Simulation for Mixing Process in the Solid Conveying Zone of a Twin-screw Extruder

Inoue, Eiichiro*/Tsuji, Tetsuharu/Kajiwara, Toshihisa/Funatsu, Kazumori/Nakayama, Yasuya

Mixing process of polymer pellets in solid conveying zone of a twin-screw extruder (TSE) is numerically investigated by using the discrete element method. It was clarified that the mixing of pellets was mainly performed in the intermeshing part of the TSE from the results of two-dimensional simulations. Moreover, a course of simulation with different conditions was performed to obtain information for improving the mixing performance. The effects of barrel property, tip-clearance, and screw-rotational speed were studied. The results suggested that the shear deformation on particle clusters at the tip-clearance is the most important factor in promoting mixing at the intermeshing part of the TSE. A preliminary result of a three-dimensional simulation with an actual geometry of conveying screws is also shown.

Key words : Twin-screw extruders/Solid conveying zone/Discrete element method

1. Introduction

A twin-screw extruder (TSE) is a type of mixing device which has been widely used in various industries including polymer processing, food industries, pharmaceutical development. In plastic industry, a TSE is used for compounding and blending polymeric materials to produce products with some desired properties. Therefore, optimizing the performance of TSEs is a key factor to improve productivity and functionality of products, and material behaviors in a TSE are of great interest. However, it is difficult to obtain information on physical process in a TSE since TSEs are often operated under severe conditions of high temperature and high pressure and a channel in TSEs in which materials are transported is highly complicated. Numerical simulation can aid in predicting material behaviors in a TSE.

In the authors' group, simulations of three-dimensional flow of a polymer melt in a TSE have been developed and successfully applied to analysis of mixing mechanisms in the assemblies of various types of screw segments^{1)~3)}. However, the analysis in melt pumping zone alone is still insufficient for evaluating the performance of a TSE. Huneault *et al.*⁴⁾ reported from experimental observation that the morphological structure of an im-

miscible polymer blend was almost determined at the melting zone which is an earlier stage than melt pumping zone. This observation implies that understanding to melting process of solid pellets is necessary. From this viewpoint, several models on the melting of solid pellets have been proposed. Potente *et al.*⁵⁾ applied a melting model developed for a single-screw extruder to the case of a TSE. However, experimental observations revealed that there existed fundamental difference in melting behaviors between a single-screw extruder and a TSE and a melting model for a single-screw extruder was found to be useless for TSEs. Vergnes *et al.*⁶⁾ modeled the melting state of solid pellets as a uniform suspension of solid/liquid mixture. Although they reported that this model could show good agreement with their experimental observations, this model cannot be applied to the individual solid pellets to start melting. To obtain better understanding of melting process, analysis including the solid conveying zone is necessary. Thus our project is to develop a model and simulation of the solid conveying zone.

In this article, we investigate the mixing process of polymer pellets in two-dimensional section of a TSE. A course of simulations by discrete element method⁷⁾ was performed and the effects of material properties of screws and barrel, size of the tip-clearance, and operational parameters were evaluated.

2. Simulation model

The discrete element method (DEM)⁷⁾ has been widely applied to simulate particulate flows^{8)~10)}. We ap-

* Department of Chemical Engineering, Kyushu University
Nishi-ku, Fukuoka 819-0395, Japan
Received May 26, 2006.

ply DEM to simulate pellet motion in the solid conveying zone of a TSE. In the framework of DEM, each particle is assumed to be spherical. In addition, we consider the monodisperse system. The motion of each particle are traced by solving the Newton's equation of motion,

$$m \frac{d^2 \mathbf{x}_i}{dt^2} = \mathbf{F}_i, \quad (1)$$

$$I \frac{d\varphi_i}{dt} = \mathbf{T}_i, \quad (2)$$

where m , $I = (8/15) \pi r^5$ are the mass and the moment of inertia of a particle of a radius r , and $\mathbf{x}_i$, φ_i , $\mathbf{F}_i$, and $\mathbf{T}_i$ are the position, angular velocity, force, and torque of the i th particle, respectively. The force includes the gravitational force and particle-particle contact force and particle-wall contact force. The contact forces are modeled according to Cundal and Strack.⁷⁾ When i th and j th particles are in contact, a spring and a dash-pot acts in the normal and tangential directions. In addition, a slider in the tangential direction works when the magnitude of the tangential force become larger than $\mu |\mathbf{F}_{ij}^n|$ where $\mathbf{F}_{ij}^n$ is the normal component of the contact force and μ the friction coefficient. This model includes five parameters concerning pair contact, *i.e.*, spring constants, damping constants for the normal and tangential directions, respectively, and the friction coefficients. Tsuji *et al.*⁹⁾ offered a way to determine the spring constants and the damping constants from the restitution coefficient, Young's modulus, and Poisson ratio. The friction coefficient is determined experimentally. For the sake of simplicity, we neglected the hydrodynamic drag and the effect of temperature on the material parameters since they are considered to have minor effect on mixing process before melting.

The geometry of the TSE studied in this paper is shown in Fig. 1 and Table 1. The radius of pellets was chosen to be 1.0 mm. Initial configuration of pellets at rest is depicted in Fig. 2(a). Resting state of particles was realized by solving Eqs.(1) and (2) with screws at rest until a resting state was obtained. For visualization of mixing process, each particle is colored by sixth different colors according to its initial positions. Initially nearby particles are marked in a color. As time progresses, differently colored particles are mixed and one can identify the mixing state by the colors. We performed a course of simulation in two-dimensional section of the TSE. The particle-particle interaction was determined from the material parameters of polyethylene which have Young's modulus of 2.0×10^6 Pa, Poisson ratio of 0.43, restitution coefficient of 0.80, and friction coefficient of 0.618. The other simulation conditions are summarized in Table 2. The material parameters of Case 1 in Table 2 is of the polyethylene-iron interaction. Iron has Young's modulus of 2.09×10^{11} Pa and Poisson ratio of 0.

Fig. 1 Geometry of the TSE used in this article : (a) top view, (b) cross sectional view.

Table 1 Parameters of the geometry of the TSE used in this article.

radius of the barrel : R_B	20.0 (mm)
radius of the flight : R_F	19.5 (mm)
radius of the screw root : R_S	12.5 (mm)
tip-clearance : δ	0.5 (mm)
calender gap : δ_c	1.0 (mm)

Fig. 2 Initial configuration (a) and snapshots from time evolution of Cases 1-3 : (b)-(d) at $t=0.5$ sec, (e)-(f) at $t=1.0$ sec. Circles in (b)-(d) indicate the difference of mixing process by shear deformation on particle clusters. In Case 3, larger friction between the wall and the particles caused larger shear stress on cluster and resulted in more notable shear deformation of cluster than Cases 1 and 2.

28. This case was chosen as a control.

An upper bound of the time increment is estimated as follows. The maximum speed of a particle is assumed to be the same as the speed of screw flight v_s . From the radius of the flight (Table 1) and the rotation speed in the

Table 2 Simulation parameters. The parameters on particle-wall interaction in Case 1 are of the polyethylene-iron interaction. The parameters of the other cases are chosen based on those of Case 1. In all cases, particles have a radius of 1.0 mm. Mass density of particles is set to be uniform except for Cases 7 and 8. In Cases 7 and 8, two kind of particles with two different mass densities were considered.

	particle-wall restitution coefficient [-]	particle-wall friction coefficient [-]	tip-clearance [mm]	screw rota-tional speed [rpm]	mass density [kg/m³]	
Case 1	0.422	5 : 45 × 10 ⁻²	0.5	60	920.0	—
Case 2	0.844	5 : 45 × 10 ⁻²	0.5	60	920.0	—
Case 3	0.422	5 : 45 × 10 ⁻¹	0.5	60	920.0	—
Case 4	0.422	5 : 45 × 10 ⁻²	2.5	60	920.0	—
Case 5	0.422	5 : 45 × 10 ⁻²	0.0	60	920.0	—
Case 6	0.422	5 : 45 × 10 ⁻²	0.5	120	920.0	—
Case 7	0.422	5 : 45 × 10 ⁻²	0.5	60	920.0	1840.0
Case 8	0.422	5 : 45 × 10 ⁻²	0.5	60	920.0	2760.0

Case 1 in Table 2, $v_s=1.23\times10^2$ mm/sec is obtained. When two particles collide with this speed, the resultant small deformation over the period Δt is $\delta=2\,v_s\Delta t$. Assuming admissible small deformation is $r\times10^{-4}$, an upper bound of the time increment is estimated to be 4.07×10^{-7} sec. In the preliminary simulations with different time increments, particle behaviors were almost unchanged when $\Delta t\leq5.0\times10^{-7}$. From these observation, the time increment used in following simulations was set to be 5.0×10^{-8} sec. Equations (1) and (2) were discretized by Euler scheme. Other details on the implementation including judgment scheme of contacting are found in the literature¹¹⁾.

3. Results and Discussions

3.1 Effect of pellet-wall interaction

The material property of the screws and the barrel is taken into account by the parameters of pellet-wall interaction in DEM. In Case 2, the pellet-wall restitution coefficient was set to be twice of that in Case 1, and in Case 3 the pellet-wall friction coefficient was set to be tenth of that in Case 1.

The snapshots of Cases 1-3 are shown in Fig.2. In the control case of Case 1, it was observed that particles were just swept and transported in the barrel except for the intermeshing part of the TSE. The substantial mixing process was occurred when the particles passed through the intermeshing part.

To quantify the mixing process, we introduce a measure of mixing

$$\langle M \rangle(t)=\frac{1}{N}\sum_{i=1}^N M_i(t), \tag{3}$$

where N is the number of particles, $M_i(t)$ is the number of differently colored particles around the i th particle within a certain radius r_M at the time t . At a initial state, $\langle M \rangle(t=0)$ is almost zero since $M_i(t=0)$ is zero for almost all the particles. The quantity $\langle M \rangle(t)$ represents a degree of mixing of whole system. $r_M/r>1$ should be

Fig.3 Time evolution of a measure of mixing for Cases 1-3.

sufficiently large to cover other particles and not to be too large so that M_i to be local quantity. Since the evolution of $\langle M \rangle(t)$ was checked to be insensitive to the choice of the radius r_M for counting M_i within 2.0 mm, 3.0 mm, and 4.0 mm, we shall show the results of $r_M=2.0$ mm.

Time evolution of $\langle M \rangle(t)$ is shown in Fig. 3. The local maxima of $\langle M \rangle(t)$ were observed at the points of time when the large fraction of particles passed through the intermeshing part. The quantity $\langle M \rangle(t)$ seemed to successfully quantify the observation stated above. This type of mixing at the intermeshing part is ascribed to the ability that the screws transport particles. Comparing Case 2 with Case 1, it was observed that there was no substantial difference in their mixing process. On the other hand, Case 3 showed the better mixing performance than Cases 1 and 2 (Fig. 2 and 3). In Case 3, larger friction between pellets and wall was assigned and during particles transported, cluster of particles was elongated at the tip-clearance before they reached the intermeshing part. This shear deformation induced by the shear stress on clusters in the tip-clearance highly promoted the mixing process. From these observations, as

Fig.4 Time evolution of a measure of mixing for Cases 4-6. For comparison, the control case of Case 1 is also drawn.

material properties for the screws and barrel, large friction should be desired for better mixing.

3.2 Effect of tip-clearance and screw-rotational speed

The results of different tip-clearance cases and a different screw-rotational speed are shown in Fig. 4. In Case 4, where the tip-clearance was set to be five times larger than that in Case 1, the enhancement of mixing was observed. Since there were many chances for pellets to pass the tip-clearance, the cluster of particles experienced much shear deformation and was apt to be elongated. This effect is similar to that in Case 3.

In Case 5, the tip-clearance was set to be zero which was chosen as the extreme case where there was no chance for particles to pass through the tip-clearance. In this case, only transporting effect of the screws was expected and almost no mixing was observed (Fig. 4). Moreover, since the pellet particles could not pass the tip-clearance and the intermeshing part, the pellets got stuck between the screws and the barrel in the intermeshing part and the simulation showed break-down. In the two-dimensional simulation, confined particles had no way to escape from this choking, which was the reason for simulation to break down. Although this choking could be avoided in three-dimensional case, this result indicated that too small tip-clearance reduced the mixing performance in the solid conveying zone.

In Case 6, the twice as much screw-rotational speed as Case 1 was tested. It is generally expected that the faster the screws revolve, the faster the pellets are mixed. In the simulation results, the point of time at which the mixing measure $\langle M \rangle(t)$ started to rise became half of Case 1 as expected (Fig. 4). However, the rate of increase of $\langle M \rangle(t)$ did not show much difference from that of Case 1. This result suggests that the faster screw rotation is not effective to enhance the mixing but

Fig.5 Time evolution of a measure of mixing for Cases 7-8. For comparison, the control case of Case 1 is also drawn.

just results proportional throughput.

From the results above, it was found that the shear deformation of particle clusters at the tip-clearance was the most important in the mixing process in the solid conveying zone of a TSE. This effect should be enhanced by making the barrel and the screws have large friction which caused larger shear stress on particle clusters and also by optimizing the size of tip-clearance itself. Moreover, it was suggested that faster screws rotation did not imply effective mixing at fixed rotation number of the screws.

3.3 Effect of mass density dispersity

In real operations of polymer processing by a TSE, mixing of different kind of pellets is a quite important task. When different materials are to be mixed, one of the important factors is difference of their inertia. We consider a mixture of light and heavy pellets as a simple model case to study the effect of mass density dispersity. In the Cases 7 and 8, the mass of heavier pellets is set to be twice and triple of the lighter ones, respectively. As an initial configuration in these cases, we set the lighter pellets in the right barrel and the heavier pellets in the left barrel.

From the measure of mixing $\langle M \rangle(t)$ in Fig. 5, it was observed that for the larger mass density ratio, mixing performance became better. By examining the motion of the particles, the collision of a heavier particle to the lighter ones expedited the dispersion of the cluster of the lighter particles.

4. Concluding Remarks

We numerically investigated the mixing process of pellets in solid conveying zone of a TSE by using the discrete element method. From the observation of particle motion in different cases, it was found that the mixing of pellets occurred when particles pass through the inter-

Fig.6 A snapshot from three-dimensional simulation of the solid conveying zone

meshing part of the TSE. In addition, the shear deformation of particle clusters at the tip-clearance enhanced the mixing. From this point of view, there found two factors to optimize the mixing performance of the TSE. One is the friction between pellets and the screws and/or between pellets and the barrel, and the other is the relative size of the tip-clearance to the size of the pellets. The shear deformation of particle clusters at the tip-clearance can be mainly controlled by these two factors.

We have performed simulations in a two-dimensional cross section of a TSE and confirmed the current simulation model works well for solid conveying zone. Application to three-dimensional systems is straightforward and a preliminary result is shown in Fig. 6. This should allow the discussion on mixing process of pellets under transport. The most important difference between two-dimensional and three-dimensional cases is the degrees of freedom of particles. The particle motion along the screw direction might result the difference of mixing behavior than the two-dimensional case, and therefore a three-dimensional simulation is an important future issue. However, in the three-dimensional case, much heavier computational resources than a two-dimensional case is required. Generally speaking, in particle simulation in its best implementation, the computation per step is proportional to the number of particles. From the preliminary computations, it seemed that a three-dimensional simula-

tion was apt to become unstable when a solid pellet passed through the intermeshing part. This instability might be ascribed to the assumption of elastic deformation in DEM. These facts suggest that an improvement on simulation scheme is necessary for a practical three-dimensional simulation. Further simulations including the effects of heating and melting of the pellets in two-and three-dimensional systems should be important future issues.

5. Acknowledgment

The simulations of this work were performed using Fujitsu VPP 5000/64 at the Computing and Communications Center, Kyushu University.

References

- 1) Funatsu, K., Kihara, S.-I., Miyazaki, M., Katsuki, S. and Kajiwar, T.: *Polym. Eng. Sci.*, **42**, 707 (2002)
- 2) Ishikawa, T., Kihara, S.-I. and Funatsu, K.: *Polym. Eng. Sci.*, **40**, 357 (2000)
- 3) Ishikawa, T., Kihara, S.-I., Funatsu, K., Amaiwa, T. and Yano, K.: *Polym. Eng. Sci.*, **40**, 365 (2000)
- 4) Huneault, M. A., Champagne, M. F. and Luciani, A.: *Polym. Eng. Sci.*, **36**, 1694 (1996)
- 5) Potente, H. and Melisch, U.: *Intern. Polym. Proc.*, **11**, 101 (1996)
- 6) Vergnes, B., Souveton, G., Delacour, M. L. and Ainsier, A.: *Intern. Polym. Proc.*, **16**, 351 (2001)
- 7) Cundall, P. A. and Strack, O. D. L.: *Géotechnique*, **29**, 47 (1979)
- 8) Kano, J. and Saito, F.: *Kagaku Kogaku Ronbunshu*, **23**, 687 (1997)
- 9) Tsuji, Y., Tanaka, T. and Ishida, T.: *Powder Tech.*, **71**, 239 (1992)
- 10) Muguruma, Y., Tanaka, T., Kawatake, S. and Tsuji, Y.: *Powder Tech.*, **93**, 261 (1997)
- 11) Funtai simulation nyumon, edited by The Society of Powder Technology, Japan, (Sangyo Tosho, Tokyo, 1998)

二軸スクリュ押出機の固体輸送部における混合過程のシミュレーション

井上栄一郎・辻 哲治・梶原稔尚・船津和守・名嘉山祥也

二軸スクリュ押出機の固体輸送部におけるペレットの混合過程を、離散要素法を用いてシミュレーション解析を行った。二次元断面のシミュレーションの結果、ペレットの混合は主にスクリュのかみ合い部で起こることがわかった。さらに、固体輸送部における混合過程の改善指針を与えるために、種々の装置条件を変えたシミュレーションも行った。その結果、ペレットがスクリュのチップクリアランス部を通過するときに受けるずりの効果が、混合過程のために最も重要な働きをすることがわかった。実際の輸送スクリュエレメントを用いた三次元シミュレーションの予備検討についても報告する。