

Simulation of transient process in melting section of reciprocating extruder[☆]

K.L. Yung, Yan Xu^{*}, K.H. Lau

Department of Manufacturing Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, People's Republic of China

Received 6 February 2001; received in revised form 11 June 2001; accepted 11 June 2001

Abstract

Plastic injection molding machine that can be classified as reciprocating extruders are among the most widely used machines in industry. However, most studies in the injector design were based on steady state models developed for extruders that involved no reciprocation. This over-simplified model leaves out the most important aspect of reciprocation. The authors of this paper have derived a transient melting model that takes care of the change from the conventional steady extrusion to that of a discontinuous transient process. This paper describes simulations conducted on the derived model to explain observation that cannot be explained by the steady extrusion model in practical experiments. The simulation was conducted by using parameters given in Donovan's experiment [Polym Engng, 11 (1971) 353]. The simulation results are found to qualitatively match with the experimental results. It proves the validity of the model. Simulation has also been conducted with the model on materials that their viscosities are temperature and shear rate dependent. The result has shown that screw rotation speed, screw axial movement speed, barrel thickness, barrel heat capacity, temperature of heater and polymer are factors affecting the melting speed and the transient effects. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Simulation; Reciprocating extruder; Polymer

1. Introduction

The simulation study of extruders with no reciprocating movement were investigated by many scientists. Studies on reciprocating extruders commonly found in plastic injection molding machine were comparatively fewer although their usage is more popular in industry [2,3].

Until recently, many studies on the inline injection process take the simpler route by assuming a steady-state extrusion. This over simplification of the in-line injection process leaves out the most important aspect of reciprocation, which changes the process model from steady extrusion to that of a discontinuous transient process. It may be the reason why there have been very little studies on optimizing the design of the plastic injection assembly. Donovan did some experiments with reciprocating extruders [1], but he used steady-state model in his works [4] which cannot explain some phenomena he observed. Rauwendaal [2,3], studied the effects of axial screw move-

ment on solids and melt conveying in injection extruders. Dormeier [5] briefly discussed the melting process when screw stops in injection extruder. However, no studies were found on simulating the transient melting process when the screw is rotating (feeding stage).

In a typical reciprocating extrusion cycle, first the screw is in the forward position in the barrel. Then the screw begins to rotate (screw recharge) in order to convey plastic material forward and develops a pressure ahead of the screw until the desired volume of the molded part is reached. The screw is then stopped at the back position while the previously injected plastic cools down in the mold. After the mold opened and the part has been ejected, the mold closes again and the screw is forced forward by hydraulic pressure, causing the newly recharged shot at the head of the screw to flow into the empty mold. A valve, such as a check ring, prevents back flow during injection. The screw then maintains pressure on the molded plastic for a specific time (holding time). Hence, the whole injection cycle can be divided into three stages. They are feeding (screw rotating and moving backwards), stop (no screw movement), and injecting (screw moving forward without rotation). The screw itself is normally divided into three parts: solid conveying, melting, and melt conveying.

In this paper, simulation of the melting process was carried out at the feeding stage which was the most dynamic part of the cycle.

[☆] This paper was originally submitted to *Computational and Theoretical Polymer Science* and received on 6 February 2001; received in revised form on 11 June 2001; accepted on 11 June 2001. Following the incorporation of *Computational and Theoretical Polymer Science* into *Polymer*, this paper was consequently accepted for publication in *Polymer*.

^{*} Corresponding author. Tel.: +852-2766-6623; fax: +852-2362-5267.

E-mail address: drxuyan@bigfoot.com (Y. Xu).

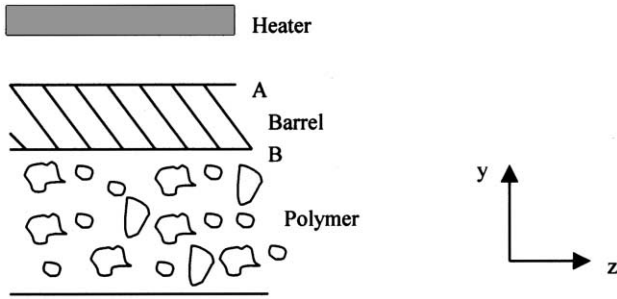


Fig. 1. Simplified structure.

2. Simulation model

The most important differences between reciprocating injector and non-reciprocating extruder are: firstly, the process in non-reciprocating extruder is continuous and stay in the steady-state over a long period of time, while processes in reciprocating extruder is short, and usually change to another stage (e.g. stop stage) before the steady-state is reached. Secondly, reciprocating extruder differs in the axial screw movement. If the model was built with coordinates of the barrel, this axial movement will only affect the velocity relationship.

To simulate the transient melting process, an analytical heat transfer model has to be developed according to the physical construction. In an injection molding machine, heat from the heater outside the barrel is transferred according to the following steps: from electric heater to fluid (air or oil), to barrel, then to polymer and screw (see Fig. 1). The heat transfer from polymer to screw can be neglected because of low heat diffusivity of the polymer. To simplify the problem, heat transfer in extruders is divided into two parts: from heater to interface of barrel and polymer, and from barrel–polymer interface to inside of polymer and cause the melting.

2.1. Heat transfer from heater to inner side of barrel

The first step in the study for the derivation of the model is to analyze the heat transfer from heaters to walls of the barrel. Assume that the barrel is a slab (Fig. 1), the heat fluxes from surface A to surface B is proportional to the temperature differences between the surface and the surrounding medium. The heater is normally surrounded by liquid (e.g. oil) and heat is transferred by convection and conduction. When the heater temperature is periodic, polymer temperature is constant and the temperature on surface B will be periodic. There will be a ‘time lag’ during the propagation of heat from outer surface A to inner surface B. The relationship between time lag and barrel heat capacity (as well as barrel thickness) is exponential [6].

When unheated polymers are being moved into the heating area, the problem becomes that of the changing polymer temperature and constant heater temperature initially at T_{b0} .

The temperature at surfaces A and B will decrease with time till it reaches a steady state. The following expression is used to describe the decrease in temperature.

$$T_b(z, t) = T_{st}(z) + (T_{b0}(z) - T_{st}(z)) e^{-At} \quad (1)$$

where z is the polymer moving direction, T_b is temperature at surface B and T_{b0} is the temperature at surface B before new polymer enters. T_{st} is steady-state temperature when $t \rightarrow \infty$. The coefficient A will be affected by the barrel thickness and barrel heat capacity. The greater the value of barrel thickness and heat capacity, the smaller will be the value of A .

In steady state, temperature at surface B will be in the form of a profile along the direction of z .

$$T_{st}(z) = T_{end} + (T_{s0} - T_{end}) e^{-Bz} \quad (2)$$

where T_{s0} is temperature at $z = 0$, T_{end} is temperature when $z \rightarrow \infty$, and coefficient B will depend on relative velocity of polymer and screw, barrel thickness and barrel heat capacity. The higher the relative velocity is the less the value of B is.

When the relative velocity between the barrel and the solid is $V_{bsz} = 0$, the steady-state temperature will be:

$$T'_{st}(z) = T_{end} \quad (3)$$

Transient temperature when $V_{bsz} = 0$ is:

$$T_b(z, t) = T_{end} + (T_{b0} - T_{end}) e^{-At}$$

so $B \propto A/V_{bsz}$.

When the screw is rotating, temperature at surface B will be (suppose $B = kA/V_{bsz}$) (from Eqs. (1) and (2)):

$$\begin{aligned} T_b(z, t) &= T_{st}(z) + (T_{b0}(z) - T_{st}(z)) e^{-At} \\ &= T_{end} + (T_{s0} - T_{end}) e^{-kAz/V_{bsz}} (1 - e^{-At}) \\ &\quad - (T_{end} - T_{b0}(z)) e^{-At} \end{aligned} \quad (4)$$

2.2. Heat transfer in melting film

In the second part of the analysis, heat transfer in polymer and melting is being dealt with. Working on the assumption that Tadmore's model [7] still stands for feeding stage of reciprocating extruder, most of the melting occurs at the interface of the melt film and solid bed. The height of the melt film does not increase and the solid bed is continuously rearranged while maintaining a constant height (this has been identified by experiment [8]). In effect, this rearrangement causes the solid inside the screw to continuously move into the interface where it melts. Consequently, the width of the solid bed is gradually decreasing as it moves down the channel, as shown in Fig. 2.

The simplified one-dimensional heat transfer model is illustrated in Fig. 3.

Heat conducted out of the melt–solid interface into the moving solid (given that the movement and temperature

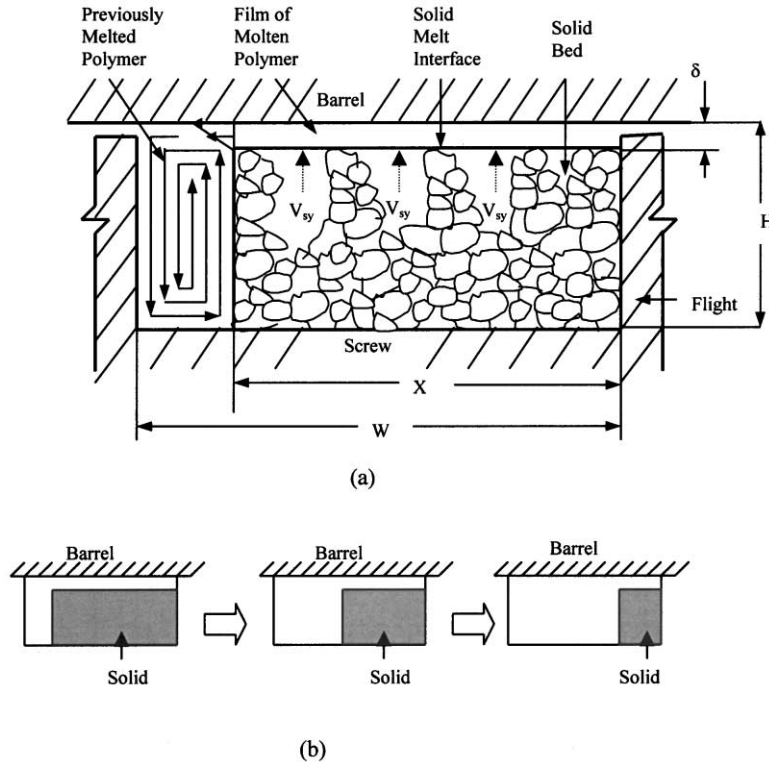


Fig. 2. Melting process.

gradient are constant) is Q_{solid} :

$$Q_{solid} = K_s \frac{\partial T_s}{\partial y} \Big|_{y=0} \quad (5)$$

Heat conducted into the melt-solid interface is Q_{mb} :

$$Q_{mb} = K_m \frac{\partial T_m}{\partial y} \Big|_{y=0} \quad (6)$$

The energy balance equation is:

$$Q_{mb} - Q_{solid} = V_{sy}(t)\rho_s\lambda, \quad (7)$$

where $V_{sy}(t)$ is the velocity of solid that moves towards the interface of melt-solid.

Transient melting speed is: $XV_{sy}(t)\rho_s$, where X is solid width and V_{sy} can be used as a measure of the rate of melting.

(from Eq. (7)). Then, temperature at interface of barrel and melt ($y = \delta$) is:

$$T_b(z, t) = T_{end} + (T_{s0} - T_{end}) e^{-kAz/V_{bsz}}(1 - e^{-At}) - (T_{end} - T_{b0}(z)) e^{-At} \quad (8)$$

Temperature at interface of melt-solid polymer ($y = 0$) is:

$$T(0, t) = T_m \quad (9)$$

Assume that initial temperature distribution in melt film is:

$$T(y, 0) = T_m + (T_{b0} - T_m)y/\delta \quad (10)$$

where $T_m < T_{b0} < T_{end}$.

The following equations are derived:

$$\begin{cases} \frac{\partial T(y, t)}{\partial t} - \alpha \frac{\partial^2 T(y, t)}{\partial y^2} = U_0 & 0 < y < \delta, t > 0 \\ T(0, t) = T_m & y = 0, t > 0 \\ T(\delta, t) = T_{end} - (T_{end} - T_{s0}) e^{-kAz/V_{bsz}}(1 - e^{-At}) - (T_{end} - T_{b0}) e^{-At} & y = \delta, t > 0 \\ T(y, 0) = T_m + (T_{b0} - T_m) \frac{y}{\delta} & 0 < y < \delta, t = 0 \end{cases} \quad (11)$$

Suppose that the solid polymer is in the form of a slab with infinite thickness and that heat absorbed from the interface Q_{solid} is constant. The time dependent characteristic of the melting rate will depend on the time dependent $Q_{mb}(t)$

where U_0 is the viscous diffusive heat per unit time caused by the relative movement between barrel and solid bed divided by the density and specific heat of melt. Assuming that the viscosity is constant, the velocity profile in the melt

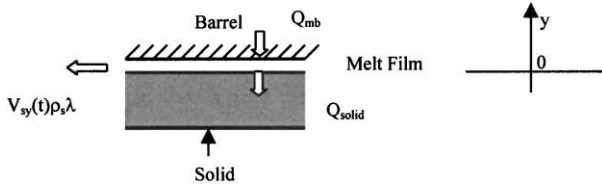


Fig. 3. Simplified one-dimensional model.

Table 1
Parameters used in calculation (polyethylene)

Property	Value	Unit
Diffusivity, α	1.97×10^{-7}	m^2/s
T_{s0}	300	K
T_{end}	450	K
T_m	380	K
T_{b0}	420	K
z	4	m
Coefficient, K	1	
Viscosity, μ	200	$\text{N s}/\text{m}^2$
Melt film thickness, δ	1.08×10^{-3}	m
Density, ρ_m	750	kg/m^3
Specific heat, C_m	2300	$\text{J}/\text{kg}/\text{K}$
Inner barrel diameter, D	0.083	m
Helix angle, θ	18	Degree

film is linear. Therefore, U_0 is constant when the rotating speed is constant.

$$U_0 = \mu(v_j/\delta)^2/\rho_m/C_m$$

Let

$$u(y, t) = T(y, t) - \{T_m + (y/\delta)[T_{\text{end}} + (T_{s0} - T_{\text{end}}) e^{-kAz/V_{bsz}} \times (1 - e^{-At}) - (T_{\text{end}} - T_{b0}) e^{-At} - T_m]\} \quad (12)$$

then:

$$\frac{\partial T(y, t)}{\partial t} = \frac{\partial u(y, t)}{\partial t} - \left(\frac{y}{\delta}\right) [(T_{\text{end}} - T_{s0}) e^{-kAz/V_{bsz}} - T_{\text{end}} + T_{b0}] (A e^{-At}) \quad (13)$$

$$\frac{\partial^2 T(y, t)}{\partial y^2} = \frac{\partial^2 u(y, t)}{\partial y^2} \quad (14)$$

Substituting Eqs. (13) and (14) into Eq. (11), we get:

$$\begin{cases} \frac{\partial u(y, t)}{\partial t} = \alpha \frac{\partial^2 u(y, t)}{\partial y^2} + U_0 + \frac{y}{\delta} [(T_{\text{end}} - T_{s0}) e^{-kAz/V_{bsz}} - T_{\text{end}} + T_{b0}] A e^{-At} & t > 0 \\ u(0, t) = 0 & t > 0 \\ u(\delta, t) = 0 & t > 0 \\ u(y, 0) = 0 & t > 0 \end{cases} \quad (15)$$

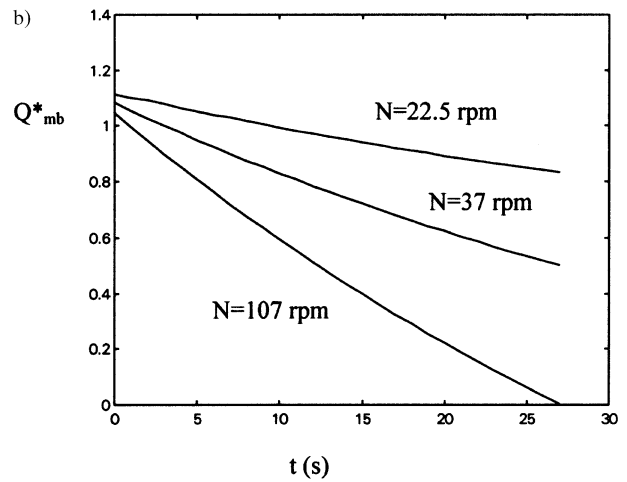
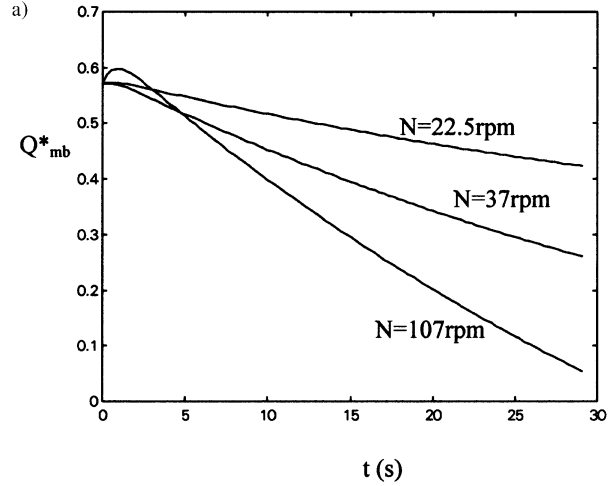


Fig. 4. (a) Result of simulation with analytical model indicates that higher rotation speed (N) causes a faster decrease in melting rate ($A = 0.02$); (b) result of numerical simulation is similar to the result of analytical model (Fig. 4a), while this one is more reasonable at the beginning part of rotation ($A = 0.02$).

$$u(y, t) = \sum_{n=1}^{\infty} u_n(t) \sin\left(\frac{n\pi y}{\delta}\right) \quad 0 < y < \delta, \quad (16)$$

where $u_n(t)$ is achieved by means of series expansion

$$T(y, t) = u(y, t) + \{T_m + (y/\delta)[T_{\text{end}} + (T_{s0} - T_{\text{end}}) e^{-kAz/V_{bsz}} \times (1 - e^{-At}) - (T_{\text{end}} - T_{b0}(z)) e^{-At} - T_m]\} \quad (17)$$

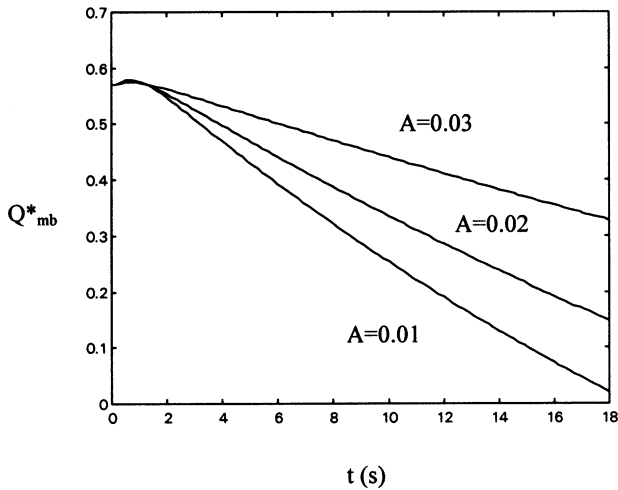


Fig. 5. Relationship between Q_{mb}^* and t at different value of coefficient A ($N = 22.5$ rpm).

$$\frac{\partial u(y, t)}{\partial y} = \sum_{n=1}^{\infty} u_n(t) \frac{n\pi}{\delta} \cos \frac{n\pi y}{\delta} \quad (18)$$

$$\begin{aligned} \frac{\partial T(y, t)}{\partial y} = & \frac{\partial u(y, t)}{\partial y} + \frac{1}{\delta} [T_{end} - T_m - (T_{end} \\ & - T_{s0}) e^{-kAz/V_{bsz}} (1 - e^{-At}) - (T_{end} - T_{b0}) e^{-At}] \end{aligned} \quad (19)$$

$$Q_{mb}(t) = K_m \left. \frac{\partial T(y, t)}{\partial y} \right|_{y=0} \quad (20)$$

The dimensionless time dependent $Q_{mb}^*(t)$:

$$\begin{aligned} Q_{mb}^*(t) = & \frac{\frac{Q_{mb}(t)}{K_m}}{\left(\frac{T_{end} - T_m}{\delta}\right)} = \left. \frac{\partial u(y, t)}{\partial y} \right|_{y=0} \frac{\delta}{T_{end} - T_m} \\ & + \left[1 - \frac{T_{end} - T_{s0}}{T_{end} - T_m} e^{-kAz/V_{bsz}} (1 - e^{-At}) - \frac{T_{end} - T_{b0}}{T_{end} - T_m} e^{-At} \right] \end{aligned} \quad (21)$$

The above equation is the model representing the relationships between the time dependent melting rate and other parameters in reciprocating extruders.

3. Simulation

The most important phenomena observed by Donovan in his experiment are that the plasticating process in reciprocating extruder is a transient process and the melting rate decrease with time during the feeding stage.

To simulate those phenomena, we used parameters of LDPE which is the material used in Donovan's experiments. The geographic parameters of screw and barrel as well as operating conditions are the same as those in Donovan's

experiments. Relationships between Q_{mb}^* and time t at different rotation speed N and coefficient A with parameters listed in Table 1 are shown in Figs. 4 and 5.

When taking into account the dependence of viscosity on temperature and shear rate, numerical methods have to be used in the calculation. A power law temperature dependent viscosity was utilized in the modeling. The representation of viscosity used in the calculation is:

$$\mu(\gamma, T) = \mu_0 \exp[m(T - T_m)] \gamma^{n-1} \quad (22)$$

where $\mu_0 = 10^4$ Pa s, $n = 0.3$, $m = -0.0007 \text{ K}^{-1}$, $T_m = 383 \text{ K}$.

The energy equation becomes:

$$\rho_m C_m \frac{\partial T(y, t)}{\partial t} - K \frac{\partial^2 T(y, t)}{\partial y^2} = \mu_0 \exp[m(T - T_m)] \gamma^{n+1} \quad (23)$$

Let $S(T)$ represents the source term:

$$S(T) = \mu_0 \exp[m(T - T_m)] \gamma^{n+1} \quad (24)$$

This source term is linearized at T_p ,

$$S(T) = S_C + S_P T \quad (25)$$

where

$$S_C = S(T_p) - \left. \frac{dS}{dT} \right|_{T=T_p} = \mu_0 \gamma^{n+1} \exp[m(T - T_m)] (1 - m) \quad (26)$$

$$S_P = \left. \frac{dS}{dT} \right|_{T=T_p} = \mu_0 \gamma^{n+1} m \exp \left[\frac{E}{R} \left(\frac{1}{T_p} - \frac{1}{T_0} \right) \right] \quad (27)$$

Eq. (23) can be discretized using Taylor expansion method. Using superscripts 0 and $'$ to represent the terms at time t and $t + \Delta t$, respectively, the resulting finite difference equation is:

$$\begin{aligned} \rho_m C_m (T_p' - T_p^0) \frac{\Delta x}{\Delta t} = & \frac{K(T_E' - T_p')}{(\delta x)_e} - \frac{K(T_E' - T_w')}{(\delta x)_w} \\ & + S' \Delta x \end{aligned} \quad (28)$$

The above is a time implicit expression. It is used to avoid problems of instability. For boundary conditions, explicit method is adopted. When Δt is small enough, errors caused by this approximation are negligible.

Eq. (28) is transformed as follows:

$$a_p T_p' = a_E T_E' + a_w T_w' + b \quad (29)$$

where

$$a_E = \frac{K}{(\delta x)_e}, \quad a_w = \frac{K}{(\delta x)_w}, \quad a_p^0 = \frac{\rho_m C_m \Delta x}{\Delta t}$$

$$a_p = a_E + a_w + a_p^0 - S_P \Delta x$$

$$b = S_C \Delta x + a_p^0 T_p^0$$

In solving this implicit problem, at each time step, the TDMA algorithm is used to solve the matrix equation.

Finally, we get different relationship between Q_{mb}^* and time t at different rotation speed N as shown in Fig. 4b which is similar to Fig. 4a.

4. Results and discussions

From Figs. 4 and 5, we can see that Q_{mb}^* will decrease as time t increases. Therefore, the rate of melting will also decrease when the screw starts to rotate from stop stage. This coincides with the phenomena observed by Donovan [1] in his experiments, that melting rate is maximum at the start point of rotating, and will decrease till steady state is reached.

When rotating speed (V_{bt}) increases and assuming that pressure ahead of screw is constant, the relative velocity between screw and solid bed (V_{bsz}) will also increase; the relative velocity between barrel and solid V_j will increase as well. The increase of V_{bsz} causes the Q_{mb}^* increase, while the increase of V_j causes the Q_{mb}^* decrease. It has been deduced [4] that the relative velocity between solid bed and barrel V_j is less for reciprocating extruders than extrusion extruders because of the axial movement, where the increase of Q_{mb}^* caused by increase of V_j is limited. Normally, the decrease of Q_{mb}^* caused by the increase of V_{bsz} overruns the increase of Q_{mb}^* caused by increase of V_j for low viscous polymers like LDPE, poly(vinyl acetate), nylon 6, polycarbonate, etc.

From Fig. 4, Q_{mb}^* is shown to be decreasing more sharply as time advances for faster rotation speed N . It induces a sharper decrease of V_{sy} . This explains higher the rotation speed, more apparent the difference of melting rate at the starting point of rotation and at the end of rotation as observed by Donovan [1].

The steady state Q_{mb}^* decreases as rotation speed increases (see Fig. 4). This will cause longer melting length, and poorer melting may be resulted [1]. Therefore, for better product quality, rotation speed should be as slow as possible and rotation time should be just long enough to get the amount of mass flow.

From Fig. 5, we can see that, the less the value of coefficient A , the longer time it will take to get to the steady-state. Therefore, the barrel heat capacity should be high while barrel thickness should be small enough to minimize this transient effect.

5. Conclusions

The axial movement of screw and the short rotation time make the reciprocating extruders totally different from the simple extruders. Simulations conducted in this paper with both analytical and numerical method explained the effects of screw rotation speed, the barrel thickness, and the barrel heat capacity on melting rate in the feeding stage of reciprocating extruder. Results of simulation agree with observations in real life [1].

Simulations have further shown that, for low viscosity polymers, higher screw rotation speed may cause longer melting length inside the screw and more apparent will be the difference of melting rate at the start of rotation and at the end of rotation. This has contributed to the understanding that the rotation speed should be as low as possible as long as it does not affect the conveyance of resin.

It is further deduced that barrels of thicker and higher heat capacity may cause stronger transient effects (longer time to get to the steady state), hence, barrels of thinner and less heat capacity will give better product quality.

Acknowledgements

The work described in this paper was fully supported by a grant from the Research Grants Council of the Hong Kong Special Administrative Region, China, and a Hong Kong Polytechnic University Central Research Grant.

References

- [1] Donovan RC, Thomas DE, Leversen LD. An experimental study of plasticating in a reciprocating-screw injection molding machine. *Polym Engng Sci* 1971;11:353.
- [2] Rauwendaal C. Melt conveying in reciprocating extruders. *Proc Annu Tech Conf — ANTEC* 1991:433 Montreal.
- [3] Rauwendaal C. Conveying and melting in screw extruders with axial movement. *Int Polym Process* 1992;7:26.
- [4] Donovan RC. A theoretical melting model for plastic extruders. *Polym Engng Sci* 1971;11:247.
- [5] Dormeier S, Panreck K. Dynamic behavior of the temperature during extrusion. *Kunststoffe Germ Plast* 1990;80:32.
- [6] Asan H, Sancaktar YS. Effects of wall's thermophysical properties on time lag and decrement factor. *Energy Build* 1998;28:159.
- [7] Tadmor Z, Klein I. *Engineering principles of plasticating extrusion*. Malbar, FL: Krieger, 1970.
- [8] Robert RN, Fenner RT. *Proc ANTEC* 1978;24:72 San Francisco, CA.