# DESIGN OPTIMIZATION OF MADDOCK MIXERS FOR SINGLE-SCREW EXTRUSION USING NUMERICAL SIMULATION

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## Abstract

Maddock-style mixers are used extensively on single-screw extruder screws to disperse materials into the molten resin matrix. Since the time LeRoy invented the device and Maddock perfected and commercialized it, the device has undergone several innovations. The goal of this paper is to describe the optimal flute geometry and mixing undercut dimension for a Maddock mixer with the goal of mitigating degradation gels and maximizing dispersive mixing efficiency.

## Introduction

Maddock mixers are used extensively on single-screw extruder screws to disperse solid particle agglomerates and trap and melt solid polymer particles. A well designed device works well at dispersing these particles, and their construction is relatively simple and low cost. Many of the screws with Maddock mixers that are in service today, however, have flute designs that are less than optimal, leading to the degradation of thermally sensitive resins and long purge times for material changes.

The fluted mixer is one of the most widely used mixing device for single-screw extrusion. Gene LeRoy at the Union Carbide Corporation (UCC) Research Center in South Charleston, West Virginia invented this device and received a patent in 1969 [1-3]. Bruce Maddock of UCC perfected the design in 1973 [4,5] and then commercialized the device. Others invented and patented similar devices including the Dray mixer [6] and Gregory's spiral mixer [7] in 1974.

The device was constructed by cutting several pairs of fluted channels into the screw in the axial direction, as shown in Figure 1. Each pair was designed with an in-flow flute and an out-flow flute. Between these flutes was a mixing flight that was undercut from the main flight. The mixing flight trapped solid particle fragments and dispersed them into the molten resin matrix. The number of flute pairs depends on the diameter of the screw. The device was positioned in the metering channel of the screw.

Solid polymer fragments [8] and unmixed gels for PE resins [9] can be removed from a molten resin stream by subjecting the flow to a one-time high shear stress field.

Unmixed gels are highly-entangled material that is typically high molecular weight polymer chains that are entangled and thus difficult to disperse during the extrusion process. When made into films, these unmixed gels solidify first and produce a gel that looks like a solid polymer fragment. In past experiences, the stress levels required to disperse PE unmixed gels are about 200 kPa [9].
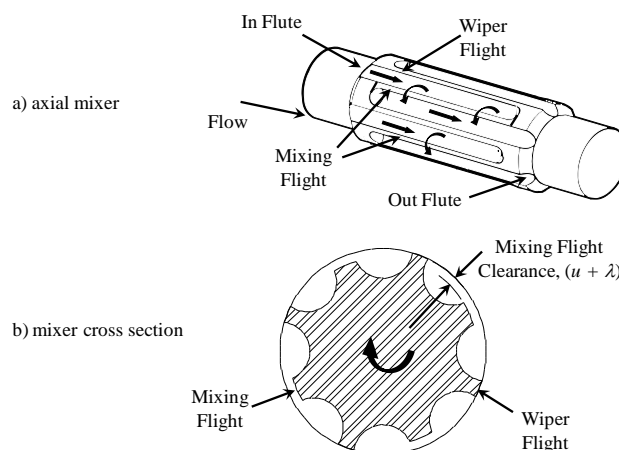


Figure 1. Schematic of a Maddock mixer [3].

The shear stress that the material experiences for flow across the mixing flight of a Maddock mixer can be estimated using Equations 1 and 2. The shear stress level is responsible for breaking up the entangled species and trapping and dispersing solid polymer fragments. This calculation is based on screw rotation physics [3].

$$\dot{\gamma}_M = \frac{\pi(D_b - 2u - 2\lambda)N}{(u + \lambda)} \qquad (1)$$

$$\tau_M = \eta\dot{\gamma}_M \qquad (2)$$

where $\dot{\gamma}_M$ is the average shear rate for flow over the mixing flight in 1/s, $N$ is the screw rotation rate in revolutions/s, $\eta$ is the shear viscosity at the temperature of the mixing process and at shear rate $\dot{\gamma}_M$, $D_b$ is the barrel diameter, $u$ is the undercut distance on the mixing flight, $\lambda$ is the main flight clearance, and $\tau_M$ is the shear stress that the material will experience for flow over the mixing flight.

Many designers will specify the mixer undercut at 1% of the barrel diameter. This is acceptable for applications that require a moderate level of dispersive mixing. Some designers use even larger undercuts with the purpose of reducing heat generation, typically up to 1.5% of the barrel diameter. This is likely to compromise the function of trapping and dispersing the solid polymer fragments and unmixed gels.

Many innovations have occurred to the mixer since it was first described. One of the innovations was to increase the depth of the flute channels to mitigate pressure consumption and energy dissipation. However, if the flutes are made too deep, resin can become stagnant at the root and lead to resin degradation and gels. Photographs of two spiral Maddock mixer designs are shown in Figure 2. The mixer in Figure 2a is poorly designed with the depth of the flutes being too large, creating flutes that will cause resin to stagnant and degrade. Degraded resin is observed in this mixer as black hard material, and gels were observed in the product film. The mixer in Figure 2b is much better with the depth of the flute set at half of the width of the flute [10]. Another innovation is to cut the flutes in a spiral path rather than straight. This design does enhance the pumping capability of the screw. However, this could potentially lead to longer residence times for resin flow and make the resin more prone to degradation.
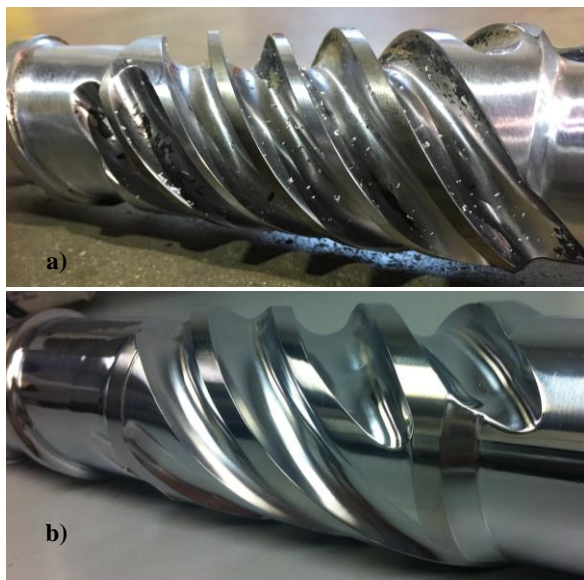


Figure 2. Photographs of spiral Maddock mixers: a) mixer with very deep flutes and evidence of resin degradation, and 2) a properly designed mixer where the depth of the flute is set at half of the width of the flute [10].

Numerous researchers have developed computer models for Maddock mixers using the flow analysis network (FAN) method [11-14] and the finite element method (FEM) [15]. We have conducted a study on the design of a spiral Maddock mixer channel depth [10]. The numerical simulation results matched well with the experimental data and observations. It reveals that improper flute channel depth design could lead to excessively long residence times for the resin.

This paper is an extension of the previous study [10]. Three major design parameters of a Maddock mixer were investigated: mixing flight undercut, flute lead length, and the flute channel depth. Four Maddock mixer designs with variations in the aforementioned parameters were numerically simulated. The results enable the development of guidelines for the flute geometry with the goal of mitigating resin gels.

## Maddock Mixer Designs

The single-screw extruder simulated had a 63.5 mm barrel inner diameter. The segments of the screws simulated in this study included the Maddock mixer sections as well as the metering sections and the screw tips downstream, as shown in Figure 3.
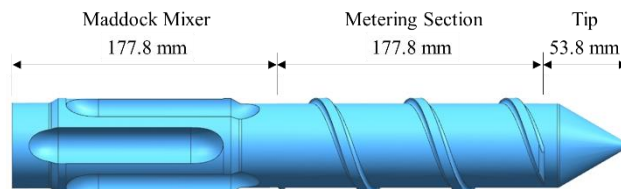


Figure 3. 3D sketch of the Maddock mixer and screw segment simulated.

Four Maddock mixer designs were investigated by numerical simulation in this study, which were named Mixers 1-4, as shown in Figure 4. Mixer 1 is a standard straight-flute Maddock mixer. It had a flute depth-to-width ratio (H/W) of 0.5, and an undercut of 0.46 mm (0.72% of the barrel diameter). Mixers 2, 3, and 4 were variants to Mixer 1 in regard to the flute lead length, mixing undercut, and depth-to-width ratio, respectively: Mixer 2 was a spiral flute Maddock mixer with a flute lead length of 345 mm; Mixer 3 has a mixing undercut of 0.76 mm, which is 1.2% of the barrel diameter; Mixer 4 has a flute depth of 12.83 mm, and a H/W ratio of 0.58.

## Material

A linear low density polyethylene (LLDPE) with a melt index (MI) of 1 dg/min (190°C, 2.16 kg) was used in this study. The rheological properties of the LLDPE polymer melt used in the simulation were obtained by curve fitting the viscosity data measured by a parallel plate rheometer. A generalized Cross fluid model was used. The viscosity data and the fitted curves are shown in Figure 5.
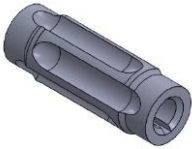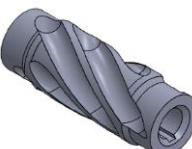
## Mixer 1



| | |
|---|---|
| Flute depth (mm) | 12.32 |
| Flute width (mm) | 24.64 |
| Flute lead (mm) | Straight |
| Undercut (mm) | 0.46 |

## Mixer 2



| | |
|---|---|
| Flute depth (mm) | 11.02 |
| Flute width (mm) | 22.23 |
| Flute lead (mm) | **345** |
| Undercut (mm) | 0.46 |

## Mixer 3



| | |
|---|---|
| Flute depth (mm) | 11.02 |
| Flute width (mm) | 22.23 |
| Flute lead (mm) | 345 |
| Undercut (mm) | **0.76** |

## Mixer 4



| | |
|---|---|
| Flute depth (mm) | **12.83** |
| Flute width (mm) | 22.23 |
| Flute lead (mm) | 345 |
| Undercut (mm) | 0.46 |

Figure 4. Specifications of different Maddock mixer designs investigated in this study.
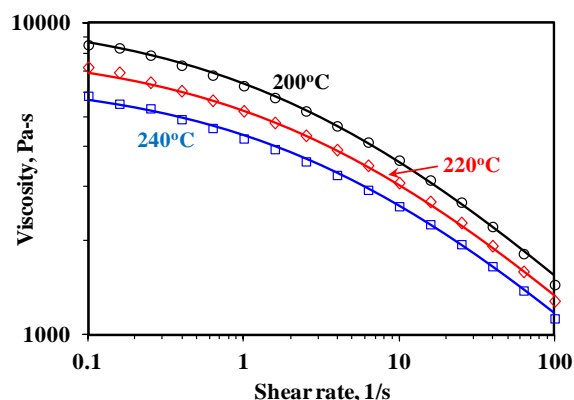


Figure 5. Viscosity data for the LLDPE resin.

## Simulation

Three dimension (3D) finite element numerical simulations were conducted using StarCCM+ to model the polymer flow momentum and energy balances. The following assumptions were made: 1) non-isothermal laminar flow; 2) the polymer flow is incompressible; 3) the influences of inertia, gravity, and elasticity of the melt are negligible; and 4) no-slip boundary conditions. Screw rotation dynamics were applied in the simulation; i.e., the barrel wall was held stationary while the screw boundaries were moving at the designated rotational speed. The validity of the numerical simulation technique has been verified by experimental data. More details can be found in our previous publication [10].

The boundary conditions of the simulation are based on the experimental configuration of a 63.5 mm diameter extruder in our lab. The barrel wall temperature was set at 220ºC and the entry pressure was 19.3 MPa. The screw was rotated at 70 rpm. The mass rate was 50.8 kg/h, which correspond to a specific rate of 0.73 kg/(h rpm).

Key outputs of the numerical simulation include the pressure and temperature profiles along this segment of screw, as well as the mixing quality using the passive scalar tracking method. The polymer flow field simulated was the melt layer between the screw and the extruder barrel wall. This layer was meshed with approximately 5,500,000 polyhedral elements.

## Results

### Impact of Mixer Design on Temperature

The temperature, pressure, and mixing quality results computed by the numerical simulation are discussed in this section for the four mixer designs. The target is to understand the influence of the three key design parameters of a Maddock mixer: the mixing flight undercut, the flute depth, and the flute lead length.

The temperature profiles yielded by the simulation of the four Maddock mixer designs are shown in Figure 6. The temperature profiles of Mixer 1 and 2 almost overlap. Mixer 3 exhibits the lowest temperature along the mixer section due to a larger undercut and less shear heating. Mixer 4 also leads to a slightly lower temperature than Mixer 1 and 2 because of the deeper flute channels.

Despite that different mixer designs yield different temperature profiles along the mixer section, the difference diminishes along the metering section. It is because the melt temperature at the discharge of the metering section is self-correcting. A higher melt temperature at the entry of the metering section would reduce the melt viscosity and lead to less shear heating to be generated, and thus less temperature increase, and vice versa, such that the temperature at the discharge is relatively insensitive to the entry temperature to the metering section. As the metering sections and tip geometry is the same for all four designs, the temperature difference at the entry does not lead to significant difference at the discharge, as shown in Figure 6.

For this reason, increasing the mixing flight undercut is not a viable way to reduce the discharge temperature.
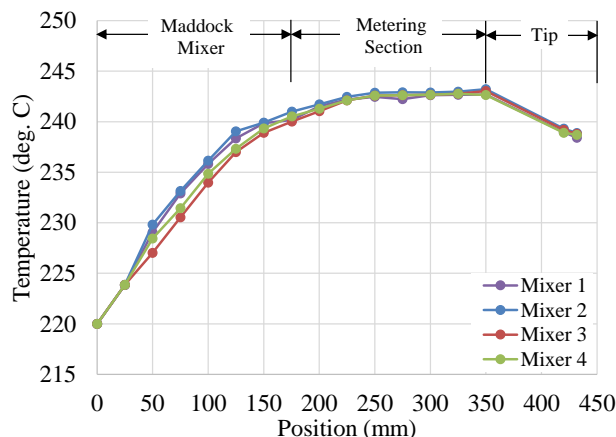


Figure 6. Temperature profiles of different designs of Maddock mixer for a rate of 50.8 kg/h at a screw speed of 70 rpm.

### *Impact of Mixer Design on Pressure*

The pressure profiles of the four mixer designs are shown in Figure 7. The pressure gradients along the metering section and tip are almost identical for all the designs, and the major difference is reflected along the Maddock mixer section. A comparison between the pressure profiles of Mixer 1 and 2 reveals that a spiral flute channel design provides additional conveying capability compared with the straight flute design, that the pressure change along Mixer 2 is approximately 1 MPa less than Mixer 1. Mixer 4 is also a spiral Maddock mixer with even deeper flute channels than Mixer 2. The purpose of cutting the flutes deeper was to further improve the conveying capability. The pressure profiles show that Mixer 4 does further reduce the pressure change, but not a useful amount.

Mixer 3 exhibits the best conveying capability among all four designs, showing a pressure gain of about 0.7 MPa rather than pressure decrease along the mixer section. This comparison indicates that the mixing flight undercut is the main restriction to the polymer flow along the mixer, such that increasing the undercut is much more effective than deepening the flute channels in regard to improving the conveying capability of the screw. Our previous study [10] indicates that a deep flute design such as Mixer 4 will lead to excessively long residence times of resin flow, and could potentially cause resin degradation. Therefore, if the conveying capability is of great importance when designing a Maddock mixer, it is more advisable to increase the mixing flight undercut than cutting the flute channels deeper.
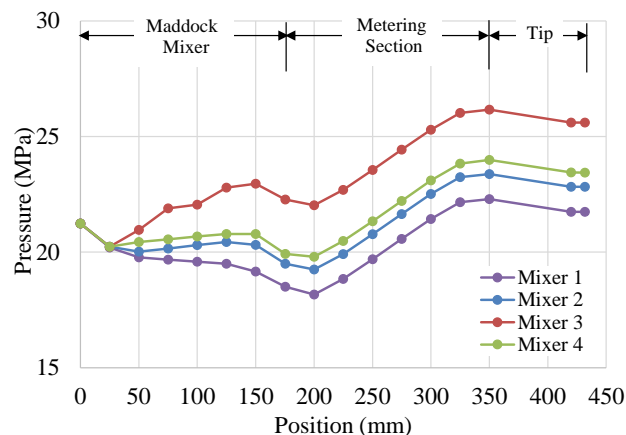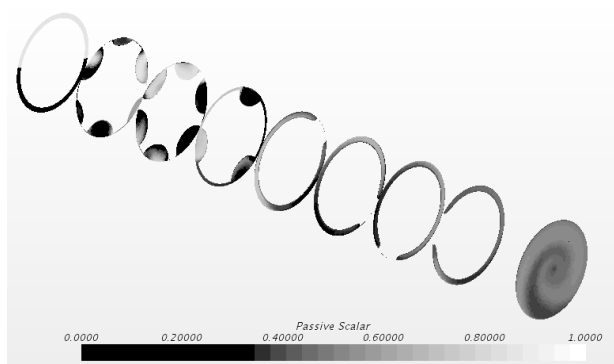


Figure 7. Pressure profiles of different Maddock mixer designs at a rate of 50.8 kg/h at a screw speed of 70 rpm.

### *Impact of Design on Mixing*

In order to evaluate the influence of the mixer designs on the mixing quality, a passive scalar tracking method was applied to the flow simulation. The passive scalar can be regarded as a massless tracer in the polymer flow. At the entry of the Maddock mixer, half of the entry surface was given a passive scalar value of 1, while the other half was valued at 0. This defines a condition that at the entry of the mixer, two streams of polymer with identical rheological behavior are completely unmixed, and each occupies 50% of the flow, which are marked in black and white color in Figure 8a. As the polymer flows through the mixer, the passive scalar is able to track the displacement of the elements in each of the two flow streams, and estimate the mixed pattern and quality. The standard deviation of the passive scalar at the cross sections along the screw is used as an index of the mixing quality. At the entry, 50% of the elements are given the value 1, while the other half is 0, and therefore, the standard deviation is 0.5 at the entry. The standard deviation decreases as the polymer blend becomes more homogeneous as it flows along the mixer section. A perfectly homogenous mixture would have an average passive scalar value of 0.5 and a standard deviation of 0.
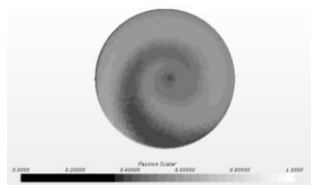
The passive scalar standard deviation profiles along the screws are plotted in Figure 9. Mixers 1, 2, and 4 exhibit similar mixing performance, while Mixer 3 yields the highest passive scalar standard deviation. Mixer 3 has a much larger undercut (0.76 mm, 1.2% of the barrel diameter) compared with the other three designs (0.46 mm, 0.72% of the barrel diameter). At the discharge, the standard deviation of Mixer 3 is 0.11, about 5 times as high as the standard deviation for the other three designs. This implies that the undercut plays a dominant role in determining the mixing quality as expected. The large mixing flight undercut of Mixer 3 reduces the shear rate and shear stress, which leads to relatively poor dispersive mixing of the polymer.

(a) Multi cross-section view



(b) Entry plane



(c) Discharge plane

Figure 8. Passive scalar tracking for mixing pattern at (a) multi cross section view, (b) entry, and (c) discharge
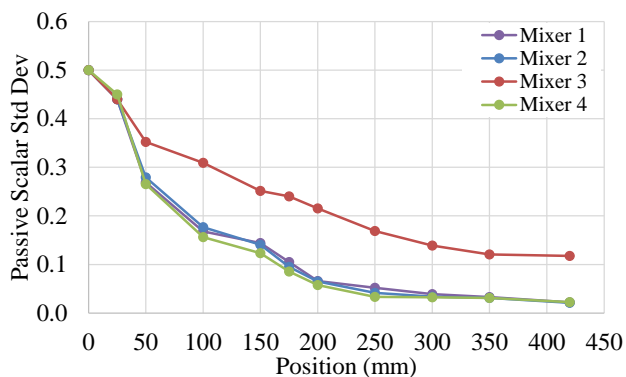


Figure 9. Passive Scalar standard deviation profiles of different Maddock mixer designs at a rate of 50.8 kg/h at a screw speed of 70 rpm.

Another key function of the Maddock mixer is to disperse the highly entangled gels in the polymer melt. It requires a considerably high level of shear stress in order to disentangle the gels. As described in Equations 1 and 2, the shear stress is determined by the shear rate, which is a function of the flight undercut and the screw speed. Using Equation 2 and the rheological model shown in Figure 5, the shear stress levels at different mixing flight undercuts and screw speed levels are plotted in Figure 10.

A general guideline for polyethylene extrusion is that it is preferable to have a shear stress level of about 200 kPa or higher in order to reduce the entangled gel content to an acceptable level in the extrudate. More detailed experimental study of the correlation between shear stress level and PE film gel content can be found in [10]. For these four mixer designs in this study, the shear stress levels are calculated using Equations 1 and 2. As shown in Figure 10, the shear stress correlates negatively to the undercut. If the undercut is set at or beyond 1% of the barrel diameter, the 200 kPa stress level is not able to be achieved even with a screw speed as high as 70 rpm. At 70 rpm screw speed, the highest average cross-sectional temperature in the barrel is already above 240°C. Further increase in screw speed is likely to overheat the polymer and could potentially cause resin degradation or other issues in the downstream processes.

As previously discussed, many designers set the undercut for the mixing flight at 1% of the screw diameter. While this undercut level is acceptable for applications where only a moderate level of dispersive mixing is required, for many applications where a large amount of entangled gels need to be dispersed, this undercut level will not provide a high enough level of shear stress.
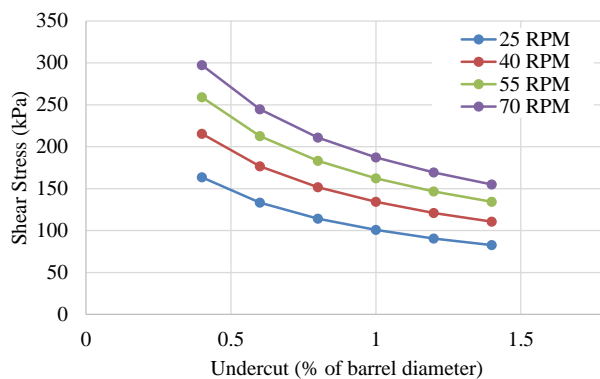


Figure 10. Shear stress levels at different mixing flight undercut.

### Impact of Design on Residence Time for the Resin

The residence time distributions of the resin flow in different mixer designs were calculated using the passive scalar method in the StarCCM+ simulation. As shown in Figure 11a, on average, Mixer 1 had the shortest residence time of 6.1 s, while the average residence time for Mixer 2 and Mixer 3 were 8.2 s and 8.4 s, respectively. This slight increase in residence time is due to the spiral flute design: the resin needs to travel a longer distance along the helical trajectory compared with straight flutes, which requires a longer period of time. Mixer 4 yields the highest residence time of 39.8 s. Figure 11b revealed that the residence time distribution of Mixer 4 is much broader than Mixers 1 - 3, and the long tail of the distribution toward right implies that at certain locations of the flute channels, the residence time for the resin is excessively long. It was observed on Figure 12d that at the bottom of the flutes near the trailing side, the

residence time is much longer than the rest of the flute channels, and at certain locations, the residence time could be as long as 780 s. The flow is almost stagnant in these regions. This coincides with our field observations of excessively deep Maddock mixers, as shown in Figure 2a; i.e., degraded resin was found at similar locations.
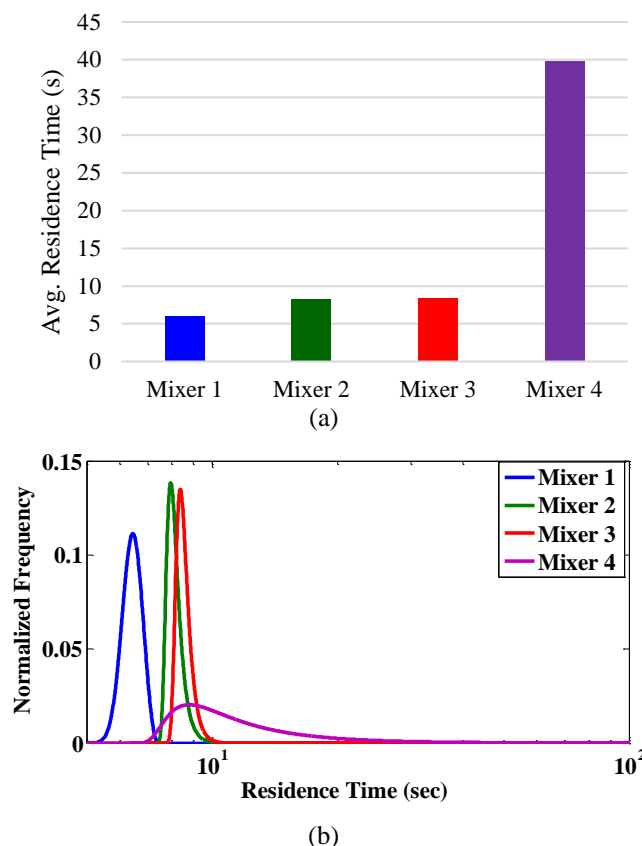


(a)



(b)

Figure 11. (a) average residence time and (b) residence time distribution of Mixers 1 to 4.

While deep flute channel helps mitigate the pressure consumption incrementally, the risk, however, for deep flutes is resin degradation. The optimal approach is to keep the flute depth at half of the flute width and then increase the screw speed by 1 or 2 rpm to offset the pressure consumption of the properly designed flutes.

## Summary

This study investigated the impact of three major design parameters of a Maddock mixer using numerical simulation. Mixer design guidelines were developed based on the results, which allow the design of Maddock mixers that are streamlined such that they do not cause resin to degrade and they provide a higher level of dispersive shear stress. To achieve a satisfactory level of shear stress for optimal mixing quality, it is recommended to use a mixing flight undercut smaller than 1% of the barrel diameter.

Meanwhile, a smaller undercut will limit the conveying capability as a tradeoff, as discussed previously. Therefore, when designing a Maddock mixer, both factors need to be taken into consideration to achieve a balanced result. It is also recommended to keep the mixing flute channel depth at about half of the flute width in order to prevent stagnant flow and resin degradation.
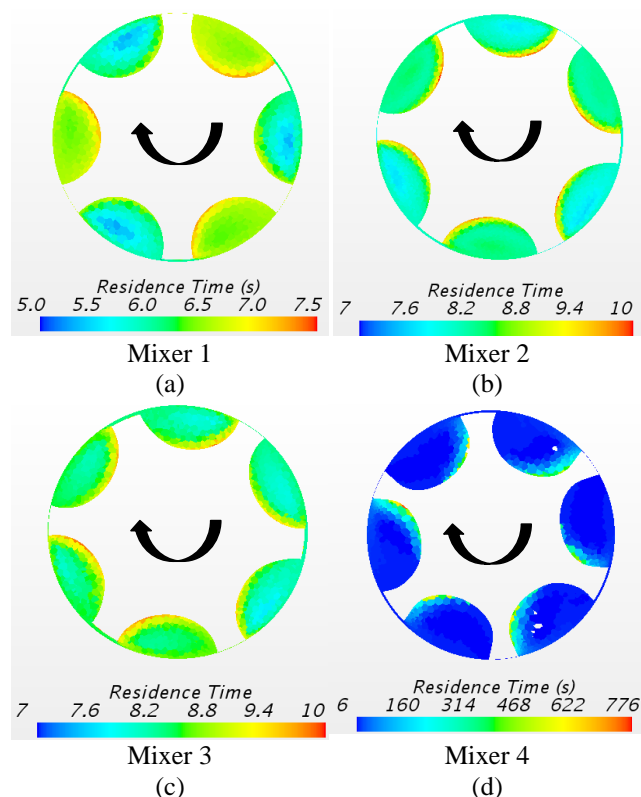


Figure 12. Residence time of the cross section near the end of the fluted section for Mixer design 1 to 4

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