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Extension rate distribution and impact on bubble size distribution in Newtonian and non-Newtonian fluid in a twin screw co-rotating mixer

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A R T I C L E I N F O

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A B S T R A C T

Extension rate distributions have been calculated in a twin screw mixer for Newtonian and non-Newtonian fluids because they strongly affect dispersion of bubbles and the maximum stable diameter estimated from calculations of the Capillary number. Extension rate calculations were made using the ratio of the third invariant of the strain rate tensor to the second invariant of the strain rate tensor following the classical work of Debbaut and Crochet (1988). The extension rate was quite significant and represented 15–25% of the magnitude of the shear rate depending on location in the mixer and mixer speed. The center of the mixer where the two sets of paddle elements intermesh displays high extension and shear rates. Critical capillary numbers and maximum stable bubble diameters depended much more on extension than shear rate. Maximum stable bubble diameters were calculated at different locations in the mixer from numerical predictions of the critical capillary number and they were mapped inside the geometry of the mixer for the first time. The results offer important insights on how to design a mixer to achieve a desired bubble size distribution.

1. Introduction

Extensional flows during mixing are very important in the deformation and breakup of droplets and bubbles which in turn are very important to foaming processes in the chemical and food industries. (Vyakaranam and Kokini, 2012; Cisneros and Kokini, 2002; Huang and Kokini, 1999). While shear rate distribution calculations are routinely made, extension rate calculations have never been made in a complex geometry since the classical work of Debbaut and Crochet (1988) showed that extension rate is equal to the ratio of six times the third invariant to the second invariant of the strain rate tensor. This is true despite the importance of extension rate in the transportation and quality of products composed of two phase dispersed systems such as aerated wheat flour doughs, direct extension rate distribution studies have not been conducted in any complex geometry. Fundamental studies of extension rate generally used simplified geometries such as abrupt contractions (Debbaut and Crochet, 1988; Keunings and Crochet, 1984; Debbaut et al., 1988) or expansions (Dheur and Crochet, 1987), flow around a sphere, and circular die swell (Debbaut and Crochet, 1988). Extension rate is important in complex flows but it occurs in tandem with shear rate and most flows are combined shear and extension. In their rigorous theoretical studies Debbaut and Crochet (1988) examined extensional flows for generalized Newtonian (White-Metzner and Bird-Carreau) and viscoelastic fluids (upper-convected Maxwell).

Janssen and Meijer (1993) noted that fluids in practical mixing devices experience bubble break-up beginning with the elongation of threads rather than stepwise break-down of larger bubbles under equilibrium conditions. Consistent with our current work they showed that transient mechanisms resulted in smaller droplets and allowed a finer morphology at a higher viscosity ratio. They found that 2D elongation was more effective than simple shear flow. In fact, the critical capillary number (Ca_{cr}) was lower for the thread scenario than that for a drop. A greater stretching rate caused a thinner thread before break-up and thus smaller resulting drops.

Emin and Schuchmann (2013) investigated the role of extruder configuration and operation on bubble break-up during starch extrusion and found that increasing screw speed did not lead

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directly to smaller bubbles, due to a simultaneous increase in both bubble break-up and coalescence. On the other hand, increasing feed rate increased blend viscosity and decreased coalescence leading to smaller droplets. Increasing mixer speed increased the maximum capillary ratio (Ca/Ca_{cr}), while changes in blend viscosity and flow rate had no significant influence. Reverse-oriented kneading blocks increased the number of particles with a high maximum Ca/Ca_{cr}, promoting dispersive mixing. The researchers found good agreement between their experimental and numerical results using particle tracking.

Previous work in our research group (Vyakaranam and Kokini, 2012) examined bubble breakup as a function of flow type (shear vs. extension) using a Newtonian fluid in a Readco continuous mixer utilizing the magnitude of the Manas-Zloczower mixing index given by:

$$\lambda_{MZ} = \frac{|\mathbf{D}|}{|\mathbf{D}| + |\Omega|} \tag{1}$$

where **D** is the strain rate tensor and **Ω** is the vorticity tensor and the index ranges from 0 for pure rotation to 1 for pure elongation and 0.5 for pure shear flow (Cheng and Manas-Zloczower, 1990). Consistent with the earlier fundamental studies of Grace (1982) and Khakhar and Ottino (1986) and using the indications offered by the Manas-Zloczower index, it was shown that extensional flows are key in the breaking of air cells during mixing. Better dispersive mixing was seen when elongational flows, as predicted by the Manas-Zloczower mixing index, were strong. Elongational flow was particularly observed in the intermeshing region above and below the paddle, as well as the middle of the C-shaped section between the barrel and the paddle. The behavior in the intermeshing region is of particular interest, as it is critical for dispersive mixing. Elongational flow was not observed in the nip region between the paddle tip and the barrel surface, where the highest shear rate is seen. Staggered paddles were shown to disrupt the axial flow and reduced elongational flow. Only the FLAT configuration allowed apparent squeeze flow in the intermeshing region as the fluid passed between two paddles inducing motion in opposite directions. This effect was fragmented with the introduction of staggered paddles.

The objective of this paper is to gain further in-depth understanding of the bubble dispersion process and predict critical bubble diameter by calculating the extension and shear rate profile for Newtonian and non-Newtonian fluids and mapping the extension rate and shear rate distribution in different parts of the geometry of a commercial pilot twin screw continuous mixer, an important model continuous mixer for automated operations. Quantitatively predicting the contribution of extensional flows is valuable in estimating and predicting bubble dispersion.

2. Materials and methods

2.1. Description of the numerical simulation

A 360° isothermal simulation was run on the full nine-paddle mixing section of a co-rotating twin-screw Readco mixer (Fig. 1) with the mesh used previously by Rathod et al. (2015) and Vyakaranam et al. (2012). Additional detailed simulation methodology can be found in these papers. A closer view of the xy mesh is shown in Fig. 2.

In order to enable simulation of the fluid dynamics in moving elements mesh superposition was used (Vyakaranam et al., 2012; Rathod and Kokini, 2013). The mixer speed was initially set at 100 rpm and the fluid inflow rate was set at 55.31 cm^3/s. A 2% Carboxymethyl cellulose solution was used as a model power law fluid where $K = 15.74\ Ns^n m^2$, $n = 0.397$, $\lambda = 1$ and the density is $1.0068\ g/cm^3$.

Mixer speeds of 50 rpm, 100 rpm, and 150 rpm and fluid inflow rates of 20 cm^3/s, 55.31 cm^3/s, and 100 cm^3/s were used. In addition to the non-Newtonian fluid two Newtonian fluids with viscosities of 120 Pas and 60 Pas were modeled.

Simulations were run on a Dell Precision 690 workstation with Dual core Xeon processors and 16 GB RAM using the Polyflow suite of programs from ANSYS, Inc.$\dot{\varepsilon}$ (extension rate – Equation (2)) was calculated and studied for all locations in a plane.

2.2. Simulation of extension rate

Extension rate ($\dot{\varepsilon}$) was numerically calculated from the rate of deformation tensor (**D**) (Debbaut and Crochet, 1988), after calculation of the second invariant (*II*) and the third invariant (*III*) of the rate of deformation tensor, using Equation (2) below:

$$\dot{\varepsilon} = 6\frac{III}{II} \tag{2}$$

$$II = tr\left(\mathbf{D}^2\right) \tag{3}$$

$$III = \det(\mathbf{D}) \tag{4}$$

Twelve planes were sliced at z = 1.92 (Plane 1), z = 4.475 (Plane 2), z = 5.82 (Plane 3), z = 7.165 (Plane 4), z = 8.51 (Plane 5), x = 0 (Plane 6), x = 0.5 (Plane 7), x = −0.5 (Plane 8), x = 2 (Plane 9), x = −2 (Plane 10), x = 4 (Plane 11), and x = −4 (Plane 12) (Fig. 3). The positive y values refer to the upper half of the mixer while the positive x values refer to the right-hand half of the mixer. As the values of z increase, fluid is approaching the front of the mixer.

Planes 2, 3, 4, and 5 are locations in the center portion of the mixer, in the gap between the individual paddles. This allows examination of the maximum number of fluid points as data collection is not constrained by the location of the paddle. It also affords a view of activity in a very narrow area bounded by moving parts. Planes 6–12 were chosen to view changes along the axial length of the mixer. Both extension rate and shear rate were calculated and compared.

2.3. Calculation of critical capillary number and maximum stable bubble diameter

A flow strength criterion (α_f) was defined using Equation (5) to account for the combination of shear and extensional flows. When extension rates are negligible α_f is 0, while at high extension rates α_f is 1.

$$\alpha_f = \frac{\dot{\varepsilon}}{\sqrt{\dot{\varepsilon}^2 + \dot{\gamma}^2}} \tag{5}$$

Critical capillary number (Ca_{cr}) is the capillary number above which bubbles become unstable and break (Vyakaranam and Kokini, 2012). In theoretical and experimental studies in model geometries it was shown that extensional flows are more effective in bubble dispersion. Equation (6) was developed and verified for mixed shear and extension flow (Bentley and Leal, 1986). In order to incorporate both shear and extension rates the alternate elongational flow strength parameter α_f, defined in Equation (5), is used in