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A STUDY OF THE KENICS STATIC MIXER VIA HIGH-PERFORMANCE PARALLEL FLOW SIMULATIONS

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ABSTRACT

Detailed numerical simulation and analysis of laminar flow in a Kenics static mixer have been undertaken. Flow computations have been performed using a conventional Eulerian approach to resolve the governing Navier-Stokes equations, while an examination of the mixing process has been conducted using a Lagrangian approach involving particle tracking. Numerical simulations performed for a range of Reynolds number have elucidated the mixing processes that occur in different flow regimes. It is shown that high-performance parallel computing provides the possibility not only to obtain detailed and accurate solutions, but also enables design optimization of the mixer geometry.

INTRODUCTION

There exists a wide range of industrial applications for fluid mixing, 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 (Pahl and Muschelknautz, 1982; Cybulski and Werner, 1986). The present study considers the Kenics static mixer, manufactured by Chemineer, Inc., which consists of alternately twisted elements inserted into a cylindrical pipe (see Fig. 1).

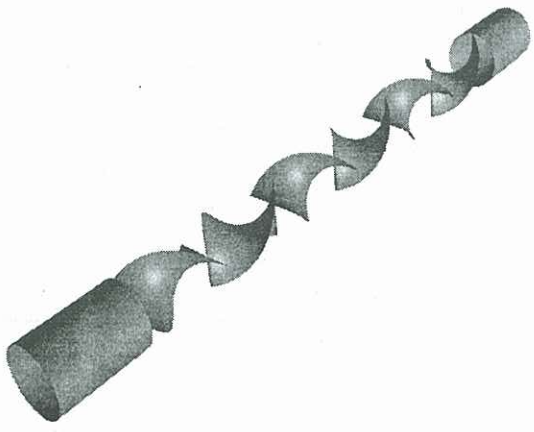

Figure 1: Perspective cutaway view of a six-element Kenics mixer.

The numerical simulation of the flow and mixing in a Kenics mixer is made difficult by the complexity of the flow behaviour and mixing processes. To solve accurately the Navier-Stokes equations requires substantial computational resources. 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 (Khakhar et al., 1987; Ling, 1993), which can be considered as a simplification of the Kenics mixer where the twist of successive mixing elements is not alternated. Creeping flow in a twisted-tape mixer has also been studied (Arimond and Erwin, 1985; Ling and Zang, 1995) using a superposition of fully-developed flows calculated for an infinitely long mixing element.

More recently, computations have been performed by solving the complete three-dimensional Navier-Stokes equations for the flow in the Kenics mixer (see, e.g., Byrde and Sawley, 1996; Byrde, 1997; Hobbs and Muzzio, 1997, 1998). While some of these studies have been restricted to creeping flow conditions, preliminary studies of the more complex flow and mixing behaviour at higher Reynolds number have also been considered.

The present paper reports on a detailed study of different laminar flow conditions, corresponding to Reynolds numbers in the range $0.01 \leq Re \leq 320$ (Re based on the mixer radius and inlet axial flow velocity). The simulations have 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.

To overcome limitations associated with the compute-intensive nature of the simulations, high-performance parallel computer systems have been employed. This has provided three distinct advantages. Firstly, sufficiently refined computational meshes (with up to 3 million mesh cells) have been used to compute accurately the flow fields, this being particularly important for flows with higher Reynolds number. Secondly, it has allowed a large number of particle trajectories (up to 2 million) to be calculated in a reasonable time, which is essential to obtain statistically significant measures of the mixing efficiency. Finally, it has rendered feasible a design optimization study of the Kenics mixer.

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NUMERICAL METHOD

Flow Computation

Two different parallel flow solvers have been employed in the present study, depending on the Reynolds number of the flow. The same block-structured computational mesh (Byrde and Sawley, 1998), comprised entirely of hexahedral cells, was used with both solvers.

For $15 \leq Re \leq 320$, a multiblock incompressible flow solver developed within our laboratory has been used (Marx, 1991). The numerical method is based on a cell-centred finite volume discretization with an artificial compressibility method to couple the pressure and velocity fields. A spatial discretization following the MUSCL approach is employed, using a second-order upwind κ scheme and the approximate Riemann solver of Roe. A "diagonal" form of the ADI method is used to solve the set of discretized equations.

For $0.01 \leq Re \leq 15$, a parallel version of the commercial flow solver FLUENT/UNS has been used (Fluent, 1996). This code is based on a cell-centred finite volume discretization on an unstructured mesh, with a second-order upwind scheme. The discretized equations are resolved using a Gauss-Seidel method coupled with a multigrid technique to accelerate convergence.

The parallelization of both flow solvers is based on domain decomposition techniques (Sawley and Tegnér, 1995). The computational domain is subdivided into a number of subdomains and the flow in each subdomain computed on different processors in a concurrent manner. Load balancing is achieved by ensuring that each subdomain has an equal, or approximately equal, number of mesh cells. Two different parallel computer systems installed at the EPF-Lausanne have been employed for the present study, a 256-processor Cray T3D (for the multiblock solver) and a 32-processor Silicon Graphics Origin2000 (for FLUENT/UNS). Good performance scalability with increasing number of processors was measured for both flow solvers, up to the maximum number of processors available (Byrde, 1997).

In principle, each of the above solvers could be used to cover the entire range of flow conditions considered. Nevertheless, it was found that for $Re < 15$, the multiblock code required an excessive number of iterations to obtain a converged solution. This behaviour is attributed to the ADI method employed to resolve the discretized equations; this has been confirmed by initial tests using an iterative matrix solver. Nevertheless, this solver provided higher levels of parallel performance and was therefore used whenever practicable.

A uniform velocity profile is assumed at the entry of the inlet pipe section, while 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.

Particle tracking

Unfortunately, it is not possible to analyze the mixing of liquids exhibiting low physical diffusion by the resolving the species continuity equations, due to the domination of numerical diffusion. A Lagrangian approach is therefore employed, involving the tracking of particles in the computed velocity field. Some care must be taken in integrating the equation describing the particle motion in order to retain sufficient accuracy, and thus limit the number of particles that are "lost" by leaving the domain or being trapped at the walls. In the present study, using a fourth-order Runge-Kutta scheme reduced the loss to 1 - 5%, depending on the Reynolds number of the flow and the mixer geometry.

Since the particles are assumed to be non-interacting, their trajectories can be calculated in an independent manner leading, in principle, to simple parallel implementation and high computational efficiencies. Nevertheless, due to the different underlying data structures of the flow computations and particle tracking calculations, attention must be paid to maintaining good load balancing and low communication and synchronization overhead (Byrde and Sawley, 1998).

RESULTS

Validation studies

A number of different tests have been conducted to verify the accuracy of the numerical flow simulations. Firstly, the solutions computed using the two flow solvers for the same flow conditions have shown excellent agreement (Byrde, 1997). Secondly, mesh convergence studies have been performed to determine the computational mesh necessary to obtain solutions of the required accuracy. These studies have shown that while the pressure drop along the mixer is rather insensitive to the number of mesh cells, the mixing quality – as determined from the structure radius – can only be determined by the use of a sufficiently fine computational mesh (Byrde and Sawley, 1998). To ensure mesh-converged solutions, computational meshes containing up to 3 million cells were used. Thirdly, the computed pressure drop along the mixer has been compared with experimentally-determined values (Byrde, 1997). While good agreement has been found across the range of flow conditions considered, the numerical values are slightly less than those measured; this is attributed to the neglect of mixer element thickness in the numerical simulations. Finally, the numerically-determined velocity fields have been compared with experimental data obtained using a non-invasive NMR imaging technique (Rombach and Blümler, 1998); preliminary results are considered to be encouraging.

Flow and mixing characteristics

By comparing the solutions computed for flows with different Reynolds number, a number of observations can be made. For the range of Reynolds number considered in the present study ($0.01 \leq Re \leq 320$), three distinct regimes, exhibiting different flow and mixing behaviour, can be distinguished: creeping flow ($Re \lesssim 1$), intermediate regime ($1 \lesssim Re \lesssim 50$), and high Reynolds number regime ($Re \gtrsim 50$).

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

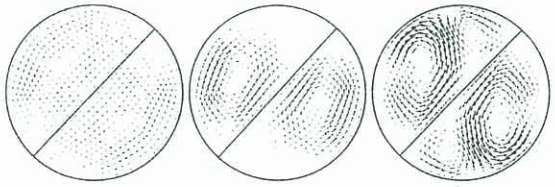

Figure 2: Crosswise velocity computed towards the end of the fifth mixing element for Re = 0.01 (left), Re = 25 (centre), and Re = 100 (right).

(Byrde, 1997). Figure 2 shows plots of the computed crosswise velocity for representative conditions in each of the three above-mentioned flow regimes. For creeping flow conditions, the crosswise velocity fields exhibit a single symmetric vortex on each side of the mixing elements. For the intermediate regime, the observed single vortices are asymmetric across the mixing element. For the high Reynolds number regime, both primary and secondary vortices are observed on both sides of the mixing element.

As shown in previous studies, mixing in the Kenics mixer occurs via chaotic advection (Ottino, 1989) associated with the stretching and folding of the fluid structures in the flow. To study in detail this mixing process, the trajectories of 262,656 particles, initially located in the right-half of the mixer cross-section (corresponding to diametrical feeding of the mixer), have been calculated. Figure 3 shows the particle positions computed at three different axial locations for each of the three flow regimes. For creeping flow, characteristic striations are apparent, the number of striations doubling with the passage through each mixing element. Such behaviour is confirmed by experimental observations (Chemineer, 1988). At higher Reynolds number, such regular, parallel striations are not observed, but rather more complex structures that exhibit large spatial variations in size and shape. For the high Reynolds number regime, these structures – which clearly are determined by the complex vortical flow behaviour – are much finer than those observed for the flows in the intermediate regime.

A more detailed analysis of the mixing process can be obtained by numerically determining the function that maps a particle position at the beginning of a mixing element to that at its end. Repeated application of this map (corresponding to a very long mixer) leads to the construction of Poincaré sections. Figure 4 shows the Poincaré sections computed for each of the three flow regimes. While no clear structure is apparent for the creeping flow and high Reynolds number regimes, for the intermediate regime four distinct stable island structures

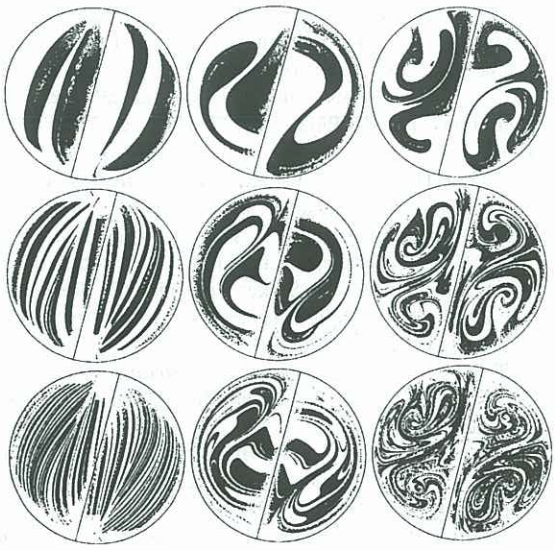

Figure 3: Particle position computed near the end of the second, fourth and sixth mixing elements for Re = 0.01 (left), Re = 25 (centre), and Re = 100 (right).

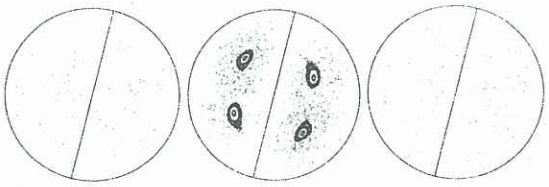

Figure 4: Poincaré sections computed for Re = 0.01 (left), Re = 25 (centre), and Re = 100 (right).

are observed. These stable islands are associated with the large flow structures seen in Fig. 3 for this flow regime.

The above observations indicate that the mixing efficiency of the Kenics mixer is dependent on Reynolds number, with poorer mixing occurring for the intermediate flow regime. Indeed, in the absence of diffusion, the Poincaré sections computed for the intermediate regime indicate that complete mixing in not attained, independent of the number of mixing elements employed.

The mixing efficiency can be defined as the ratio of the mixing quality divided by the axial pressure drop along the mixer. In the present study, the mixing quality of a fluid containing two species is determined by considering the 2D structure radius at the mixer outlet, defined as 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 dependence of mixing on Reynolds number can be analyzed more quantitatively from the plots shown in Fig. 5. These show that the pressure drop in the Kenics

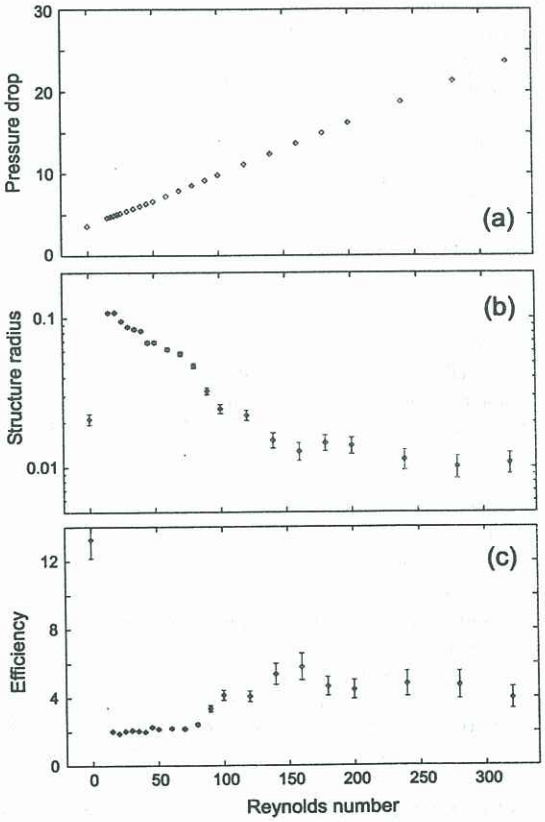

Figure 5: Dependence on Reynolds number of (a) the pressure drop along the mixer, (b) structure radius at the mixer outlet, and (c) resulting mixing efficiency.

mixer (normalized to that in an empty pipe) increases with increasing Reynolds number, while the structure radius exhibits a peak for Re ≈ 20. The resulting mixing efficiency is therefore lower in the intermediate flow regime compared with the creeping flow and high Reynolds number regimes. This result is consistent with experimental observations (Hartung and Hiby, 1975), which indicate that more mixing elements are required to obtain adequate mixing for the intermediate flow regime.

Design studies

Numerical simulations have been undertaken for a series of Kenics mixers having the same geometry except for the twist angle of the mixing elements. Due to the large amount of computer time required for this study (a total of 8640 processor-hours on the Cray T3D), only one flow condition, Re = 100, has been considered. The results presented in Fig. 6 show that the pressure drop (normalized to the dynamic pressure at the mixer inlet) increases with increasing twist angle, while the structure radius decreases. As a consequence, a maximum efficiency is determined for a twist angle of approximately 180°. This value is the same as that of the standard Kenics design. Nevertheless, given the complexity of the mixing process and its irregular dependence on Reynolds number, some caution must be taken as to the generality of this result for all operating conditions.

CONCLUSION

Numerical simulations of the flow in a Kenics static mixer using high-performance parallel computers has provided increased insights into the mixing process over a range of operating conditions. Three different flow regimes have been revealed, distinguished by different flow behaviour and resulting mixing efficiency. A design optimization study has shown that for Re = 100 flow maximum mixing efficiency is achieved for the standard element twist angle of 180°.

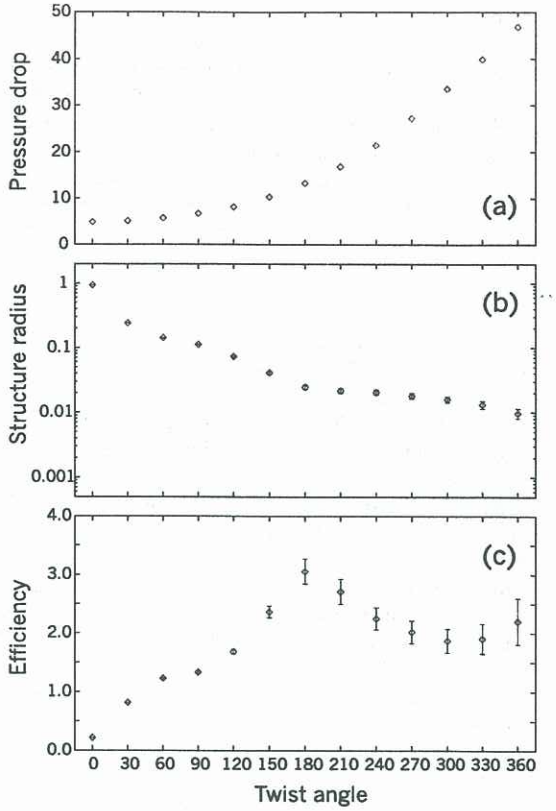

Figure 6: Dependence on the twist angle of (a) the pressure drop along the mixer, (b) structure radius at the mixer outlet, and (c) resulting mixing efficiency.

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