# Validation of the ORCA CFD Software Using SMX and Kenics Static Mixer Elements

**E.S. Szalai and F.J. Muzzio**
Department of Chemical and Biochemical Engineering, Rutgers University,
PO Box 909, Piscataway, NJ 08855

**K.J. Bittorf***
Dantec Dynamics Inc., 777 Corporate Drive, Mahwah NJ, 07430
*Corresponding Author: e-mail Kevin.Bittorf@Dantecdynamics.com

Static mixers are commonly used for blending and heat transfer applications involving viscous fluids are used in a variety of products within the pharmaceutical, chemical, personal product, and food industries. Static mixers or inline mixers are often used in series, parallel, or other configurations within piping networks. Completing extensive experimental work on these complete systems is nearly impossible.

Optimization of these processes becomes critical as margins lower; product consistency and product quality are essential. Many food, pharmaceutical and health products industries use batch processes in which the same equipment is utilized for a variety of products. Within these industries, change over time must be reduced by minimizing the residence time of remaining products. In the pharmaceutical industry it is crucial that products are consistent from batch to batch, as slight impurities can result in failure to comply with FDA testing.

Computational fluid dynamics (CFD) offers an alternative technique to traditional experimental methods for accelerating equipment design and optimization while gaining additional fundamental understanding of mixing processes. The ability to analyse potential problem areas and test various solutions efficiently presents a myriad of beneficial possibilities. Once validated, CFD can be utilized for design purposes.

Before CFD can be used confidently, the results must be validated against experimental values and from such validation, inline mixer systems can be designed with confidence. The primary benefit of CFD models lies within their capacity for testing and optimizing numerous scenarios quickly compared to designing and building an experimental/laboratory model.

The pressure drop and mixing characteristics were computationally determined using the ORCA CFD package and the results were between compared two types of static mixers: the Koch-Glitsch SMX static mixer and the Chemineer® Kenics mixer. The ORCA CFD package provides accurate solutions in a timely manner utilizing a novel solution technique in the area of mixing fluid dynamics. The results attained form ORCA are validated against two detailed experimental studies using the SMX mixer and Kenics mixer. The comparison shows excellent agreement between the CFD and the experimental data.

## I. ORCA CFD Software

ORCA uses Galerkin Least-Squares finite element technology, a novel approach to computer aided modeling and optimizing mixing processes. Computer aided mixing, modeling, and analysis involves Lagrangian and Eulerian analysis for relative fluid stretching, and energy dissipation concepts for laminar and turbulent flows. High quality, conservative, accurate, fluid velocity, and continuity solutions are required for determining mixing quality.

The ORCA CFD package, based on a finite element formulation, solves the incompressible Reynolds Averaged Navier-Stokes (RANS) equations. Though finite element technology has been well used in areas of heat transfer, solid mechanics, and aerodynamics for years, it has been applied only recently to the area of fluid mixing. While most commercial technologies solve the resultant Partial Differential Equations (PDEs) as discretized approximate solutions using finite volume or finite difference techniques, ORCA uses the Galerkin Least-Squares (GLS) finite element technology. The GLS finite element formulation presented provides another formulation for numerically solving RANS based fluid mechanics equations.

The Galerkin finite element method serves as the basis of the formulation but is insufficient to yield a stable solution for the incompressible Navier-Stokes equations. Instabilities in the finite element technique arise from the continuity equation and the convective term in the momentum equations.

However, the added least-squares operators provide rigorous mathematical stability and convergence without sacrificing accuracy. The GLS finite element technology, a central difference operator that uses weighted residual methodology for momentum, energy and turbulence equations, minimizes error in the approximating functions while satisfying all conservation equations (heat, energy, momentum), both locally on the elements and globally on the entire system, while maintaining system stability. Conservation principles are specifically formulated and solved. The GLS technique provides the basis of the confidence, robustness, accuracy, convergence, and stability of ORCA. It provides 4th order accuracy with respect to the spatial discretization and 2nd order accuracy with respect to time. This method ensures extremely accurate solutions for a wide variety of flows, as shown in the following validation studies.

The ORCA CFD code runs on a Linux platform to optimize memory usage for the computations. Presently (2002), a typical system consists of one to four desktop computers in parallel, each with 515 GB Ram and Intel® or Athlon® processors. Solution times on a 3 million tetrahedral mesh typically vary from ten minutes to five hours depending on problem complexity. In this study, the typical solution time was one hour for solutions with an accuracy or residual ratio of $10^{-4}$ for both pressure and velocity.

## II. Validation Flow and Mixing in the SMX Static Mixer

The continuous mixer design considered is a Koch-Glitsch SMX static mixer, a device that is commonly used for blending and heat transfer applications involving viscous fluids. The four-element SMX static mixer assembly shown in Figure 1 is arranged axially in a pipe so that the series of crossing blades repeatedly divide the fluids into layers and distribute them over the pipe cross-section. Each mixer element has a diameter, $D_m$, of 0.07715 m and a length-to-diameter ratio equal to one. The thickness of each blade is 0.001928 m. The mixer assembly is located inside an open tube with a diameter, $D_t$ , of 0.07872 m.

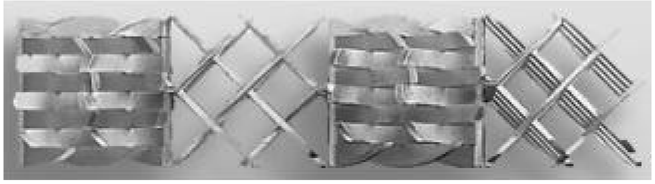


**Figure 1. The geometry of an SMX static mixer manufactured by Koch-Glitsch. Fluid mixing is accomplished by inserting a series of criss-crossing blades in a tube, and the energy for the mixing process is derived from an increase in pressure drop.**

In the simulations, the fluid chosen possesses the same physical properties as a water/glycerine solution; the viscosity, μ, is taken to be 0.4 kg/(m*s) and the density, r, is 1.247 kg/($m^3$). The flow condition in the static mixer can be represented by the static mixer Reynolds number, $\mathrm{Re}_{SM}$, which as customary is computed according to:

$$\mathrm{Re}_{SM} = \frac{r \langle v_x \rangle D_t}{m}$$

Subsequently, results at different inlet velocity conditions are reported in terms of this dimensionless parameter. Here, $\langle v_x \rangle$ is the mean axial velocity and the various Reynolds numbers are simulated by altering this value.

### *Validation of Results by Pressure Drop Measurements*

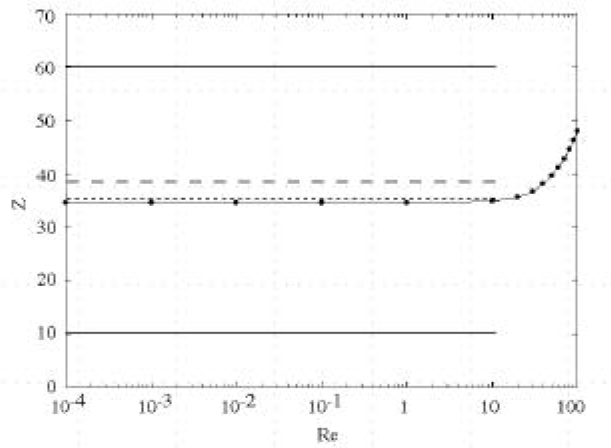
For the system examined here, comparison of numerical and experimental results for pressure drop comprise a vital element of validation because direct comparison of velocity vectors is extremely difficult due to a dearth of experimental information. Experimental measurement of planar velocity components in the SMX mixer is further hindered by the complex geometry of the device. For each flow condition, the average pressure is computed at 10,000 uniformly distributed points on an axial cross-section 1 mm upstream of the first mixer element and on a plane 1 mm downstream of the fourth mixer element. The pressure drop for each flow field is simply defined as the difference between the average values at these two axial positions.

The pressure drop across the mixer elements increases with increasing $\mathrm{Re}_{SM}$. For $\mathrm{Re}_{SM} < 10$, the pressure drop is linearly proportional to the Reynolds number. However, this relationship becomes nonlinear once $\mathrm{Re}_{SM}$ exceeds 10. The increase in pressure that occurs when mixer elements are inserted in a tube to enhance mixing is measured by a parameter called the Z factor. This is the ratio of the pressure drop in the static mixer to the pressure drop in an open tube:

$$Z = \frac{\Delta P_{SM}}{\Delta P_{OT}}$$

Here, $DP_{SM}$ is the pressure drop across the four static mixer elements and $DP_{OT}$ is the pressure drop for a flow in a pipe for equivalent conditions.

The Z factor is virtually independent of Reynolds number for $\mathrm{Re}_{SM} = 10$ but Z increases nonlinearly with increasing Reynolds number for $\mathrm{Re}_{SM} = 10$ in the SMX mixer. Many of the experimental results for Z available in the literature apply only to cases in which $\mathrm{Re}_{SM}$ £10 and under these conditions, inertial effects are insignificant. In Figure 2, simulation results for the Z factor are compared with the manufacturer's data. To compute the Z factor based on the simulation results, the open tube pressure drop was calculated from the analytical flow solution. The calculated Z factors are 34.6 for all Reynolds numbers inclusive of 1 and increase beyond that, reaching a value of 48.0 for $Re_{SM}$ = 100. The manufacturer's data from Koch-Glitsch indicate that Z = 35 for $Re_{SM}$ < 10 for this equipment and the current numerical results deviate by only 1.4%. Other researchers have reported experimental values of the Z factor between 10 and 60 (Pahl and Muschelknautz, 1982) and 38.7 (Alloca, 1982).



The Reynolds number is a dimensionless measure of flow conditions. If glycerine, a viscous fluid is processed in the device, a value of Re=100 corresponds to a flowrate of 1.94 L/s.

**Figure 2.**
**Experimental and computational values of the pressure drop in an SMX static mixer. (●) the computational values as a function of Reynolds number are compared with manufacturer data (– ––) and to results obtained by other researchers: (—–—) Alloca, 1982; (——) Pahl and Muschelknautz, 1982.The pressure drop is normalized by the pressure drop in an equivalent-size empty tube at the same flowrate, showing the increase due to the insertion of mixing elements in the tube.**

### *Mixing of equal volumes of fluids*

Industrial applications of the SMX static mixer include the blending of two fluids that possess similar fluid properties. Such a scenario may exist when trying to blend differently colored pigments, for instance. To examine the mixing of two similar fluids, one stream is dyed red and the other blue. Initially, the interface between the two fluids, the inter-material contact area, occurs at the center of the mixer along the pipe diameter. The local micro-mixing intensity can be measured by the increase in the inter-material contact area.

Results for Reynolds number of 1 are shown in Figure 3. Illustrations correspond to cross-sections at the end of 0.25, 0.5, 0.75, 1.0, 1.5, and 2.0 mixer elements shown in Figures (3a) through (3f) respectively. By the end of 0.25 mixer elements the interface between the red and blue tracers has increased significantly. At this point, 'spade-like' structures of blue tracer extend into the originally red area and vice-versa. Similar structures exist at the end of 0.5 mixer elements (Figure (3b)). However, the 'spade-like' structures are now more elongated than in (Figure 3a) and tracer particles of both colors span most of the pipe diameter in the direction normal to the initial interface. More complex structures are created as the fluid streams are split by the mixer blades in the second half of the first element, as shown for the end of 0.75 mixer elements (Figure 3c) and at the end of the first mixer element (3d). By the end of 1.5 mixer elements (Figure 3e), a layered structure similar to that after 0.5 mixer elements (Figure 3b) exists, except that at this point a greater number of fluid layers exists. However, the local orientations of the boundary between the red and blue tracer particles are identical (after a 90° rotation) at both of these cross-sections. Such self-similarity is a fingerprint of chaotic mixing behavior that has never before been identified in the SMX static mixer. By the end of two mixer elements (Figure 3f), numerous alternating layers of red and blue tracer exist as a result of the stretching and folding during the mixing process.

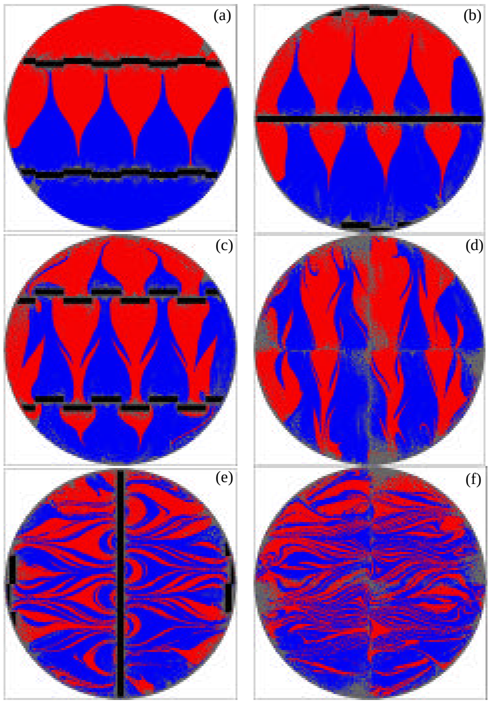


**Figure 3. Mixing patterns generated by Reynolds number 1 flow in the SMX static mixer are shown at the end of 0.25 (a), 0.50 (b), 0.75 (c), 1.00 (d), 1.50 (e) and 2.00 (f) mixer elements. The cross-sectional view of the mixer is seen as a circle with parts of the impeller blades in the plane colored in black. (From Zalc 2000)**

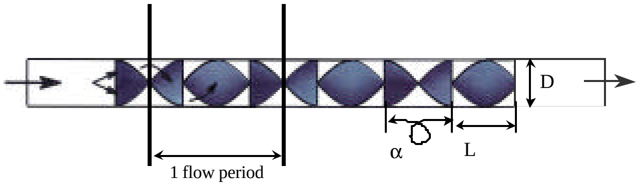
### *Discussion*

The objective was to assess flow and mixing characteristics of the SMX mixer at low and moderate Reynolds numbers. For that purpose, numerical simulations with the ORCA CFD package were conducted in a very fine (>3.5 million tetrahedra), unstructured mesh. Each simulated flow field converged within 1 hour of CPU time, where the residuals in velocity and pressure decreased below $10^{-4.}$ Results for laminar flow were presented for multiple flow conditions, and the computational results for the pressure drop factor, Z, agree very well (< 1.5 % difference) with experimental data from the manufacturer. The flow appears to be essentially independent of Re for Re = 1, while substantial deviations occur at increasingly higher Reynolds numbers, where inertial forces are significant.

The distributive mixing performance of the SMX was described for two fluid streams with equal volume, and the evolving pattern of striations revealed a self-similar mixing process. The mixing rate, based on the relative standard deviation, was computed and compared with experimental data in a six-element SMX. Excellent agreement is obtained between the computational and experimental data set for a 10% centerline injection. The exponential decrease of the relative standard deviation at three different flow rates is further evidence for the existence of chaotic flow and mixing in this static mixer. Furthermore, a trend of decreasing rates of relative standard deviation with increasing flow rate in the SMX was observed, suggesting that lower flow rates produce more effective mixing at more modest energy cost. Thus, the lowest practical flow rates are recommended for use in viscous mixing applications.

## III. Validation for Flow and Mixing in a Kenics Static Mixer

Fluid flow and mixing in the Kenics mixer, a static mixer geometry designed by Chemineer®, is examined here. Static mixers generally consist of a series of mixing elements, which are inserted in a pipe with a specific degree of rotation between successive elements. The Kenics mixer is comprised of helix-shaped, twisted elements that are arranged with a $90^{o}$ rotation with respect to one another. Each element in the standard design has a twist angle of 180o and a length to diameter ratio of 1.5 (Figure 4).



Some Important Geometric Features:
2 mixer elements = 1 flow period
Element length to diameter ratio = L/D
Twist angle per element = a

**Figure 4.**
**Geometry of a six-element Kenics static mixer. The element length-to-diameter ratio (L/D) is 1.5 and the twist angle is 180 degrees in the standard design.**

The mixing action in static mixers is accomplished by the periodic cutting and reorientation of fluid elements . The energy derived from fluid pressure drop across the inlet and outlet regions is utilized to create flow, as opposed to mechanical agitation. This is advantageous in processes where cleaning and maintenance is significant. Beyond heat and mass transfer applications, polymer processing, or distributing additives in fluids with high viscosity ratios, static mixers have been also employed in fermentations and bioprocesses, which are traditionally associated with stirred tank reactors (Junker 1994). The absence of moving agitators can be beneficial when shear damage of the mixture components is a concern.

Numerous designs on the market for static mixers depend on the particular supplier. The most common geometries include the Koch-Sulzer SMX and SMV mixer, the Lightnin Inliner mixer for turbulent flows, and the Kenics static mixer by Chemineer Inc. Due to the variety in geometric construction and the long list of design parameters, equipment selection, sizing and scale-up is just as difficult for static mixers as for more traditional impeller-agitated mixing tanks. A limited number of predictive methods are available for a limited range of operating conditions and applications, based mainly on statistical correlations; however, process and equipment design is often based on experience and/or trial-error procedures.

Experimental investigations of static mixers have traditionally measured bulk flow properties, such as pressure drops, residence time distributions, and power consumption (Nigam 1985; Pustelnik 1986; Kemblowski 1988; Naumann 1991). Non-intrusive flow visualization in these devices is often difficult as a result of their complex geometry. One intrusive optical method developed for static mixers is based on flowing a suspension of particles through the device, which are then illuminated by a laser beam and photographed at the exit (Jaffer 1998).

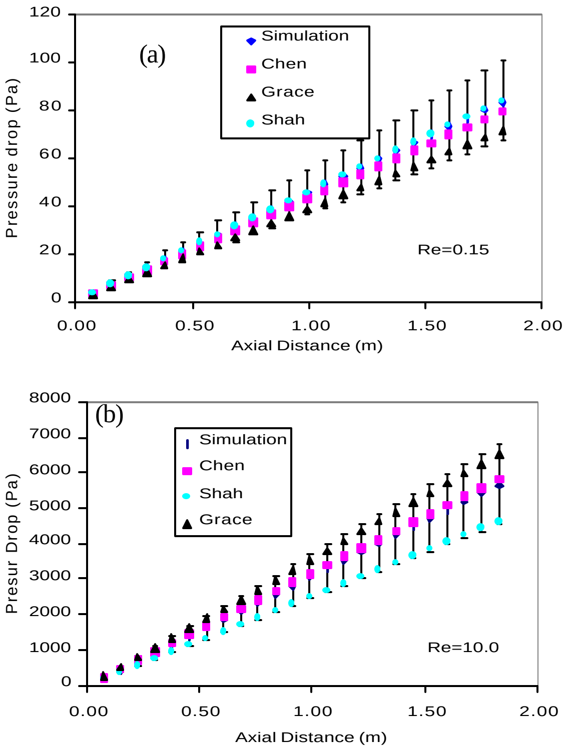
### *Pressure Drop Calculations*

This example illustrates relevant characteristics of flow and mixing analyzed in a 24 element standard Kenics static mixer using Newtonian fluids.. In most three-dimensional flows, fully 3D simulations are necessary to enforce mass and momentum conservation, and consequently the computational meshes are detailed and extensive. A 24-element

Kenics mixer geometry was modeled with 6.11 million tetrahedral elements and 1.85 million nodes. The velocity and pressure solutions, from the ORCA CFD package, converged just under 1 hr of CPU time, using 1.44 GB memory. Velocity/pressure data was obtained at a low (Re = 0.15) and at a moderate flowrate (Re = 10.0), both well within the laminar flow regime.

To assess the validity of the simulations, the pressure drop computed by ORCA is compared with pressure drop correlations from published experimental data. Because of the additional obstruction in the path of the flowing fluid, a greater pressure drop is needed to maintain the same flowrate when mixer elements are inserted in a pipe. The increase in pressure drop is measured in terms of the Z factor described in the introduction.

The available experimental correlations contain significant variability, partially due to slight differences in geometry, different measurement locations, or variations in the methods for correlating the data. Despite the slight differences, the computed pressure drop compares well with numerous experimental correlations. In Figure 5, the pressure drop in the Kenics mixer as a function of axial length is examined at two flowrates: (a) at an average velocity of 0.0012 m/s and (b) 0.38 m/s. $\mathrm{DP}_{SM}$ after each mixer element was computed as an average of 1000 measurements. Despite the variability, the simulation data falls within the range of values predicted by other researchers for the two flow conditions considered.



**Simulations:** ◆

**Experimental data from correlations:**

**(1)○ Shah & Kale; (1991)** **(2)● Wilkinson & Cliff; (1977)**

**(3)■ Chen; (1973)** **(4)▲ Grace; (1971)**

**Figure 5.**
**Pressure drop across a 24 element Kenics mixer compared to experimental data from various researchers. Two different flowrates are considered: (a) low flowrate, viscous effects only (b) moderate flowrate, where inertial effects are also important.**

### *Stretching*

Mixing of different fluids is achieved by increasing the contact area between the mixture components. Material and energy is transported across that interface, which is known as intermaterial contact area. The deformation and folding of this interface can be related to its length increase, or stretching. The stretching field, which describes the amount of interfacial area in each region of the flow, measures local mixing intensities. For practical applications, the stretching field is a sound indicator for good or poor injection locations when dispersing additives. Material injected to areas of high stretching will spread much faster and more uniformly throughout the mixer than material injected into a low stretching region. If reactive materials are mixed, spatial non-uniformities in reaction rates or selectivity can also be foreseen by examining the stretching field. A non-uniform stretching distribution indicates that different portions of fluid experience varying extents of mixing at the same time. Areas in low stretching regions contain little interfacial area, and therefore diffusion in those regions is significantly slow-

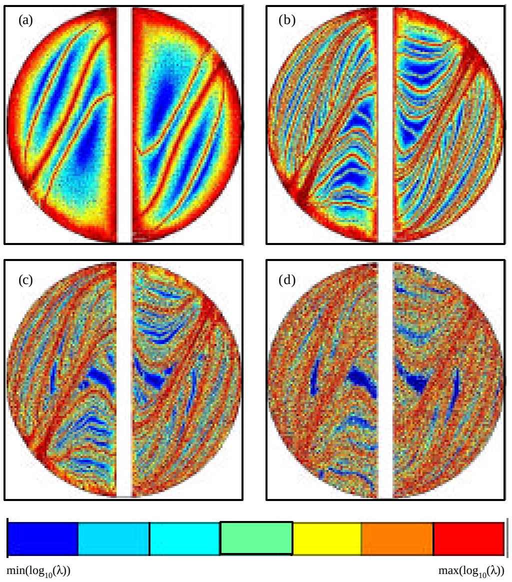


**Figure 6.**
**Contours of the stretching field in the standard Kenics mixer at a moderate flow rate (an average downstream velocity of 0.176 m/s). The cross-sectional planes correspond to axial distances after (a) 2 (b) 6 (c) 10 (d) 22 mixer elements.**

er. The spatial variations in interfacial area and in reactant concentration ultimately reflect in non-uniform reaction rates and selectivities.

Figures 6a-d depicts the cross-sections of the Kenics mixer at four downstream positions: after 2, 6, 10 and 22 elements. The cross-section of the tube appears as a circle and each mixer element appears as a line along the tube diameter. The amount of stretching that each fluid particle experiences is color-coded based upon magnitude.
Red represents areas that experience high stretching (i.e. mix rapidly) and blue represents slowly mixing areas in the device. It is immediately apparent that a spectrum of mixing intensities occurs at each downstream location. A pattern of well-mixing and slow-mixing areas emerges in the Kenics as a function of mixer elements. Materials injected in the blue regions remain separated from the rest of the mixture. Comparison of the four different locations reveals that the field of mixing intensities forms a self-similar pattern. The general features appear early and new details, folds, and filaments are added after each subsequent element. However, the overall appearance remains unchanged. Thus, the non-uniform mixing intensities (the definite pattern of multiple colors) represent a permanent feature of the flow, and will not diminish over time.

### *Relative Standard Deviation*

One frequently encountered application for static mixers involves blending a small amount of material as an additive into the main fluid component in a process. Examples of this application include blending a flavoring substance into syrup, mixing a coloring material into a batch during the manufacturing process of a polymer, or neutralizing a stream of acidic waste material by adding base to it before disposal. Non-uniform mixing can have undesirable effects on the process in all of these cases, with consequences ranging from the creation of a non-uniform product, as in the first two examples, to having unreacted waste material that cannot be removed, as in the last example.

To examine the mixing process, passive, colored tracers were injected at the inlet of the Kenics and their position followed in time ($\underline{x}$) by integrating along the velocity field: $d\underline{x}/dt = \underline{v}$. The passive tracers follow the motion of the fluid closely without altering the flow field. An injection of 10% by volume of dark-colored tracers is simulated to match available experimental data. 200,000 particles are placed at the centerline of the mixer for each simulation and their positions are recorded after 4, 8 12, 16 and 20 mixer elements (Figure 7). The dye forms thinner and thinner striations as it spreads through the mixer and the mixture appears to be nearly homogeneous after 20 Kenics elements.

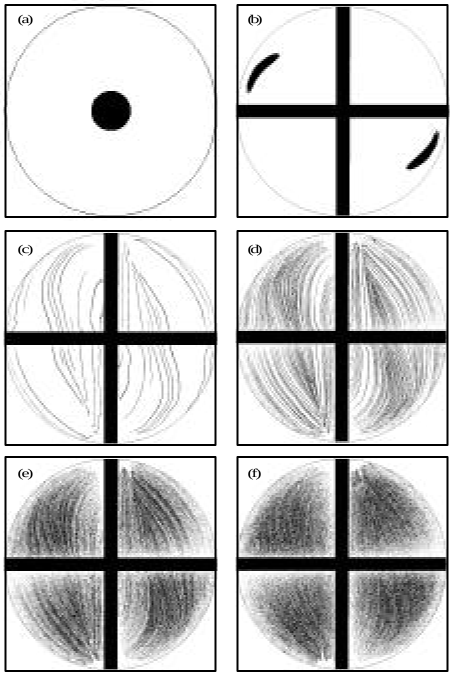


**Figure 7.**
**Tracer spreading in the standard 24 element Kenics: (a)-(f) Inlet condition and after 4, 8, 12, 16, and 20 elements.**

Building on the intensity of segregation concept (Danckwertz, 1952), the homogeneity of the system can be assessed based on statistical analysis of samples from the mixture. One such statistical method involves computing the decrease in the relative standard deviation (rsd). In short, this measures the size the light/dark striations of material in the mixture at a given time. Experimental methods can measure the quality of a mixture in a similar manner, and can be used to directly compare the simulated mixing process to physical experiments.

The relative standard deviation (rsd) at each axial cross-section is computed as:

$$\text{rsd} = \sqrt{\frac{\left(\sigma_N^2 - \sigma_\infty^2\right)}{\overline{N}^2}} \qquad \text{where} \qquad s_N = \sqrt{\frac{\sum_{i=1}^{\text{ncells}}\left(N_i - \overline{N}\right)^2}{\text{ncells} - 1}}$$

Here, $s_{¥}$ represents the residual value of the number-based standard deviation at the end of ten mixer elements, $N_i$ is defined as the amount of one-color dye in each sample *i*, and N is the overall average amount of dye in the system. Smaller values of rsd indicate that the mixture becomes increasingly homogeneous. In an ideal situation, the amount of dark dye in each mixture would correspond to the average in the total amount processed.

Figure 8 reveals the comparison between experimentally measured values of rsd and values computed from tracer spreading simulations. Both the experimental data (by Pahl and Muschelknautz, 1982) and the simulated data were fitted by regression. A logarithmic scale is most appropriate for rsd as a function of axial distance, because chaotic flows, such as flow in the Kenics, produce exponentially decaying values. Comparing the slope of the curves shows that the experimental mixing rate is nearly identical to the computed rate (experimental mixing rate = 0.159 and simulated mixing rate = 0.163).

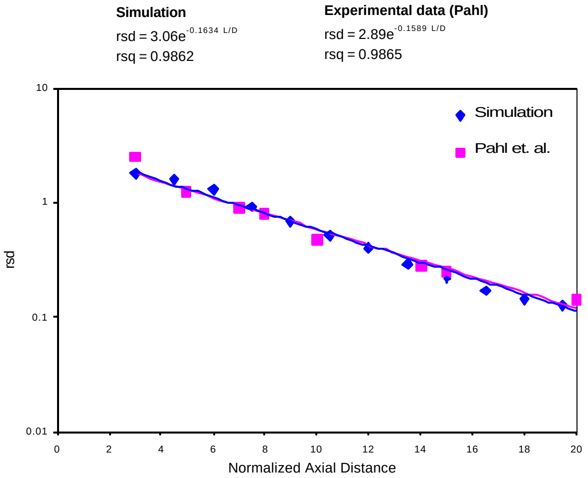


**Figure 8.**
**The relative standard deviation (rsd) compared to experimental data in a standard Kenics static mixer at Re = 0.15.**

When each sample from the mixture has a variation of less than 5 % (i.e. rsd < 0.05), the commonly used arbitrary definition of a "well-mixed" stream has been satisfied. The number of mixer elements needed to reach that state can be set as a process requirement in a particular application. Both the simulations and the experiments for the Kenics at this flow rate predict a total of 25 elements.

### *Discussion*

The Kenics static mixer was the subject of a computational analysis using the ORCA software package. Despite significant variability in the available experimental data, the computed pressure drop compares well with numerous experimental correlations. The pressure drops obtained from ORCA fall well within the range of values predicted by other researchers for the two flow conditions considered.

The mixing performance was examined in the standard geometry (L/D = 1.5 and twist angle = $180^{\circ}$) by computing the spectrum of mixing intensities at various axial locations. Segregated zones appeared in the flow, where mixing is very slow. These regions represent significant barriers to mixing, because materials can only enter or leave these regions by painfully slow diffusion. The range of mixing intensities created by the flow converged to a self-similar distribution, which remained highly non-uniform for the entire length of the device. This observation directly impacts processes, where additives or reactants are distributed in the bulk fluid during the mixing process. Selecting the proper injection location is crucial, because the mixing rate can be several orders of magnitude less in some locations, retarding reaction rates and product selectivity.

Tracer mixing patterns were also computed using post-processing algorithms in ORCA based upon a 10% by volume dye injection along the center of the mixer housing. This initial condition was chosen to match a set of experiments conducted by other researchers. The mixture was sampled at multiple axial distances and compared to the experimental data. The two methods predicted essentially the same mixing rate, establishing confidence in the computational techniques.

## IV. Conclusions

Computational fluid dynamics (CFD) is an alternative technique to traditional experimental methods for accelerating equipment design and gaining additional fundamental understanding of mixing processes. Experimental validation is needed before one can rely mostly on computational tools. However, evaluating design parameters, such as flow rate or geometry, becomes a reasonably simple task once the techniques are developed.

The ORCA CFD package is accurate within experimental variation for both the SMX and Kenics mixers. As computational power increases, solution times will decrease and the capacity to solve more complex problems will become possible. This will enable the design of complex systems of inline mixers and will allow the optimization of residence time, pressure drop and blend time. The CFD is an excellent tool for engineering design and optimization work and will help reduce inconsistency in products, reduce change over time, and improve productivity.

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