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Optimization of a Kenics static mixer for non-creeping flow conditions

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Abstract

Computational Fluid Dynamics (CFD) has been employed for the optimization of the mixing efficiency of a Kenics static mixer. A series of numerical simulations has been undertaken for non-creeping flow conditions to determine the optimal twist angle of the mixing elements. The mixer efficiency has been assessed by considering the computed pressure drop along the mixer and the size of the fluid structures remaining at the mixer outlet. Contrary to the results of previous investigations for creeping flows, it is shown that for the present non-creeping flow conditions, the twist angle of 180° employed in the standard Kenics design is optimal. It is demonstrated that CFD provides an invaluable tool for mixer design optimization, despite the significant computational resources necessary to undertake the present study.

Keywords: Computational Fluid Dynamics; Kenics static mixer; Non-creeping flow conditions

1. Introduction

A wide range of industrial applications for fluid mixing exists, using a variety of constituent fluids, physical mixing methods and underlying mixing processes. While mechanical agitators are commonly employed for batch mixing, static mixers are often preferred for continuous mixing applications. Static mixers generally consist of a series of motionless elements inserted into a length of pipe, with the energy for mixing being derived from the pressure loss incurred as the process fluids flow through the elements. Since the range of applications for static mixers is very broad, a variety of element designs is available from various manufacturers [1–3].

In the present study, we will restrict our attention to the mixing of fluids in the Kenics static mixer (manufactured by Chemineer, North Andover, MA) [4]. This mixer design has been employed in the chemical process industry since the mid-1960s, mainly for the in-line blending of liquids under laminar flow conditions. The standard Kenics mixer is comprised of a series of mixing elements, each consisting of a short helix of length L equal to three times the pipe radius a (i.e. aspect ratio $L/a = 3$) with a twist angle of 180°. The mixing elements are arranged in pairs, each pair comprised of a right-handed and left-handed element arranged alternately in the pipe. The leading edge of each element is at 90° to the trailing edge of the preceding element. For the present study, a Kenics mixer with six elements (i.e. three element pairs) is considered, as illustrated in Fig. 1.

A number of experimental investigations of the Kenics mixer have been undertaken, generally with the purpose of measuring the pressure drop along the mixer [1–8]. Limited experimental data are available that provide insight into the flow behaviour when the velocity (or alternatively, flow rate) is sufficiently small. For such creeping flows, for which the Reynolds number is small ($Re \ll 1$), it has been observed that the flow division at the leading edge of each mixing element leads to an exponentially increasing number of essentially parallel striations [5,9]. Nevertheless, detailed quantitative measurements of mixing efficiency for different mixer geometries and flow conditions have not been reported. The geometrical characteristics of the Kenics mixer have therefore been determined by empirical considerations. For example, an angle of 90° between elements is considered optimal because each mixing element cuts the striations perpendicularly.

The numerical simulation of fluid mixing is of increasing interest to the process industry. Interest in Computational Fluid Dynamics (CFD) as a design tool has been spurred both by recent performance increases in computer hardware,

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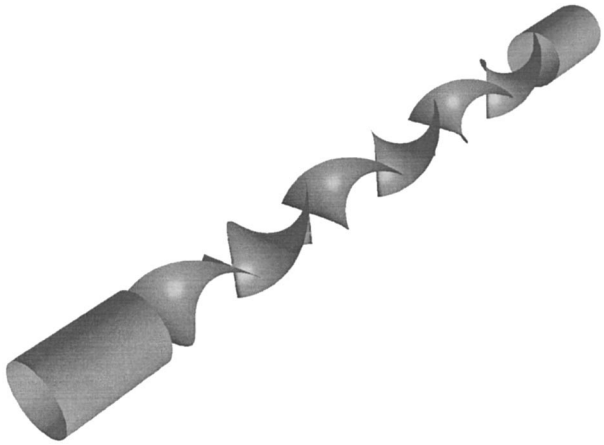

Fig. 1. Perspective cutaway view of the six-element Kenics static mixer.

and by the availability of advanced software packages for complex flow simulation. The numerical simulation of fluid mixing in static mixers can be performed by resolving the governing Navier–Stokes equations to determine the flow velocity and pressure, while the mixing process is best analyzed by calculating the trajectories of a large number of particles through the mixer.

To solve accurately the Navier–Stokes equations governing the complex three-dimensional flow in a Kenics static mixer requires substantial computational resources. (Indeed, the analysis of one flow condition for a single specified geometry can require many hours of computational time on a modern workstation.) A number of studies have therefore considered simplifications to the mixer geometry and/or governing flow equations to render the computations more tractable. For example, fully-developed creeping flow has been considered in a partitioned pipe mixer [10–12], which can be considered as a simplification of the Kenics mixer where the twist of successive mixing elements is not alternated. An analytical solution for the velocity field could be derived, which enabled detailed studies of the chaotic flow behaviour. A number of studies [13–15] have also treated creeping flow in a twisted tape mixer as a superposition of the fully-developed flows calculated for an infinitely long element. The velocity fields were determined using helical coordinates, with special conditions applied for matching at the interface between two mixing elements. The application of such calculations is therefore restricted to mixer geometries for which the elements are sufficiently long and the influence of the junctions between elements is small.

More recently, computations have been performed by solving the complete three-dimensional Navier–Stokes equations for flow in the Kenics mixer [16–22]. While the majority of these studies have been restricted to creeping flows, laminar flow at higher flow rates, for which inertial effects are important, has also been considered [17,18,20]. Flow in the Kenics mixer has been observed to be differ substantially for different Reynolds number regimes, with non-creeping flows being dominated by complex vortical flow features. Not surprisingly, fluid mixing under these conditions has been shown to exhibit significantly different characteristics, although it appears that chaotic advection [23] is still responsible for mixing.

Due to the above-mentioned computer resource limitations, mixer design optimization studies to date have generally been undertaken using the simplified theory for the twisted tape mixer [13–15]. In particular, it has been suggested that an element twist angle less than the standard 180° [13], or an aspect ratio smaller than the standard value of $L/a = 3$ maintaining the standard twist rate [15], would provide better mixing. These conclusions, however, should be considered with caution, due to the underlying assumptions of the theory employed. In particular, the use of approximate matching conditions at the interfaces between mixing elements may significantly influence the determination of vortical structures at the leading edge of the elements. As previously indicated [18,19], the greatest contribution to mixing efficiency in fact occurs within the developing flow in the vicinity of the element interfaces. In addition, solutions of the complete Navier–Stokes equations [18,19] suggest that the velocity field in a Kenics mixer is far from that of fully developed flow, especially in the first three and last elements.

To overcome these potential problems, a recent study has been reported [21] of the optimization of a Kenics mixer for creeping flow conditions based on the resolution of the complete Navier–Stokes equations. It was determined that, maintaining the standard twist rate, an element twist angle of around 120° was required for optimal mixing, corresponding to a smaller aspect ratio than for the standard Kenics mixer. It was also determined in [21] that for constant total twist angle, the mixing efficiency is independent of the element aspect ratio; combined with the previous result, this indicates that for a given total mixer length, the mixing efficiency is maximized for an element twist angle of around 120°. These conclusions are in qualitative agreement with the earlier above-mentioned results based on a twisted tape mixer.

It should be emphasized, however, that all previous optimization studies have been restricted to creeping flow conditions. Since the flow and mixing process are significantly different for higher flow rates, the optimal values of mixer design parameters are not necessarily the same as for creeping flow.

In the present paper, a numerical study is presented with the aim of optimizing the mixing efficiency of the Kenics mixer for non-creeping flow conditions. In principle, the optimization of a number of different design parameters would be of interest (e.g. element length and twist angle, flow rate, fluid properties), since it would provide a complete operational diagram for the mixer. However, due to computational resource limitations, only the optimal value of twist angle of the mixing elements has been determined keeping all other geometrical characteristics unchanged,

and for only one flow condition. In fact, the sizeable computational resources necessary for this study has only been available through the use of modern high-performance parallel computer hardware and software. In Section 2, the numerical methods employed to compute the flow and mixing characteristics are described. The qualitative and quantitative results obtained are presented and discussed in Section 3.

2. Numerical methods

The numerical simulation of the flow and mixing in the Kenics mixer has been performed via a two-step procedure. In the first step, the flow velocity (and pressure) is computed. These values are then used as input to the second step that consists of the calculation of the particle trajectories within the computed flow fields.

2.1. Flow computation

The parallel flow solver used in this study is based on a multi-block code developed for the numerical simulation of the 3D steady/unsteady, laminar/turbulent, incompressible flow of a Newtonian fluid [18,24]. This code uses a conventional Eulerian approach to solve the Reynolds-averaged Navier–Stokes equations on block-structured computational meshes.

The numerical method is based on a cell-centered finite volume discretization with an artificial compressibility method to couple the pressure and velocity fields [25]. For steady, laminar flow, as considered in the present study, the Navier–Stokes equations can be written as

$$\frac{\partial}{\partial t}\int_V \boldsymbol{IQ}\,\mathrm{d}V + \int_{\partial V} \boldsymbol{F}\vec{n}\,\mathrm{d}S = \int_{\partial V} \boldsymbol{G}\vec{n}\,\mathrm{d}S \tag{1}$$

where $\boldsymbol{I} = \mathrm{diag}(1/c^2,1,1,1)$, $\boldsymbol{Q} = (p/\rho, u, v, w)^{\mathrm{T}}$ is the vector of the primitive variables, and $\boldsymbol{F}$ and $\boldsymbol{G}$ are the flux matrices of the convection and diffusion terms. The artificial compressibility coefficient c^2 is set equal to $3\max\{u^2 + v^2 + w^2\}$, which has been observed to provide optimal convergence rates. A spatial discretization following the MUSCL approach [26] is employed, using a second-order upwind κ scheme and the approximate Riemann solver of Roe [27] for the convection terms, while the diffusion terms are discretized using a central approximation. A 'diagonal' form of the ADI method [28] is used to solve the set of discretized equations. Full details regarding the numerical method employed in the present study can be found in [18].

Parallelism is achieved by dividing the computational domain into a number of sub-domains, each sub-domain being covered by a structured hexahedral-element mesh. The flow equations are resolved concurrently on this block-structured mesh by assigning the computation for one block to one processor. Communication between processors is necessary to exchange data at the interface of neighbouring blocks. The communication overhead is minimized by data localization using two layers of halo cells surrounding each block. Data are exchanged between blocks using message passing via the PVM library, since this provides a good combination of performance and portability [29]. Load balancing is achieved by ensuring that each block has an equal, or approximately equal, number of mesh cells. Employing these techniques, a high parallel computational efficiency has been attained [18,22].

Taking account of the two-fold rotational symmetry of the mixer geometry about its axis, preliminary computations [18] have shown that for the flow conditions considered in the present study, the flow fields are also symmetric. Flow computations have therefore been performed only in half of the mixer. The computational meshes used in the present study consist of a H-type mesh in the core of the pipe and an O-type mesh near the pipe wall (see [18,22] for more details). The mesh is composed of 784 cells in the cross-section of each half of the mixer, with 60 cells in the axial direction of each element. For the 6-element mixer considered in the present study, this corresponds to a total of 376 320 hexahedral cells for half the mixer geometry.

A uniform velocity profile is assumed at the entry of the inlet pipe section, with a parabolic velocity profile characteristic of Hagen–Poiseuille flow being established at the leading edge of the first mixing element. At the exit of the outlet pipe section a constant pressure profile is imposed. No-slip boundary conditions are applied at all the solid wall surfaces.

2.2. Particle tracking

To determine the efficiency of a chemical mixer, it is necessary to establish means by which the fluid mixing can be gauged both qualitatively and quantitatively. In the present study, this was achieved by calculating the trajectories of fluid particles in the flow field of the mixer. This method avoids the problem of excessive numerical diffusion that is observed if the species continuity equations are solved [18].

For steady flow, as considered in the present study, particle trajectories correspond to streamlines. Some care must be taken in integrating the equation describing particle motion in order to retain a sufficient degree of accuracy. Preliminary tests have indicated that while lower order schemes appear to provide acceptable results, they accentuate the problem of 'lost' particles, that is, particle trajectories that are trapped near a solid wall (where the local velocity is zero) or leave the computational domain. For the results presented in this paper, therefore, a four-stage Runge–Kutta scheme was employed. In addition, to avoid problems near stagnation points, the numerical integration of the streamline equation was performed using a fixed spatial increment rather than a fixed time step. For the chosen value of the spatial increment, a minimum of

12 000 integration steps were required to calculate each particle trajectory through the mixer. With these considerations, the number of lost particles was reduced to 1– 5%, depending on the Reynolds number of the flow and the mixer geometry. No attempt was made to recuperate lost particles by re-injection into the flow field, since this may unduly perturb the mixing analysis.

To obtain an accurate global evaluation of the mixing, the study of the trajectories of a large number of particles has been undertaken via the use of a high-performance parallel computer system. Since the particles are assumed to be non-interacting, their trajectories can be calculated in an independent manner, leading to simple parallel implementation and high computational efficiencies. A detailed discussion regarding parallelization issues for the calculation of particle trajectories in the static mixer can be found in [18,22]. Using this procedure, a total of 262 656 particles (for each constituent fluid) has been considered in the present study.

At the entry of the inlet pipe section, the particles were distributed uniformly in the half disc delineated by the line traversing diametrically the mixer pipe at an angle of 90° to the front edge of the first mixing element. This can be viewed as a simplified model for the diametrical feeding of the mixer with two component fluids. Particle trajectories corresponding to only one of the fluids are calculated (and plotted in the present paper); the trajectories associated with the second fluid can be determined by two-fold rotational symmetry about the mixer axis.

2.3. Numerical solution accuracy

It is important that the accuracy of numerical solutions be analyzed before confidence in the predictive ability of the numerical techniques can be justified. For the present study of mixing under non-creeping flow conditions, there is unfortunately an absence of experimental data sufficiently detailed and accurate to undertake a complete validation of the numerical results.While comparison with certain experimental values of the pressure drop across the mixer measured for the standard element twist angle shows good agreement over a range of flow conditions ($15 \leq Re \leq 280$) [18], wide variations in published experimental data [1–8] render such comparisons unsuitable for detailed validation purposes. More significantly, good agreement with experimental data for such a global measure is not sufficient to ensure that the complex mixing process has been accurately simulated.

Two complementary approaches have therefore been employed to provide an adequate level of confidence in the computed flow fields. Firstly, independent numerical simulations have been performed – on the same computational mesh – using a commercially-available CFD software package, Fluent/UNS, for a selected number of flow conditions. A comparison of the resulting velocity fields has shown excellent agreement [18]. Secondly, a detailed mesh convergence study [22] has indicated that the computational meshes employed in the present study are sufficiently refined to provide good numerical resolution. In addition, a study conducted using different numbers of particles for the mixing analysis [22] has demonstrated, as required, that the results remain unchanged if the number of particles is increased.

It is noted that the number of mesh cells used to compute the flow fields, and the number of particles employed in the mixing analysis, is considerably greater than used in most previous investigations. This is associated with the greater complexity of the flow for non-creeping flow conditions. Indeed, coarser meshes are not able to resolve adequately the complex vortical flow behaviour, and can lead to a significant loss of particles in the particle tracking calculations. In addition, the use of an inadequate number of particles to analyze mixing can lead to the false illusion of good mixing in the presence of the fine flow structure observed under non-creeping flow conditions.

2.4. Computational resources

For the non-creeping flow conditions considered in the present study, both the flow computation and particle tracking steps require sizeable computational resources to provide adequate accuracy in the numerical simulations. For the present study, the 256-processor Cray T3D system installed at the EPF-Lausanne was used. Generally, 64 processors were used for the flow computation and 128 processors for the particle tracking. To obtain the results for the optimization study presented in this paper, approximately 4800 processor-hours were required for the flow computations, and 3840 processor-hours for the particle tracking. This corresponds to a total wall-clock time on the Cray T3D of slightly greater than 4 days, or approximately 1 year on a modern workstation.

3. Numerical results

Numerical simulations have been performed for a Kenics mixer with the characteristics listed in Table 1. (Note that non-dimensional units are employed by the flow solver.) The empty inlet and outlet pipe sections were both chosen to

Table 1
Geometrical and flow characteristics used in the present study

Radius	a
Element length	$L = 3a$
Element thickness	0
Number of elements	6
Mixer length	$18a$
Inlet pipe	$3a$
Outlet pipe	$3a$
Total length	$24a$
Twist angle	$0° \leq \Theta \leq 360°$
Reynolds number (based on radius)	100

have the same length as the mixer elements. The elements were considered to be infinitely thin, both to facilitate mesh generation and to avoid excessive mesh refinement at the leading and trailing edges of the elements necessary to capture the associated fine-scale flow behaviour. (Preliminary tests have indicated that this simplification has little influence on the results obtained.) Due to the large computational resources required, only one flow condition has been considered (i.e. $Re = 100$, based on the inlet axial velocity and pipe radius). Thirteen different values of twist angle Θ between 0° and 360° have been considered; since the total mixer length and the number of elements have been kept constant in these studies, this corresponds to 13 different values of element twist rate.

A detailed study [18] using various dynamical system techniques (e.g. Poincaré sections, finite-time Lyapunov exponents) has shown that for the standard twist angle of 180°, the flow is globally chaotic for the chosen conditions. No regular islands (consisting of segregated non-chaotic regions) are apparent, as are observed for non-creeping flows with lower Reynolds number (e.g. $Re \approx 25$). Such observations are in qualitative agreement with those of [20]. (Note that in [20], the authors define Re based on the pipe diameter and not its radius.)

3.1. Flow fields

The flow in the Kenics mixer is best represented by the crosswise velocity in a helical coordinate system that accounts for the local twist of the mixing elements [18]. In Fig. 2 are shown plots of the crosswise velocity computed at an axial location near the end of the fourth mixing element (i.e. end of second element pair) for six of the 13 twist angles considered. For this axial location, it has been determined that the velocity fields are not influenced by either the inlet or outlet conditions. The plots shown in Fig. 2 are therefore representative of the crosswise velocity fields that arise at the end of each mixing element pair in a mixer containing a larger number of elements.

From the plots presented in Fig. 2, it can be seen that the rotation of the fluid in the sense opposite to the local helical twist of the mixing elements leads to the creation of a vortical structure. Contrary to that observed for creeping flow [12–16,19,21], a secondary vortex is also seen to develop on the suction side of each element. This secondary vortex, which is not apparent for small twist angles, progressively grows as Θ is increased, and eventually dominates the crosswise velocity plot.

3.2. Particle distributions

The particle distributions computed near the end of the last (i.e. sixth) mixing element for six of the 13 twist angles considered are presented in Fig. 3. Comparing these plots with those presented in Fig. 2 shows that the flow structures roll-up around the vortices. Such behaviour is similar to that observed in a blinking vortex mixer [23]. As observed in the crosswise velocity plots, these rolled-up flow structures, which are virtually non-existent for small twist angles, grow as Θ is increased, and eventually dominate the cross-sectional particle distribution plots. The increased rolling of the structures around the flow vortices results in thinner, more elongated structures for larger twist angles. Qualitatively, Fig. 3 therefore suggests that a higher degree of fluid mixing is achieved for mixers with larger twist angle.

3.3. Quantitative mixing evaluation

A number of measures can be proposed to obtain a quantitative evaluation of the efficiency of the mixing

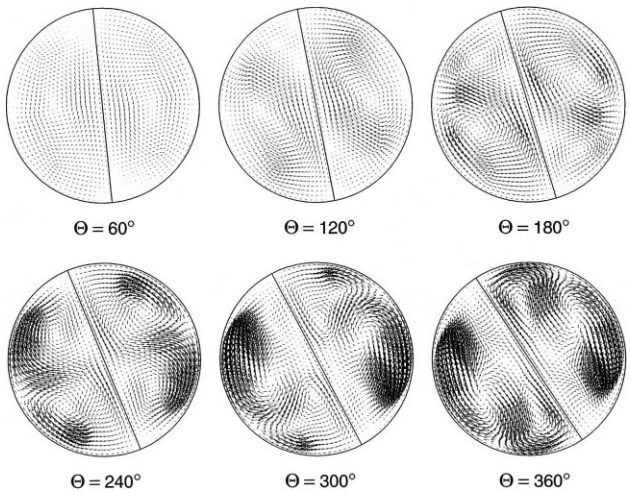

Fig. 2. Crosswise velocity vectors in the helical coordinate system at an axial location near the end of the fourth mixing element computed for mixers with different twist angles.

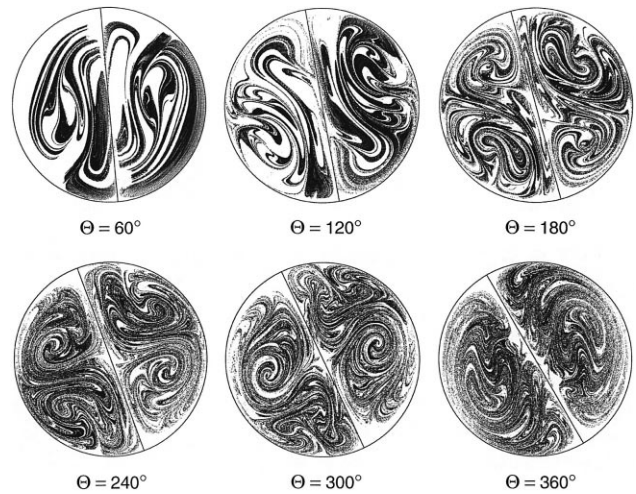

Fig. 3. Plots of the positions of 262 656 particles at an axial location near the end of the last (i.e. sixth) mixing element computed for mixers with different twist angles.

process. The efficiency can be related to the ratio of the mixing quality and the energy required to perform the mixing. We take the total pressure drop along the mixer (defined as the difference between the average pressures at the inlet and outlet planes of the mixer) as a measure of the energy consumption. In many mixing applications, one is concerned with the size of the largest unmixed region that exists in the fluid. A practical measure of the quality of the mixing can then be obtained by defining the 2D structure radius at a given axial location, normalized to the pipe radius, to correspond to the radius of the largest circle that can be drawn around a particle of one of the component species that does not contain any particles of the second species. The structure radius is thus related to the size of the flow structures, and corresponds to the striation thickness generally measured experimentally.

The mixing efficiency can then be defined as

$$E = (-\Delta p\, r_s)^{-1} \tag{2}$$

where $-\Delta p$ is the total pressure drop along the mixer, and r_s is the structure radius at the end of the last (i.e. sixth) mixing element.

As indicated above, Eq. (2) is not the only means of defining the mixing efficiency, the most appropriate choice being determined by the specific requirements of the mixer. Rather than be concerned with the largest unmixed regions, a more global value of the mixing quality may be appropriate, based for example on the crossection-averaged structure radius. Alternately, measures of mixing quality based on average rates of deformation of the fluid may be appropriate, as employed in [19,20]. Such measures may provide the most useful measure of mixing quality under conditions for which large regions of segregated non-chaotic flow exist. Since for the conditions considered in the present study the flow is not dominated by regular islands (although Fig. 3 suggests their presence for small twist angles), the use of either local or global measures has been found to lead to the same general conclusions [18].

Fig. 4(a) shows the computed dependence of the pressure drop on the twist angle. As expected, for larger twist angle the pressure drop along the mixer is greater, due to the increased resistance of the fluid flow through the mixer pipe. This is a consequence of both the increased energy required to generate the internal vortical fields, and the increased frictional drag associated with the larger surface area of the mixer elements.

Fig. 4(b) shows that as the twist angle is increased the structure radius decreases substantially (note the logarithmic vertical scale). This is in agreement with the qualitative observations of the particle distribution plots shown in Fig. 3.

As a result of the dependencies on twist angle of the pressure drop and structure radius, Fig. 4(c) shows that a clear maximum in the mixing efficiency E is computed near $\Theta = 180^\circ$. For this value of twist angle, the mixer provides close to its maximum mixing quality for a relatively modest energy input.

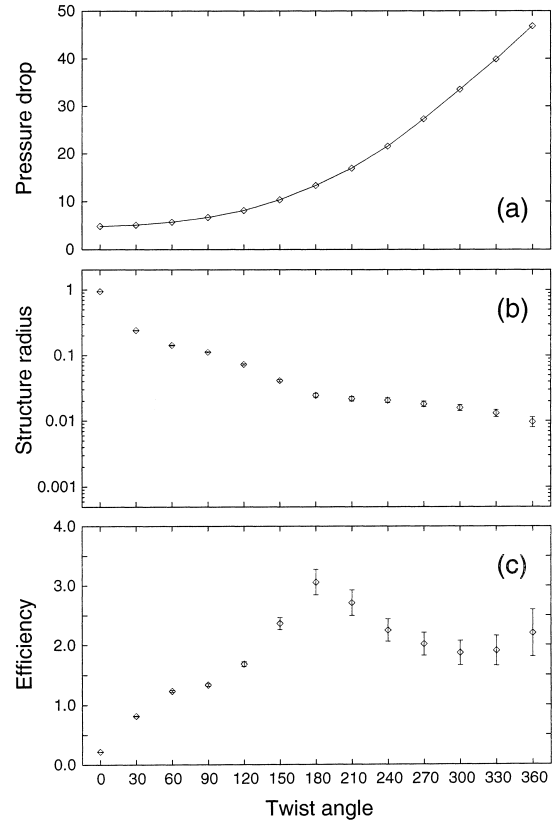

Fig. 4. Dependence on the twist angle of (a) pressure drop along the mixer, (b) structure radius at the mixer outlet, and (c) resulting mixing efficiency.

4. Conclusion

In the present study, advanced CFD techniques have been used as a design optimization tool for the Kenics static mixer. The results obtained from a series of numerical simulations for non-creeping flow with $\mathrm{Re} = 100$ have shown that an optimal value of twist angle exists for which the mixing efficiency is maximized. This optimal value is close to the standard design angle of 180°. It should be stressed that such a result is by no means obvious. Given the complexity of the mixing process and its irregular dependence on Reynolds number [18,20], some caution should be taken as to the generality of this result for all operating conditions. Indeed, previous optimization studies for creeping flow conditions [13,15,21] have concluded that a twist angle significantly less than 180° provides optimal mixing. A more complete parametric study is therefore required to reveal the inherent complexity in the optimal operating conditions of the Kenics mixer. Such a study would benefit from the inclusion of other design parameters of interest, such as aspect ratio, number of mixing elements, Reynolds number and fluid properties.

By resolving the complete Navier–Stokes equations for three-dimensional flow in the mixer, the present results avoid the approximations and uncertainties associated with

some of the previous numerical design studies. Unfortunately, this is at the expense of greatly increased computational costs. For the non-creeping flow conditions considered, to obtain accurate numerical results in a reasonable time necessitated the use of state-of-the-art computational resources that are generally not available in the chemical process industry. Nevertheless, the current rapid increase in affordable computational hardware together with the growing capability of commonly-available CFD software packages, should enable numerical design studies such as that of the present paper to be performed on a regular basis in the near future.

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