SIMULATION OF DISTRIBUTIVE AND DISPERSIVE MIXING IN A CO-ROTATING TWIN-SCREW EXTRUDER

L. Cong and M. Gupta
Michigan Technological University, Houghton, MI, 49931

Abstract

Simulation results for mixing of two different polymers in a co-rotating twin-screw extruder are presented. Velocity distribution predicted by a three-dimensional simulation of the flow is used to predict the change in the spatial distribution of initially segregated particles as well as the reduction in radius due to erosion. The predicted particle distribution is used to estimate the increase in Shannon entropy due to dispersive and distributive mixing along the extruder channel.

Introduction

Dispersive mixing refers to the break-up of the minor component of a mixture into smaller size particles or droplets, whereas distributive mixing leads to a homogeneous spatial distribution of the minor component into the polymer matrix [1]. A three-dimensional simulation of the flow can be exploited as an excellent aide for analysis of dispersive as well as distributive mixing in screw extruders. The predicted velocity distribution along with a particle tracing scheme for finding path lines can be employed to predict the mixing efficiency in screw extruders. In references [1, 2], this methodology was applied to study the mixing in single-screw extruders. Implementation of a particle tracing algorithm for a single-screw extruder is relatively simple because a time-independent flow field can be obtained by keeping the screw stationary and rotating the barrel in the direction opposite to the screw rotation direction. In comparison to single-screw extruders, the flow in twin-screw extruders is much more complicated. Besides the increased complexity of geometry, the time-dependent flow in a twin-screw extruder cannot be transformed into a steady state flow by fixing the coordinate frame on a screw. Because of the time-dependent nature of the flow, the predicted velocity distribution for a single configuration of the two screws cannot be used to trace the path lines in a twin-screw extruder. However, in a reference frame moving with axial velocity \( V_{ax} = LN \) towards the exit, where \( L \) is the screw lead and \( N \) is the rotational speed in revolution per second, the flow field in a twin-screw extruder is time independent. In the present work, a particle tracing scheme was developed to trace path lines in this translating reference frame. Quality of distributive mixing in a co-rotating twin-screw extruder was evaluated by finding the change in the spatial distribution of initially segregated particles. For the same twin-screw extruder, quality of dispersive mixing was determined by using the erosion model of Manas-Zloczower et al. [1, 2].

Shannon Entropy of a Mixture

Following the approach of Manas-Zloczower and co-workers [1], in the present work Shannon entropy [3] is used as a measure of the quality of mixing. For mixing of two different types of particles (red and blue), if the flow domain at each cross section is divided into \( M \) equal-sized bins, Shannon entropy \( S \) is in defined as

\[
S = \sum_{c=1}^{M} \sum_{j=1}^{M} P_{c,j} \ln P_{c,j}
\]

where \( c \) represents the particle type (red or blue) and \( P_{c,j} \) is the probability of finding particle of color \( c \) in bin \( j \).

To estimate the homogeneity of color, Manas-Zloczower et al. [1] subtracted the entropy associated with the overall spatial distribution of particles (irrespective of the type of particles) \((- \sum_{j=1}^{M} P_j \ln P_j )\) from the Shannon entropy, resulting in a quantity called color homogeneity index (CHI).

\[
\text{CHI} = (S + \sum_{j=1}^{M} P_j \ln P_j )/\ln(2)
\]

where \( P_j \) is the probability of finding a particle (irrespective of color) in bin \( j \) and the division by \( \ln(2) \) is used to normalize the index such that its value lies between 0 and 1.

Erosion Model for Porous Agglomerate

Two different types of mechanisms, namely, rupture and erosion, are often employed to analyze dispersive mixing. Rupture refers to break-up of a particle or drop into two parts of comparable size. For erosion, the original particle or drop is modeled as an agglomerate of smaller particles or droplets, which are detached or ‘peeled’ off the agglomerate surface. The erosion model developed by Scurati et al. [4, 5] is employed in the present work to predict the quality of dispersive mixing. Scurati et al. [4, 5] postulated that reduction in radius \( (R) \) of an agglomerate in a shear flow is proportional to the shear rate \( (\dot{\gamma}) \) and the difference between the hydrodynamic \( (F_h) \) and cohesive \( (F_c) \) forces.

\[
\frac{dR}{dt} = K(F_h - F_c) \frac{\dot{\gamma}}{2}
\]

where \( K \) is the proportional coefficient. Scurati et al. [4, 5] assumed that during erosion the agglomerate maintains a