# Turbulence in Flocculators: Comparison of Measurements and CFD Simulations

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Researchers have shown a different equilibrium floc-size distribution with increasing tank size when the unit mass energy dissipation rate ($\bar{\epsilon}$) = constant (Oldshue and Mady, 1978; Ducoste and Clark, 1998a,b). Further, researchers have also observed changes in flocculation performance using different kinds of mixing impellers when $\bar{\epsilon}$ = constant (Ducoste and Clark, 1998a,b). Ducoste and Clark showed that accurate models of coagulation kinetics must not only include $\bar{\epsilon}$, but also must include information on the frequency of passage of floc through the impeller region and the rms velocity fluctuations in the anisotropic impeller region. Hence, there is growing evidence that a complex relationship exists between particle agglomeration/breakup and the fluid mechanics generated in flocculation reactors that cannot be fully parameterized by $\bar{\epsilon}$ alone.

A previous article (Ducoste et al., 1997) showed that the measured turbulence in square flocculation reactors is both scale- and impeller-geometry-dependent (when $\bar{\epsilon}$ = constant). These results help explain the variation in flocculation performance in different scale systems or in same scale systems with different impeller geometries. However, the experimental methods used to measure the fluid mechanics require sophisticated and expensive equipment and a dedicated laboratory.

In recent years, major advances in computer technology and computational mechanics have made it possible to use computational fluid dynamics (CFD) to analyze flows. The intent of this study was to evaluate the effectiveness of a commercial CFD code in modeling flocculator fluid mechanics.

## Finite Element Formulation and Boundary Conditions

A general purpose CFD code called FIDAP (Fluid Dynamics International, Evanston, IL) was used in this study. It is a finite-element code based on the Galerkin method of weighted residuals. The model is based on a simple geometric representation of a submerged mixing impeller in a square-stirred reactor. The impeller was modeled as a cylinder whose diameter and height matched that of the Rushton turbine or A310 foil impeller. Due to its complexity, a free surface was not included. The free surface was approximated as a free-slip wall boundary. Reactor sizes of 5- and 28-L were modeled with both the Rushton turbine and A310 foil impeller.

The Rushton turbine and A310 fluid foil impellers generate a complex, three-dimensional turbulent flow field in a square reactor. A two-equation $k$-$\epsilon$ turbulence model was used to describe the transport of the kinetic energy and the length scale of the large energy containing eddies throughout the stirred reactor. Other transport models (that is, zero-equation or one-equation mixing-length models) are not capable of modeling the wide range of length scales found in stirred reactors. A description of the $k$-$\epsilon$ model is described by others (Rodi, 1984).

Dirichlet boundary conditions for velocity $k$ and $\epsilon$ were established for the Rushton turbine and the A310 foil impellers using the LDV measurements (Ducoste et al., 1997). For the radial flow Rushton turbine, a polynomial reconstruction of the measured mean radial and tangential velocities was used with radial and tangential components originating from the cylindrical impeller region. In the case of the axial flow A310 foil impeller, a polynomial reconstruction of the axial velocity component from the LDV measurements in the impeller region was used. In all the simulations, the fluid properties (viscosity, density) were defined at a temperature of 20°C. All solid surfaces were assumed to have no-slip velocity boundary conditions. The turbulent boundary conditions for the Rushton turbine and the A310 foil impeller were set using a polynomial reconstruction of the kinetic energy and energy dissipation rate profiles from the LDV experiments.

For the two reactors mixed with the A310 impeller, 18,880 elements were used to discretize the flow domain in the 5-L

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square reactor, and 108,072 elements were used to discretize the 28-L reactor. To discretize the flow domain in the 5- and 28-L square reactors mixed with the Rushton turbines, 22,640 and 139,032 elements were used, respectively. More elements were required for the larger reactor size to maintain an equivalent average mesh density between the 5-L and 28-L reactor. The average mesh size was fine enough to produce a grid independent solution of the mean and turbulent flow fields. A higher local mesh density was used in the impeller discharge zone to permit resolution of the turbulence field in the impeller region.

## Results

### *Mean velocity flow pattern*

FIDAP predicts the four-quadrant circulation pattern indicative of a Rushton turbine (Oldshue, 1983). The model predicted the location of the center of the circulation in the bottom right quadrant at $r/R = 2.0$ and $z/R = 1.8$. The radial location of the circulation center is in good agreement with the LDV results in the previous article. The vertical location was slightly higher than the value found experimentally (experimental $z/R = 1.5$). However, insufficient resolution in the experimental measurement points in the vertical direction may cause inaccuracies in determining the actual location of the circulation center. A very similar fluid velocity pattern was found in the 28L reactor. As in the experimental study, the model results showed that the mean velocity was proportional to the tip speed, regardless of reactor size.

Figure 1 displays the mean velocity pattern for the A310 fluid impeller in the 5-L reactor. This flow pattern is not typical of axial flow patterns found in studies of cylindrical reactors (Oldshue, 1983). So, the patterns shown in Figure 1 are apparently characteristic of flows generated by axial flow impellers in square reactors. In the plane perpendicular to the reactor wall, the mean velocity flow pattern seems to indicate circulation only in the bottom half of the reactor. A similar result was also found in the LDV experimental results (Ducoste et al., 1997). Figure 2 displays the mean velocity pattern in the plane that bisects the 5-L reactor corner (a region not studied in the work of Ducoste et al., 1997). Here, the fluid flow circulates in the reactor corners and seems to feed the upper part of the square reactor. Ducoste et al. (1997) reasoned that in order to satisfy continuity, the fluid flow from the reactor corners must be feeding the top of the reactor. The results from FIDAP validate this speculation. Parallel results were found in the 28-L reactor.

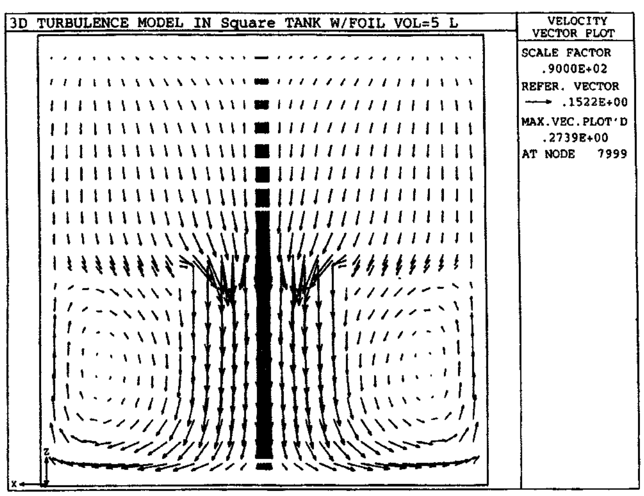


**Figure 1. FIDAP mean velocity flow pattern for the A310 foil impeller in the plane perpendicular to reactor wall $T = 5$L.**

Vectors are nondimensionalized with tip speed; tip speed = 57.85 cm/s.

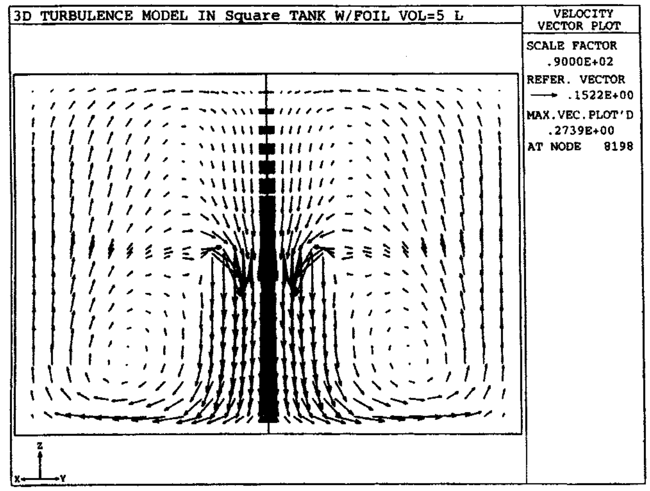


**Figure 2. FIDAP mean velocity flow pattern for the A310 foil impeller in the plane bisecting the reactor corners $T = 5$L.**

Vectors are nondimensionalized with tip speed; tip speed = 57.85 cm/s.

### *Turbulent energy dissipation rate*

Figures 3 and 4 compare the local energy dissipation values between the model and experiments for the Rushton turbine in the impeller discharge zone for the 5- and 28-L reactors. In the impeller discharge region, the model overpredicted the local energy dissipation rate values at points closest to the Rushton blade tip, and slightly underpredicted these values at points further away from the impeller blade tip. In the 28-L reactor, the model also overpredicted the local energy dissipation rate in the region closest to the blade tip ($r/R = 1.1$, 1.444). The model seemed to do a better job of predicting the local energy dissipation rate in the rest of the impeller discharge region of the 28-L reactor. However, the model did not match the experimental results exactly. The inability of FIDAP to predict the local energy dissipation produced by the Rushton turbine might be due to the existence of vortices trailing the impeller blades.

Figure 5 compares simulated and measured local energy dissipation rates for the A310 foil impeller in the 28-L reactor. Here FIDAP does not seem to accurately predict the local energy dissipation rate. In the lower part of the reactor, the model overpredicts the experimental values of the local energy dissipation rate in the impeller discharge region ($r/R$

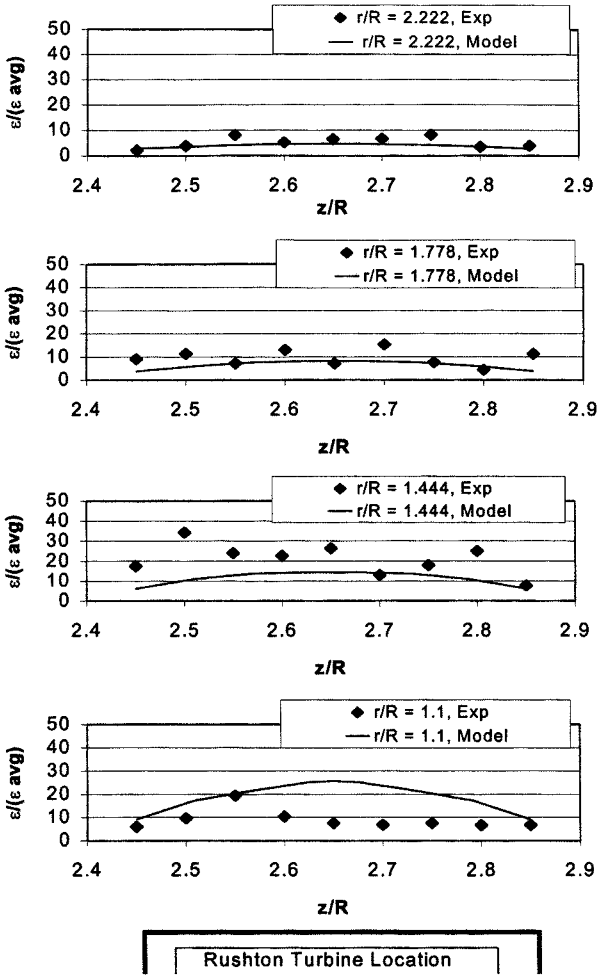


**Figure 3. Turbulent energy dissipation rate for the Rushton turbine: comparison between FIDAP model and experimental results in the impeller discharge zone $T = 5$L, $\epsilon$ avg. = 0.0016 m²/s³.**

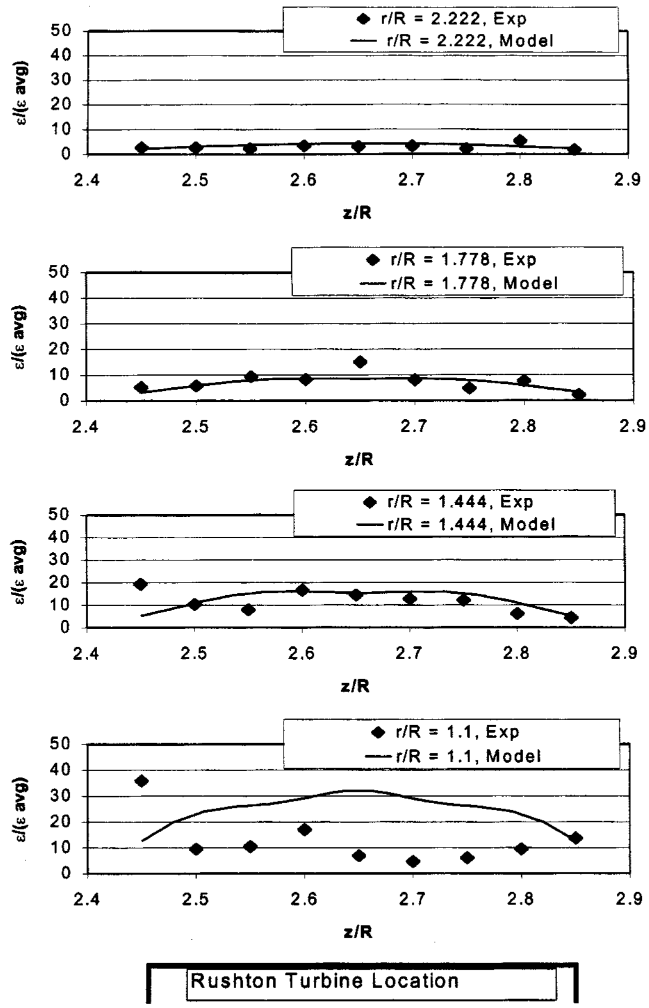


**Figure 4. Turbulent energy dissipation rate for the Rushton turbine: comparison between FIDAP model and experimental results in the impeller discharge region, $T = 28$ L, $\epsilon$ avg. = 0.0016 m²/s³.**

$= 0.2 \rightarrow 1.0$, Figure 5). Figure 5 also shows that the model tends to underpredict the local energy dissipation rate between $r/R = 1.25$–$2.25$. The inability of the model to exactly match the measured energy dissipation rate might be due to improper boundary conditions or limitations of the $k$-$\epsilon$ turbulence model.

## Discussion

The CFD simulations of the Rushton turbine and A310 foil impellers in square reactors were able to replicate qualitatively the spatial variation turbulent flow. Mean circulation patterns were verified. Many researchers have applied the $k$-$\epsilon$ model to simulate the flow pattern and turbulence produced in a stirred vessel (Middleton et al., 1986; Renade and Joshi, 1990; Kresta and Wood, 1991; Luo et al., 1993; Armenante and Chou, 1996). For the most part, reasonable agreement between experimental results and CFD simulations have been found by most researchers in the bulk region with slight variation in the turbulent results in the impeller discharge region.

FIDAP did not accurately match the experimental results for energy dissipation rate in the Rushton reactor. In the impeller discharge region, the model overpredicted energy dissipation at $r/R = 1.1$ and underpredicted dissipation values at $r/R = 1.444$, 1.778, and 2.222. Two possible reasons for the lack of agreement:

(1) As Ducoste et al. (1997) and Van der Molen and Van Maanen (1978) suggested, the local energy dissipation rates are influenced by the energy contained in the trailing vortices. Since trailing vortices were not modeled with FIDAP, the simulations would tend to underpredict the experimental energy dissipation rate values.

(2) The method used to calculate $\epsilon$ from the experimental results is not accurate at the turbulence intensities typically found in stirred reactors.

The first explanation focuses on the possible importance of energy transfer from the trailing vortices to the small-scale

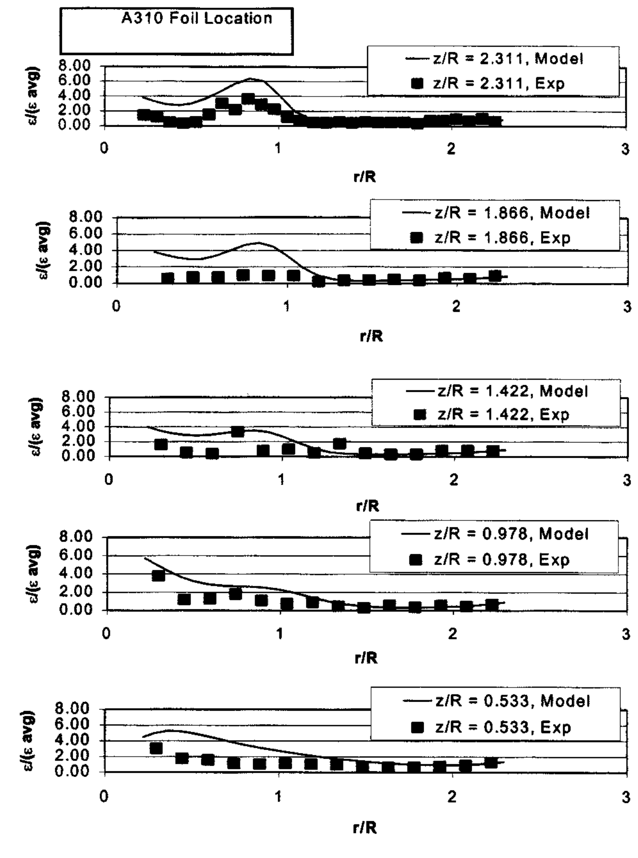


**Figure 5. Turbulent energy dissipation rate for the A310 foil impeller: comparison between FIDAP model and experimental results in the impeller discharge zone $T = 28L$, $\epsilon$ avg. = 0.0016 $m^2/s^3$.**

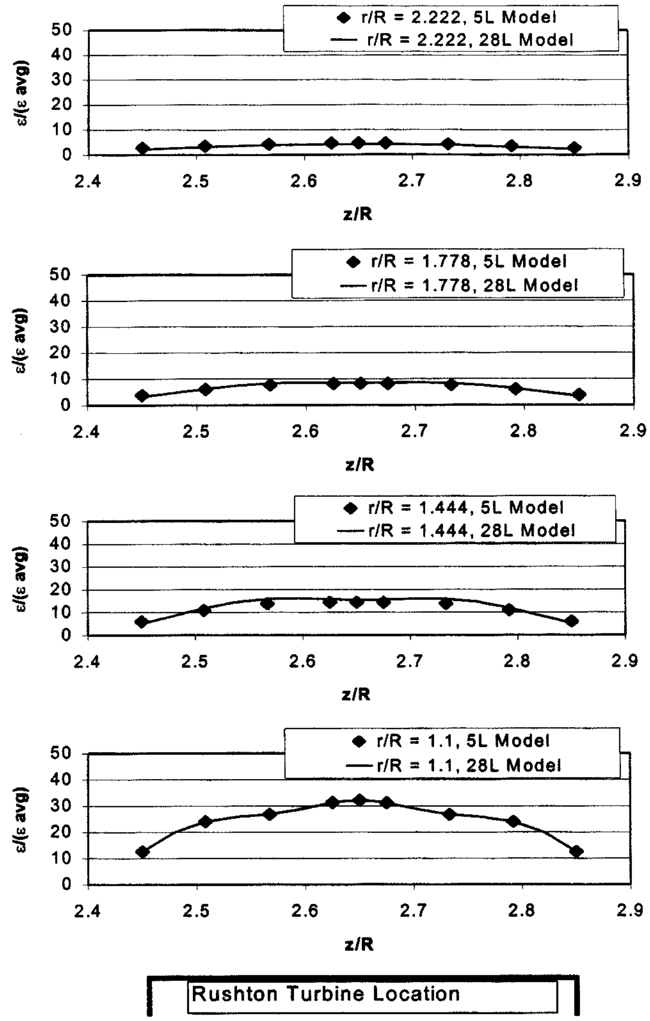


**Figure 6. Turbulent energy dissipation rate for the Rushton turbine: comparison between 5L and 28L FIDAP models.**

eddies. Ducoste et al. (1997) speculated that the reduction in the local energy dissipation rate values with increasing reactor size is due to a decreasing energy contribution from the trailing vortices to the small-scale eddies at the measured locations. If there were no trailing vortices in the flow domain, then the local energy dissipation rate would not be a function of reactor size since the power per unit volume is constant with reactor size. Therefore, if we compare the FIDAP results for local energy dissipation rates in the 5- and the 28-L reactors and observe no difference between the two simulations, then the assumption that the trailing vortices influence the rate of energy dissipation at the small-scale eddies may be plausible. As seen in Figure 6, the FIDAP model predicts no significant change in the local energy dissipation rate with reactor size.

The second explanation is based on the fact that indirect methods are always used to estimate dissipation, and these methods might be in error under certain circumstances. One question is whether Taylor's frozen field hypothesis is valid in the reactors studied. Taylor's hypothesis states that the velocity fluctuations at a fixed point in a homogeneous turbulent flow with a constant mean velocity in one direction may behave as if the whole turbulent flow field passes that point with a constant mean velocity. However, Taylor (1938) proposed this hypothesis for a case in which the magnitude of the turbulent fluctuating velocity was 5% of the mean velocity. In reactors mixed with impellers, the fluctuating velocity can be as much as 50% of the mean velocity (Weetman and Oldshue, 1988). Under these conditions, Taylor's hypothesis may not be valid. Unfortunately, there is currently little alternative to Taylor's hypothesis.

Overall, CFD qualitatively confirmed results from the experimental study, demonstrating that constant $\bar{\epsilon}$ does not ensure the same turbulence characteristics in different scale systems or in same scale systems with different impeller geometries. Finally, it should be pointed out that the CFD simulations were quite useful in understanding the complex flow generated by rotating impellers in square tanks. Although experimental studies cannot in general be replaced (and in fact, were required in this work to establish the impeller boundary conditions), the time and expense of experiments needs to be considered in light of the accessibility of efficient and general CFD codes, and fast workstations.

## Acknowledgments

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