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Fluid Flow and Distributive Mixing Analysis in the Cavity Transfer Mixer

Giovanna Grosso,* Martien A. Hulsen, Andrew Overend, and Patrick D. Anderson

In the polymer industry good mixing is essential to guarantee the characteristics of finished products. However, optimizing mixing devices is often difficult because mixing mechanisms are the result of the complex interaction between the moving elements and the non-Newtonian fluids used. Full 3D simulations are computationally expensive and the complexity of the problem is often split into approximated subproblems. The present work focuses on a simplified 2D model of the Cavity Transfer Mixer, investigating stretching and folding mixing actions. Several geometrical and functioning parameters, such as cavity speed, cavity shape, intercavity distance, rotor–stator clearance, and fluid rheology are varied. Mixing is analyzed in terms of Poincaré maps and by simulating the evolution of fluid blobs. The intercavity distance is found to play a major role, enabling and governing the stretching actions inside the mixing device.

1. Introduction

The blending of different materials is an important process in many industrial applications and in particular in polymer industry, where good mixing is essential to guarantee adequate performances of the finished product.1–4 In the 1980s a new device called the Cavity Transfer Mixer (CTM) was invented and patented by Gale at Rapra Technology Limited,5 as an add-on to be mounted downstream of existing extruders in order to improve distributive mixing. The invention followed the theoretical work of Spencer & Wiley6 and the experimental work by Ng and Erwin.7 The CTM consists of two concentric cylinders, the rotor and the stator. Both of them are provided with staggered rows of hemispherical cavities as shown in Figure 1. The motion of the rotor changes the relative position of the hemispherical cavities of the rotor and of the stator, generating a different geometrical configuration for each degree of rotation. At the same time the pressure imposed upstream pushes the fluid through the mixer. The result of the interaction between the moving geometry and the imposed pressure load is the generation of a complex flow field inside the device, characterized by helical flow paths developing between the inlet and the outlet of the mixer.

Because most of the CTM industrial applications involve non-Newtonian fluids, mixing modeling and optimization are a rather difficult task.8,9 Mixing processes are indeed the result of the combination between the complex flow field generated by the device and the properties of the molten polymers used.10–14 For this reason, a fast and efficient technique able to guide the development and optimization of the CTM is still missing and the modeling itself is not straightforward. In fact, simulations have to be able to properly represent a multiplicity of complex aspects: the moving geometry, the non-Newtonian fluid behavior, and the mixed fluid interaction.

In Grosso et al.,15 the authors presented a fully 3D analysis of the CTM and show how the material shuffling among the cavities is the dominant mixing mechanism. Such a mixing mechanism has a strong 3D character and hence can be only properly captured by 3D simulations, which are computationally very expensive. For this reason, in order to solve the problem in a reasonable calculation time, the fluid was limited to be of Newtonian rheology. In this way, it is possible to run a number of simulations and investigate the mixing dynamics in different CTM configurations, the results of which confirm how the fluid shuffling and redistribution among the cavities are the major mixing drivers. Actually shuffling is generally recognized as one of the main mechanisms of material mixing16 and it is usually combined with cutting16,17 to mix granular systems, while stretching and folding18 are considered typical of fluid systems. However, recent works19,20 investigate cases in which combined stretching-and-folding and cutting-and-shuffling actions take place. In particular, Smith et al.19 propose an analysis of fluid flows containing Lagrangian discontinuities (like valves and free-slip boundaries), which introduce fluid cutting, and they nicely show how cutting can have a strong effect on mixing, allowing an extra degree of topological freedom. The study is focused on a fluid flow where cutting and shuffling are dominant, but stretching and folding take place as well. It demonstrates how the combination of these actions produces mixing dynamics which are not found in systems where only cutting and shuffling or stretching and folding are present.

Even if the finite size of the gap between the rotor and the stator of the CTM does not allow true cutting, the high shear...
concentrated in this very thin fluid region might enable cutting-like actions. Smith et al.\[20\] also expect that in the presence of a finite thickness flowing layer, the cutting-and-shuffling action is replaced with a localized shear and similar structures should appear (see also Zaman et al.\[21\]). At the same time, because of the finite size of the gap between the CTM rotor and stator, stretching and folding actions can also develop inside the cavities, which do not dominate mixing dynamics, but can still play a role in radial and longitudinal direction. In order to investigate this particular aspect of CTM mixing mechanisms and to better analyze the effect of the gap size both as thickness and as length of the land between the cavities, also in the case of non-Newtonian fluids, the fully 3D model proposed by Grosso et al.\[15\] reveals to be computationally too expensive. For this reason, in this work we introduce a simplified and computationally inexpensive 2D model of the mixer, which can be used to run a broad range of simulations assessing the effects on mixing of many different factors, like geometrical dimensions, operating conditions or the rheology of the fluid.\[8,9,22–24\]

In particular, the simplified 2D geometry is based on the assumption to move along one of the flow helical paths inside the CTM, so that the complex 3D system can be approximated as a sequence of cavities. In particular, a path is chosen such that it always cuts the cavities in their middle section. The sequence of spherical cavities encountered along the path can then be approximated as a row of circumferential cavities. A similar approach was used by Woering et al.\[25\] in 1999, who proposed a study of mixing in a 2D CTM. In their case, however, the cavity shape was assumed to be rectangular, quite a simplification of the 3D spherical cavities of the device; we show in the following how even small differences in the cavity shape can give rise to differences in Poincaré maps - see Section 4.1.

In order to analyze mixing features, two approaches are followed: Poincaré maps and the study of the evolution of a blob of fluid inside the mixer, following pioneering concepts of Hassan Aref\[18,26\] and Julio Ottino\[27\] and co-workers and later many other researchers.\[22,28–37\] Through these two tools, the impact of the mentioned factors on the approximated 2D mixer efficiency is assessed. Regarding the rheological properties of the mixed fluids, the present work focuses on determining the influence of a shear-dependent viscosity, by using the Carreau model.\[23\] Section 2 presents the methodology used, Section 3 shows results of flow simulations, Section 4 focuses on mixing results and Section 5 draws conclusions and gives an outlook on future work.
in the device, the flow can be considered semi-stationary, i.e., at each position of the upper cavity, a steady state flow solution is computed independently of the previous ones, by solving the following set of stationary Stokes equations

\begin{align}
\nabla \cdot (2\eta \mathbf{D}) - \nabla p &= 0, \quad \text{in } \Omega(t) \\
\nabla \cdot \mathbf{u} &= 0, \quad \text{in } \Omega(t)
\end{align}

where \( \mathbf{u} \) is the fluid velocity vector, \( p \) is the pressure, \( \eta \) is the fluid viscosity, \( \mathbf{D} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2 \) and \( \Omega \) is the 2D flow domain as shown in Figure 3. Periodic boundary conditions for the velocity are implemented coupling the inlet \( \Gamma_{\text{in}} \) and the outlet \( \Gamma_{\text{out}} \). A zero pressure difference \( \Delta p \) between the inlet and the outlet is also imposed. At the walls, Dirichlet boundary conditions are applied, imposing a zero velocity at the stator \( \Gamma_{\text{stat-wall}} \) and the desired translation velocity at the rotor \( \Gamma_{\text{rot-wall}} \). The numerical solution is obtained via the finite element method \([39]\) both for Newtonian fluids and for shear–thinning fluids. In the latter case, the Carreau–Yasuda model \([40]\) is implemented

\[ \eta = \eta_\infty + \left(\eta_0 - \eta_\infty\right) \frac{1}{(1 + (\lambda\dot{\gamma})^{1-n})^a} \]

where \( \eta_0 \) is the viscosity at zero shear rate, \( \eta_\infty \) is the viscosity at infinite shear rate, \( a, \lambda, \) and \( n \) are parameters to specify different rheological characteristics and \( \dot{\gamma} \) is the shear rate. Triangular Taylor–Hood elements \( (P_2/P_1) \) are used: six nodes (corners, and mid-sides) for velocity with biquadratic base functions and three nodes (corners) for pressure with bilinear base functions. Because the viscosity is shear–rate dependent, the nonlinear equations are solved using a Picard iteration.

Figure 3. Possible configurations of the computational domain \( \Omega \) depending on the position of the upper cavity.

After getting an accurate flow solution, mixing characteristics are investigated by using Poincaré maps and by studying the evolution of a blob of fluid during the mixer operation. \([41,42]\) Both techniques require the computation of material point trajectories, which are obtained by integrating in time the point material coordinates

\[ \frac{d\mathbf{x}}{dt} = \mathbf{u}(x, t) \]

by using a fifth-order Runge–Kutta method with monitoring of local truncation error to ensure accuracy and adjustable
step size (see Press et al.\cite{43}). Here the source of any chaotic behavior inside the system is provided by the time dependence of $\mu$. Because small changes in the velocity field can give rise to different advection patterns, accurate flow field solutions are fundamental. As the velocity field is available only at positions inside a moving domain and at discrete times, an accurate interpolation is also required to compute the velocity at any location and time during the trajectory integration process.

While Poincaré maps provide an asymptotic picture of mixing and a topological breakdown of chaotic and linear mixing regimes, simulating the advection of fluid elements gives a direct overview of the mixing efficiency in the domain, but only for the limited area initially occupied by the fluid elements.\cite{41} This is the reason why we propose here a combination of these two techniques.

The present work investigates the impact on mixing of the following variables: cavity shape, distance between cavities, rheological properties of the mixed fluid, cavity speed, and size of the clearance of the gap between rotor and stator. Here, the distance between cavities is the distance the upper cavity must travel before it starts overlapping again with the lower one. This length is called hereinafter displacement. Following Woering et al.,\cite{25} a nondimensional displacement is defined as follows (see Figure 4)

\[
\xi = \frac{S}{2D} = \frac{S}{2D/U} = \frac{S}{2D/U} = 2D
\]

where $S$ is the displacement and $D$ the width of the cavity. Because we propose a 2D simplification of the real 3D geometry, in the definition of displacement we must also properly account for 3D effects. In fact, while in 2D the displacement is simply the distance over which the fluid is stretched inside the narrow gap between the two cavities, in 3D a much more complex scenario takes place. One cavity of the rotor interacts with more than one cavity of the stator at the same time and the fluid is stretched among all of them in multiple direction. In order to properly capture this phenomenon, we propose here the introduction of the following equivalent 2D displacement:

- we obtain the 3D nondimensional displacement ($\xi_{3D} = 0.73$) by dividing the total area of stator and rotor covered by cylindrical walls by the total area of stator and rotor covered by cavities, and
- given the 3D nondimensional displacement and the cavity width, by applying equation (5), we calculate the 2D equivalent displacement $S_{\text{equiv}}$, i.e., the equivalent length of the pipe between the cavities.

The obtained 2D equivalent displacement is quite larger than the actual distance between cavities ($\xi_{3D} = 0.73$ versus $\xi_{\text{actual}} = 0.0045$) but seems to give a more realistic picture of mixing, as shown in the following sections of this article. Other values of the displacement are also tested, in order to assess the effect of this parameter.

In the following sections the period $T$ is defined as the time required by the cavity system to travel from one complete overlapping configuration to the next one (see Figure 4).

3. Flow Characteristics

In this section we show some flow simulation results for both Newtonian and shear-thinning fluids. In particular, Figure 5 shows comparisons of relative $x$-velocity profiles obtained along the lower cavity vertical middle section by using fluids with
different rheology and a displacement $\xi = 0.0045$. Figure 6, instead, gives the impact of displacement on the relative $x$-velocity profile for a shear–thinning fluid with $n = 0.3$. Please note that for $t = T$, all four profiles coincide, while for $t = 1/2 T$, only the profiles obtained with $\xi = 0.5$, $\xi = 0.73$, and $\xi = 1$ coincide.

Actually no large differences can be seen in the obtained flow fields, but the effect on mixing of these small differences is relevant, as shown in the following sections. In particular, the effect of increasing the displacement is not that of really varying the flow field inside the cavities, but that of increasing the distance in which the fluid is stretched inside the narrow passage between cavities. For what has been found in the present 2D analysis, this distance has major effects on stretching and folding actions inside the CTM, as presented in Section 4.2.

4. Mixing Characteristics

We show here the effect on mixing of the cavity shape, of the displacement, of the rheological properties of the mixed fluids, of the cavity speed, and of the size of the clearance between the rotor and the stator.

4.1. Effect of the Cavity Shape

We analyze the differences between Poincaré maps obtained by using the ideal—perfectly circular—shape and Poincaré maps obtained by using the real cavity shape (two lowered half circles). The comparisons are made for a set of different situations, in terms of displacement and rheology. In Figure 7, Poincaré maps showing the effects of cavity shape are presented for both a Newtonian and a shear–thinning fluid.

The cavity shape effect is visible in terms of the number and shape of unmixed islands and is stronger for larger values of the displacement and for shear-thinning fluids. In particular, for a Newtonian fluid and $\xi = 0.0045$, the concentric islands in the top and bottom cavity are less numerous and much larger in the real geometry (note that the same number of points is used in both simulations), while for a Carreau fluid with $\eta = 0.3$ and $\xi = 1$ the two central unmixed islands appearing with the ideal shape are not present in the real shape cavities, but an unmixed island is generated in the outer part of the rotor cavity. This last effect is recognizable in all cases using the real geometry, but it must be noted that this might not reflect the 3D behavior. Figure 8 shows again the Poincaré maps obtained with the ideal and the real geometry and $\xi = 1$ for a Carreau fluid with $\eta = 0.3$, where some red points are initially positioned inside the unmixed islands. The maps show that the points keep falling inside the islands at the end of each period, demonstrating how the fluid contained in the islands does not get mixed with the rest of the fluid inside the mixer.

4.2. Effect of Displacement

Let us verify how displacement affects mixing by comparing Poincaré maps obtained with different values of $\xi$. Simulations are performed by using the actual geometry and one value of the cavity speed ($0.4$ m s$^{-1}$). In Figure 9, examples of the impact of displacement on Poincaré maps are given for a shear–thinning fluid. It can be clearly seen how increasing the displacement, the number of unmixed islands dramatically decreases: the case with $\xi = 0.0045$ has a large number of concentric islands in the top and the bottom cavity, but already with $\xi = 0.23$ the concentric unmixed islands get reduced and restricted to a smaller portion of the cavities, even if two new islands appear on the middle axis. Moving to $\xi = 0.5$ further improves mixing and with $\xi = 0.73$ the most homogeneous Poincaré map is obtained. Further increasing the displacement to $\xi = 1.0$ gives rise to a new family of unmixed islands.

Mixing performances are also investigated by modeling the evolution of a blob of fluid, by tracking the movement of its contour points. If the blob is initially positioned in an unmixed island, it can get deformed, but it can never exit the island boundaries. Hence, it cannot undergo any strong stretching and folding action. On the other hand, if the blob is initially
positioned in a regular mixing zone, it will be stretched and folded during the mixer operation and its length after a certain number of periods can be taken as a measure of mixing efficiency. For this reason we show here the evolution in time of the contour line length of a blob initially positioned in the middle of the mixer (regular mixing zone) and we use it to compare mixers with different displacements operated with fluids with different rheological characteristics (see Figures 10 and 11). From Figure 11 it is evident how larger values of the displacement give rise to higher stretching actions and hence much faster line length growth. On the contrary, the rheology seems to have only a limited effect on the blob evolution and differences between the Newtonian fluid and the shear-thinning one can be seen only with $\xi = 0.5$.

In conclusion, it can be stated that in 2D the displacement plays a major role in mixing efficiency, because it is the main...
Figure 9. Comparison of Poincaré maps obtained with the real geometry for a Carreau-Yasuda ($n = 0.3$) fluid and different values of the displacement.

Figure 10. Stretching after one period of a blob of fluid initially located in the middle of the mixer: a) $\xi = 0.0045$ and b) $\xi = 0.5$. 
cause of fluid stretching inside the mixer. In particular, for low values of the displacement, the fluid simply rotates inside the cavities and many unmixed islands are generated. On the other hand, when the value of the displacement increases, stretching actions can take place and the quality of mixing noticeably improves, up to an optimum. Too large values of the displacement negatively affect mixing as well.

4.3. Effect of Rheology

In Figures 12 and 13, the effect on mixing of fluid rheological characteristics is shown in terms of Poincaré maps for the real geometry and a fixed value of the displacement and of the rotor cavity speed. In particular, from Figure 12 ($\xi = 0.23$), it can be seen how for small values of the displacement, the rheology has a very limited effect on mixing. Only the most shear-thinning fluid shows slightly smaller unmixed islands, while the Poincaré maps of the other three fluids look all very similar. On the other hand, if the displacement is larger (see Figure 13), the effect of the rheology is more evident in Poincaré maps: unmixed islands change in size and in radial position, when changing the fluid characteristics and the most homogeneous mixing is obtained with the Newtonian fluid.

Figure 14, instead, shows the impact of rheology on the evolution of a blob of fluid initially positioned in the middle of the upper cavity. The graph shows that the blob of fluid gets much more elongated with a low shear-thinning fluid or with a Newtonian one. It must be noted that in all considered cases the blob is not originally positioned in an unmixed island of the Poincaré map. Actually, the blob gets elongated and stretched in all four simulations, but much more intensely when the fluid has a Newtonian or quasi-Newtonian character. Indeed, the Poincaré maps corresponding to these last two cases show unmixed islands which are smaller and closer to the cavity walls.
In conclusion, it can be stated that the fluid rheology reveals to influence mixing characteristics only when the displacement is large enough to allow stretching actions. Positive or negative effects of shear-thinning features depend strongly on the configuration tested.

4.4. Effect of Cavity Speed

Introducing a non-Newtonian fluid behavior makes the system of governing equations nonlinear. Thanks to this nonlinearity, other parameters like the cavity speed can play a role on mixing, as shown in Figure 15. Here the displacement is $\xi = 0.73$ and the fluid is shear-thinning with $n = 0.3$ in the Carreau–Yasuda model. Varying the cavity speed from 0.1 to 0.4 and 0.8 m s$^{-1}$ changes considerably the size and shape of the two unmixed islands inside and also slightly affects the size of the unmixed island in the outer region of the rotor cavity. In general, it can be stated that each combination of displacement, rheology, and cavity shape presents a different optimal value of the cavity speed. The impact of the cavity speed is more relevant for stronger shear-thinning fluids, but the displacement has to be large enough to allow rheology effects and, consequently, cavity speed effects on mixing.

4.5. Effect of Rotor–Stator Clearance Size

In this section we investigate the effect on mixing of the rotor–stator gap radial size. It has to be noted that in 2D, the gap size is defined as the height $p$ of the narrow pipe connecting the cavities. The importance of such an analysis stems from the fact that simulating the real rotor–stator gap size is particularly computationally expensive, because of the very small grid cell size required to discretize it. Simulations with a bigger gap size can have much bigger mesh elements and can consequently

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**Figure 13.** Comparison of Poincaré maps obtained with the real geometry and $\xi = 1.0$ for a Carreau with $n = 0.3, 0.5, 0.8$ and a Newtonian fluid.

**Figure 14.** Evolution in time of the nondimensional length of the contour line of a blob of fluid initially positioned in the middle of the upper cavity for $\xi = 0.73$ and for a Newtonian fluid and a Carreau-Yasuda fluid with $n = 0.3, 0.5,$ and $0.8$. 

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run much faster. In Figures 16 and 17, the impact on mixing of the nondimensional rotor–stator gap radial size \( p = p^*/(2D) \) is shown in terms of Poincaré maps for a shear-thinning fluid with \( n = 0.3 \). In particular, \( p = 0.0028 \) corresponds to the real size of the gap, while \( p = 0.017 \) is the value used in all our simulations (to speed up computations). The gap size has indeed an effect on mixing, especially for large displacement values, as shown in Figure 17. Here, increasing the pipe height \( p \) changes noticeably the size of the unmixed islands. However, it can be stated that the value we choose to approximate our system still gives representative results of the real configuration in terms of number, location, and size of unmixed islands in the Poincaré maps. On the other side, increasing even more the rotor–stator clearance \( p = 0.034 \) leads to quite different mixing features.

5. Conclusions

The present work proposes a single fluid simplified 2D mixer model of the CTM, which specifically aims at capturing stretching-and-folding mixing actions inside the device and assessing the impact on them of geometrical and operational variables. This work is related to Grosso et al.,\(^{[15]}\) where the authors present a fully 3D model of the same mixer and show how the main mixing mechanism inside the device is the fluid splitting and shuffling among the cavities. Notwithstanding the dominant role played by these mixing actions and because of the finite size of the gap between the rotor and the stator, stretching-and-folding actions are also expected to have an effect on mixing, especially in radial and longitudinal directions. In order to specifically investigate the latter actions inside the CTM and the effect on them of the rotor–stator gap size (both as thickness and as intercavity distance) and of the rheology of the fluid, a simplified 2D model was proposed. This resulted in much faster simulations and, as a consequence, the possibility to investigate a larger set of CTM configurations with respect to the fully 3D model.\(^{[15]}\) As such, the simplified 2D model of the CTM here proposed must be seen as a supplementary tool, which aims at investigating a particular aspect (namely the stretching-and-folding actions) of CTM mixing mechanisms. In this respect, the model was used to run a broad range of simulations assessing the effects of many different factors, like geometrical dimensions, operating conditions, and the rheology of the fluid.

By analyzing the results of the simplified 2D simulations, it is evident that a dominant role is played by the intercavity distance (or displacement), which reveals the stretching actions and determines their entity. In fact, for low values of the displacement the fluid simply rotates inside the cavities and many unmixed islands result, while for larger displacements stretching actions can take place and the quality of mixing noticeably improves, up to an optimum. After that, further increasing the displacement worsens again mixing performances. Other parameters such as the cavity shape, the cavity speed, the size of the rotor–stator clearance, and the rheology of the fluid have secondary effects on mixing, which become relevant only if the displacement is large enough to enable fluid stretching. In particular,
Figure 16. Comparison of Poincaré maps obtained with the real geometry and $\xi = 0.0045$ for a Carreau fluid with $n = 0.3$ and different values of the pipe height $p$.

(a) $p = 0.0028$, $\xi = 0.0045$, $n = 0.3$  
(b) $p = 0.017$, $\xi = 0.0045$, $n = 0.3$  
(c) $p = 0.034$, $\xi = 0.0045$, $n = 0.3$

Figure 17. Comparison of Poincaré maps obtained with the real geometry and $\xi = 0.73$ for a Carreau fluid with $n = 0.3$ and different values of the pipe height $p$.

(a) $p = 0.0028$, $\xi = 0.73$, $n = 0.3$  
(b) $p = 0.017$, $\xi = 0.73$, $n = 0.3$  
(c) $p = 0.034$, $\xi = 0.73$, $n = 0.3$
by comparing results obtained with an ideal—perfectly circular—shape and with the real cavity shape (two lowered half circles), differences were found in terms of number, location, and shape of unmixed islands in Poincaré maps. These differences are for larger values of the displacement and for shear-thinning fluids. Rheological characteristics of the fluid also affect mixing features, in a way which strongly depends on the tested configuration: in some cases better mixing is obtained with Newtonian fluids, in other cases with shear-thinning ones. In addition, for non-Newtonian fluids, the cavity speed can also play a role in mixing performances and effects are more evident for stronger shear-thinning fluids. There is not a general optimal value of the cavity speed, but it depends on the specific combination of displacement, rheology and cavity shape. In the end, the thickness of the gap between the rotor and the stator is also shown to have an effect on mixing, which reveals itself to be independent of the fluid rheology. Using the actual value of this gap is computationally very expensive because of the very small elements needed to discretize it. For such a reason, in the present work most of the simulations were performed with an approximated value of the rotor–stator clearance. Such a value is shown to give results still representative of the real configuration in terms of Poincaré map number, location, and size of unmixed islands.

In conclusion, because of the complex interaction of the fluid rheology with the moving geometry, it is not possible to identify a priori optimal configurations of the mixer, but for a given set of parameters simulations have to be run to find the optimal values of other parameters (like the cavity distance and the cavity speed). In this regard, the simplified 2D model presented here has the advantage of being a fast and inexpensive computational tool for the device optimization. Even if results can only account for the effects on stretching-and-folding actions of parameter variations, they can be used in order to run a selected number of fully 3D simulations giving the global picture of mixing performances. Indeed future work will focus on combining the 2D and the 3D model, in order to precisely investigate the role played by cutting-and-shuffling actions in combination with stretching-and-folding ones on global mixing performances. This will provide a complete picture of CTM mixing mechanisms and will allow identifying a best modeling practice for the mixer optimization, properly integrating 2D and 3D simulations.

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Conflict of Interest
The authors declare no conflict of interest

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cavity transfer mixer, mixing, Poincaré map, shear-thinning fluid

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