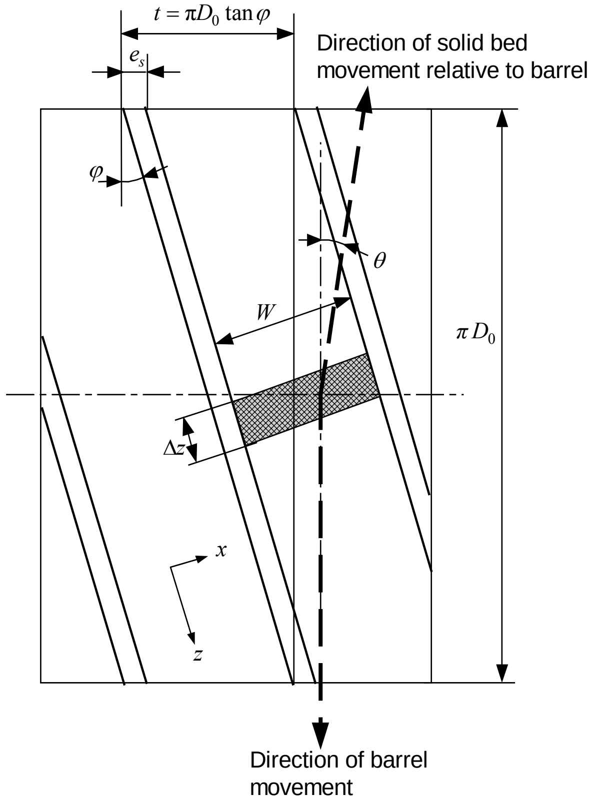

Fig.2 Unwrapped screw channel

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, φ is the helix angle of the screw flight, θ 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 Δz 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 Ω is

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

where M is the melting efficiency, ρ_m is the melt density and U_{sb} is the relative velocity of the solid bed to the barrel.

M is given as follows:

$$M = \left(\frac{\delta_0}{X_0}\right) \cdot \left\{\frac{A}{G(a)} + \sigma \cdot H(a) \cdot A^3\right\} \qquad (2) \qquad [P. 232, (4.147)]$$

where δ_0 is the characteristic melt film thickness, X_0 is the solid bed width measured along the direction of the solid bed movement relative to the barrel and σ 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

$$M = \left(\frac{\delta_0}{X_0}\right) \cdot \left\{\frac{A}{G(a)}\right\} \qquad (3) \qquad [P. 231, (4.142)]$$

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

$$U_{sb} = \pi N D_0 \cdot \frac{\sin\varphi}{\sin(\theta + \varphi)} \qquad (4) \qquad [P. 201, (4.3)]$$

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 θ, the screw geometry and the screw speed N.

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

The solid conveying angle θ 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.

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

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),

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

The characteristic melt film thickness δ_0 is give as follows:

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

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 ΔH is the enthalpy necessary to convert the solid to the melt at T_f. The solid bed width X_0 at the start is

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

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

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

The reduced pressure σ is

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

where P_0 is the local pressure. The characteristic viscosity η_0 is given by making the reference temperature $T_0 = T_b$ and $T = T_b$ in the following power-law equation.

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

$$\eta_0 = m_0\big|_{T_b} \cdot \left(\frac{U_{sb}}{\delta_0}\right)^{n-1} \qquad (10) \quad \text{[P.356, Nomenclature]}$$

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 η_0, the following Eq. (10a) can be used too.

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

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

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

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

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

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

$$A = \sqrt{\frac{2G(a)}{5/_6 \mathrm{Gr}} \cdot \ln\left[1 + \frac{5}{6} \mathrm{G_r} \cdot \left(1 + \frac{\mathrm{B_r}}{2} \right) \right]} \tag{14}$$ [P. 232, (4.144)]

Graetz number and Brinkman number are

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

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

In Eq. (16), when the unit of η_0 is Pa·s and the unit of k_m is cal/cm·s°·C, the following equation should be used.

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

When the unit of η_0 is g-force · s/cm^2 and the unit of k_m is cal/cm·s°·C, the following equation should be used.

$$\mathrm{B_r} = 2.343 \times 10^{-5} \frac{\eta_0 \cdot {U_{sb}}^2}{k_m \cdot \left(T_b - T_f\right)} \tag{16b}$$

The enthalpy necessary to convert the solid to the melt ΔH is

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

where C_{ps} is the specific heat of the solid, λ 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:

$$T_{ss} = C_0 \cdot T_{s0} + \left(1 - C_0\right) \cdot T_f + \frac{(1 - C_0)}{C_{ps}} \cdot \lambda \tag{18}$$

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

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

where ρ_s is the solid density and ρ_{sb} is the apparent density of the solid bed.

Volumetric melting rate of the solid bed during a small increment Δz is

$$\Delta Q_s = \Omega \cdot W_s \cdot \Delta z / \rho_s \tag{20}$$

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

$$T_b = B_0 \cdot (1 - B_1 \cdot \mathrm{e}^{-B_2 \cdot l}) \qquad (21)$$

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.

$$F_s = \tau_s \cdot A_s \qquad (22) \qquad [\text{P.277, (4.227a)}]$$

where τ_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 τ along the solid bed velocity U_{sb} is

$$\tau = S \cdot \tau_0 \qquad (23) \qquad [\text{P.214, (4.76)}]$$

where τ_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) τ_0 is expressed by

$$\tau_0 = m_0 \big|_{T_b} = m_0 \cdot \exp[-b(T_b - T_0)] \qquad (24)$$

The stress efficiency S is

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

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

When not considering the effect of pressure, S becomes

$$S=\left(\frac{U_{sb}}{\delta_0}\right)^n\cdot\left\{\frac{a}{A\cdot\left(1-e^{-a}\right)}\right\}^n\cdot\left(\frac{2}{2-n}\right) \qquad (27) \qquad [P.232, (4.143)]$$

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

$$\Delta F_s = S\cdot\tau_0\cdot\cos\theta\cdot W_s\cdot\Delta z \qquad (28)$$

The motor power ΔM_p for the same increment is

$$\Delta M_p = \Delta F_s\cdot U_s \qquad (29)$$

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 τ_0 in Eq. (28) is Pa and that of ΔM_p is W, Eq. (29) becomes

$$\Delta M_p = 1.0\times10^{-6}\Delta F_s\cdot U_s \qquad (29a)$$

when the unit of τ_0 is $\mathrm{G/cm^2}$ and that of ΔM_p is W, Eq. (29) becomes

$$\Delta M_p = 9.8\times10^{-5}\Delta F_s\cdot U_s \qquad (29b)$$

The screw velocity U_s is

$$U_s = \pi N D_0 \qquad (30)$$

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.

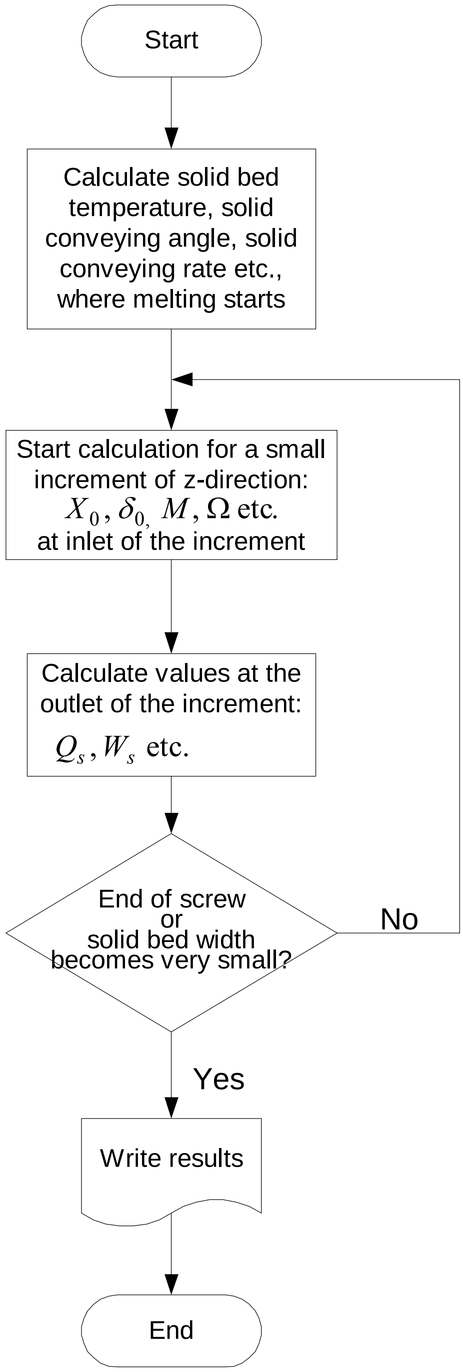

Fig.3 Program flow chart

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 metering	= 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 ($^\circ$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 ($^\circ$C)	= 290.0
Density of solid ρ_s (g/cm^3)	= 1.34
Density of melt ρ_m (g/cm^3)	= 1.20
Specific heat of solid C_{ps} (cal/g$\cdot^\circ$C)	= 0.40
Heat of fusion λ (cal/g)	= 17.7
Specific heat of melt C_{pm} (cal/g$\cdot^\circ$C)	= 0.48
Thermal conductivity of melt k_m (cal/s$\cdot$cm$\cdot^\circ$C)	= 0.000520
Melting point T_f ($^\circ$C)	= 265.0
Solid temperature at inlet T_{s0} ($^\circ$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$\cdot$s/cm^2])

Fig. 4 shows the calculation result.

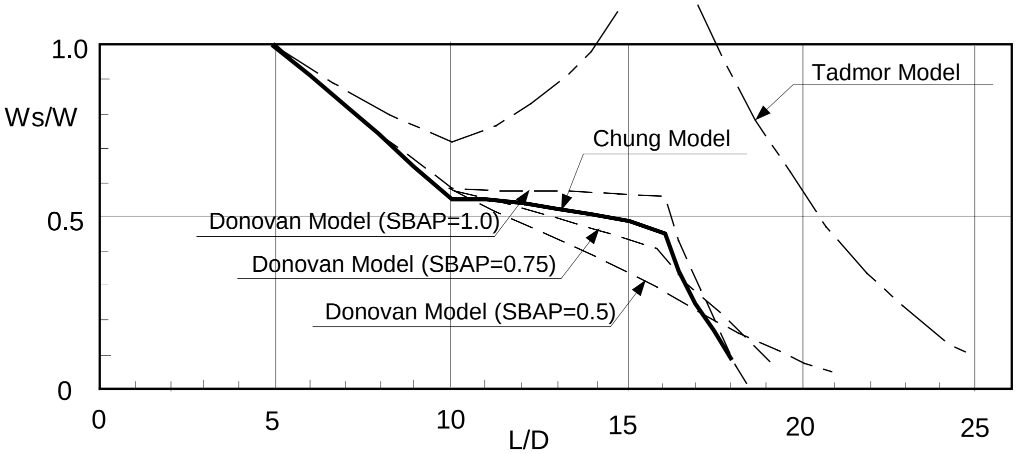

Fig.4 Solid bed profile (PET: 150ϕ, 300kg/hr, 38rpm)

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

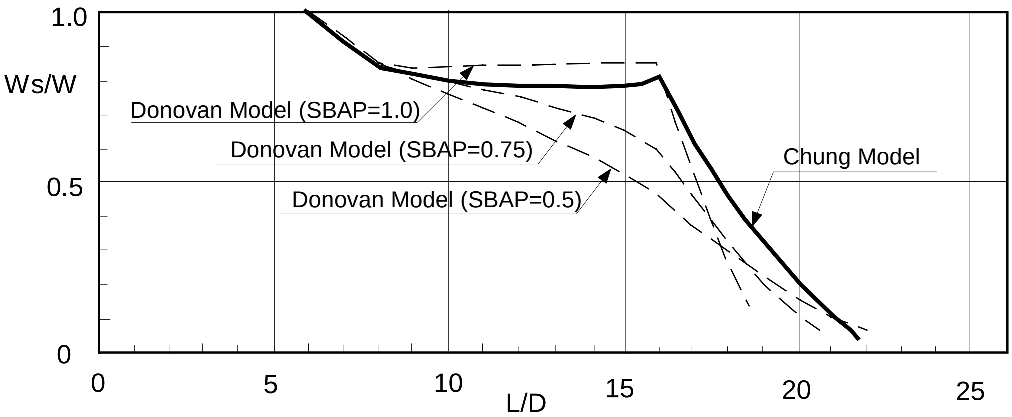

Fig.5 Solid bed profile (N66: 65ϕ, 57kg/hr, 52rpm)

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 δ_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

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