THE USE OF GLOBAL MIXING INDICES TO ASSESS MIXING EFFICIENCY IN SINGLE SCREW EXTRUSION

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Abstract: Mixing indices can be derived from descriptions of morphology evolution of liquid-liquid or solid-liquid systems coupled to computations of flow and temperature along a plasticating screw (thus, including in the analysis the melting and melt conveying stages). In the case of liquid-liquid systems, distributive mixing depends essentially on droplet stretching and residence time, while dispersion takes into account the opposed effects of drop break-up and coalescence. Distributive mixing of solids-liquid systems depends on residence time and location (calculated via entropy), while dispersive mixing considers rupture and erosion phenomena.

Introduction

Generally, single screw extruders are required to pump at the highest possible rate a homogeneous melt, i.e., a well distributed and well dispersed media, which might contain two or more polymers, additives, or fillers. Both the screw configuration and the operating conditions play a role in mixing efficiency. Given the importance of the topic, several attempts have been made to understand the physics of mixing and to develop corresponding mathematical descriptions applicable to extrusion (for example [1,2]).

The present work uses the above concepts to evaluate the mixing ability of extrusion screws. In order to demonstrate the sensitivity of the method, the effects of geometrical and operational parameters are discussed.

Mixing Indices

Mixing a two-phase system involves distribution or/and dispersion of the additive component (liquid or solid) in the melted matrix [1, 2]. Quantification of mixing must be approached differently in each liquid/solids additives system [3].

Liquid Additives

The system containing liquid additives forms drops in the micro-scale, which can suffer break-up (splitting into two smaller drops) or coalescence (two drops joining together). Both phenomena depend on various parameters, such as relative viscosity, viscous forces, surface tension and residence time [4].

Dispersive mixing is quantified by computing the change in drop diameter (d) relative to its original size (d_i), at any location. A global mixing index is defined, taking into account the existence of N drops [3]:

$$mix_{disp} = \frac{\sum_j^N \left[\left(\frac{d}{d_i} \right)_j \times \left(1 - \frac{d}{d_i} \right)_j \right]}{\sum_j^N \left(\frac{d}{d_i} \right)_j} \qquad (1)$$

Distributive mixing is assessed using the concept of affine deformation, which depends on shear rate and residence time. The respective mixing index is a function of the drop width (B) and of the initial drop diameter (d_i) [3]:

$$mix_{dist} = \frac{\sum_j^N \left[\left(\frac{d}{d_i} \right)_j \times \left(1 - \frac{B}{d_i} \right)_j \right]}{\sum_j^N \left(\frac{d}{d_i} \right)_j} \qquad (2)$$

Both mixing indices are dimensionless, ranging in the interval [0, 1]. For both cases, value 1 corresponds to perfect mixing.

Solid Additives

Solid additives are usually made up of agglomerates, which, in turn, are formed by aggregates, these comprising several indivisible particles. Agglomerates can rupture (into a few large fragments) or erode (detachment of small particles from the agglomerate surface), depending on the hydrodynamic forces induced by the flow and on the agglomerate cohesive forces [5, 6].

Agglomerate dispersion depends on the breakup probability (related with the agglomerate surface) and on residence time [6]. Equation (1) can be used to estimate the degree of dispersion if d is now the agglomerate/aggregate/particle diameter and d_i the original agglomerate size [3].

To quantify the agglomerate distribution in the system an entropic measure is applied using the Shannon entropy [7, 8]:

$$S = -\sum_{j=1}^{M} p_j \, log \, p_j \tag{3}$$

where p_j is the probability of finding a particle in bin j and M is the total number of bins in which the screw channel section is divided. Normalizing S ($S_{norm} = S/\log(M)$), Shannon entropy ranges also in the interval [0. 1]. S is maximum when the probability of finding a particle is identical on every bin, i.e., $S_{max} = \log(M)$.

Case study

An extruder with a screw diameter of 30 mm and an L/D of 30 was considered. The channel depth of the feed and metering sections is 5 and 2 mm, respectively, and the length of the feed, compression and metering sections (i.e., L_1, L_2 and L_3) is identical (10D).

A High Density Polyethylene was taken as the matrix. Ten thousand drops with a radius of 10 μm were inserted progressively and uniformly distributed in the channel cross-section, as melting was taking place. The viscosity ratio between these and HDPE was taken as 1. In the case of the solid-liquid system, 10.000 silica agglomerates were inserted as above, corresponding to a concentration of 2.1%. Each agglomerate contains 100 aggregates and each aggregate 100 single particles. The agglomerates had a cohesive strength of 1000Pa.

Results and Discussion

Effect of Screw Speed

Since screw speed influences deformation, residence time and mass output, it has a profound effect on mixing efficiency. Upon increasing screw speed, shear rate and mass output increase (Figure 1), and residence time for melting and for melt conveying diminishes (Figure 2).

Figure 3 shows the influence of screw speed on the dispersive and distributive mixing indices, in the case of liquid systems. In spite of the higher shear rates associated with higher screw rotations, dispersive and distributive mixing decrease due to the decrease in the overall residence time for mixing.

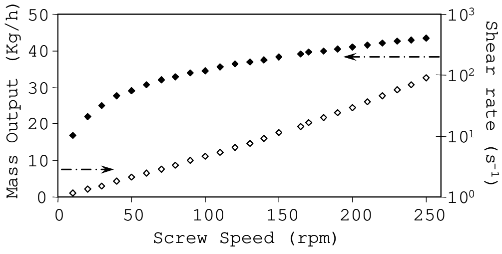

Figure 1 – Variation of mass output and shear rate with screw speed.

In the case of solid additives (Figure 4), the dispersive mixing index increases up to 60 rpm due to the higher hydrodynamic forces, but beyond that value the particles residence time becomes too short to achieve a good dispersion. The distributive mixing, quantified via Shannon entropy, decreases also, thus reflecting the decrease in residence time.

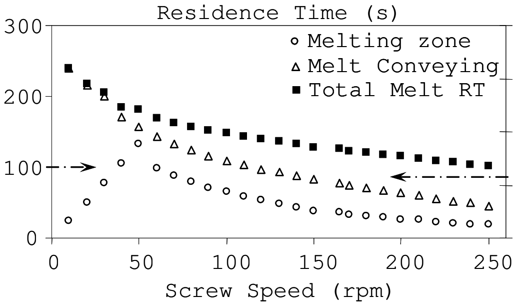

Figure 2 – Variation of Residence time for melting, melt conveying and total residence time (RT) with screw speed.

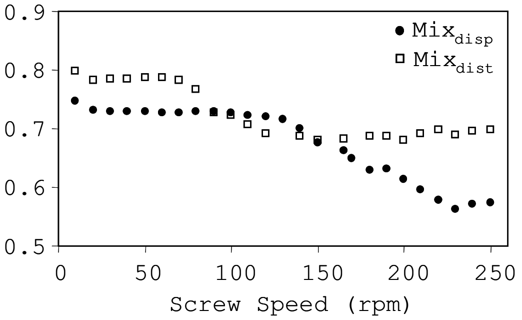

Figure 3 – Dispersive and distributive mixing indices for a liquid-liquid system.

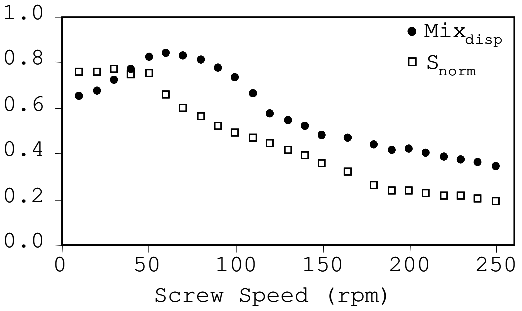

Figure 4 – Dispersive and distributive (Shannon entropy) indices for solid-liquid system.

Effect of Screw Geometry

To illustrate the effect of screw geometry on mixing, the length of the metering section was changed, i.e., numerical simulations were also carried out for a screw with a metering length, L_3, equal to 20D. As anticipated and shown in Figure 5, the residence time increases essentially in the melt conveying zone, while mass output and shear rate decrease (see Figure 6).

Thus, in the case of liquid additives, dispersive and distributive mixing indices are improved with the longer screw (see Figures 7 and 8). Figure 9 shows the evolution of the dispersive mixing index for the solid-liquid system. Dispersion is higher, because the residence time of the particles is higher. The same behavior was observed for the distributive mixing index, as seen in Figure 10.

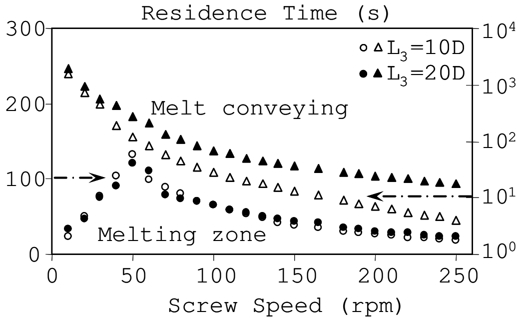

Figure 5 – Residence time for melting and melt conveying for screws with distinct metering lengths.

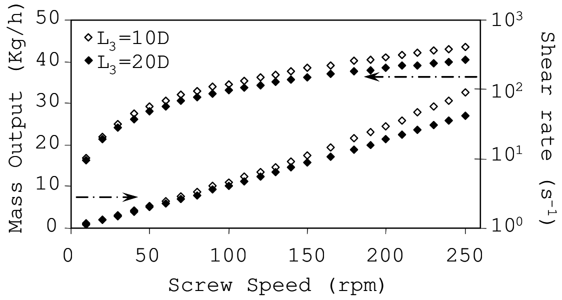

Figure 6 – Mass output and shear rate for screws with distinct metering lengths.

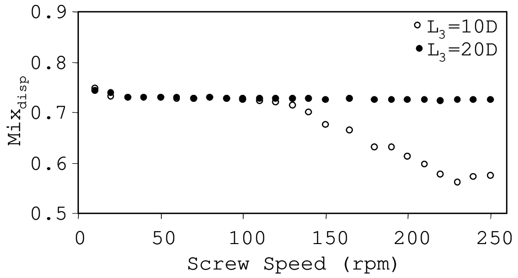

Figure 7 – Dispersive mixing for screws with distinct metering lengths (liquid-liquid system).

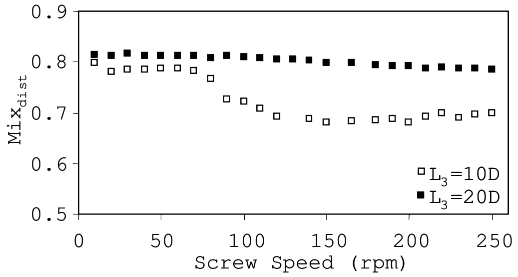

Figure 8 – Distributive mixing for screws with distinct metering lengths (liquid-liquid system).

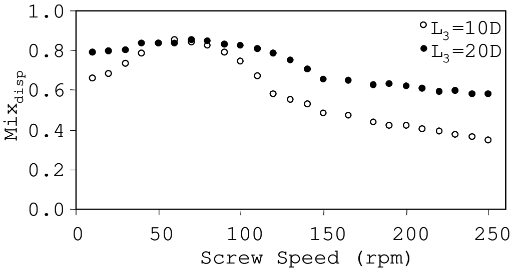

Figure 9 – Dispersive mixing for screws with distinct metering lengths (solid-liquid system).

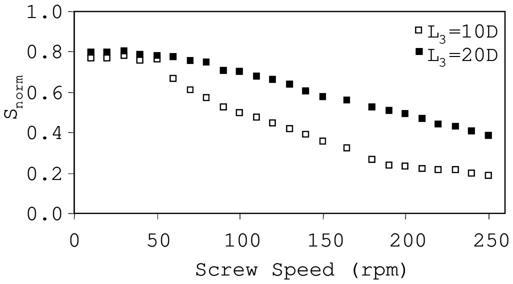

Figure 10 – Normalized Shannon entropy for screws with distinct metering lengths.

Conclusions

Dispersive and distributive mixing in single screw extruders can be estimated considering systems containing liquid or solid additives. The indices range in the interval [0,1], which facilitates the comparison of the mixing efficiency of different screws.

Mixing efficiency depends on material properties, operating conditions and screw geometry, the methodology being sensitive to all these parameters.

Acknowledgements

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