Mixing processes in the cavity transfer mixer: a thorough study

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Mixing Processes in the Cavity Transfer Mixer: a Thorough Study

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Abstract

In many industrial applications, the quality of mixing between different materials is fundamental to guarantee the desired properties of products. However, properly modelling and understanding polymer mixing presents noticeable difficulties, because of the variety and complexity of the phenomena involved. This is also the case with the Cavity Transfer Mixer (CTM), an add-on to be mounted downstream of existing extruders, in order to improve distributive mixing. The present work proposes a fully three-dimensional model of the CTM: a finite element solver provides the transient velocity field, which is used in the mapping method implementation in order to compute the concentration field evolution and quantify mixing. Several simulations are run assessing the impact on mixing of geometrical and functioning parameters. In general, the number of cavities per row should be limited and the cavity size rather big in order to guarantee good mixing quality.

Topical Heading: Soft Matter: Synthesis, Processing and Products.

Keywords: Cavity Transfer Mixer, polymer mixing, finite element

solver, marker tracking, mapping method.

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Introduction

Mixing processes have been the object of thorough investigations for several decades, because of their relevance in many industrial and natural fields. Even if in many cases mixing is associated with turbulent flows, laminar mixing also covers a wide range of important applications, such as polymer blending and food processing. Here the high viscosity of the employed fluids restricts the flow to the laminar regime, where chaotic mixing is the only possible mechanism for mixture blending. In all these cases, one way of obtaining efficient mixing is the application of the baker's transformation, i.e. a repetitive stretching, folding, re-orienting and stacking of the material, see Ottino¹. An implementation of this mixing technique can be found in static and dynamic mixers: see Meijer et al.² and Singh et al.³ for a deep illustration of the former and the works of Ottino et al.¹, Chella et al.⁴, Elemans et al.⁵ and Sarhangi Fard et al.⁶ for the latter.

A variant of this principle is applied in the Cavity Transfer Mixer (CTM), where mixing is achieved by smart shuffling of material between the many cavities composing the device. The CTM was invented and patented in the

1980s by Gale at Rapra Technology Limited⁷, and is often an add-on to be mounted downstream of existing extruders in order to improve distributive mixing. The invention followed the theoretical work of Spencer & Wiley⁸ and the experimental work by Ng and Erwin⁹. The CTM consists of two concentric cylinders, the rotor and the stator. The rotor rotates, while the stator remains still. 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 at each degree of rotation. At the same time the pressure imposed upstream of the CTM, pushes the fluid through the mixer. The result of the combination 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 CTM. The combination of such a flow field with the properties and mutual interaction of the used materials drives the mixing mechanisms inside the device.

Because of the variety of the involved phenomena, a clear and complete understanding of CTM mixing processes is still lacking and the system development and optimization encounter noticeable difficulties. In particular, the only comprehensive work found in literature about the Cavity Transfer Mixer, is the three-dimensional flow field analysis published in 1994 by Wang and Manas-Zloczower¹⁰, where the potential use of the CTM for dispersive mixing is discussed on the basis of flow field results. A more specific and quantitative mixing analysis is proposed by Woering et al.¹¹, but only on a two-dimensional approximation of the device, where two rectangular cavities interact between each other.

In this paper we demonstrate the essential three-dimensional nature of

(a)

(b)

Figure 1: View of the geometry of the CTM. In (a) the stator is made transparent so that the inner rotor is better visible. The rotor is cylindrical and provided with rows of concave hemispherical cavities. The diameter is reduced at the inlet and outlet via conical junctions in order to facilitate the in- and out-flow. The arrows indicate the rotation of the rotor around its axis. In (b) the stator is fully visible and the arrows indicate the mass flow entering the annulus comprised between the rotor and the stator. The stator is provided with rows of convex hemispherical cavities and it is stationary.

CTM mixing processes, which rules out any two-dimensional analysis. In fact, in the two-dimensional framework presented by Woering et al.¹¹, mixing results to be driven by stretching and folding processes and the CTM main mixing mechanism, i.e. the three-dimensional material shuffling between the cavities, cannot be intrinsically captured. For this reason, in the present work we propose a thorough investigation of mixing processes taking place inside the CTM, by the development and implementation of a fully three-dimensional model of the device, including not only a fully three-dimensional modelling of the flow field inside the mixer, but also a fully three-dimensional volumetric mapping method implementation (see Meijer et al.² and Anderson and Meijer¹²) simulating the evolution of the concentration field. In addition, the developed model is used to assess the impact on CTM mixing performances of geometrical parameters and operating conditions. Section Methods describes the employed methodology, Section Results presents the modelling results and Section Conclusion draws some conclusions about CTM performances.

Methods

The main mixing mechanism inside the CTM is material shuffling between cavities, which is dominantly three-dimensional. As such an appropriate CTM mixing modelling must be fully three-dimensional. Hence, a volumetric implementation of the mapping method is chosen. Such a method is based on tracking the evolution of the material inside the device, by using fully three-dimensional flow field solutions, and on constructing a specific matrix, called the mapping matrix, by which transformations of the concentration field can be simulated. In this work we assume that the two fluids to be mixed are both Newtonian and have the same material prop-

erties. In summary, the three-dimensional CTM model is composed by the following parts: the finite element flow solver, reproducing the complete three-dimensional flow field inside the mixer; the particle tracking algorithm, which uses the flow solution in order to track the material transport during the CTM operation; the algorithm constructing the mapping matrix on the basis of the computed material transport inside the mixer; the application of the mapping matrix in order to simulate the evolution of the concentration field; post-processing algorithms quantifying mixing performances. All these parts will be described in detail in the following sections.

Flow Simulations

As mentioned above, the CTM consists of two concentric cylinders provided with staggered rows of hemispherical cavities. The rotation of the rotor changes the relative position of the hemispherical cavities of the rotor and of the stator, generating a different geometrical configuration at each degree of rotation. At the same time the pressure imposed upstream of the CTM, pushes the fluid through the mixer (see Figure 1). In order to simulate such a complex flow field, the domain of which changes continuously in time, discrete steps of one degree of rotation are used. At each degree of rotation, the corresponding geometry is created by properly rotating the rotor surfaces Γ_{rot} (see Figure 2) and creating the fluid domain $\Omega(t)$ included in the domain boundaries Γ_{in} , Γ_{out} , Γ_{rot} and Γ_{stat} . A second-order tetrahedral computational grid (see Figure 3) is then generated for the obtained geometry. The geometry and the mesh are constructed by using a combination of the commercial software GAMBIT and of the meshing software GMSH¹³.

Figure 2: Geometry and boundaries of the CTM. Here Γ_{in} indicates the inlet boundary, Γ_{out} the outlet boundary, Γ_{rot} the rotor surface and Γ_{stat} the stator surface.

Figure 3: Second-order tetrahedral mesh of the CTM. The typical number of nodes for this kind of geometry with four rows of cavities on the stator is around 1.2 million.

Because of the high viscosity of the fluid used, advective inertial forces can be neglected and the transient flow field generated during the CTM rotation can be approximated as a sequence of stationary Stokes flows, satisfying the following set of equations:

$$\nabla \cdot (2\mu \mathbf{D}) - \nabla p = 0, \quad \text{in } \Omega(t) \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega(t) \quad (2)$$

where $\mathbf{u}$ is the fluid velocity vector, p is the pressure, $\mathbf{D} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$, Ω is the fluid domain and μ is the fluid viscosity. In case of Newtonian fluids, the latter is just a parameter for the solution and it is taken equal to $100 \text{ Pa} \cdot \text{s}$ in all the simulations here presented. At the walls Γ_{rot} and Γ_{stat} , Dirichlet non-slip boundary conditions are applied, imposing a zero velocity at the stator and the rotation speed at the rotor. Periodic boundary conditions for the velocity field are applied between the inlet Γ_{in} and the outlet Γ_{out} of the CTM. A pressure equal to zero is also imposed at a point in the middle of the mixer (in the centre of the gap between the rotor and the stator and at half the length of the device). This is needed only to set a pressure level for the solution. The pressure drop across the mixer is, indeed, independent of this value and is a result of the simulation. Actually the pressure difference between the inlet Γ_{in} and the outlet Γ_{out} of the CTM is computed as the one which gives the desired flow rate, imposed as a constraint at the inlet by using Lagrange multipliers. The numerical solution is obtained over the computational mesh by applying the finite element method¹⁴, with a generalized minimal residual solver (GMRES)¹⁵, in conjunction with an incomplete LU-decomposition for the preconditioner. The computational domain is discretized with Taylor-Hood (P_2/P_1) tetra-

hedral elements and the 6th-order integration over tetrahedra is performed by using a 24-point Gauss rule¹⁶.

Marker Tracking and Mapping Matrix

The mapping method was originally proposed in a restrictive form by Spencer and Wiley⁸. It describes the transport of a conservative quantity, like concentration, from one state to another by means of a so-called mapping matrix. The elements of the matrix contain the discretized fractions of the fluid transported from an initial cross section to a final one (for spatially periodic flows) or from an initial time to a final time (for time periodic flows). In 2001 Kruijt et al.¹⁷ proposed a new version of the mapping method to analyze the long term efficiency of distributive mixing in Stokes flows. Differently from previously existing methods, which usually give limited results or are highly memory and time consuming and mostly implicit, the mapping method offers an efficient way to investigate the influence on overall mixing quality of different mixing protocols or of different geometrical configurations and operating conditions in real mixing devices, see Kruijt et al.¹⁷. The mapping method was successfully applied to optimize prototypical and industrial mixing flows, as illustrated in Singh et al.³, Sarhangi Fard et al.⁶, Galaktionov et al.¹⁸, Kruijt et al.^{19,20} and Singh et al.²¹.

In the mapping method, the quantitative description of material transport is stored in a matrix called the mapping matrix, which summarizes all the material transport taking place inside the mixer during one period of operation, where one period is defined as the time required by the device to rotate from one geometrical configuration to an equivalent one. For example, in a CTM with five cavities per row, one period of rotation can be defined as $1/5$ of 360° . In fact, in this case after each 72° of rotation the

geometrical configuration is equivalent to the initial one.

In order to build the mapping matrix, a computational mesh must be generated for the fluid domain $\Omega(t_0)$, where t_0 is chosen as the reference time. Note that the mapping mesh is not the same as the finite element method mesh used for flow simulations. In the present work, the mapping mesh is a first-order tetrahedral one, coarser than the one used to compute the flow field. For details on the effect of the mapping grid, the reader can refer to Singh et al.²². Once the whole domain $\Omega(t_0)$ is divided into a large number N of discrete cells, each i^{th} cell is filled with a number of markers, uniformly distributed inside the single cells, with a number of markers proportional to the volume of the cell Ω_i . To determine where the material originally contained in the cells is transported during a period of rotation of the mixer, all markers of each cell are tracked during a period from $t = t_0$ to $t = t_0 + \Delta t$ (where Δt is the period duration). If the number of markers in the donor cell j is M_j at $t = t_0$ and the number of markers found in the recipient cell i after tracking is M_{ij} at $t = t_0 + \Delta t$, the mapping coefficient is computed as

$$\Phi_{ij} = \frac{M_{ij}}{M_j}, \quad (3)$$

with $\Phi \in \mathbb{R}^{N \times N}$, where N is the number of elements of the mapping matrix (typically for a CTM with four rows of cavities on the stator $N \approx 600$ thousands). In order to track the markers, the calculated Eulerian three-dimensional flow field is employed and the position of each marker (x, y, z) after a certain time Δt is computed from the initial position of the marker (x_0, y_0, z_0) by integrating in time the velocity according to the following equations

$$x = x_0 + \int_0^{\Delta t} v_x(x, y, z, t) d\tau, \quad (4)$$

$$y = y_0 + \int_0^{\Delta t} v_y(x, y, z, t) d\tau, \quad (5)$$

$$z = z_0 + \int_0^{\Delta t} v_z(x, y, z, t) d\tau. \quad (6)$$

Equations (4), (5) and (6) are solved numerically by using a fourth-order Runge-Kutta Bulirsch-Stoer scheme with an adaptive step size selection (see Galaktionov et al.²³). In order to find the value of the velocity at the position visited by a marker at time t , i.e. $\mathbf{v}(x, y, z, t)$, the velocity field computed at the two discrete time steps t_s and t_{s+1} , with $t_s \leq t \leq t_{s+1}$, has to be interpolated:

$$\mathbf{v}(x, y, z, t) = \mathbf{v}(x, y, z, t_s) + \frac{\mathbf{v}(x, y, z, t_{s+1}) - \mathbf{v}(x, y, z, t_s)}{t_{s+1} - t_s} (t - t_s), \quad (7)$$

where $\mathbf{v}(x, y, z, t_s)$ and $\mathbf{v}(x, y, z, t_{s+1})$ are the interpolated velocities at the position (x, y, z) at the discrete time steps t_s and t_{s+1} respectively, obtained from the computed numerical solution in the mesh nodal values by applying the basis functions of the second-order tetrahedral finite element.

Concentration Field Evolution and Mixing Performance Evaluation

Once the mapping matrix is generated, it can be easily used to compute the evolution of scalar quantities like the concentration vector $\mathbf{C} \in \mathbb{R}^{N \times I}$. In fact, if the initial concentration vector $\mathbf{C}^0$ at time $t = t_0$ is given, the evolved concentration vector $\mathbf{C}^1$ after a period Δt can be obtained by

$$\mathbf{C}^1 = \Phi \mathbf{C}^0. \quad (8)$$

Here $\mathbf{C}$ represents a coarse-grained description of the volume fraction (dimensionless concentration) of a marker fluid in a mixture of two marker fluids with identical material properties, and its component C_i describes the concentration (volume fraction) locally averaged in the cell Ω_i , with $0 \leq C_i \leq 1$. In case of time periodic flows, during the following periodic interval, the new concentration vector $\mathbf{C}^1$ is subjected to the same transformation summarized in Φ . That means that, after each periodic interval

$$\mathbf{C}^{i+1} = \Phi \mathbf{C}^i. \quad (9)$$

Hence the final concentration vector after n periodic motions of the mixer can be computed as:

$$\mathbf{C}^n = \underbrace{(\Phi(\Phi(\dots(\Phi \mathbf{C}^0))))}_{n \text{ times}}. \quad (10)$$

Thus, the mapping matrix Φ is computed only once and is applied repetitively to simulate the concentration evolution. The computation of the mapping matrix is quite expensive, and may take several CPU hours, but, once calculated, the necessary matrix–vector multiplication is very fast. Furthermore, the mapping matrix calculation can be easily parallelized, in order to speed up simulations.

By applying the above described mapping method, it is possible to simulate the concentration field evolution in different CTM configurations and operating conditions. The concentration initial condition is that the whole CTM is empty. During the simulation, the CTM is filled by the material coming from the inlet section, where the boundary condition is a 45° wedge of red fluid and the rest of blue fluid (see Figure 4). After a certain number of rotations (depending on the ratio between the throughput and the

rotation speed), the CTM is completely full of fluid and the concentration field reaches an asymptotic state. Qualitative comparisons can then be performed by visual inspection of different final concentration fields. In order to quantitatively compare different mixing states, instead, mixing measures need to be defined. Relevant measures for the mapping method are usually functions of the moments of the concentration distribution. Here we choose the discrete intensity of segregation integrated over a two-dimensional plane given by a cross-section:

$$I = \frac{1}{A\bar{C}(1-\bar{C})} \sum_{i=1}^N (C_i - \bar{C})^2 A_i, \quad (11)$$

where A is the area of the cross section, N is the number of the mapping mesh cells intersected by the cross section, C_i is the concentration in the i^{th} cell intersected by the cross section, A_i is the fraction of the cross-section area belonging to the i^{th} intersected cell and

$$\bar{C} = \frac{1}{A} \sum_{i=1}^N C_i A_i \quad (12)$$

is the cross-section surface weighted averaged concentration. The intensity of segregation is a measure of the deviation of the local concentration C_i from the ideal situation of perfectly homogeneous mixture. In the perfectly mixed section $I = 0$, while in the completely segregated section $I = 1$. The cross section surface integrated intensity of segregation can be computed at the inlet, at the outlet and at several cross sections inside the CTM.

Figure 4: Concentration at the inlet of the CTM. Two fluids with the same material properties enter the domain. The two fluids are given two different colours in order to distinguish them in the visual representation. The majority of the section is occupied by the blue fluid, while the red fluid is confined to a 45° wedge.

Results

In this section results of the fully three-dimensional modelling of the CTM are presented: first some flow simulations are shown, then the impact on mixing of geometrical and functioning parameters is illustrated by comparing results of different mapping calculations.

Flow Simulations and Validation

As a validation of the numerical flow field simulations, a test case is chosen (mass flow rate 0.006kg/s, rotation speed 5rad/s) and the mesh-size independence of the solution is assessed. In order to minimize the computational cost of the validation phase, the smallest CTM unit is taken as a test case for the model, i.e. a CTM configuration with only two cavity rows on the stator (see Figure 5). Velocity and pressure are sampled along a line crossing the CTM longitudinally and at a specific location inside the mixer (see Figure 6). The results obtained with three different mesh sizes (see Table 1) are compared: a coarse mesh case, a mesh twice refined and a mesh four times refined (the same degree of refinement used in all flow field simulations presented in this work). Figure 7 and Figure 8 compare the results obtained with the three different meshes. The coarsest mesh presents some pronounced peaks, while the two refined meshes not only keep a nice smooth behaviour, but also appear very similar to each other. In addition to the mesh-size convergence of the numerical solution, Figure 7 and Figure 8 give an interesting insight into the flow field behaviour. Along the sampling line, the pressure and the velocity magnitude trends reflect the non constant size of the flow cross section determined by the relative position of rotor and stator cavities. At the sampling point, the same variables clearly show the periodicity of the flow field generated by the mixer rotation.

Figure 5: Geometry of the validation test case (longitudinal cut).

Table 1: Number of elements of the three meshes: the second mesh has elements twice smaller than the coarse one, while the third one has elements four times smaller than the coarse one.

mesh	# elements
coarse	14836
2ref	71089
4ref	404102

Figure 6: Sampling locations for the solution validation. The line (a) lies inside the rotor–stator gap and crosses twice the interface between rotor and stator cavities. The point (b) lies inside a stator cavity but rather close to the rotor.

Figure 7: Pressure (a) and velocity magnitude (b) are sampled along the line shown in Figure 6a at one of the time steps of the solution (in this case the zero degree of rotation one). Results are given for the three different meshes.

Figure 8: Pressure (a) and velocity magnitude (b) are sampled at the point shown in Figure 6b during a periodical rotation of the CTM unit (in this case one fifth of the full rotation with steps of one degree, i.e. 72 steps). Results are given for the three different meshes.

In Figure 9 and Figure 10, results of three-dimensional simulations are shown for a CTM with four rows of cavities on the stator. It can be noted that the z -velocity is negative at some locations inside the mixer. This is due to the continuous change in the size of the opening window between rotor and stator cavities during rotation. When the opening window becomes smaller, little back-flow is generated inside the cavities.

Figure 9: Pressure (Pa) in the CTM on an x -axis parallel plane (a) and velocity magnitude (m/s) in the CTM on a y -axis parallel plane (b).

Figure 10: Axial velocity (m/s) in the CTM on a y -axis parallel plane (a) and axial velocity (m/s) in the CTM on a z -axis parallel plane (b).

Particle Tracking

The particle tracking algorithm implemented to compute the mapping matrix can be also used to obtain visual representations of the material transport during CTM operations. In Figure 11 and Figure 12, for example, results obtained by tracking a spherical cluster of one thousand particles initially located at the inlet of the CTM are shown both as visual position of the single particles and as percentage distribution of their residence time (in this test case the mass flow rate is 0.006kg/s and the rotation speed is 5rad/s). It can be clearly seen how the particles, initially very compact and close to each other, get redistributed in the CTM volume during the mixer operation and finally leave the mixer at quite different moments in time (see Figure 12). After passing through the conical inlet, the volume of fluid is immediately transferred to the first row of rotor cavities. Here, while still moving forward because of the pressure load, the volume of material gets redistributed by the device rotation to the first row of stator cavities. Such a mechanism is then repeated for all following rows of overlapping rotor-stator cavities, so that the initial volume of material is split in many small volumes, which are mixed and shuffled in the cavities. Good mixing is obtained when the fluid moving from the inlet to the outlet of the device is sufficiently redistributed and the resulting sub-volumes are sufficiently shuffled along the device to produce a uniform final reorganization of the material elements.

Figure 11: Transport of a spherical cluster of particles initially located at the inlet of the CTM.

(a)

Figure 12: Percentage distribution of the residence time of the spherical cluster of particles in terms of number of rotations from inlet to outlet.

Mapping Simulations

In this section, results of mapping simulations are given, both in terms of evolution of the concentration field and of the behaviour of the cross-section integrated intensity of segregation. The effect on them of several geometrical and functioning parameters is also presented. First of all the role of the rotor-stator gap size is tested. In particular, mixing simulation results obtained with the real gap size and with a gap three and six times larger than the real one are compared. However, using the real gap size not only implies working with huge meshes (because of the very small element size required to discretize the gap region), but it also gives quite some numerical problems. In fact, in the narrow region between the rotor and the stator points can easily land outside the mixer during the tracking for mapping simulations and this fact gives rise to a leakage of mass in the system and to inaccuracy in the mapping matrix. On the other hand, using a three or a six times bigger gap, gives quite similar results in mixing simulations (see Figure 13 and Figure 14), confirming the limited influence of the gap size on mixing performances. Indeed, this is not particularly surprising since the fluid inside the gap is almost in rest and does not contribute to the mixing process. For this reason, the three times larger gap size is chosen for mapping simulations when possible, i.e. in CTM configurations with four rows of cavities on the stator. For larger configurations like the ones with six rows of cavities on the stator, the six times larger gap is employed in order to limit the already huge size of the problem.

Figure 13: Concentration at the inlet, at the outlet and at four intermediate cross sections cutting the stator cavities in the middle (zoom on the last two sections) in the three times larger gap case (a) and in the six times larger gap case (b). All simulation conditions are the same in both simulations - mass flow rate 0.006 kg/s, rotation speed 5 rad/s.

Figure 14: Intensity of segregation at the CTM outlet as a function of time obtained with different gap sizes (a). Intensity of segregation at the final asymptotic state as a function of the non-dimensional axial coordinate z^* obtained with different gap sizes (b).

Among the operational variables, the ratio between the flow rate through the mixer and the rotation speed seems to be one of the dominating factors influencing mixing performance. Such a ratio regulates the shuffling mechanism between cavities: in fact, while the axial velocity moves the fluid toward the outlet, the rotation distributes it azimuthally among the cavities. The optimal ratio is the one which allows the fluid to pass through the mixer in a reasonable time, but it also allows it to get shuffled enough through the subsequent cavity rows. If this ratio is too high, the fluid passes quickly and compactly from one rotor cavity row to the next stator cavity row and vice versa and the content of each cavity in a row is only little mixed with the content of the other cavities in the same row. On the other hand, if the ratio is too low, the fluid remains isolated rotating in the same cavity row, moving from rotor to stator cavities and vice versa and not proceeding downstream. In order to summarize this ratio in a non-dimensional number, we define the variable k , as the ratio between the axial and the tangential velocity of the fluid at the inlet at the rotor radial coordinate, i.e.

$$k = \frac{Q}{A_{\text{inlet}}} \frac{1}{(\omega R_{\text{rotor}})} = \left| \frac{v_z}{(v_t)_{\text{rotor}}} \right|_{\text{inlet}}, \quad (13)$$

where Q is the volumetric flow rate (mass flow rate divided by density) in m^3/s , A_{inlet} is the area of the inlet in m^2 , ω is the rotor rotation speed in rad/s and R_{rotor} is the rotor radius in m . Typical values of k are between 0.04 and 0.6.

If the value of the non-dimensional variable k is changed (while keeping the same geometry), noticeable differences can be seen in mixing behaviour, as shown in Figures 15, 16 and 17. Here the geometry has four rows of cavities on the stator and four (Figures 15 and 17a) or eight cavities per

row (Figures 16 and 17b). It can be seen that for the four cavities per row case, there is an optimal value of the parameter k around 0.077, for which the intensity of segregation decreases rapidly and smoothly along the CTM, reaching an outlet value of about 10^{-8} . On the other hand, a too low value of k does not reveal to improve mixing, as shown by the case with $k = 0.043$: the intensity of segregation initially decreases a lot, but then remains almost constant until the fluid gets finally reunified in the outlet cone, where again a steep decrease of I takes place. Even if the final value of the intensity of segregation at the outlet is very low (10^{-10}), the CTM functioning does not look optimal, since the central rows do not contribute to improve mixing. Increasing k over 0.4, instead, clearly worsens CTM performances. On the other hand, in the eight cavities per row case mixing quality is in generally worse than in the four cavities per row one: the best performances are obtained with $k = 0.077$ with a final intensity of segregation at the outlet of 10^{-4} . Anyway, the same trend of the intensity of as a function of the parameter k can be recognised: increasing the value of k worsens mixing performances with the intensity of segregation at the outlet going from 10^{-4} for $k = 0.077$ to 10^{-1} for $k = 0.4$ (the case with $k = 0.639$ is not even simulated, because mixing quality is already very poor with $k = 0.4$).

Figure 15: Concentration at the inlet, at the outlet and at cross sections cutting in the middle the stator cavities (zoom on the last two sections) in the $k = 0.114$ case (a) - mass flow rate 0.006 kg/s, rotation speed 3.14 rad/s - and in the $k = 0.639$ case (b) - mass flow rate 0.083 kg/s, rotation speed 8.38 rad/s - for a CTM with four cavities per row.

Figure 16: Concentration at the inlet, at the outlet and at cross sections cutting in the middle the stator cavities (zoom on the last two sections) in the $k = 0.077$ case (a) - mass flow rate 0.006 kg/s, rotation speed 5 rad/s - and in the $k = 0.4$ case (b) - mass flow rate 0.02 kg/s, rotation speed 3.14 rad/s - for a CTM with eight cavities per row.

Figure 17: Intensity of segregation as a function of the non-dimensional axial coordinate z^* obtained with different ratios between the flow rate and the rotation speed ($k = 0.043$, $k = 0.077$, $k = 0.114$, $k = 0.2$, $k = 0.4$ and $k = 0.639$ in the geometry with four cavities per row (a) and in the geometry with eight cavities per row (b). Please note that the case with eight cavities per row and $k = 0.639$ is not simulated because of the already low performances obtained with $k = 0.4$. The points on the graph are computed at the axial coordinates of the stator cavities middle cross sections.

Comparisons can be also made between simulations having the same value of the variable k , but a different geometry. For example, on the same CTM configuration (number of rows of cavities on the stator, diameter of the rotor and stator, land between cavities) the number of cavities per row can be varied. It has to be noted that this implies changing the size of the cavities as well, since the diameters of the rotor and of the stator are fixed, such as the land between the cavities. Hence, increasing the number of cavities makes them smaller and vice versa. In Figure 18 results are shown of simulations with four, five or eight cavities per row. Here the geometry has four rows of cavities on the stator and a fixed value of the variable $k = 0.077$. It can be seen how the four and five cavities per row geometries behave quite similarly, while the eight cavities per row case shows much worse mixing performances. Table 2 directly compares the final intensity of segregation at the outlet of the mixer for the cases with four and eight cavities per row and different values of the parameter k . The cases with four cavities per row always perform better than the equivalent eight cavities per row ones.

Figure 18: Concentration at the inlet, at the outlet and at cross sections cutting in the middle the stator cavities (zoom on the last two sections) in the four cavities per row case (a), in the five cavities per row case (b) and in the eight cavities per row case (c). All simulation conditions are the same in all simulations - mass flow rate 0.006 kg/s, rotation speed 5 rad/s. Intensity of segregation as a function of the non-dimensional axial coordinate z^* for the three cases (d). Here the points on the graph are computed at the cross sections shown in figures a, b and c.

Table 2: Final intensity of segregation at the outlet for the cases with four and eight cavities per row and different values of the parameter k .

Case	I_{out} 4 cav	I_{out} 8 cav
$k = 0.043$	1.0×10^{-10}	1.0×10^{-5}
$k = 0.077$	1.6×10^{-8}	8.4×10^{-5}
$k = 0.114$	2.0×10^{-7}	9.4×10^{-4}
$k = 0.2$	4.6×10^{-4}	5.0×10^{-3}
$k = 0.4$	5.5×10^{-3}	7.0×10^{-2}

A similar behaviour can be also observed in Figure 19, where the intensity of segregation is plotted for two cases with six rows of cavities on the stator. “Case c” has five cavities per row, while “case d*” has six cavities per row (all other geometrical and functioning parameters are the same). Also in these cases, the solution with a lower number of cavities per row reveals to have better performances, as it can be recognised both by the concentration field visualization (Figures 19a and 19b) and by the intensity of segregation decrease along the mixer (Figure 19c).

In conclusion, more, and hence smaller, cavities per fixed CTM diameter and length seem to produce a less effective mixing, probably because of their smaller opening time and because they contain less material, which is rather compactly transferred to the next cavity instead of being split into many other cavities. In this case, changing the value of the parameter k has a limited effect on mixing performances. Hence, for real industrial applications, where the flow rate is determined by production requirements, first an appropriate cavity size or number of cavities per row must be found, then the rotation speed must be adjusted in order to obtain the optimal ratio k . Other geometrical parameters like the cavity depth (i. e. using cavities obtained as different portions of a sphere than its half) or the cavity shape can be varied in order to improve mixing. However, given the cost of the fully three-dimensional numerical simulations, we focus the present analysis only on the case of perfectly hemispherical cavities.

Figure 19: Concentration at the inlet, at the outlet and at cross sections cutting in the middle the stator cavities (zoom on the last two sections) in “case c”, with five cavities per row (a) and “case d*” with six cavities per row (b). All simulation conditions are the same both simulations - mass flow rate 0.006 kg/s, rotation speed 2.09 rad/s. Intensity of segregation as a function of the axial coordinate z^* for the two cases (c). Here the points on the graph are computed at the cross sections shown in figures a and b.

Finally, let us consider the impact of the number of rows on mixing efficiency. Figure 20 shows the results of simulations run with the same geometrical and functioning parameters, but with a different number of cavity rows. In particular, cases with four rows and cases with six rows of cavities on the stator and with $k = 0.114$, $k = 0.2$ and $k = 0.4$ are compared. It can be seen how simulations differing only by the number of cavity rows behave similarly in the first four rows and that, in general, adding two more rows of cavities does not improve mixing performances. Further confirmation is given by Table 3 and Figure 21, where results are given of simulations of different CTM configurations, all with six rows of cavities on the stator. As shown in the first column of Table 3, the cases differ in the diameter of the CTM, in the number of cavities per row and in the value of the parameter k . Figure 21 shows the intensity of segregation at the asymptotic state as a function of the non-dimensional axial coordinate z^* for the different cases. (It has to be noted that the not perfectly monotone decrease of I along z^* is due to the fact that the intensity of segregation is computed at individual cross-sections along the mixer and that it can happen that the cross section locally presents a more homogeneous concentration than its surrounding volume.) On the basis of the same data plotted in Figure 21, the third column of Table 3 provides ΔI_{tot} , i.e. the common logarithm of the decrease of the intensity of segregation along the CTM between the first and the last stator cavity row middle cross sections (i.e. excluding the inlet and outlet cone). The fourth and fifth column show the percentage of ΔI_{tot} lost respectively in the first and in the second half of the mixer. It can be clearly seen how the first part of the CTM already determines mixing quality and that the second part provides a further improvement of the concentration homogeneity only if the first part is effective enough. On

the contrary, if mixing is rather poor in the first part, adding more cavity rows does not seem to be beneficial. Not finding a huge improvement in mixing performance by adding more cavity rows to the mixer seems indeed reasonable: since only very little backflow takes place inside the mixer and given the very high viscosity of the fluid, the flow downstream has almost no influence on the flow upstream. As a consequence, it is possible to decompose the CTM in a series of equal mixing moduli, in which the same flow field repeats periodically. If the operating mode (variable k) or the geometry of the single modulus do not provide good conditions for the material splitting and shuffling inside the modulus, increasing the number of moduli cannot noticeably improve mixing performances. For this reason, in order to increase mixing effectiveness, optimizing the number of cavities per row and the ratio between the throughput and the rotation speed looks more appropriate than increasing the length of the mixer by adding mixing units. However, it has to be noted that in a real two-phase system, the length of the mixer might have to be increased in order to make the residence time long enough to fully allow the second-phase droplet break-up. Because of the too expensive numerical cost of two-phase three-dimensional simulations, these cases are not considered in the present study.

Figure 20: Concentration in the CTM in two cases with four (a) and six rows (b) of cavities on the stator and $k = 0.4$. Intensity of segregation as a function of the axial coordinate z for cases with four and six rows of cavities on the stator and $k = 0.114$, $k = 0.2$ and $k = 0.4$. The points on the graph are computed at cross sections cutting in the middle stator cavities.

Table 3: Behaviour of different CTM configurations in terms of decrease of the intensity of segregation. The third column gives the common logarithm of the decrease of the intensity of segregation along the CTM between the first and the last stator cavity row middle cross sections (i.e. excluding the inlet and outlet cone). The fourth and fifth column show the percentage of ΔI_{tot} lost respectively in the first and in the second half of the mixer.

Case		ΔI_{tot}	ΔI_{first}	ΔI_{last}
case m	$D_{\text{rot}} = 37$ 4 cav/row $k = 0.043$	5.3	60.6%	39.4%
case c	$D_{\text{rot}} = 75$ 5 cav/row $k = 0.025$	1.1	81.7%	18.3%
case d	$D_{\text{rot}} = 75$ 6 cav/row $k = 0.038$	0.4	83.9%	16.1%
case e	$D_{\text{rot}} = 150$ 7 cav/row $k = 0.030$	2.6	103.9%	-3.9%
case f	$D_{\text{rot}} = 150$ 9 cav/row $k = 0.041$	1.9	100%	0%

Figure 21: Intensity of segregation as a function of the non-dimensional axial coordinate z^* for the cases with six rows of cavities on the stator given in Table 3. The points on the graph are computed at cross sections cutting in the middle stator cavities.

Conclusions

In this work a fully three-dimensional modelling of the Cavity Transfer Mixer is presented. The continuous motion of the mixer is taken into account by discretising it in small steps, for each of which the relative geometry is built and the flow solution computed by using a finite element solver. Velocity field results are used in a mapping method implementation in order to compute the concentration field evolution and evaluate mixing quality. The developed model is used to run a broad set of simulations, assessing the impact on mixing of several geometrical and working parameters, where comparisons between different cases are performed both via visual inspection of the concentration field and via evaluation of the cross-section surface integrated intensity of segregation, a measure of the concentration homogeneity over an area. Simulation results show that the main mixing mechanism taking place inside the CTM is not the classical stretching and folding of static and dynamic mixers, but the material splitting and shuffling between cavities, the character of which is dominantly three-dimensional. This confirms the importance of having a fully three-dimensional model, in order to properly simulate mixing dynamics inside the CTM.

A very important parameter for CTM mixing effectiveness is the ratio between the fluid throughput and the device rotation speed. The optimal ratio is the one which allows the fluid to pass through the mixer in a reasonable time, but it also allows it to get shuffled enough through the subsequent cavity rows. In order to account for that, a non dimensional variable k is introduced as the ratio between the axial and the tangential velocity of the fluid at the inlet at the rotor radial coordinate. It is demonstrated that cases having different values of the fluid throughput and of the rotor speed, but having the same value of the parameter k perform exactly in the same way.

On the other hand, variations of the parameter k can give rise to noticeable differences in mixing performances, where an optimum can be found via simulations.

Another important factor is the number of cavities per row, where bigger and less cavities per row seem to guarantee a more effective mixing. In fact, bigger cavities, containing a larger volume of material and having a larger opening time, look more efficient for the splitting and shuffling mixing mechanism. This effect overcomes the role of the parameter k : in case of a not appropriate cavity size, changing the value of the parameter k gives a limited improvement of mixing performances. As a consequence, for real industrial applications, where the flow rate is determined by production requirements, first an appropriate cavity size or number of cavities per row must be found, then the rotation speed must be adjusted in order to obtain the optimal ratio k .

On the other side, increasing the number of cavity rows of the mixer seems to provide a very limited mixing improvement in the cases in which a quite inhomogenous concentration field is obtained. In fact, the first few rows of the CTM are already decisive for mixing quality and if mixing is poor inside them, increasing the length of the mixer cannot produce the desired concentration field homogeneisation. This looks reasonable: the CTM is made of modular repeating elements and if the number of cavities per row or the functioning parameters are not properly designed to provide a good splitting and shuffling of the material inside a single module, no mixing improvement is obtained by increasing the number of modules, because the same poor material reorganization takes place inside the added parts.

It has to be noted that other geometrical parameters like the cavity depth (i. e. using cavities obtained as different portions of a sphere than its

half) or the cavity shape could be also varied in order to improve mixing. However, given the cost of the fully three-dimensional numerical simulations, the present analysis is focused only on the case of perfectly hemispherical cavities.

In conclusion, we can state that mixing mechanisms taking place inside the CTM are rather complex and that mixing efficiency is the result of the very complicate flow field developing between rotor and stator cavities during the operation of the device. Because of the strong three-dimensional character of mixing dynamics, fully three-dimensional simulations are essential to assess the performances of each CTM configuration and no simple rule can be found to quickly identify an optimal design. In general, we can say that the number of cavities per row should be kept rather low, because more and smaller cavities perform in general worse than less and larger ones. In addition, mixing is rather sensitive to the value of the non-dimensional parameter k , where an optimum value has to be found. On the other hand, if the number of cavities per row is inadequate, changing the value of the variable k or increasing the number of cavity rows cannot improve mixing performances.

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