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Characterization of melt-mixing in extrusion: finite-time Lyapunov exponent and flow pattern structure

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Abstract. We discuss the mixing characteristics of different kneading blocks based on the numerical simulation of non-isothermal polymer melt flow. The distributive and dispersive mixing is assessed by using finite-time Lyapunov exponent and the mean stress during residence. In addition, the flow patterns associated with the different geometry of the mixing elements are quantified by the strain-rate state. Our approach is found to be useful to evaluate essential difference of mixing characteristics between the conventional kneading discs element and pitched-tip kneading discs elements.

Keywords: Mixing, Twin-screw extrusion, Finite-time Lyapunov exponent
PACS: 83.50.Xa Mixing and blending

INTRODUCTION

The mixing of polymeric fluids, such as polymer blends and composites, is a key process in extrusion processes because homogenization of distributions of temperature and additives, as well as of the size of filler materials are mainly achieved by melt-mixing [1, 2, 3]. In single/twin-screw extrusions, since the geometry of the mixing elements mainly determines the characteristics of the mixing process, various types of mixing elements have been developed [2, 3]. Understanding the relation between the channel geometry and the mixing characteristics is a key issue in the development of a mixing element. For this purpose, the fluid dynamical characterization of the mixing process is required.

In general, mixing processes are discussed from two viewpoints of distributive and dispersive mixing, so the relative contribution of these effects defines the mixing characteristics of a process. For the discussion of distributive mixing, the distribution of residence time is often used experimentally and numerically. However, the residence time distribution only reflects the mixing in axial direction. In order to assess the mixing ability in three-dimensional space, different approach is required. The distributive mixing requires the divergence of the nearby trajectories and the resulting disappearance of positional correlation of fluid particles. This process can be measured with the finite-time Lyapunov exponent (FTLE) for the transient flow in extrusion processes. On the other hand, the general aspect of the dispersive mixing can be measured with the distribution of the mean stress during the residence in the melt-mixing zone. In this article, the mixing characteristics of different kneading blocks are evaluated based on the numerical simulation of non-isothermal polymer melt flow, and the variation of the mixing characteristics by the element geometry is discussed.

CHARACTERIZATION OF FLOW AND MIXING

Fluid particles starting from the different locations in the inlet of the kneading zone take different paths. Kinematic histories of all the paths constitute the mixing process. FTLE, denoted as λ_t, measures the exponential growth rate

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over a finite time interval, t, of the distance between two initially nearby points, $|\boldsymbol{l}|$, namely, $|\boldsymbol{l}|(t_0+t) = |\boldsymbol{l}||(t_0)\ \exp(\lambda_t t)$. Positive λ_t indicates the disappearance of positional correlation is faster for larger value of λ_t, while zero or negative λ_t indicates the sustained positional correlation. Since λ_t changes along an individual path, the mean value over the residence time represents the mixing potential of the path, and the statistical distribution of the mean FTLE during residence over the all the paths characterize the overall mixing ability of the kneading zone.

Difference in the distributive/dispersive mixing for different channel geometry comes from the flow pattern dominated by the mixing element. Local flow pattern, including planar flow, converging and bifurcating flows, can be conveniently identified by the strain-rate state $\beta = 3\sqrt{6}\det \boldsymbol{D} / (\boldsymbol{D}:\boldsymbol{D})^{3/2}$ which is a scalar quantity and an invariant of the strain-rate tensor $\boldsymbol{D} = (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)/2$ [4]. Positive and negative values of β respectively indicate the converging and bifurcating flow, while $\beta = 0$ indicates the planar flow. The spatial distribution of β helps to understand the geometry-driven flow pattern of each mixing element.

SCREW MODELS AND SIMULATION

Figure 1 shows five kinds of kneading blocks (KD) used in this study. Forward kneading discs element (FKD) is a conventional KD, while the others are pitched-tip KDs (ptKD) [5, 6]. In ptKDs, the tips of each disc are twisted with respect to the screw axis. For a conventional KD, the pumping ability and flow pattern are primarily determined by the disc-stagger angle. In contrast, for a ptKD, the channel geometry is modified by pitched tips, leading the combination of tip angle and disc-stagger angle determines the flow characteristics. The combination of forward or backward tip (Ft or Bt) with forward or backward disc-stagger (Fs of Bs) defines four different types of ptKD shown in Fig. 1.

Figure 2 shows the screw configuration used in this study. In the kneading block zone in Fig. 2, we set either KD shown in Fig. 1. The diameter of the barrel, D, is set to 28 mm. The whole domain of the melt-mixing zone of Fig. 2 is $L/D = 3.28$, while the KD zone is $L/D = 1.5$.

The flow of a polymer melt is modelled by Stokes equation, $0 = -\nabla p + \nabla \cdot \boldsymbol{\tau}$, with the incompressibility condition, $\nabla \cdot \boldsymbol{v} = 0$, and the heat equation, $\rho c_p \boldsymbol{v} \cdot \nabla T = k \nabla^2 T + \boldsymbol{\tau} : \boldsymbol{D}$. The fluid is assumed to be a viscous shear-thinning fluid, $\boldsymbol{\tau} = 2\eta \boldsymbol{D}$, where the viscosity is modelled by Cross–Arrhenius model. The specific values of the parameters are from Ref. [6]. The barrel and the screw surfaces are non-slip, the temperature at the inlet and the barrel surface is set to be 473.15 K, the volume flow rate and the screw rotation speed are respectively set to $10 cm^3/s$ and 100-200 rpm. The set of equations was solved by the SIMPLE method using a commercial software, "R-FLOW" (R-flow Co., Ltd., Saitama, Japan). The trajectories of the passive tracers were calculated by integrating the solved velocity field, and were analyzed for characterization of the mixing process of each KD.

RESULTS AND DISCUSSION

Figure. 3 shows the average pressure drop across the kneading block as a function of the screw rotation speed under a flow rate of $10\ cm^3/s$. Fs-Bt, Bs-Ft, and Bs-Bt ptKDs shows positive pressure drops, indicating a negative pumping ability. in contrast to the positive pumping abilities of Fs-Ft ptKD and FKD.

Figure 4 shows the average temperature profile along the extrusion direction. For the five different KDs, the average temperature increases with the axial position. The variation by KD types is at most 5 K, suggesting the temperature does not have a significant effect on the mixing ability.

For an evaluation of the development of converging and bifurcating flows, the section-average of the strain-rate state as a function of the axial position is drawn in Fig. 5. In Fig. 5, the strain-rate state is decomposed as $\beta = \beta_+ + \beta_-$ so that $\beta_+ > 0$ and $\beta_- < 0$ in order to evaluate the converging and bifurcating flows separately. FKD and Fs-Bt ptKD basically have a similar $\beta\pm$ profile: the converging flow increases at the upstream side within individual disc regions, while the bifurcating flow increases at the downstream side, but the development of these non-planar flow is more enhanced in Fs-Bt ptKD. The occurrence of the non-planar flows as well as the axial variation of them is most prominent in Bs-Ft ptKD. The development of the converging/bifurcating flows is responsible for the mixing ability in low-strain-rate region of the channel [4]. This fact suggests that the flow pattern driven by Fs-Bt and

Bs-Ft ptKDs is more effective in distributive mixing than in FKD. In contrast, for both Fs-Ft and Bs-Bt ptKDs, both the converging and bifurcating flows are substantially suppressed compared to FKD, indicating the circumferential planar flow is prevailing in Fs-Ft and Bs-Bt ptKDs.

Figure 6 shows the probability density function (PDF) of the time-averaged FTLE during residence in the kneading block zone, under a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm. We observe that PDF of mean FTLE is bimodal for FKD, indicating that a large fraction of the trajectories takes positive FTLE but a certain small fraction takes negative FTLE. This fact suggests that mixing by FKD at this condition have a large inhomogeneity due to the negative FTLE portion. In contrast, for four types of ptKD, PDF of mean FTLE is unimodal, suggesting that pitched tips on KD are effective to reduce the inhomogeneity in the mixing process. For Fs-Ft and Bs-Bt ptKDs, although the mean FTLE is positive on average, some fraction of trajectories takes negative value of mean FTLE, indicating that the mixing ability is rather suppressed. In contrast, for Fs-Bt and Bs-Ft ptKDs, the fraction of negative mean FTLE almost vanishes and the average value of the mean FTLE is larger than FKD, suggesting more homogeneous and enhanced mixing ability than that of FKD.

Figure 7 shows the joint PDF of the mean FTLE and mean stress during residence under a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm. For FKD, we observe that the trajectories with lower mean stress take negative or positive but small values of FTLE, indicating this portion causes both distributive and dispersive mixing by FKD largely inhomogeneous. In contrast, for four types of ptKDs, the joint PDFs in Fig. 7 are unimodal, suggesting the uniformities in distributive as well as dispersive mixing by ptKDs are improved in comparison with those by FKD. In addition, the levels of the mean FTLE and the mean stress are different for different ptKDs, showing the balance between the distributive and dispersive mixing can be tuned by modifying the combination of pitched-tip and disc-stagger angles in the ptKD keeping a level of homogeneity of mixing.

CONCLUSIONS

The mixing characteristics of a conventional kneading discs (KD) element and four types pitched-tip KD elements are evaluated by using the numerical simulation of the melt flow. For direct evaluation of distributive mixing ability, finite-time Lyapunov exponent (FTLE) is used, and the distribution of the mean FTLE during residence turns out to be useful to quantify the mixing characteristics of different mixing elements. The inhomogeneity as well as the average level of distributive and dispersive mixing are clearly evaluated by the joint PDF of the mean FTLE and mean stress during residence. The results indicate that inhomogeneity of mixing by a conventional FKD can be suppressed by using either pitched-tip KD. Underlying mechanism for different mixing characteristics originates from the flow pattern driven by the geometric shape of the mixing elements. In an assessment of the relation between flow pattern and the channel geometry, the qualitative change in the flow pattern by geometries are reflected in the distribution of the converging and bifurcation flows, which can be conveniently quantified with the strain-rate state.

Understanding the relation between the channel geometry and the flow pattern behind the different mixing characteristics of different mixing elements is an essential issue in the optimization and the development of mixing processes. In this line, the approaches used in this study can be applied to other mixing devices, including twin- screw ones as well as single screw ones, in order to discuss the geometry effects on the mixing characteristics.

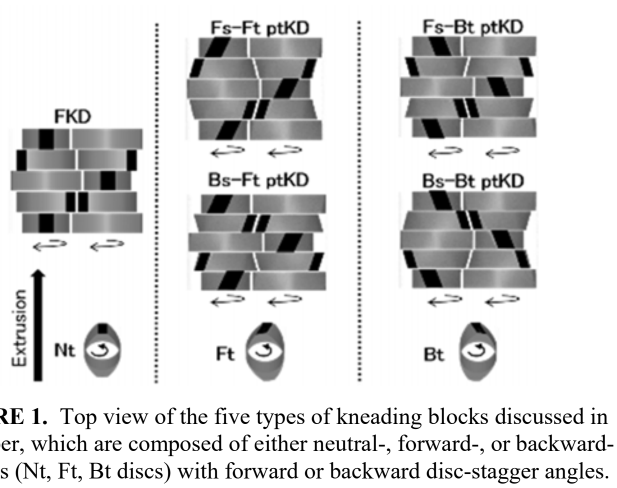

FIGURE 1. Top view of the five types of kneading blocks discussed in this paper, which are composed of either neutral-, forward-, or backward-tip discs (Nt, Ft, Bt discs) with forward or backward disc-stagger angles.

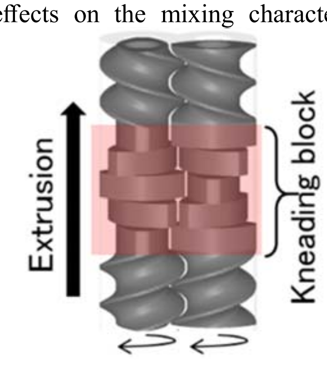

FIGURE 2. Screw configuration of the melt-mixing zone. From the inlet (bottom of the figure), forward conveying element, kneading block, and backward conveying element are configured. The arrows indicate the extrusion direction and the rotation direction.

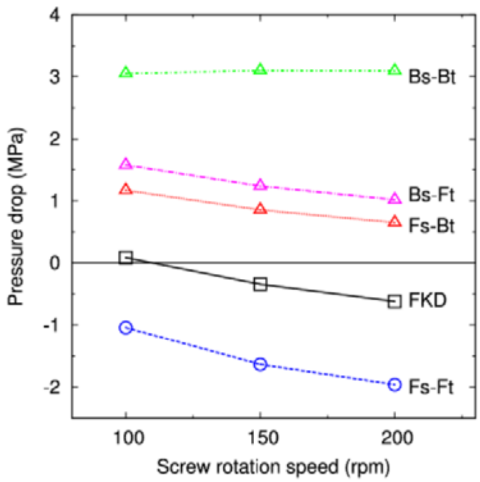

FIGURE 3. Average pressure drop in the kneading block zone over a section and one screw rotation under a flow rate of 10 cm^3/s as a function of screw rotation speed.

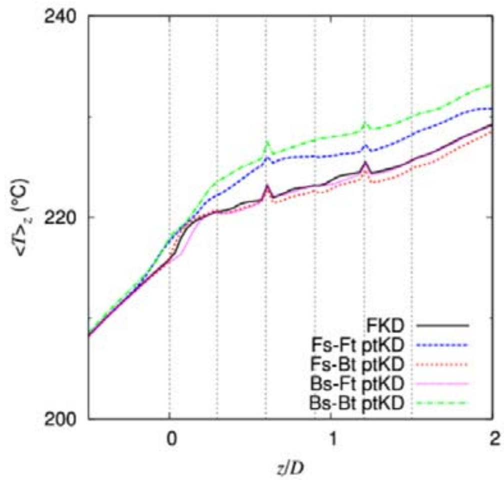

FIGURE 4. Average temperature over a section and one screw rotation as a function of the axial position with a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm for five types of kneading blocks. The vertical dashed lines indicate the locations of the ends of the discs in the KDs.

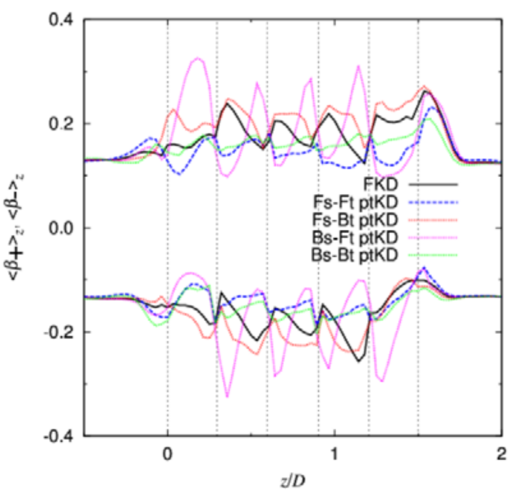

FIGURE 5. Average strain-rate state over a section and one screw rotation as a function of the axial position with a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm for five types of kneading blocks. $\beta_{\pm}$ respectively represent positive and negative values of β, which correspond to the converging and bifurcating flows. The vertical dashed lines indicate the locations of the ends of the discs in the KDs.

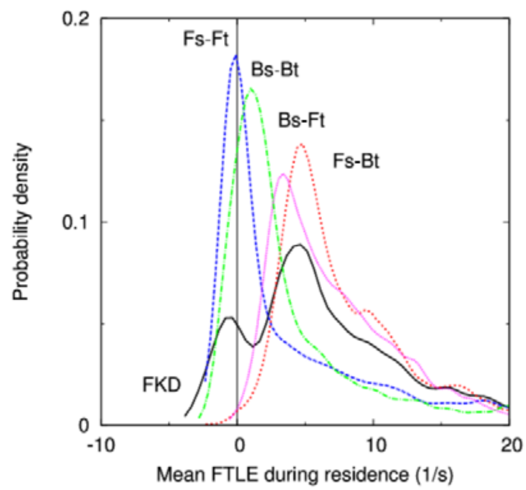

FIGURE 6. Probability density of the mean FTLE during residence with a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm.

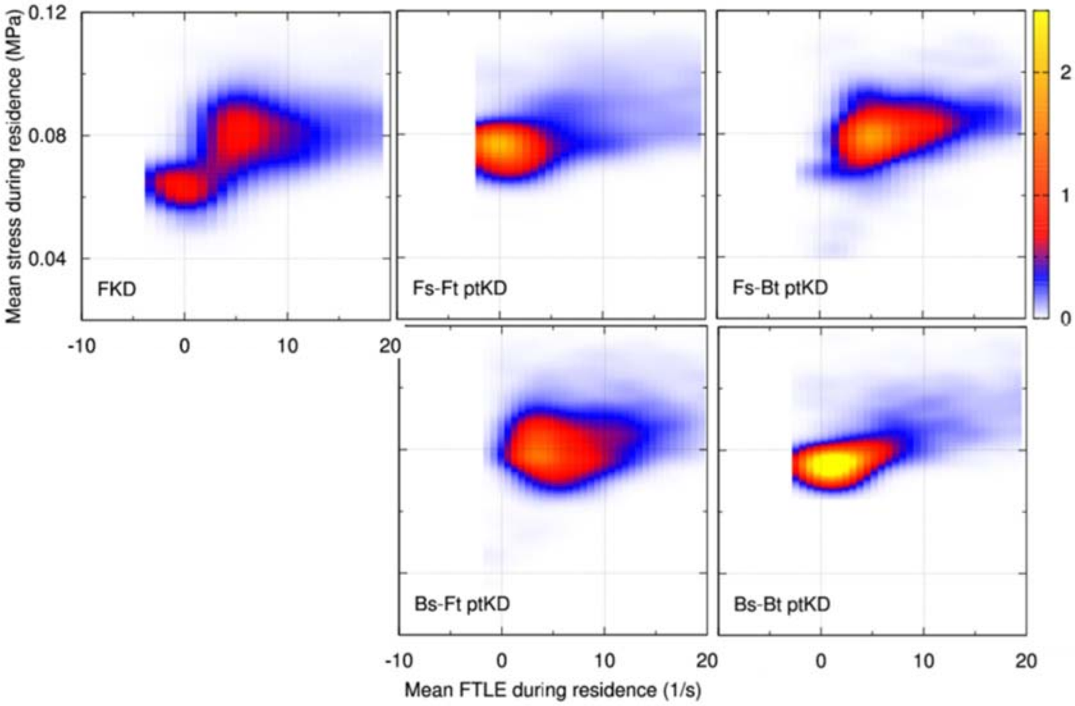

FIGURE 7. Joint probability density of the mean FTLE during residence and the mean stress during residence in the kneading block zone with a flow rate of 10 cm^3/s and a screw rotation speed of 200 rpm.

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