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Numerical simulations of mixing in an SMRX static mixer

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Abstract

The present work focuses on the flow characteristics and mixing induced by Sulzer SMRX static mixers. It is observed both experimentally and numerically that pressure drop increases linearly with velocity for this mixer type and that, as expected, this effect is amplified when multiple mixers are placed in the flow field. It is further shown numerically that the slope of the pressure drop versus velocity curve increases for increasing internal mixer tube crossing angles. Moreover, it is found that mixing efficiency is a strong function of the internal tube crossing angle. Finally, analysis of the pressure drop results, particle patterns at the reactor outlet, streamlines, and the intensity of segregation suggests that the optimum configuration of an SMRX mixer is one with a 90° internal tube crossing angle. It also shows to what extent the use of two static mixers provide enhanced mixing compared to one.

Keywords: SMRX static mixers; Numerical simulations; Mixing

1. Introduction

Owing to their simplicity, tubular reactors used for homogeneous polymerization are common in industrial environments. However, the polymerization reactions which occur therein often display a large increase of viscosity with monomer conversion. It has been shown that static mixers considerably improve heat transfer in a viscous medium and avoid the broad residence time distribution normally observed for laminar flow (Refs. [1,2]). Although these facts indicate something about macroscopic mixing, they do not yield information on microscopic mixing which is equally important. The full-scale problem of flow in a static mixer reactor consists of a combination of mixing (diffusion and convection), chemical reaction (polymerization) and heat transfer, in addition to fluid mechanics. As a first step to understanding this complex process, a fundamental understanding of fluid flow behavior in static mixers is clearly of both academic and industrial interest.

Although many different static mixer geometries exist in practice, the point that they all have in common is that there are no moving parts, as opposed to traditional stirred tank reactors. Mutsakis et al. [3] have shown that Sulzer SMR-type mixers are particularly effective in providing radial mixing in polymerization reactors. For the purpose of numerical simulation, the static mixer of interest in this work is of type SMRX (Ref. [4]), a simplified version of the proprietary SMR-type mixer manufactured by Sulzer Chemtech of Switzerland. Its complex geometry consists of a series of solid crossing tubes, placed inside a rectangular tubular reactor (Fig. 1).

As a result of the geometric and flow complexities described above, researchers to date have approached this problem primarily from an experimental perspective. Villermaux et al. [5], Fleury et al. [6], and Meyer and Renken [7] and [8], respectively, have obtained empirical relationships describing micromixing times, polymerization rates, and segregation rates of polymers in tubular reactors containing static mixers. Meyer et al. [9] have shown generally that reactor mixing times are substantially reduced when static mixers are used, and Villermaux et al. [5] showed that the mixing time is a function of the ratio of viscosity to the rate of energy dissipation.

To date, few researchers have performed computer modeling of static mixers. Using the finite element code FLUENT, Bakker and LaRoche [10] studied flow and mixing for

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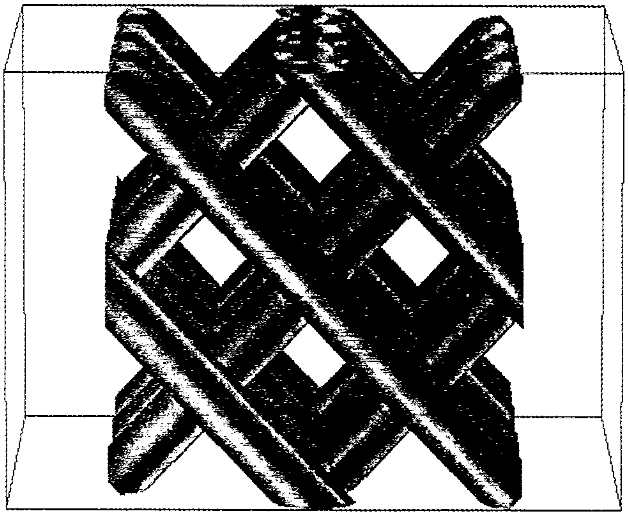

Fig. 1. A single static mixer of type SMRX in a rectangular reactor. Flow direction is from left to right.

Kenics (KM helical) mixers. With this same mixer type, Gyenis and Blickle [11] performed stochastic simulations of unsteady state particle flows. More recently, Bertrand et al. [12] investigated the residence time distribution in LPD and ISG (Ross Engineering) mixers. As for SMRX static mixers, Tanguy et al. [13] produced a preliminary analysis of flow in these devices, hence providing a starting point for the present work.

Although there are several mutually competing physical phenomena occurring in this system, computational fluid dynamics, which captures the primary dynamic features and allows for quick modification of system parameters, can be a cost-effective and enlightening alternative to experimental studies. Nevertheless, it is imperative that preliminary numerical calculations be ones which can be verified experimentally. The experimental results of van Dijck et al. [14] regarding pressure drop across SMRX static mixers, which will be discussed in more detail later, provide a source of comparison for the present numerical simulations. The goal of this study is to broaden current understanding of flow in static mixers through the use of numerical simulations and to provide an optimum design for an SMRX static mixer.

2. Numerical method

The flow in an SMRX static mixer Ω is governed by the steady-state Navier-Stokes equations:

$$\text{div}\ \tau + \rho v \cdot \text{grad}\ v + \text{grad}\ p = 0, \quad \text{in}\ \Omega \tag{1}$$

$$\text{div}\ v = 0, \quad \text{in}\ \Omega \tag{2}$$

where v and p denote the velocity and the pressure respectively, and where ρ stands for the density. In these equations, the stress tensor τ is a function of the rate-of-strain tensor $\dot{\gamma} = \frac{1}{2}[\text{grad}\ v + (\text{grad}\ v)^T]$ through a rheological model:

$$\tau = -2\eta(|\dot{\gamma}|) \tag{3}$$

In this article, a Newtonian model is considered:

$$\eta(|\dot{\gamma}|) = \mu \tag{4}$$

where μ stands for the viscosity.

These equations can only be solved numerically because of the complexity of the geometry. In the present work, the finite element method is used.

The complex design of the SMRX mixer makes mesh generation especially challenging. Mesh creation was attempted using several commercial grid generators unsuccessfully. One reason for this shortcoming is imputable to the crossing points where the mixer tubes touch and where degenerate elements often occur. Consequently, a mesh generator was specially developed for this problem. The grid generator divides the mixer volume into enriched $P_1{}^+$-P_0 type tetrahedral elements composed of 8 nodal points each. This element type is chosen because of its flexibility. It allows for linear velocity, discontinuous constant pressure, and conservation of mass within the element (Bertrand et al. [15]).

RheoTek's finite element program POLY3D solves the Navier-Stokes equations for flow past a single static mixer or multiple mixers. The solver is based on an augmented Lagrangian formulation and the iterative Uzawa method which decouple the velocity field from that of the pressure field (Robichaud et al. [16]). An entire calculation requires two pre-processing (mesh generation) steps which were run on a Silicon Graphics (SGI) computer, two processing phases which were accomplished on a Cray Y-MP, and two post-processing steps which were completed on an SGI.

The present authors used this program to calculate pressure drop as a function of fluid velocity for 1 and 2 static mixer elements, in addition to streamlines and various profiles. Depending on the exact geometry, the program divides the volume of a single static mixer into roughly 19,000 tetrahedral elements (Fig. 2) and two mixer elements into about 36,000 tetrahedral elements, resulting in as many as 100,000

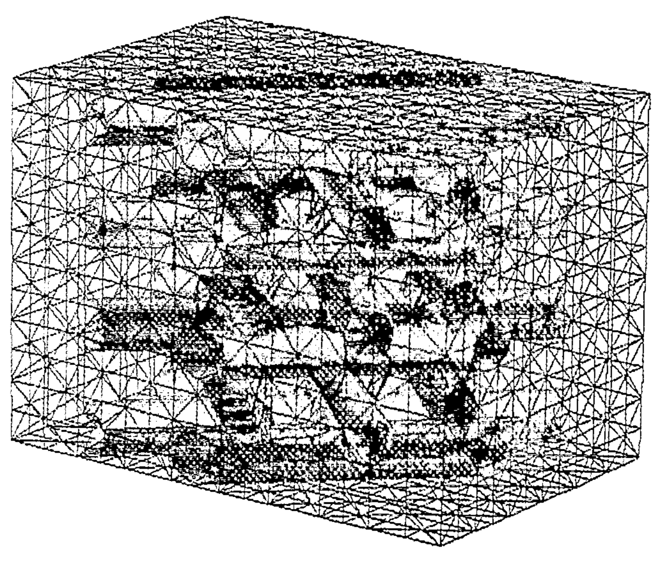

Fig. 2. Example mesh for a single static mixer element of type SMRX in a rectangular reactor.

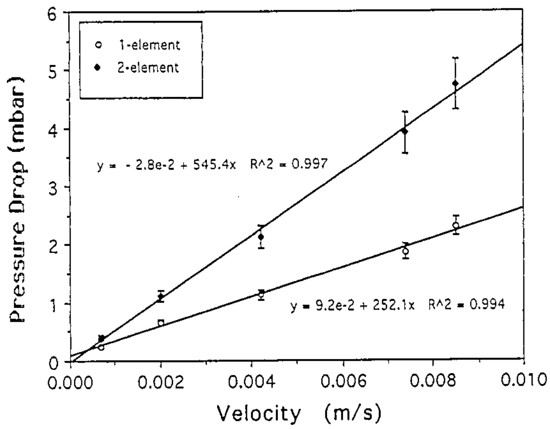

Fig. 3. Experimental data of van Dijck under conditions of viscosity = 1.46 Pa·s, density = 1053 kg m^{-3}, and angle = 90°.

Table 1
Mixer, velocity, and physical values

Mixers		
Number of static mixer elements	1	2
Total number of tubes in mixer	21	42
Tube crossing angle (90° for simulations related to van Dijck's experiments)	Variable	Variable
Velocity		
Velocity profile at inlet	Fully developed	Fully developed
Reference velocity	Variable	Variable
Physical		
Newtonian viscosity	1.46 Pa·s	
Density	1053 kg m^{-3}	

and 200,000 velocity equations respectively. The solution to these equations, obtained by using the iterative Uzawa method, requires approximately 70 MB of memory space for one element and 130 MB for two elements. This information translates to roughly 30 CPU min on a Cray Y-MP for a single element calculation and 60 CPU min for a two element case.

The physical parameters chosen for the numerical calculations correspond to those of the experiments of van Dijck et al. [14] who performed pressure drop measurements across 1, 2, and 10 static SMRX mixing elements in a rectangular tubular reactor at differing flow velocities of a 31 wt.% polyethylene glycol (PEG) solution in water. Their experimental data are shown in Fig. 3. It is mentioned that the 10 element case studied by van Dijck et al., although hypothetically possible to solve using POLY3D capabilities, pushes the numerical limit of Cray memory space presently allotted to individuals. Similarly, numerical accuracy could be improved by the use of finer meshes, but the mesh sizes described above were the densest possible within the hardware limitations.

Mixer, velocity, and physical information provided to the program is presented in Table 1. Exact geometric specifications may not be given, as they are proprietary. It is noted that the velocities, viscosity, and density used for these calculations correspond to those of van Dijck's experiments, and yield Reynolds numbers, based on the reactor channel width, of the order of 10^{-2}. Moreover, it is mentioned that the values given in Table 1 may be altered to mimic other mixer specifications, or to satisfy other fluid properties. The convergence criteria chosen for these studies were tested and found to be the minimum values required for accurate results.

3. Pressure drop verification

The experimental results of van Dijck et al. [14] mentioned above may be used to validate the numerical code used in this work. Fig. 4 shows both experimental and numerical results for pressure drop versus velocity for the case of 1 static mixer element enclosed in a rectangular-shaped tubular reactor (as shown in Fig. 1). The experimental data have an estimated systemic error of 7% in the pressure drop coordinate, as a true error analysis of the data was not performed. A linear fit of both experiment and computation suggests a 20% discrepancy in slope between the two. The y-intercept in both cases is small (10^{-4} to 10^{-2}) indicating a slight error compared to the theoretical y-intercept of zero. Numerical error can propagate quickly because pressure is calculated from the divergence of the velocity. Thus, a 20% variation between experiment and calculation is considered quite acceptable, for such a complex geometry.

Fig. 5 depicts the commercial configuration of 2 static mixer elements in a rectangular reactor. It is hereby noted that for multiple mixer arrangements every other element is generally rotated by 90° about the flow axis. The pressure drop results for 2 elements are displayed in Fig. 6. Here, the measurements have an estimated error of 9% in the y-coordinate. Again, a regressed line fit suggests a 16% error in slope between calculations and experiment, with small y-intercepts for both.

It is interesting to note that there exists a factor of 2 between the slope of the 1 element case and that found for 2 elements. Van Dijck et al. also found a factor of 2 in slope (with a 2%

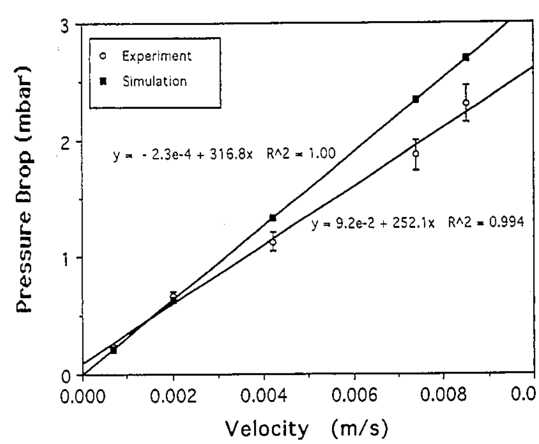

Fig. 4. Pressure drop versus velocity for a single static mixer in a rectangular reactor. Viscosity = 1.46 Pa·s, density = 1053 kg m^{-3}, and angle = 90°.

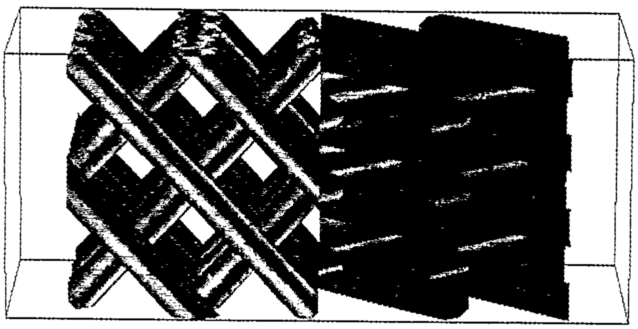

Fig. 5. Commercial configuration of two SMRX static mixers in a rectangular reactor. The second mixer is rotated by 90° with respect to the flow axis. Flow direction is from left to right.

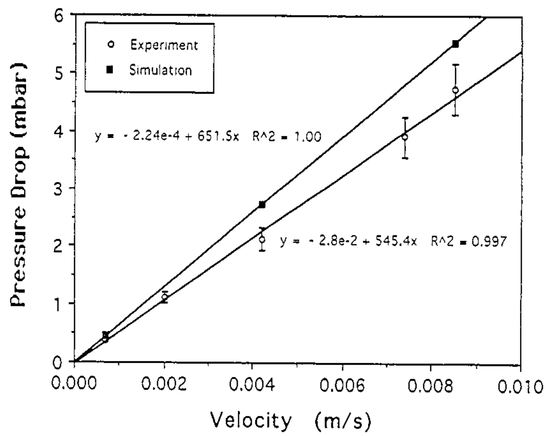

Fig. 6. Pressure drop versus velocity for two static mixers in a rectangular reactor. Viscosity = 1.46 Pa·s, density = 1053 kg m^{-3}, and angle = 90°.

error) between 1 and 2 elements. From a theoretical standpoint, the slope factor between 1 and 2 elements is expected to be 2 exactly if we neglect the gap between these two elements. The direct proportionality between pressure drop and velocity found for laminar flow in a duct follows from a classic derivation (Ref. [17]). This two-fold factor increase in slope implies that the pressure drop is nearly twice as large (at the same fluid velocity) for two mixer elements as for one.

The discrepancy between experimental and simulation results is attributed to three factors. Firstly, accurate pressure drop measurements were difficult to carry out in the experimental system. Secondly, viscosity, taken as constant in the numerical model, displays slight variations for uncontrolled temperature conditions during experiment. Thirdly, numerical error is introduced by the very process of geometric discretization. However, despite these shortcomings the numerical results provide an adequate representation of the experimental data.

4. Effect of angle on pressure drop

The effect of tube crossing angle (Fig. 7) on pressure drop for an SMRX mixer, keeping all other parameters constant, was also studied. Fig. 8 shows the results of pressure drop versus velocity for several crossing angles of a single mixer element. The graph indicates that the pressure drop increases with an increasing angle at a constant velocity. However, as suggested by the closeness of the lines for 30° and 60°, this increase is not linear but rather S-shaped (Fig. 9). This nonlinear behavior can be attributed to the fact that for any angle the mixer tubes are trimmed such that they always fit into a fixed volume. Moreover, an asymptotic behavior is expected as the crossing angle approaches 180°, at which point the flow is blocked completely.

Fig. 10 shows the same trend as Fig. 8 for two static mixers in the commercial configuration. Substantially higher pressure drops are noted for 150° and 120° than for smaller crossing angles. For example, both graphs show that the pressure drop for 120° is about 80% higher than that for 90° at an inlet flow velocity of 0.0085 m s^{-1}. High pressure drops are industrially undesirable because they increase operating costs, and low pressure drops are an indication of mixing inefficiency. Hence, effective mixer design requires a proper compromise between minimizing pressure drop and maximizing mixing.

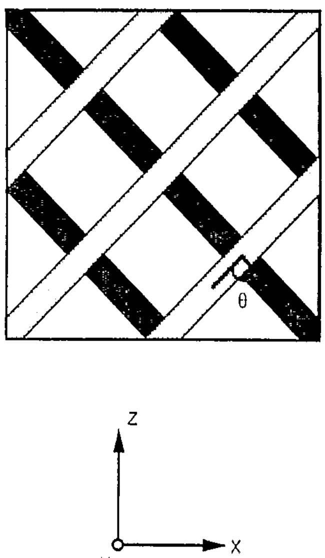

Fig. 7. Mixing element in 2-D, where θ is the internal tube crossing angle and Z is the flow direction.

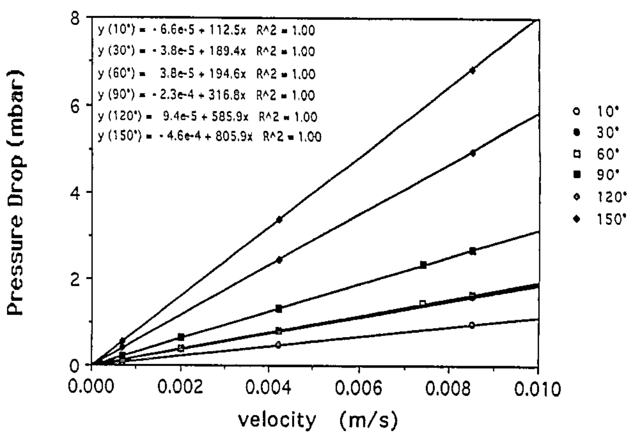

Fig. 8. Effect of angle on pressure drop versus velocity for a single static mixer in a rectangular reactor.

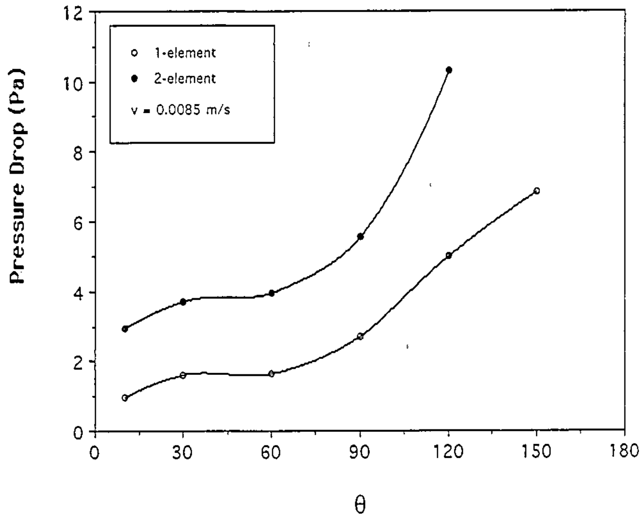

Fig. 9. Pressure drop versus crossing angle for a fixed velocity of 0.0085 m s^{-1}.

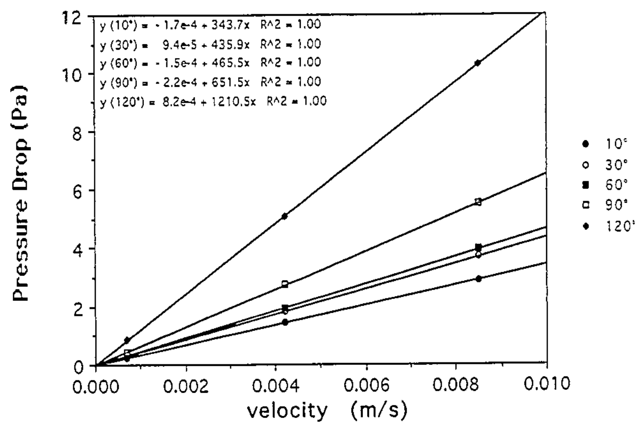

Fig. 10. Effect of angle on pressure drop versus velocity for two static mixers in the commercial configuration.

5. Visualization of mixing

Visual representations of mixing are particularly useful in understanding mixing phenomena. Using the procedure described in Bertrand et al. [12] to determine the residence time distribution (RTD), mass-less fluid particles may be tagged and then tracked as they proceed through a static mixer. Table 2 contains the parameters used to determine particle distributions. The study begins by looking at a single mixer of type SMRX enclosed in a rectangular reactor (Fig. 1). The basis for study is 10,000 evenly distributed particles at the reactor inlet (Fig. 11). All of the particles entering on the left hand side of the reactor's vertical center-line are represented by black dots and all of the ones entering on the right hand side are denoted by grey dots. The final positions of the particles were obtained by integrating the velocity field over time using a second order Runge-Kutta scheme. Step sizes were varied until stable results were obtained, thus establishing an optimum step size.

If no static mixer is placed in the reactor, regardless of its length, the particles remain segregated. In other words, no mixing occurs, which is expected. However, as soon as a mixer is introduced into the flow field, mixing is observed.

The degree of mixing achieved depends strongly on the crossing angle of the internal mixer tubes (Fig. 7). Fig. 12 (a)–(e) show the outlet results for a single static mixer element and several angles. Fig. 12(a) shows that for a 10° crossing angle, mixing is mild and proceeds by forming a sort of zigzag close to the reactor's center-line. At 30° (Fig. 12(b)), veritable fingers or striations (Mohr et al. [18]) are observed. At 60° (Fig. 12(c)), the striations extend horizontally until by 90° (Fig. 12(d)) many of the particles that were originally on the left-hand side have migrated close to the left reactor wall and vice versa. By 120° (Fig. 12(e)), a void region is noted about the vertical reactor center-line suggesting that mixing is no longer effective. The aforementioned results were for a reactor entrance velocity of 0.0007 m s^{-1}. However, the same mixing effects were observed for 0.0042 m s^{-1} and 0.0085 m s^{-1}.

Table 2
Parameters used in the computation of particle distributions

Geometric parameters	
Flow axis	3 (Z)
No. of particles along first axis	100
No. of particles along second axis	100
Initial position along flow axis	Inlet of mixer element
Final position along flow axis	Outlet of first element for single mixer or outlet of second element for 2 mixer case
Numerical parameters	
Maximum no. of iterations	50,000
Time step	0.01

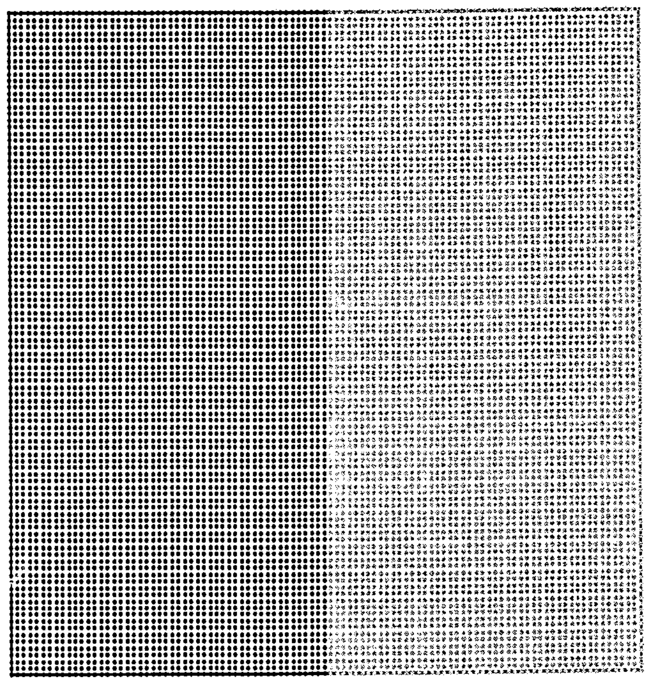

Fig. 11. Initial configuration of 10,000 marked particles at reactor inlet. The particles are segregated by the vertical center-line.

Simulations were also performed for the situation where 10,000 evenly distributed particles at the reactor inlet were separated by the horizontal center-line (i.e. particles tagged by grey dots above and black dots below this center-line). For a single static mixer, little to no vertical mixing at the outlet was observed for all of the crossing angles and velocities studied here.

Mixing is less effective for smaller crossing angles because the mixer tubes are more closely aligned with the flow field. For example, Fig. 13 shows that for a 30° crossing angle, the fluid flows by with little resistance. In contrast, for larger angles, the fluid must displace itself more vigorously in order to bypass the obstacles in its path, and mixes as a result. Fig. 14 shows this phenomenon for a 120° angle. Therein, the regions where streamlines approach each other are those where fluid mixing would occur for heterogeneous fluids. Moreover, streamlines which were originally near one another may take completely different paths to reach the outlet. However, for any given geometry, the streamlines are regular and do not look chaotic in nature [19]. Although streamlines indicate something about fluid mixing in a static mixer, it is important to keep in mind that they suggest noth-

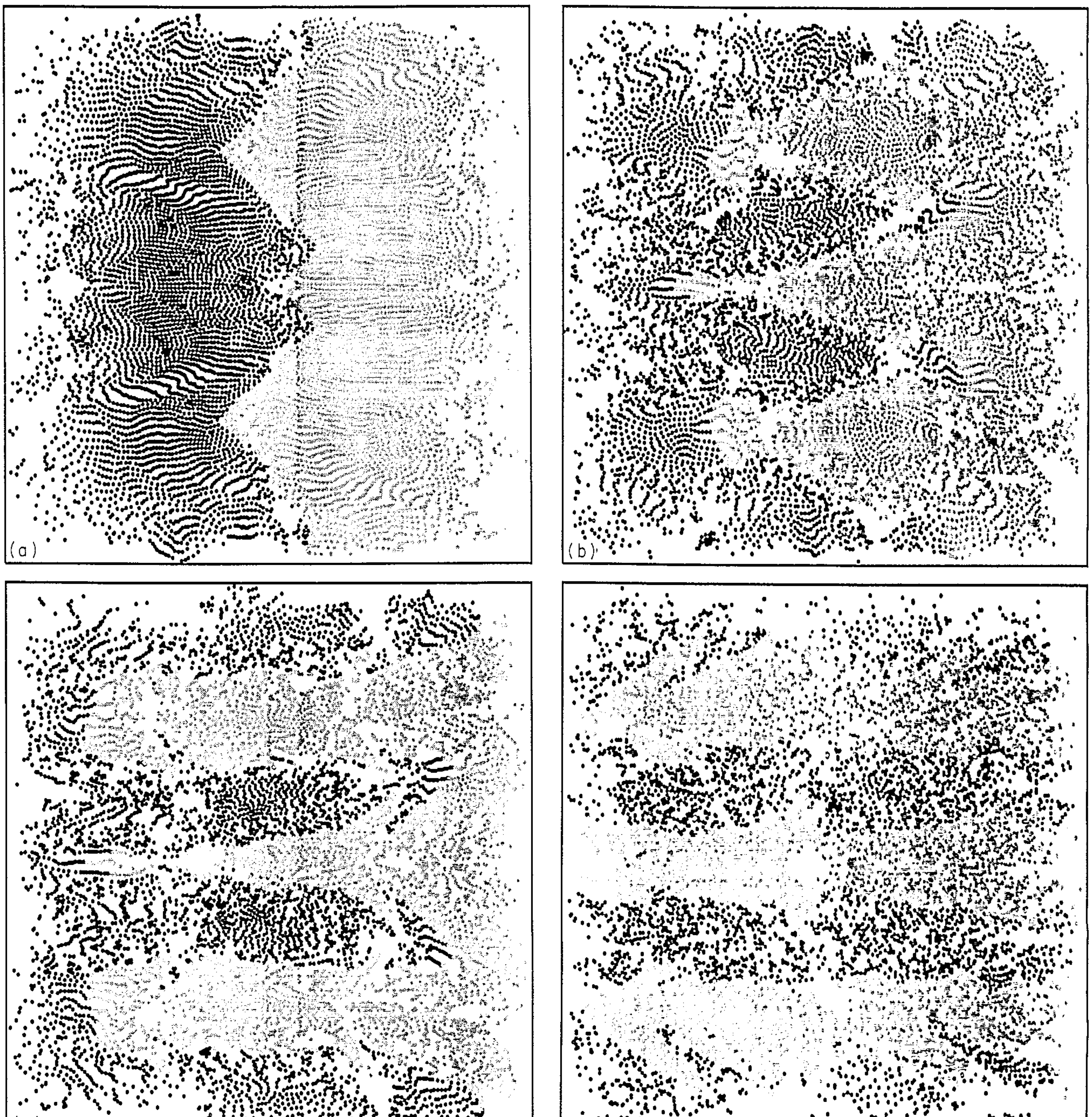

Fig. 12. (*continued*)

Fig. 12. Particle configuration at reactor outlet for a single static mixer with various crossing angles: (a) 10°, (b) 30°, (c) 60°, (d) 90°, (e) 120°.

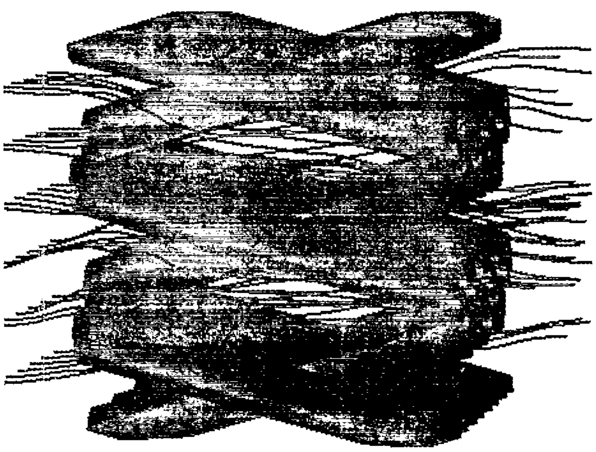

Fig. 13. Streamlines for a static mixer with a 30° crossing angle. Internal tubes are nearly parallel with the flow and provide little resistance.

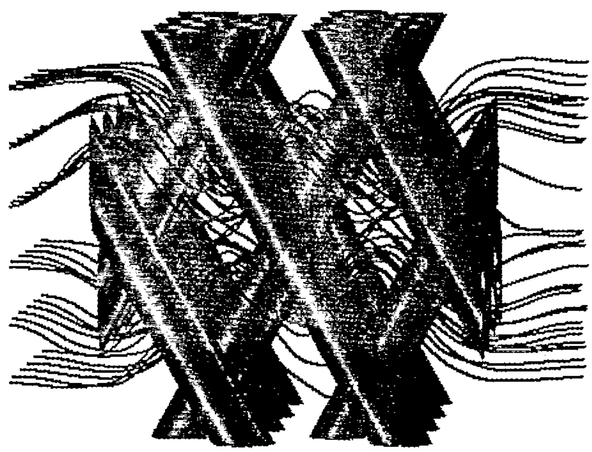

Fig. 14. Streamlines for a static mixer with a 120° crossing angle. Obstacles in the flow path impose more fluid displacement and induce mixing.

ing about the diffusion and heat transfer that occur simultaneously in the real system. Nevertheless, the streamlines capture the salient dynamic features of the system.

For two static mixers in the commercial configuration shown in Fig. 5, the mixing effect is enhanced. It is mentioned that the inlet configuration of the 10,000 particles is exactly as it was shown in Fig. 11. Visualization of the reactor outlet (past the second mixer) shows that striations are no longer easily observable, although a much larger number of particles would reveal small-scale structures. Nevertheless, the second mixer rotates the flow axially by 90° and suggests that, for more than one static mixer, both axial (horizontal) and vertical mixing are appreciable.

Fig. 15(a)–(e) shows the particle configurations at the reactor outlet for different inner tube crossing angles at an inlet velocity of 0.0007 m s^{-1}. Compared with their corresponding single element cases, these images show enhanced mixing. However, the trend of increased mixing with increasing crossing angle that was noted for a single static mixer is still valid. Inlet velocities of 0.0042 m s^{-1} and 0.0085 m s^{-1} were also studied and showed the same behavior. As before, a void region occurs at 120°, but this time it is about the horizontal center-line (Fig. 15(e)).

The conclusion drawn here is that the mixing phenomena for an SMRX mixer is affected primarily by the inner tube crossing angle. As expected, inlet velocities remaining in a laminar range have little to no effect on mixing. Enhanced mixing is observed for two mixers compared to one. Based on these results and the pressure drop considerations made in the previous section, the most effective mixing angle for an SMRX mixer would appear to be greater than 60°, but less than 120°. The rest of this paper is devoted to determining this optimum angle.

6. Residence time distributions

Residence time distributions (RTDs) provide one measure, amongst others, for evaluating the "quality" of mixing. Ideally, to avoid accumulation and the presence of hot spots, all fluid elements should have the same residence time. This fact implies that the RTD function should be nearly vertical, as for a piston flow.

The residence time distribution function versus dimensionless residence time $\bar{t}$ for one and two static mixer elements respectively were plotted, as well as the probability density function $E(\bar{t})$. The results are not presented herein because clustering of the curves near the x-intercept made analysis both difficult and inconclusive. Although RTDs are commonly used to assess the quality of mixing, they are not particularly useful in static mixing problems [12]. However, the residence time distribution is only one criterion which can be used to assess mixing efficiency. As a result, it is desirable to use a clearer quantitative method to assess mixing quality.

7. Intensity of segregation

In this section, the quality of mixing will be quantified using the "intensity" approach developed by Danckwerts

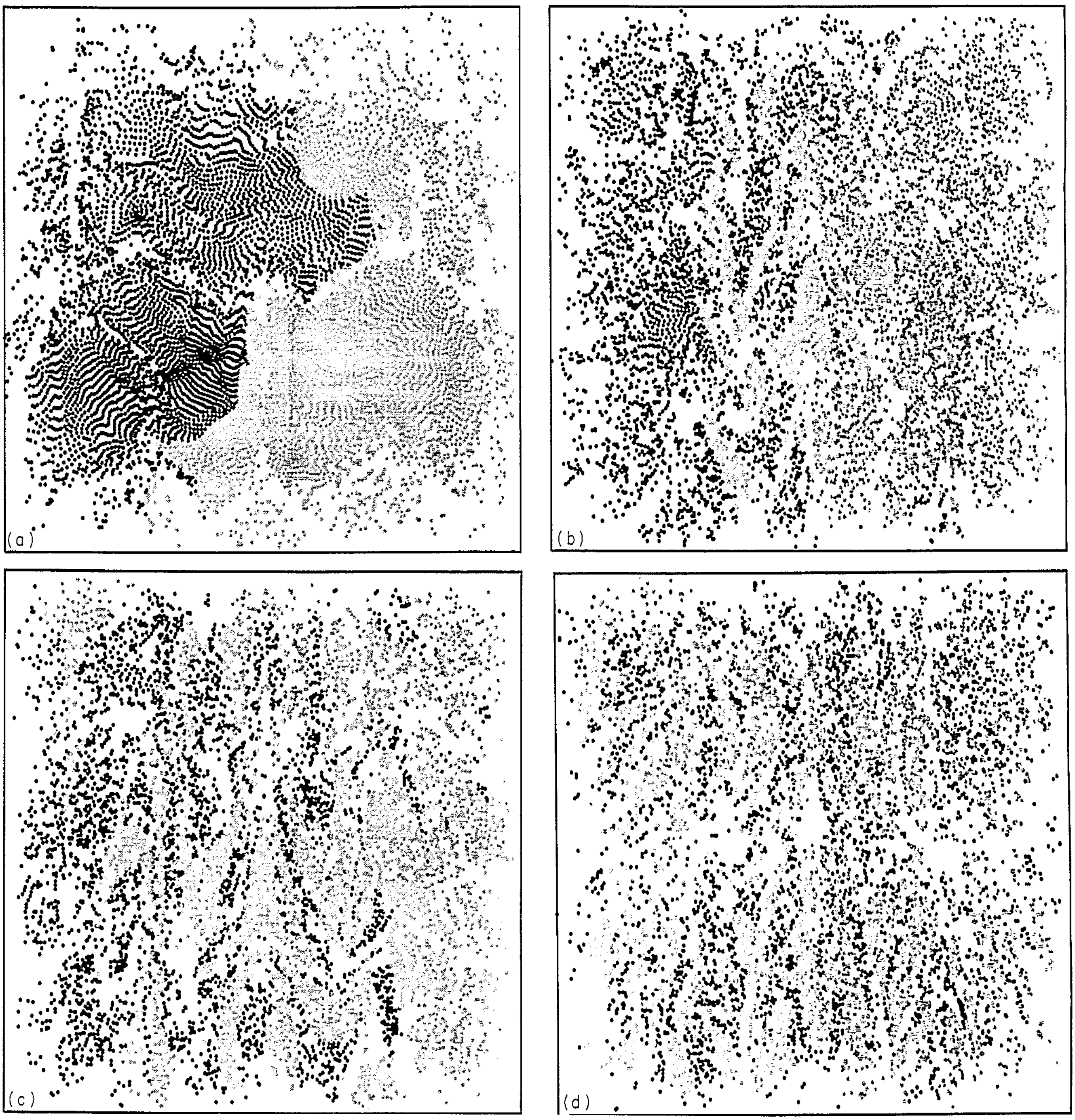

Fig. 15.

(*continued*)

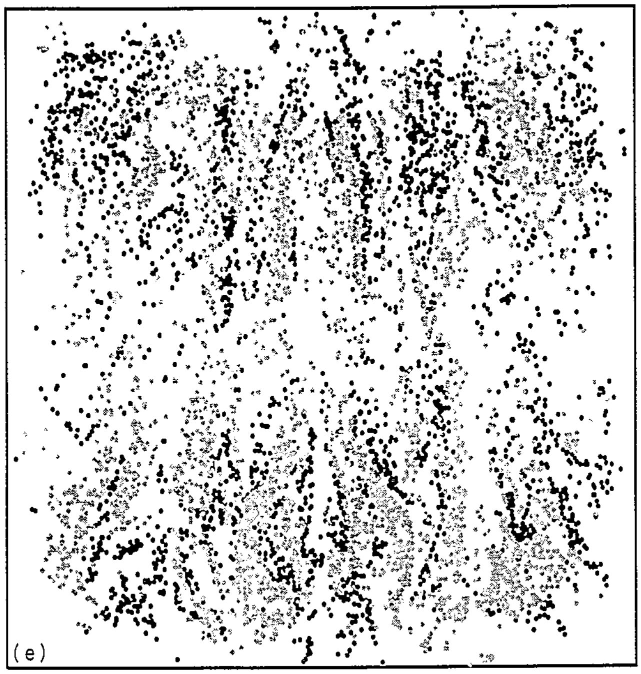

Fig. 15. Particle configuration at reactor outlet for two static mixers with various crossing angles: (a) 10°, (b) 30°, (c) 60°, (d) 90°, (e) 120°.

[20]. Using the notation given in Middleman's book [21], the average concentration of a system may be determined by randomly sampling the concentration C_i in a given system N times. That is,

$$C_{avg}=\frac{1}{N}\sum_{i=1}^{N} C_i \tag{5}$$

This definition requires that one component be chosen as primary in a binary system. The choice of the major component is arbitrary, and we will choose the particles denoted by the black dots to be major. Thus, we define C_i to be the quotient of the number of particles given by the black dots divided by the total number of particles.

One measure of the homogeneity of a mixture is the variance (s^2) of the concentration at different regions of space compared to the mean concentration, written

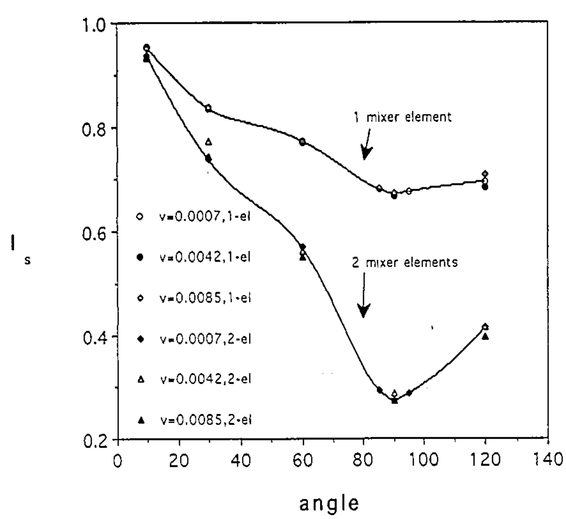

Fig. 16. Intensity of segregation versus crossing angle for 1 and 2 static mixers and several velocities. In both cases, the minimum occurs at 90°.

$$s^2=\frac{1}{N-1}\sum_{i=1}^{N}(C_i-C_{avg})^2 \tag{6}$$

The maximum variance (s^2_{max}) occurs when all the elements are segregated:

$$s^2_{max}=C_{avg}(1-C_{avg}) \tag{7}$$

The normalization of the variance to its maximum value is called the intensity of segregation, I_s, where

$$I_s=\frac{s^2}{s^2_{max}} \tag{8}$$

The value of the intensity ranges from 1 (complete segregation) to 0 (perfect mixing).

This statistical measure of mixing was incorporated into the RTD computations. The particle tracking portion of the program eased the burden of counting particles and of finding their outlet location, values which are needed to implement the Intensity Method.

Division of the outlet into a grid of 16×16 cells was determined to yield a representative sampling because this is where the value of the intensity stabilized. Fig. 16 shows a plot of the intensity parameter I_s versus inner tube crossing angle for one and two static mixer elements. For all velocities of the single element cases studied, the intensity slowly decreases to a value of about 0.69 at a crossing angle of 90° and then rises again slowly.

For the two static mixer configuration, the drop in intensity is amplified. The minimum value (that is, $I_s=0.28$) occurs at 90°, thus indicating that the optimum crossing angle for an SMRX static mixer is 90°.

8. Conclusions

As a first step, the numerical calculations were verified against van Dijck's pressure drop versus fluid velocity data, within 20% accuracy. It is found, both experimentally and computationally, that pressure drop increases linearly with velocity for SMRX static mixers, and that the slope for two mixing elements is twice that for one. The veracity of this statement for multiple mixers as well as for non-Newtonian fluids is still in question, and may be a point for further study. Furthermore, it has been demonstrated, for both case one and two static mixers, that pressure drop increases with increasing crossing angle.

Finally, it has been shown both visually and quantifiably that an SMRX mixer with a 90° inner tube crossing angle provides the most efficient mixing. Small crossing angles do not provide enough obstacles in the flow path to induce mixing and large angles block flow and create high pressure drops. Mixing efficiency is enhanced for two mixers in the commercial configuration compared to one.

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