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Research Article

Numerical Simulation of Temperature and Mixing Performances of Tri-screw Extruders with Non-isothermal Modeling

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Abstract: Tri-screw extruders are new extrusion equipments for food and polymer processing. Especially, there is one special circumfluence exists in center region only at cross section. In this study, the 2D transient and non-isothermal modeling of a tri-screw extruder is established by using Finite Element Method (FEM) with particle tracking technology to reduce the axial effects. The transient temperature and flow fields are calculated with a commercial code, Polyflow. Moreover, the effect of temperature rise due to viscous heating on the flow and mixing characteristics such as mixing index, segregation scale, mean and instantaneous time-averaged efficiency of mixing for the tri-screw extruder are carried out. The results show that in the special center region, the velocity and mixing index is small and viscosity and temperature are relatively big, indicating the poor mixing efficiency. When the heat transfers due to self-heating is considered, the dispersive mixing of the tri-screw extruder decreases, but the distributive mixing and stretching mixing efficiency all increase for the tri-screw extruder. In particular, the stretching effect of the fluid particles in the tri-screw extruder decreases due to the decrease of viscous dissipation when the non-isothermal model is employed.

Keywords: FEM, mixing efficiency, non-isothermal model, tri-screw extruder, viscous dissipation

INTRODUCTION

Tri-screw extruders are new equipment for food and polymer processing, which is different from traditional single and twin screw extruders in flow and mixing mechanism. A tri-screw extruder has three intermeshing regions and one dynamic center region. Because the tri-screw extruders have more complex geometrical structures than twin screw extruders, they have complex flow and mixing behaviors (Jiang and Zhu, 2001). At present, the tri-screw extruder has attracted more and more attentions and widely studied on their flow and mixing mechanism due to its high mixing efficiency. However, because of the complexity of geometrical structures and mixing mechanism, the studies about tri-screw extruder are still in the immature conditions.

So far, many studies of numerical simulations researches have been employed for the flow and mixing mechanism in tri-screw extruders (Hu and Chen, 2006; Zhu *et al.*, 2007, 2009). But most studies on the tri-screw extruder are emphasis on the flow and mixing mechanisms using isothermal model. The temperature rise due to viscous dissipation has significant effects on the polymer properties, thermal degradation and reaction rate in screw extruders. Many studies about the single and twin screw extruder with non-thermal modeling have been employed to the temperature fields due to viscous dissipation. For example, Ishikawa *et al.* (2001) studied the three-dimensional and non-isothermal flow simulations in the kneading disc regions of twin screw extruders using FEM. They found that the temperature becomes higher with increasing rotation speeds due to high viscous dissipation. Bai *et al.* (2011) simulated a non-isothermal transient process of temperature increase for an internal batch mixer using Polyflow codes to obtain the temporal temperature distribution and characterize the heat transfer between polymer melt and mixer wall. Khalifeh and Clermont (2005) study steady non-isothermal flows in a single-screw extruder with two viscoelastic models and a finite volume method. However, the reported studies with non-isothermal modeling about screw extruders and other mixers seldom performance the effects of temperature fields on mixing efficiency. Evaluation mixing efficiency, such as distributive and dispersive mixing is an important tool to design the screw extruders. At present, many studies about the mixing efficiency for the screw extruders have been reported with isothermal modeling (Connelly and Kokini, 2007; Salahudeen *et al.*, 2011). However, it is not clear of the effects of temperature rise on the mixing efficiency for the mixers.

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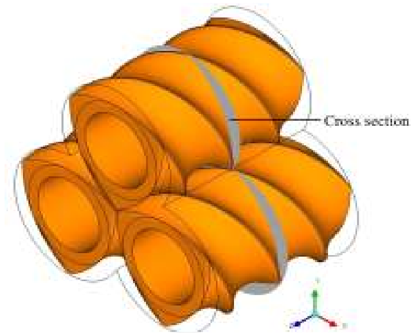
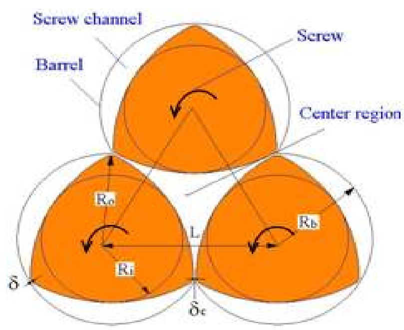


(a)



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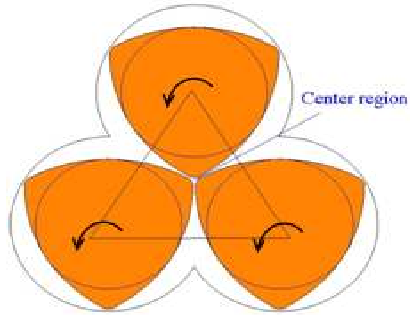


(c)

Fig. 1: Geometric model of the tri-screw extruder with different angles: (a) 3D isometric view, (b) 2D model with angle 0°, (c) 2D model with angle 120°

In this study, a 2D transient and non-isothermal model of a tri-screw extruder was established by using FEM. The transient temperature and flow fields were calculated using the commercial code, Polyflow. Moreover, the velocity, viscosity and viscous dissipation distributions of considering and ignoring temperature field were compared for the tri-screw extruder. At last, the effect of temperature rise on the mixing performances, such as mixing index, segregation scale, mean and instantaneous efficiency of mixing were carried out. The purpose of this study is to farther understand the mixing mechanism and the special contributions of center region for the whole tri-screw extruder under the effect of temperature rise due to viscous heating.

CALCULATED MODELING AND MATERIAL

The geometric and FE model: The tri-screw extruder investigated in this study appears equilateral triangle arrangement for their three screws, which has three intermeshing regions and one special center region, the 3D isometric view is shown in Fig. 1a. With three screws rotation, the center region changes continually from big to small corresponding to the typical angles of 0° and 120°, as illustrated in Fig. 1b and c. The geometric specifications in Fig. 1a are depicted as follows: $R_i = 13.0$ mm; $R_o = 17.0$ mm; $R_b = 17.4$ mm; $L = 41.0$ mm; $\delta_c = \delta = 0.4$ mm.

The simulated calculations are carried out using FEM software, Polyflow. The Finite Element (FE) models are established using Gmabit software with the Mesh Superposition Technique (MST) without re-meshing according to periodical changes. The barrel and the screw elements are meshed, as shown in Fig. 2a and b, individually. The barrel is meshed with quadrilateral element and the screws are meshed with the composite quadrilateral and triangular elements. There are 13296 elements and 13592 nodes in the FE model of the tri-screw extruder respectively, as shown in Fig. 2.

Mathematical models: In this study, the following assumptions are adopted. The non-Newtonian and laminar flow are proposed due to high viscosity of polymer melts; the flow domain is fully filled with fluid under the conditions of non-isothermal, incompressible and non-slip of surfaces; and the inertia and gravitational forces are negligible. Furthermore, the continuity, momentum and constitutive equations are given as the following formats (Polyflow, 2007).
The continuity equation can be expressed by:

$$\nabla \cdot V = 0 \tag{1}$$

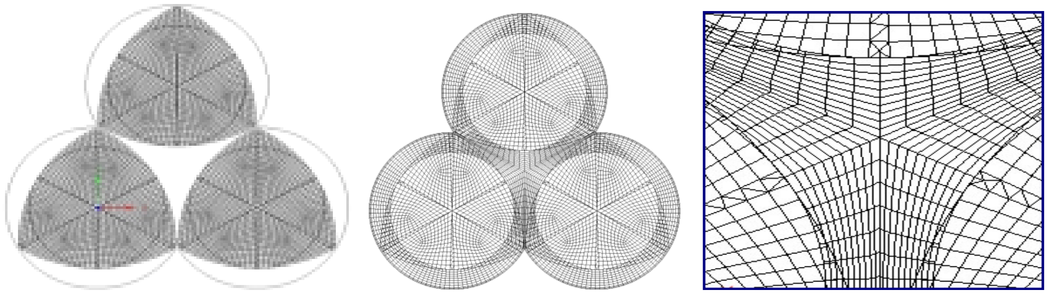
The momentum equation is defined by:

$$H\left(V-\bar{V}\right)+\left(1-H\right)\left(-\nabla p+\nabla\cdot\boldsymbol{\tau}+\rho\left(\frac{\partial V}{\partial t}+V\cdot\nabla V\right)\right)=0 \tag{2}$$

where,
H : A step function, which is 0 for fluid field and 1 for inner moving part
V : The velocity
$\bar{V}$: The local velocity of the moving part
p : The fluid pressure
ρ : The fluid density
t : The time

The equation of the non-isothermal conservation of energy is given as:

$$\rho C\left(T\right)\cdot\left(\frac{\partial T}{\partial t}+\mathbf{v}\cdot\nabla T\right)=\mathbf{T}:\nabla\mathbf{v}+r-\nabla\cdot q \tag{3}$$



(a) (b) (c)

Fig. 2: FE model of the tri-screw extruder: (a) FE model of three screws, (b) combined FE model, (c) amplified FE model of the center region

where,

C(T) : The heat capacity as a function of temperature
r : The given volumetric heat source
q : The heat flux

Viscous heating is described through the term T: Δv. The stress tensor is described by:

$$\tau = 2\eta_0 \left(\dot{\gamma}, T\right) D \tag{4}$$

In which,

η_0: The zero shear viscosity
$\dot{\gamma}$: The effective shear rate
T : The temperature
D : The rate of deformation tensor

The rheology of the polymer melt is described in terms of the Carreau-Yasuda model:

$$\eta = \eta_\infty + \left(\eta_0 - \eta_\infty\right)\left[1+\left(K\dot{\gamma}\right)^a\right]^{\frac{n-1}{a}} exp\left(-\beta\left(T-T_0\right)\right) \tag{5}$$

where,

η_∞ : Infinite shear viscosity
K : A constant parameter with units of time
n : A dimensionless constant
a : The width of the transition region between η_0 and the power-law
β : The temperature coefficient of viscosity (Bai *et al.*, 2011)

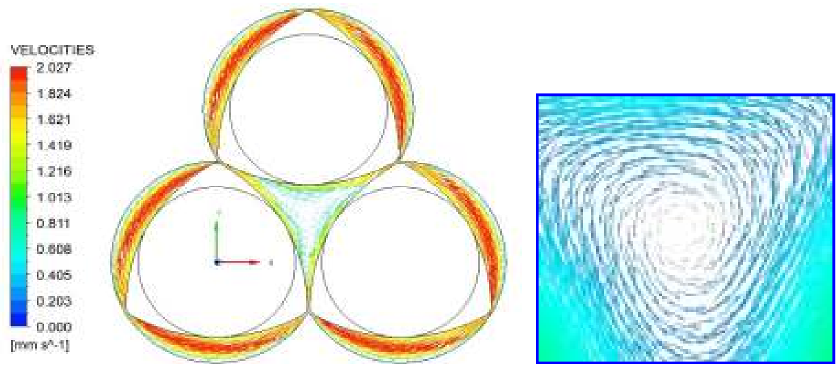
In the present study, a kind of material sensitive to temperature, Polystyrene (PS) is selected to study the effect of temperature rise on the flow and mixing efficiency of the tri-screw extruder. The parameters of this PS melts are as follows: thermal capacity is 2098 J/kg·K, thermal conductivity is 0.213 W/m·K, ρ = 882 kg/m^3, $\eta_\infty = 0$ Pa.s, $\eta_0 = 5520$ Pa.s, a = 0.669, n = 0.322, T_0 = 463 K. In order to minimize the "High Weissenberg Problem" (Connelly and Kokini, 2007), the small rotational speeds of the screws such as 1, 5 and 10 rpm are used in our simulations. The temperature boundary conditions are described as follows: Barrel surface is set with the constant temperature 463 K; the thermal capacity in the screws surface is 400 J/kg·K; the thermal conductivities of screw and barrel are 15 W/m·K.

RESULTS AND DISCUSSION

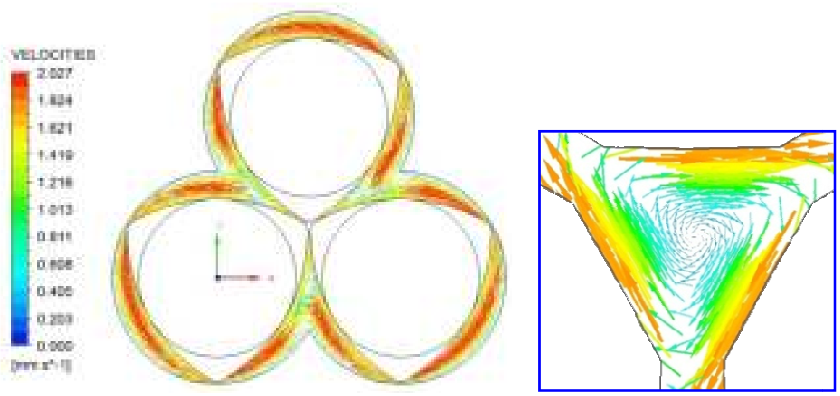
Flow patterns: The velocity vector distributions in the whole cross-section and magnified vector in center region with different angles are visualized with a rotational speed of 1 rpm, as shown in Fig. 3. As can be seen in Fig. 3b, even if the area of the center region is very small, there is still one dead flow zone in the center region. It implies the poor flow and mixing efficiency for the tri-screw extruder. Moreover, with the increase of the area for the center region in Fig. 3a, the area of triangular dead flow zone in center region also increase, in which there are small flow velocities. The dead flow zone always exists in the center of the center region for the tri-screw extruder. It is different from twin screw extruder and must have great effects on the temperature and mixing performance of the tri-screw extruder.

Temperature profile: In this study, we have emphasis on the heat generation due to viscous dissipation, so the initial temperatures of the polymer melt in tri-screw extruder are imposed to 463 k, which is equal to the fixed temperature of the barrel. The temperature and viscous dissipation changes in the middle of center region with time are shown in Fig. 4. The temperatures of polymer melt in the middle of center region increase gradually due to the viscous dissipation until the energy balance of the whole system is obtained after 400 sec with the rotational speed of 1 rpm. The maximal temperature is only about 0.36 K in the center region because the rotational speed and shear rates in the tri-screw extruder are small. Figure 4 also shows the viscous dissipation changes with time in the center region. With the increase of mixing time, the viscous dissipation decreases until the energy balance of the whole system is obtained.

The temperature rises with different rotational speeds of the tri-screw extruder due to viscous dissipation are described in Fig. 5. It can be observed that with the increase of rotational speeds, the



(a) 0°



(b) 120°

Fig. 3: Velocity vector distributions in the tri-screw extruder with different angles: (a) 0° (b) 120°

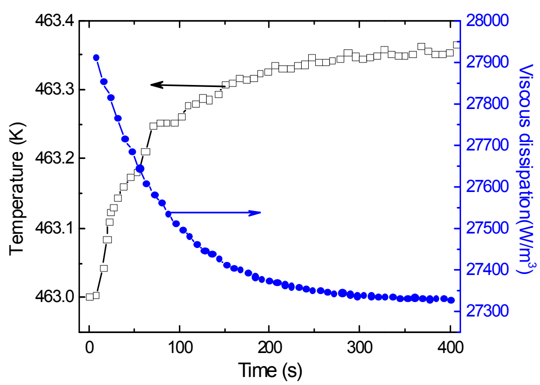


Fig. 4: Temperature and viscous dissipation changes in the middle of center region with time

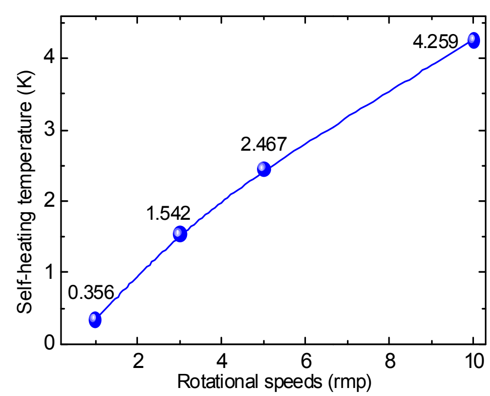


Fig. 5: Temperature increase with different rotational speeds

temperature rise due to the heat generation of viscous dissipation increases gradually. When the rotational speed increases to 10 from 1 rpm, the increasing temperatures are increase to 4.26 K from 0.356 k, because of the great shear rates with the big rotational speeds.

The temperature distributions in tri-screw extruder with different screw revolutions are illustrated in Fig. 6. With the increase of mixing time, the temperature values in the tri-screw extruder also increase gradually. When the whole screw extruder gets the energy balance in Fig. 6d, the center region has higher temperatures than other regions in the tri-screw extruder because of cooling effects from the temperature-controlled barrel and the heat transfer boundary condition on the screw surfaces. At the same time, there are three red regions with maximal temperatures in the center region of the tri-screw extruder, which are also corresponding to

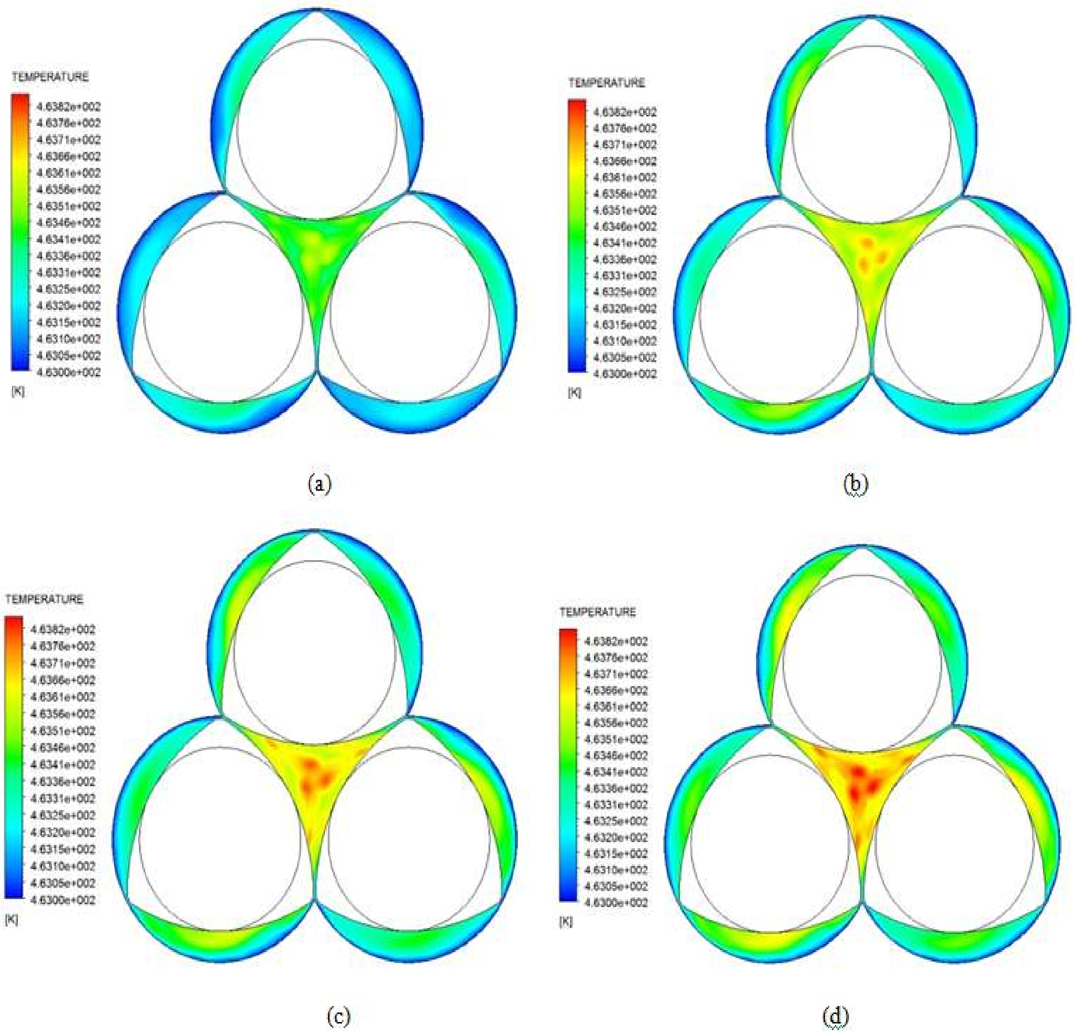


Fig. 6: Temperature distributions in tri-screw extruder with different screw revolutions: (a) 1 revolution, (b) 2 revolutions, (c) 3 revolutions, (d) 6 revolutions

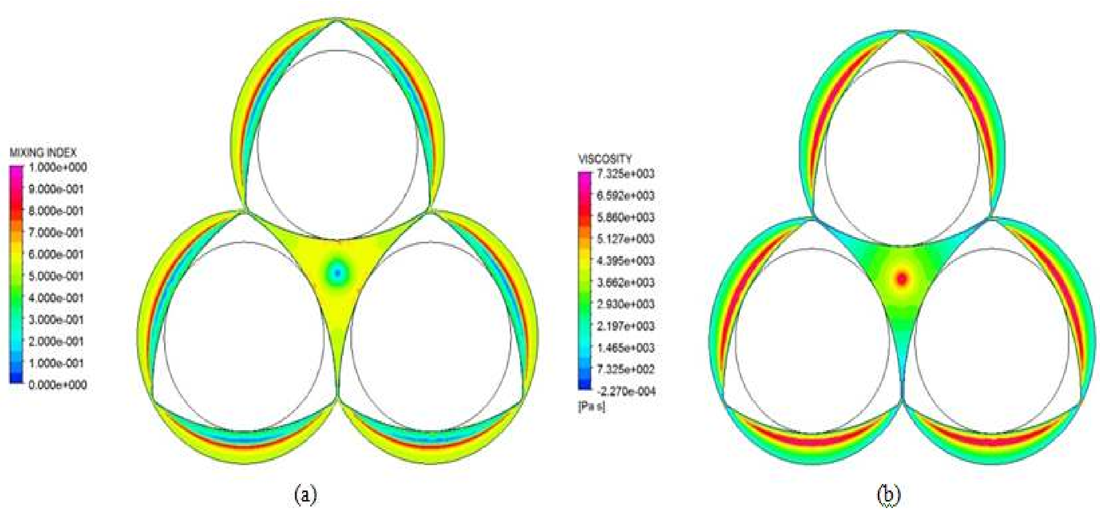


Fig. 7: Mixing index and viscosity distributions in the tri-screw: (a) mixing index, (b) viscosity

three regions with small velocities in the circumfluence. This is because the flow velocities of polymer melts are small in the center region and the heat exchange is relatively slow.

Mixing index and viscosity distributions: The mixing index and viscosity distributions in the tri-screw are described in Fig. 7. From Fig. 7a, it can be seen that the mixing index is highest in the intermeshing regions and in the middle of the screw channels. This corresponds to the areas with the highest shear rates in the screw and indicates that the dispersive mixing will be good in these regions (Fig. 7b). In addition, the mixing index is decreased from the outer to inside in the special center region. In middle of the center region, the mixing index is very small, indicating poor mixing efficiency. From Fig. 7b, it can be seen that the values of viscosity in the center region and the middle of the screw channels are all very small because of the small shear rates of fluid.

Effect of temperature rise on the flow performance: In order to learn about the effect of temperature fields due to viscous heating on the flow and mixing characteristics, we study the comparisons of different values with considering and ignoring temperature field with a rotational speed of 10 rpm in the lines L_1 and L_2 as shown in Fig. 8.

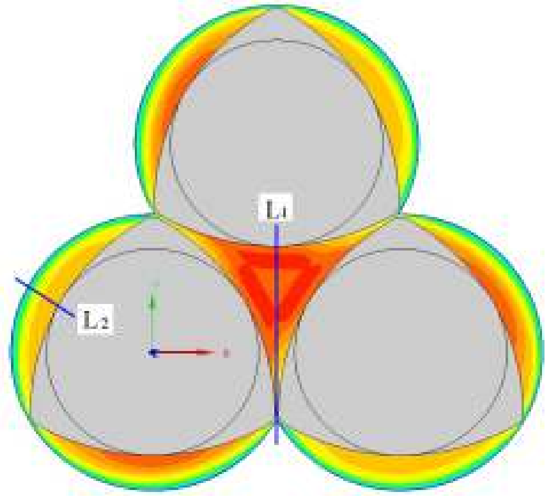


Fig. 8: Positions of different lines in the tri-screw extruder

Figure 9 describes the temperature distributions in different lines of the tri-screw extruder. It can be seen

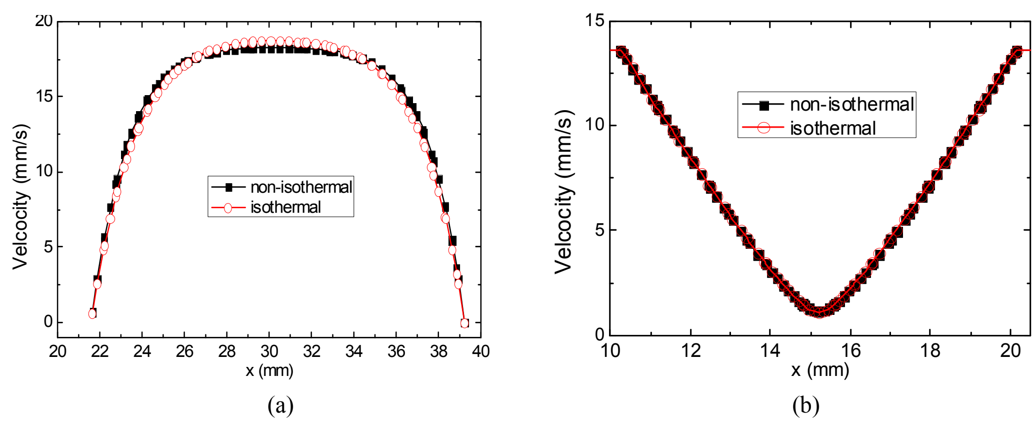


Fig. 9: Velocity distributions in different lines: (a) L_1, (b) L_2

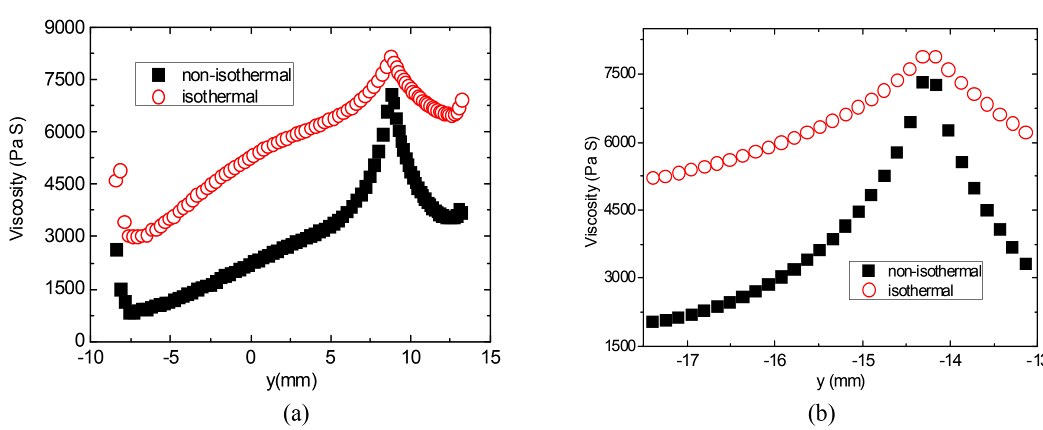


Fig. 10: Viscosity distribution in different lines: (a) L_1, (b) L_2

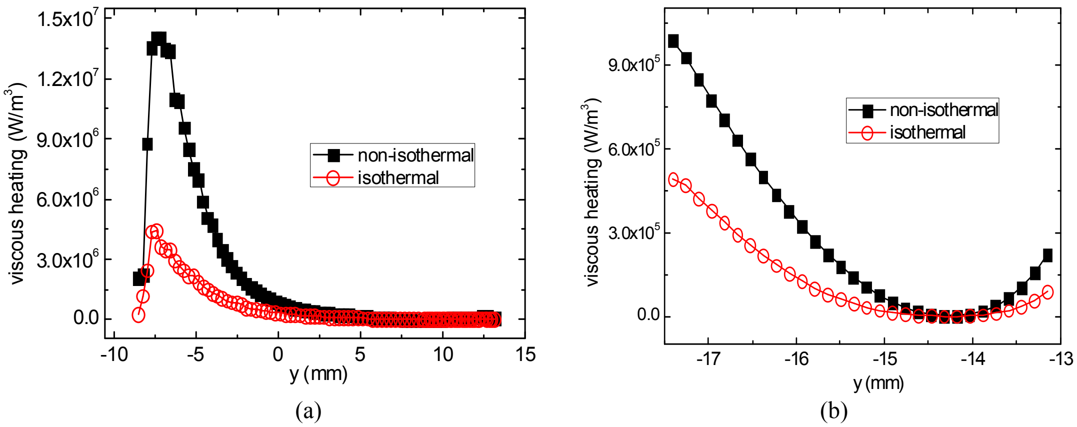


Fig. 11: Viscous heating distribution in different lines: (a) L_1, (b) L_2

that the velocities in the two lines with considering temperature field are almost equal to those with ignoring temperature field. Those illuminate that the temperature filed has little effect on the flow velocity in the tri-screw extruder.

Figure 10 displays the viscosity distributions in different lines of the tri-screw extruder. It can be seen that the viscosity distribution rules of considering and ignoring temperature field are same, but the values of considering temperature field are smaller than those of ignoring temperature field. Meanwhile, the maximal rising viscosity comes to 90% of considering temperature field in line L_1. But in middle of the center region, the viscosity rising is minimal due to the low shear rate.

Figure 11 describes the viscous heating distribution in different lines in the tri-screw extruder. It can be seen that the values of viscous heating in middle of center region and 'C' region with considering temperature field are similar to those with ignoring it, because the shear rates and viscosities are very small in those region and the temperatures are relatively high. Therefore, the temperature field has great effect on the viscous heating distribution in the tri-screw extruder.

Effect of temperature fields on the mixing efficiency: Distributive and dispersive mixing are very important parameters to design screw extruders. The scale of segregation S(t) is an important tool to evaluate the distributive mixing of laminar flow and can be expressed by:

$$S(t) = \int_0^{\zeta} R(r,t)dr \tag{6}$$

Where R(r, t) is a correlation coefficient for the concentration (Polyflow, 2007) and it gives the probability of finding a pair of random points with a relative distance *r* and with the same concentration. The segregation scale is a measure of the size of the regions of homogenous concentration and it decreases when mixing improves.

The effect of temperature field on the segregation scale of the tri-screw extruder is shown in Fig. 12. Initially, the two curves show a rapid drop to a segregation of operation due to big segregated area. After 50 sec, the segregation scale with isothermal model of the tri-screw extruder fluctuates smaller than that with non-isothermal model. At the same time, the values of segregation scale with non-isothermal model are smaller than those with isothermal model, because the viscous heating increases. It implies the better dispersive mixing in the tri-screw extruder with considering the temperature field.

In order to evaluate the extensional mixing efficiency of the flow inside the screw extruders we obtained the mixing index as defined by Polyflow (2007):

$$\lambda_{MZ} = \frac{|D|}{|D| + |W|} \tag{7}$$

where,

$|D|$: The rate of deformation tensor

$|W|$: The norm of the vorticity tensor. The extensional efficiency coefficient is equal to 0 for pure rotation, 0.5 for simple shear flows and 1 for pure elongation

λ_{MZ} : 0 for pure elongation

Figure 13 depicts the effect of temperature fields on the mixing index in the tri-screw extruder. It can be seen that the mixing index of the tri-screw extruder decreases when the temperature effect is considered. It reveals that the weak dispersive mixing of the tri-screw extruder due to the decrease of shear rate with the non-isothermal model. It will result in the decrease of dispersive mixing for the tri-screw extruder with considering temperature field.

The instantaneous efficiency is defined as a local instantaneous efficiency of mixing given by:

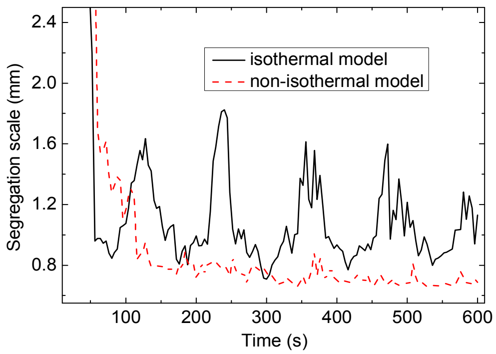


Fig. 12: Effect of temperature fields on the segregation scale

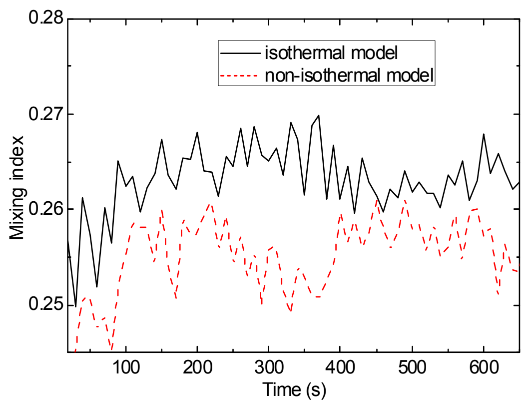


Fig. 13: Effect of temperature fields on the mixing index

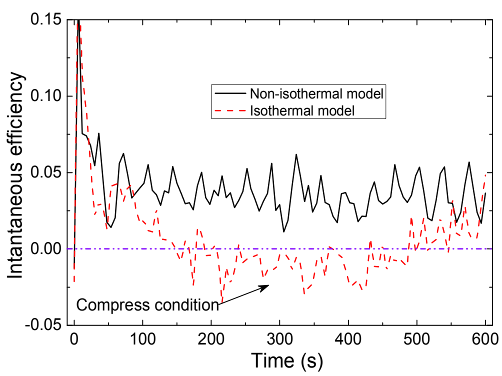


Fig. 14: Effect of temperature fields on the instantaneous efficiency

$$e_\lambda = \frac{\dot{\lambda}/\lambda}{(D:D)^{\frac{1}{2}}} \tag{8}$$

where, D is the rate of strain tensor. The instantaneous efficiency can be thought of as the fraction of the energy dissipated locally that is used to stretch a fluid element at a given instant in a purely viscous fluid (Polyflow, 2007).

Figure 14 shows the effect of temperature fields on the instantaneous efficiency of the tri-screw extruder.

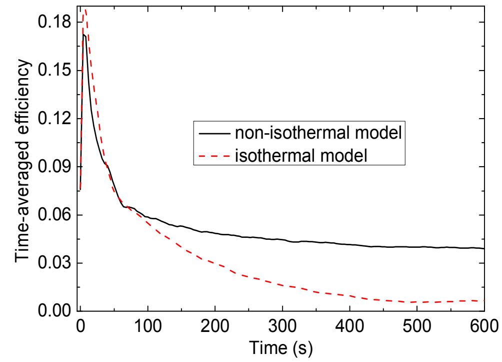


Fig. 15: Effect of temperature fields on the time-averaged efficiency

When the viscous heating is considered with the non-isothermal model, the instantaneous efficiency of the tri-screw extruder is all above zero at all times, because the splitting and folding of the flow by the screws. However, the values of instantaneous efficiency ignoring the viscous heating with isothermal model are less than zero during 60-150 sec for the tri-screw extruder. It implies that the flow particles in the tri-screw extruder are in the compressing conditions. This is not benefit to efficient laminar mixing due to the little viscous dissipations. So the instantaneous mixing efficiency of the tri-screw extruder decreases with considering the temperature effect.

The time-averaged efficiency is used to describe the stretching mixing and can be defined as Polyflow (2007):

$$(e_\lambda) = \frac{1}{t}\int_0^t e_{\lambda\, dt} \tag{9}$$

Typical time-averaged efficiency will decrease with the increase of the mixing time. Figure 15 shows the effect of temperature fields on the time-averaged efficiency for the tri-screw and twin-screw extruder. When the temperature filed is considered, the time-averaged efficiencies of the tri-screw extruder obviously increase due to the increase of viscous dissipation. For example, the time-averaged efficiency of the tri-screw extruder increases to 0.0431 from 0.0124 at 350 sec and increases to 0.0391 from 0.0278 at 600 sec. So the temperature field has great effect on stretch mixing such as time-averaged mixing efficiency for the tri-screw extruder.

CONCLUSION

- There is one dead flow zone in the center region for the tri-screw extruder, where the viscous heating are relatively small and the viscosity and temperature are relatively big, showing the poor flow and mixing efficiency in the center region.
- With the increase of rotational speeds, the temperature rise increases gradually due to the increase of shear rate. When the rotational speeds

increase from 1 to 10 rpm, the increasing temperatures also increase to 4.26 from 0.35 K. By comparison, we can found that the velocities are almost unchangeable, but in the viscosity decreases and viscous heating increases obviously, when the temperature field is considered for the tri-screw extruder. Therefore, the temperature rise has great effect on the viscosity and viscous heating distributions.

- The temperature field has great effect on the mixing performances for the tri-screw extruder. When the temperature field is considered, normalized segregation scale and instantaneous efficiency all increase, but the mixing index decreases for the tri-screw extruder. Therefore, the dispersive mixing of the tri-screw extruder decreases, but the distributive mixing increases with considering the rising temperatures due to viscous dissipation. In particular, the stretching effect of the particles in the tri-screw extruder decreases due to the decrease of viscous dissipation when non-isothermal model is employed.

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