Simulation and Visualization of Flow in a New Miniature Mixer for Multiphase Polymer Systems

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ABSTRACT: A newly designed mixer, the Alberta polymer asymmetric minimixer (APAM), was compared to the MiniMAX molder with flow simulation and flow visualization techniques to evaluate the performance of the mixers. The APAM has a unique, asymmetric design consisting of a varying clearance between the rotor blade tips and the cup wall, which enables the material to be squeezed, stretched, and kneaded in high-shear and converging zones. Flow simulation showed that substantial folding and axial movement occurred in this mixer and that the pressure and velocity profiles exhibited high values at the rotor tip with the smallest rotor tip/cup clearance. In contrast, the MiniMAX molder had very simple flow patterns, which were insufficient to induce good dispersive and distributive mixing. These results concurred with those from an earlier work that studied the structure of blends and nanocomposites processed in the APAM compared to other polymer processing equipment. © 2005 Wiley Periodicals, Inc. J Appl Polym Sci 97: 136–142, 2005

Key words: mixing; processing; simulations; blends; imaging

INTRODUCTION

The significant role of mixing in polymer processing is indisputable. Blending polymers or compounding them with fillers in melt-processing equipment gives the polymer scientist or polymer engineer a way to control the composition and structure and, thereby, obtain optimized properties. Mixing is an extremely complex process because it can involve different basic operations, such as dispersing particles, wetting solid particles by the matrix, plasticizing, and uniformly distributing the particles to obtain a homogeneous compound.[1] Many studies have analyzed the quality of mixing in multiphase polymer systems obtained by a certain mixing process[2] with flow visualization, flow simulation, or experimental techniques. This is obviously important for understanding the fundamentals of existing industrial equipment, but is also extremely useful for designing new mixers and evaluating them.

The internal mixer is an effective processing machine for polymers and rubbers mainly because of its high dispersive effect, reproducibility, and ease of material feeding.[3] A substantial amount of simulation work has been conducted on internal batch mixers, which has enabled the characterization of melting[4] and both distributive[2,5] and dispersive[5–8] mixing. Wong and Manas-Zloczower[2] performed simulation work on an internal batch mixer, characterizing the extent of mixing in relation to rotor speed ratio and initial positions. Cheng and Manas-Zloczower[6] focused on the narrow regions within an internal mixer as the intensive mixing region. Considerations such as void formation due to the partial filling of the chamber have also been taken into account.[9] Gramann and Osswald[10] used the boundary element method to analyze the flow in an internal batch mixer. Many of these results showed good correlations with flow visualization[6] observations. Flow visualization has been performed on processing equipment with glass or Plexiglas windows.[11–14]

In an earlier article,[15] we introduced a new miniature mixer called the Alberta polymer asymmetric minimixer (APAM). The design consists of a rotor with a unique, asymmetric shape spinning within a heated cup. Varying clearance between the tips of the rotor and the cup wall enables the material to be squeezed, stretched, and kneaded in high-shear and converging zones. Unlike other commercial miniature mixing devices, the APAM combines the complex flow modes required for both dispersive and distributive flow and requires a small sample mass of approximately 1–1.5 g. Experimental results have shown that well-dispersed, uniform nanocomposites and blends are obtained when samples are processed by the APAM.

In this study, we applied methods of flow visualization and flow simulation to the APAM and the

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more commonly used MiniMAX molder[16] to gain more insight about the flow mechanisms existing in these machines. The MiniMAX molder is made up of a cylindrical rotor in a stator cup. Flow visualization gives important information about the mixing process, showing the flow patterns and distribution and dispersion occurring within the mixer. Flow simulation provides data including local velocities, pressure values, and particle tracking. With these approaches, we performed a comprehensive evaluation of the mixers.

The numerical simulation of fluid mixing is of increasing interest to the process industry. Interest in computational fluid dynamics (CFD) as a design tool has been spurred both by recent performance increases in computer hardware and by the availability of advanced software packages for complex flow simulation.[17] Numerical simulation has several advantages. First, it can be used to optimize mixer design without building a new machine. This is an extremely cost-effective, flexible way to perform redesign.[1–3,5,18–23] Second, it is possible to predict performance for several different polymer systems with different properties and different mixing conditions because the fluid parameters may be easily changed.[3] Finally, with simulation, we can also conduct a comparison with industrial equipment or standard laboratory batch mixers so that we can better scale-up processing after the materials are initially processed in the APAM.[21,23] The main disadvantage of simulation is that the results rely on the accuracy of the input, that is, the accuracy of the geometry, polymer properties, flow conditions, and also, the level of meshing, proper choice of equations, and relevant approximations to reduce the complexity of the problem.[3,7]

EXPERIMENTAL

Mixers

Two mixers were used in this study: the APAM, shown schematically in Figure 1, and a MiniMAX molder.[16,24–26] The APAM rotor had a length of 25 mm and an alternating diameter around its asymmetric configuration.[15] The smallest gap between the rotor and the 13 mm diameter cup was 0.250 mm, and this was where maximum shear rates occurred. The cup had an inner diameter of 13 mm and a height of 25 mm. The rotor had a shape similar to a roller blade used in an internal batch mixer. Mixing occurred between the contoured surface of the rotor and the cup walls. The MiniMAX used the same mixing cup as the APAM, but the rotor had a simple cylindrical shape. The mixing occurred in the cylindrical volume formed between the bottom surface of the rotor and the bottom of the cup.

Design software

The APAM rotor was designed with Pro/ENGINEER (Pro/E) software (Parametric Technology Corp., Needham, MA). Pro/E is an advanced three-dimensional computer-aided design application, a feature-based, parametric, solid modeling package used for the mechanical design of parts. With this software, we created a model of the rotor. With the barrel volume, we computed the free volume of the mixer cavity to be approximately 2 cc. The data file from Pro/E was then transferred to a subsequent software package for meshing and simulation.

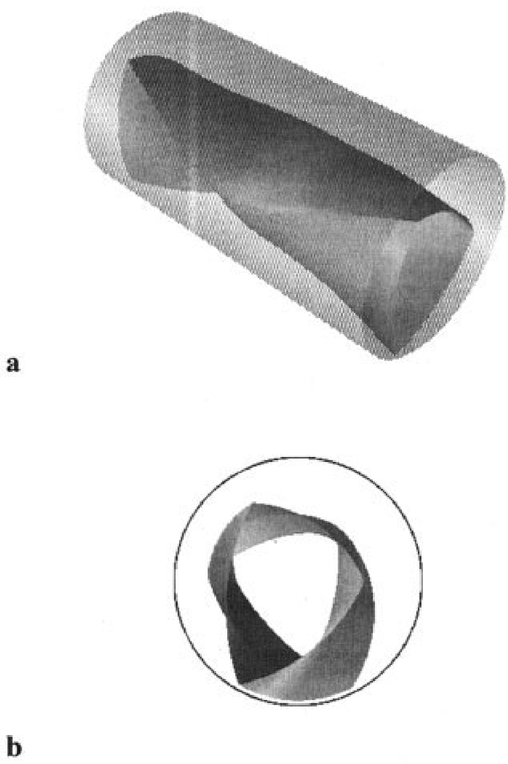

Figure 1 Geometry of the APAM: (a) axial and (b) cross-sectional views.

Simulation method

A Gambit CFD preprocessor (Fluent, Inc., Lebanon, NH) was used to build additional components of the APAM (the cylindrical cup) and the MiniMAX molder (the cylindrical rotor that fits into the cup). Thus, we were able to define the boundaries and mesh all components. The APAM rotor imported from Pro/E was also meshed with Gambit. The APAM was meshed with tetrahedral elements, whereas the MiniMAX molder was meshed with paved elements. In each case, the grid was refined until no major change in the flow pattern was seen.

Because the flow visualization was done with silicone oil (see the Materials section for its properties), the flow simulation was also conducted with this fluid's properties. The flow behavior of this oil resembled a Newtonian fluid; therefore, a Newtonian model was used to describe the rheological behavior.

Polyflow, a finite-element CFD software package from Fluent, Inc., was used to simulate flow in the APAM and MiniMAX molder. A three-dimensional analysis was used for an incompressible fluid at steady-state conditions. The fluid was considered to be isothermal throughout the mixer and to be at room temperature. The boundary conditions specified no slip at the walls. No free surfaces were defined, which implied that the mixing chamber was fully filled. The rotational speed of the mixer was set at 100 rpm. For ease of computation, a rotating frame of reference was used for the APAM, which meant that the cylindrical cup rotated around the rotor.

Postprocessing was performed with Fieldview (Intelligent Light, Lyndhurst, NJ). We obtained velocity and pressure profiles and, in addition, used particle tracking methods to create animations of particle movement within the mixers. Thus, we could see the flow patterns occurring and the distributive mixing performance of the mixers.

Materials

The flow visualization was conducted with a model material so that we could view mixing in a transparent mixing cell at room temperature. The material was a silicone fluid, phenylmethyl polysiloxane (Dow Corning 550 silicone oil; Midland, MI). The specific gravity of this silicone fluid was 1.07 at 25°C, and its viscosity was 125 cs. Red polycarbonate particles were also used to see the pathlines during the flow visualization experiment.

Flow visualization

For both the APAM and the MiniMAX molder, a few specks of red polycarbonate were placed at the bottom of the mixer. The silicone fluid was carefully injected into the mixing chamber so as not to disturb the solid dye particles. The rotors of the two mixers were then brought into contact with the fluid according to the procedures used for each of the mixers: for the APAM, the rotor was lowered until it was submerged within the fluid, and for the MiniMAX molder, the rotor was lowered until its bottom surface came into contact with the silicone liquid. A filling of approximately 70–80 vol % was used for the APAM, corresponding to the filling used when polymers are processed in internal mixers, to allow for axial flow and folding at the free surface. Mixing was conducted for 10 min at a rotation speed of 50 or 100 rpm. The entire mixing process was videotaped, and we followed the change in the distribution of the dyed polycarbonate particles as a function of time.

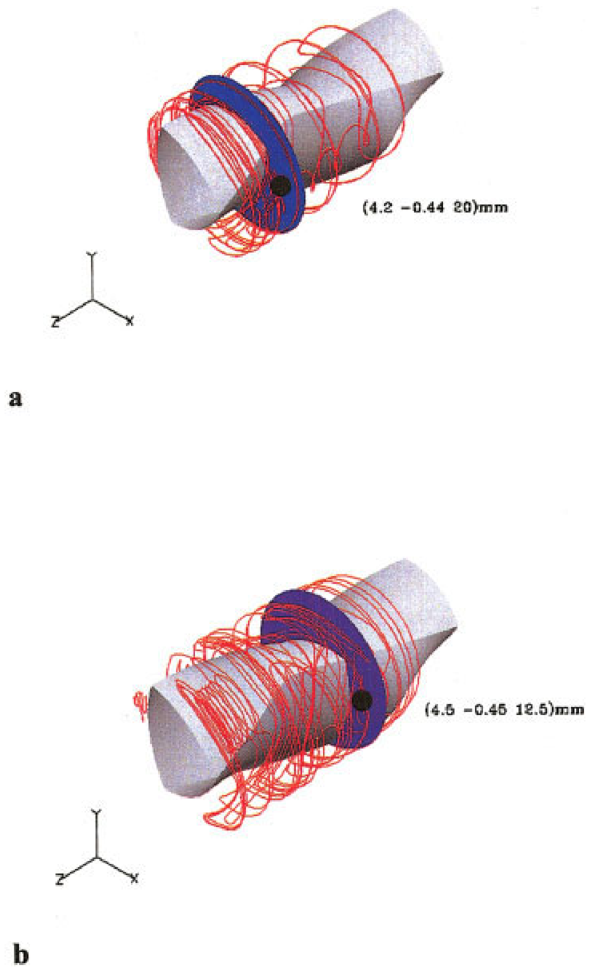

Figure 2 Particle tracking in the APAM. The initial position of the particle was different for cases (a) and (b) and is schematically shown by the black dot. The initial x, y, z position of the particle is given in the figure. The shaded cross-section is the radial plane of the initial position. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

RESULTS AND DISCUSSION

As mentioned previously, we used the flow simulation and flow visualization to see the flow patterns in the mixers and to obtain a qualitative measure of the extent of distributive mixing occurring in the APAM and the MiniMAX molder.

Flow simulation

Two paths simulating the motion of a single, massless particle within the APAM are shown in Figure 2. The theoretical particle was initially located in the position denoted by the dark circle, and its trajectory is indicated. Substantial axial movement occurred relative to the initial position; however, there were still stagnant regions that the particle did not access. The particle traveled mainly in the tangential direction, and reori-

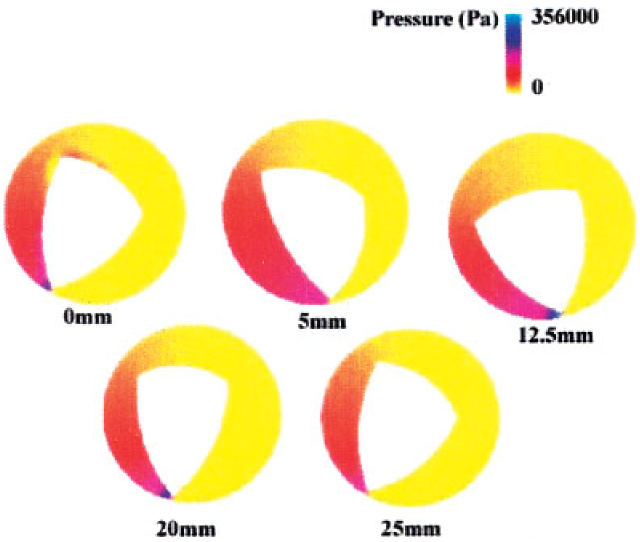

Figure 3 Cross-sectional pressure profile within the APAM at axial positions starting from the bottom: 0, 5, 12.5, 20, and 25 mm. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

entation took place through a folding mechanism in which the particle altered its direction of flow, usually in the area of the rotor nips. These observations suggest that the particle passed through many locations within the mixer, thus contributing to good distribution. The issue of stagnant regions needs to be addressed further. The simulation done here was a simplification of actual mixing because we neglected free-surface effects because of the complexity it would have added to the simulation. Therefore, we needed to determine whether stagnant regions occurred under real flow conditions. Because a fully filled mixer was used for the simulation, the extent of particle mobility may have been underestimated. When the chamber was only partially filled, the material had more freedom to move and, thus, may have accessed more areas within the mixer, resulting in a more uniform material.[22] However, if there were stagnant regions that limited uniformity, we could have iteratively used the computer-aided design software to change the rotor geometry and run the simulation with the new geometry to obtain an optimized mixer with a more uniform flow field.

Figure 3 shows the pressure profile in various cross-sections of the mixer. As expected, the pressure reached a maximum near the rotor tip that had the smallest clearance with respect to the cup. The pressure then decreased as the gap increased and had a low and uniform value in the wider gaps. The higher pressure values found in the region in front of the rotor tip and the lower pressure values found in the region behind the rotor tip were in agreement with simulated data reported previously for internal mixers.[6,8,27,28] These results indicate that in general, there was similarity between the pressure field developing in a standard internal batch mixer and in the APAM.

The velocity profiles for different cross-sections of the APAM mixer are shown in Figure 4. The simulation used a rotating frame of reference; that is, the cup was rotating rather than the rotor. Figure 4(a) shows the velocity field at the bottom of the cup, and as shown, the maximum velocity occurred just after the smallest clearance, and the velocity gradually decreased as the gap increased. This same type of velocity profile was seen for the other cross-sections, as shown in Figure 4(b–d). The regions with small clearances were high-shear regions with high pressures; therefore, intensive mixing occurred in these areas, causing agglomerate breakup, dispersion, and filler incorporation[1,20] as the material passed through these regions several times.[29] The high velocities noted in these areas were due to a combination of the drag flow due to the rotation of the rotor and the pressure flow resulting from the converging channels.[28] Another phenomenon seen in the simulations was vortices in the wider regions between the rotor tips. These vortices combined with axial flow reoriented the fluid through a folding mechanism, which enhanced the mixing significantly. The existence of extensional flow in the converging sections of the mixer, combined with repeated reorientation as observed in the simulation in Figures 2 and 4, resulted in the so-called baker's transformation, in which stretching and folding were combined to improve distribution.[30]

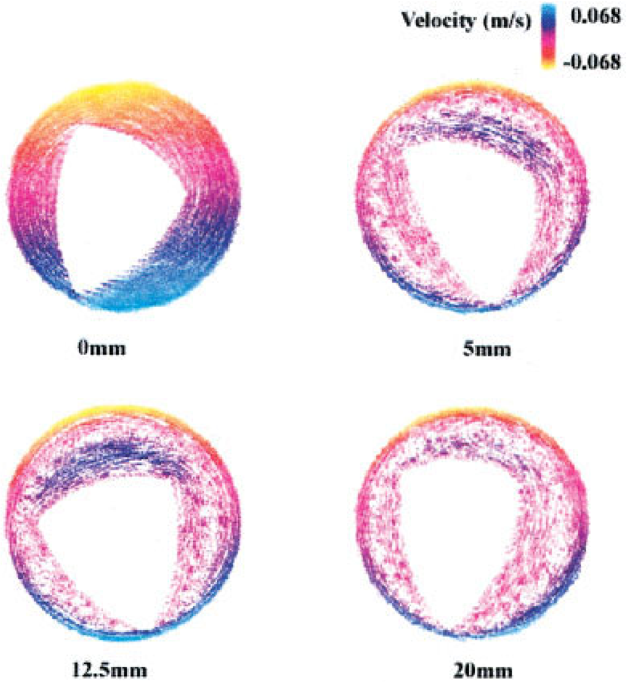

Figure 4 Cross-sectional velocity profile within the APAM at axial distances from the bottom: 0, 5, 12.5, and 20 mm. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

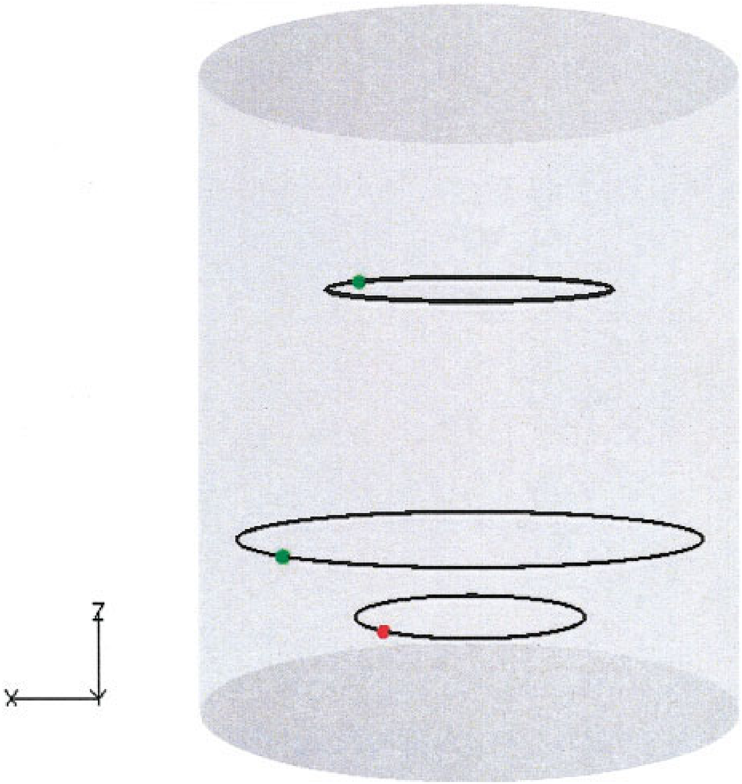

Figure 5 Particle tracking in the MiniMAX molder. The initial positions of the particles are shown by dots on the shaded cross-section, and the paths are the circles (i.e., there was no radial or axial motion). [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

A simulation was also conducted on the MiniMAX molder for purposes of comparison with the APAM. The trajectories of a few particles located at a particular cross-section within the MiniMAX molder are shown in Figure 5. According to the simulation, the particles rotated around the central axis at a constant distance; that is, they followed a simple circular path with no axial movement. This was the case for all cross-sections; therefore, only one axial location is shown. Although the flow pattern may have become more complicated if several particles collided with each other during mixing, the circular motion would have led to poor particle distribution. Minimal dispersive mixing was expected because the gap was large, and therefore, the shear rate was low. In addition, there were no converging sections, so extensional flow did not play a role in dispersion for this mixer.

Flow visualization

Flow visualization was performed to compare with the simulation and to enhance our understanding of the flow mechanisms in the APAM. Figure 6 shows still photographs obtained from mixing silicone oil with red polycarbonate tracer particles. In Figure 6(a), most of the particles are shown at the bottom of the mixer. After several seconds of mixing, the red tracer began to rise, traveling close to the surface of the rotor. After 1 min of mixing [Fig. 6(b)], the red particles had moved axially and were located along the entire length of the rotor. The mobile free surface seen during the visualization led to enhanced distribution via folding mechanisms and vortices. After 10 min of mixing [Fig. 6(c)], the red particles were well distributed within the APAM. In addition, some dispersion had taken place, as indicated by the fine red tint of the silicone oil. The visualization confirmed the result found by simulation: there was substantial axial movement, there was good distributive mixing, and dispersion took place due to the extensional flow as the material passed through small clearance regions. This correlated with the experimental results reported previously.[15]

Flow visualization was also conducted on the MiniMAX molder, and the results are shown in Figure 7. The red dye particles were initially at the bottom of the cup. Even before mixing began, when the rotor was inserted into the silicone oil, a vertical current occurred, causing some of the particles to rise [Fig. 7(a)]. This was consistent with previous studies,[24–26] where enhanced mixing was obtained in the MiniMAX molder by simply raising and lowering the rotor in the axial direction. However, it has also been noted that it is difficult to perform this operation consistently

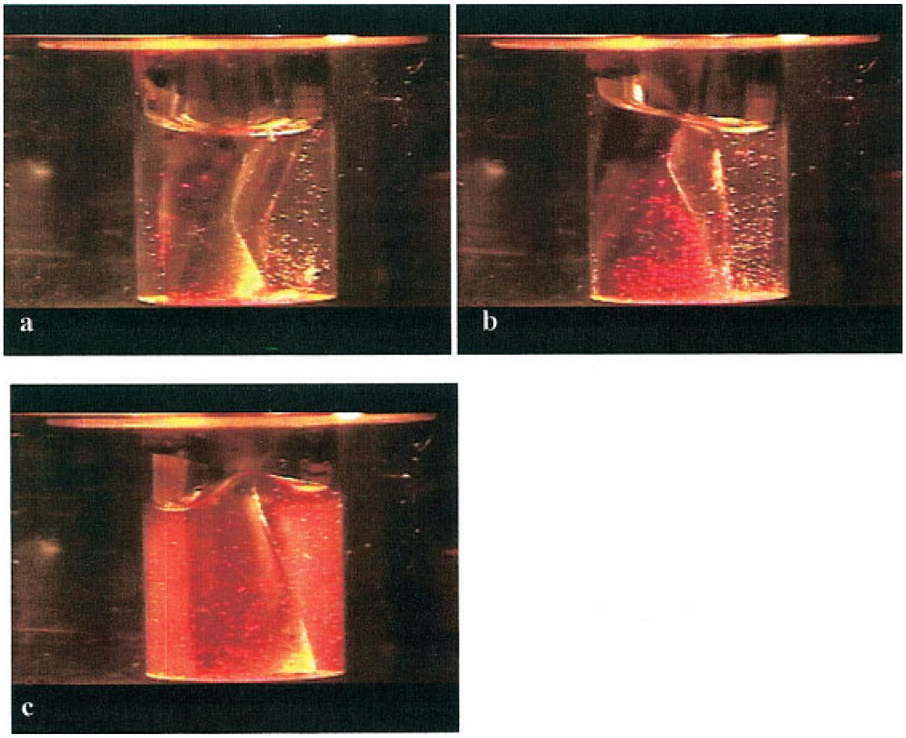

Figure 6 Flow visualization in the APAM at various mixing times: (a) 1 s, (b) 60 s, and (c) 10 min. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

even with automated raising or lowering of the rotor. After 1 min of mixing [Fig. 7(b)], the particles were better distributed, although not uniformly. There was a stagnant region at the bottom right corner of the rotor where the red color could not be seen. Uniformity improved as time passed [Figs. 7(c)], but even after 10 min of mixing, the distribution of red color was not nearly as homogeneous as that seen for the APAM mixture. At the bottom right corner of the mixer, there was still a small area where no red color was present. The rotor was not perfectly aligned, resulting in a flow pattern that should not have occurred under better alignment. In addition, there was mixing in the leakage clearances; these gaps exist to reduce the pressure within the mixer by enabling the material to seep out of the top of the MiniMAX. They are not meant to play a role in mixing; however, because this experiment used a very low-viscosity silicone fluid, this material penetrated the gap and allowed for better mixing in that region. The mixing behavior may be significantly poorer when a higher viscosity polymer is used.[24,25]

These visualization results agreed with the findings of the flow simulation; that is, that the mixing capabilities of the MiniMAX molder were inferior to those of the APAM because the MiniMAX had no axial movement, and its very simple flow patterns produced a nonuniform distribution. The results were also consistent with earlier findings showing that blends and nanocomposites processed with the MiniMAX exhibited a larger particle size and a less uniform structure than those processed with the APAM.[15]

CONCLUSIONS

Numerical simulation was used to evaluate the performance of a newly invented mixer and may be used in future to optimize geometry to improve mixing. When combined with flow visualization and the experimental results of blends or composite structures created in the machine, much can be learned about the flow mechanisms existing in the machine and the possibilities of improving it.

Flow simulation and visualization techniques were used to compare the performance of the APAM to that of the MiniMAX molder. The APAM exhibited folding flow patterns, extensional flow, high pressure at the rotor tip region, and varying velocities. These characteristics allowed the APAM to have both good dispersive and distributive mixing qualities, and the current results agreed with earlier experimental results found with this mixer.[15] The MiniMAX molder shows much simpler flow patterns and produced less uniform distributions, and this also agreed with previous findings. Axial rotor movement in the MiniMAX molder provided a small amount of axial movement, but the mixing was still insufficient, and it was difficult to consistently repeat the axial motion.

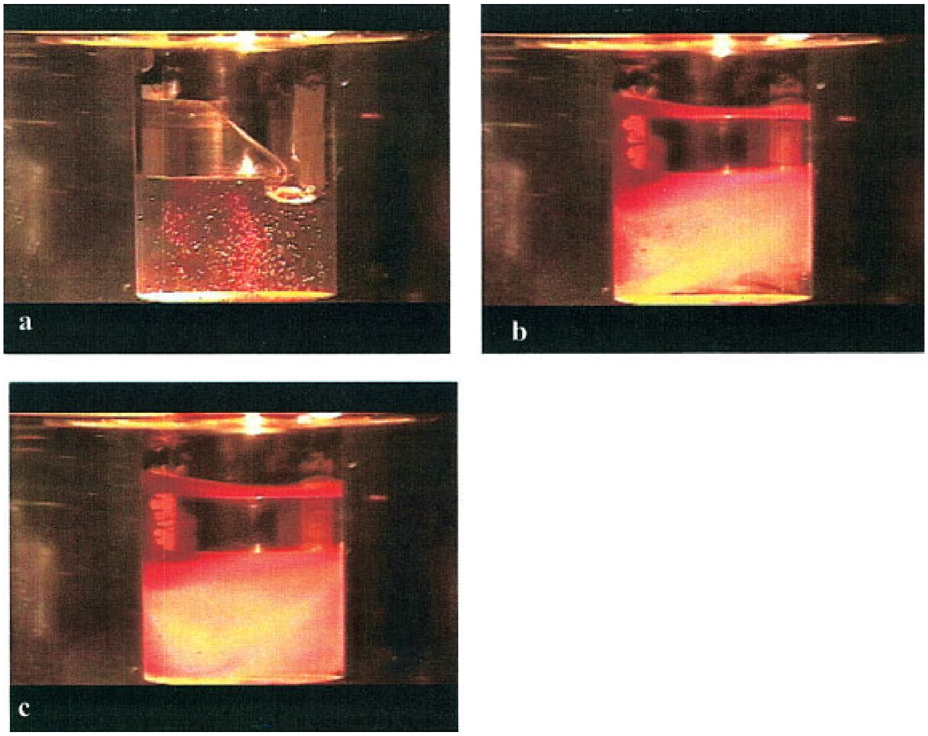

Figure 7 Flow visualization in the MiniMAX molder at various mixing times: (a) 0 s, (b) 60 s, and (c) 10 min. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

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