CHAPTER 4

CFD ANALYSIS OF THE MIXER

This section presents CFD results for the venturi-jet mixer and compares the predicted mixing pattern with the present experimental results and correlation results with injection angle $\theta$ between $45^\circ$ and $135^\circ$. Full fledged numerical simulations for quality of mixing process of two liquid streams at required proportions in venturi-jet mixer have not been reported in the literature.

Mixing of passive scalars such as heat or contaminants, is one of the significant features of the turbulent jet mixing that can be found in many practical applications. The turbulent flow simulation using a standard two-equation $k-\varepsilon$ model for venturi-jet mixer with different jet injection angles $45^\circ$, $60^\circ$, $90^\circ$, $120^\circ$ and $145^\circ$, each with Reynolds number 31917, 38301, 44684, 51068 and 57451 is carried out in this chapter.

The governing conservation equations are solved using finite volume schemes available in FLUENT [Fluent software]. This study employs the mixing model of two turbulent miscible fluids with the same viscosity and density and different tracer concentrations as such mixing is applied in mixing of water with fibre in paper industry and water with fertilizer in agricultural industry.

In the numerical investigation of turbulent mixing, it is necessary to predict the turbulent intensity, and pressure, velocity and concentration field,
simultaneously since the mixing process can be described as the interaction between a velocity and concentration field (Boersma et al. 1998).

Mixer design is slowly changing from being a complete experimental process to a partially numerical and experimental one. Numerical simulation has an advantage that analysis and optimization can be done before the device is built. Consequently, the design of new mixing devices becomes less expensive and at the same time faster.

Recently, some numerical studies have been performed on two- or three-dimensional turbulent mixing with mass or heat transfer for simple geometries (Monclova and Forney 1995). There have been several previous efforts to model the flow in transverse mixers using CFD.

Xiaodong et al. (1999) used a commercial CFD code to analyse the mixing performance of transverse mixers that was used in a silo unit for the mixing of fibre with water. Some of the recent advances in applying CFD techniques to the chemical process industry are documented by Shanley (1996).

However, very few studies are available for dealing with complex three-dimensional turbulent simulation with mass transfer (Xiaodong Wang et al. 1999).

4.1 NUMERICAL SIMULATION APPROACH

CFD is based on the numerical solutions of the fundamental governing equations of fluid dynamics namely the continuity, momentum and energy equations. Gambit 2.3.16 was used to model and mesh the mixer and Fluent 6.3.26 software package was used for analysis purpose.
The code is used for the modelling of a wide range of industrial problems involving fluid flow, heat transfer (including radiation), mixing of chemical species, multi-step chemistry, two-phase flows, moving/rotating bodies and other complex physics including turbulence flow conditions.

A finite volume, pressure based, fully implicit code solving the 3D Navier-Stokes equations governing fluid flow and associated physics was utilised to accomplish this work. The flow configuration and associated coordinates of the numerically solved venturi-jet mixer using Fluent 6.3.26 are shown in Figure 4.1.

Figure 4.1 Flow configuration and coordinate system used for simulation

The turbulent flow of a homogeneous, viscous, incompressible jet and cross-flow fluids with constant properties were considered for the present study.

The standard k - \( \varepsilon \) model has been used extensively to simulate the turbulent round jets in a crossflow (Launder and Spalding 1974). Patankar et al. (1977), Catalano et al. (1989), Hwang and Chiang (1995), He et al. (1999), and many others have predicted round turbulent jets in a weak and moderate crossflow (\( R < 2 \)) using the standard k - \( \varepsilon \) model.
In the present study a segregated, 3D, incompressible and steady solver is employed for predictions of turbulent jets in a uniform, weak and moderate crossflow in venturi-jet mixer are presented by using the standard $k - \varepsilon$ model. By representing the fluctuating parts in the eddy viscosity $\nu_t$, turbulent kinetic energy $k$, and turbulent dissipation rate $\varepsilon$, mass and momentum conservation equations can be written as (Xiaodong et al. 1999, Launder and Spalding 1974, Wilcox 1994):

$$\frac{\partial \nabla_i}{\partial x_i} = 0 \quad (4.1)$$

$$\frac{\partial \nabla_i}{\partial t} + \nu_j \frac{\partial \nabla_i}{\partial x_j} = \frac{1}{\rho} \frac{\partial \nabla_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu + \nu_t \right) \frac{\partial \nabla_i}{\partial x_j} \quad (4.2)$$

where $\rho$, $\nu$, $\nu_t$, $\nu_i$ and $\nabla$ stand for fluid mass density, kinematic viscosity, eddy viscosity, time-average fluid flow velocity in direction $x_i$, and time average pressure, respectively.

The turbulent quantities $k$ and $\varepsilon$ for the standard $k - \varepsilon$ model are obtained by solving the following transport equations:

$$\frac{\partial k}{\partial t} + \nu_j \frac{\partial k}{\partial x_j} = \frac{1}{\rho} \frac{\partial \nabla_j}{\partial x_j} \left( \nu + \nu_t \right) \frac{\partial k}{\partial x_j} + \nu \frac{\partial k}{\partial x_j} - \frac{k}{\rho} \quad (4.3)$$

$$\frac{\partial \varepsilon}{\partial t} + \nu_j \frac{\partial \varepsilon}{\partial x_j} = \frac{1}{\rho} \frac{\partial \nabla_j}{\partial x_j} \left( \nu + \nu_t \right) \frac{\partial \varepsilon}{\partial x_j} + a_1 \frac{1}{\rho \varepsilon} \nu \frac{\partial \phi}{\partial x_j} - a_2 \frac{1}{\rho \varepsilon} \quad (4.4)$$

where $\phi$ denotes the inner product of velocity strain tensor $2e_{ij}e_{ij}$ with

$$e_{ij} = \frac{\frac{\partial \nabla_i}{\partial x_j} + \frac{\partial \nabla_j}{\partial x_i}}{2} \quad (4.5)$$
And the turbulent time scale $T$ and viscosity $\nu_i$ are expressed as

$$T = \frac{k}{\varepsilon} + \sqrt{\frac{\nu}{\varepsilon}},$$

(4.6)

$$\nu_i = c_\mu kT$$

(4.7)

The terms $a_1$, $a_2$, $\sigma_k$, $\sigma_c$, and $c_\mu$ are constants of the turbulence model. The values of these constants are found elsewhere (Xiaodong et al. 1999). The tracer conservation equation to model the mass transfer phenomena in the turbulent flow can be written as

$$\frac{\partial c}{\partial t} + \sum_j \left( v_j \frac{\partial c}{\partial x_j} \right) = \left( \nu/Sc + \frac{\nu}{\sigma_c} \right) \frac{\partial}{\partial x_j} \left( \frac{\partial c}{\partial x_j} \right)$$

(4.8)

where $c$, $Sc$, and $\sigma_c$ are the time-average concentration of tracer, Schmidt number, and a selected constant.

The values of constants are chosen as $a_1 = 1.44$, $a_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_c = 1.3$, $c_\mu = 0.09$, $Sc = 1.64 \times 10^6$, and $\sigma_c = 0.9$ (Xiaodong et al. 1999). The governing equations – the continuity, momentum, tracer concentration and turbulence closure are formulated in strong conservation form and coupled together using the artificial compressibility method (Chorin 1967).

### 4.2 COMPUTATIONAL DETAILS AND BOUNDARY CONDITIONS

The venturi-jet mixer modelled in this work contains a converging part, a throat and a diverging part. The computational domain further consists of an inlet section and an outlet section of pipe and also inlet section of the jet. These three sections are included to ensure that the inlet and outlet boundary conditions required for the solution of the governing equations do...
not contaminate the computed flow fields in the vicinity of the jet (Jones et al. 2002).

Length of the pipe is designated to be sufficiently long for the crossflow and jet fluid to have fully developed flow condition. The numerical simulations were carried out using the commercial flow solver FLUENT 6.3.26 based on the finite volume method.

The momentum and energy equations were discretized using the second-order upwind scheme and other transport equations were discretized using the power law scheme. The discretized equations were solved using the SIMPLE algorithm.

Similar to the experiment, crossflow fluid properties were set to the physical and thermodynamic properties of water at 303K. Jet fluid with a diffusive species (tracer) was introduced at a concentration of 0.3.

Physical and thermodynamic properties of tracer were also set to water at 303K, and the binary diffusion coefficient of tracer in water was set to $D_{AB} = 2.8 \times 10^{-9} \text{ m}^2\text{s}^{-1}$. No slip wall condition was applied to the walls of the mixer.

At the inlet of the crossflow domain, a uniform velocity profile, hydraulic diameter and the turbulence intensity were specified from a separate calculation for fully developed, turbulent flow in a pipe at each Reynolds number used for the study.

For the jet inlet pipe, a pressure inlet condition was set and outflow condition was set for boundary of exit of the mixer. The implicit and segregated solver was used for the solution of the system of governing
equations. All the variables (u, v, k, and ε) were under-relaxed at each iteration.

The monitored flow parameters were always converged after the sum of the imbalance of the transport equations between iterations for over all cells in the computational domain fell below $10^{-3}$ and normal residual of energy equation was $10^{-6}$. The iterative convergences at every time step are checked and all residuals are dropped below four orders ($10^{-4}$) in 1,200 iterations.

The computations were performed on an Intel Core 2 Duo machine with 2 GB RAM, 2 GHz processor speed. Commercial package Gambit 2.1.6 was used to generate the geometry and mesh for the computational domain.

![Computational mesh](image)

**Figure 4.2 Computational mesh used in the present study (346,000 cells)**

The computational mesh is mainly structured and consists of hexahedral elements shown in Figure 4.2. The use of structured mesh near the jet exit and wake region provides easier handling of variation in mesh size and relatively higher computational efficiency, provided by the finite volume method in FLUENT (Li et al. 2006).
Figure 4.3 Grid dependence test based on turbulent kinetic energy profiles at the jet centre plane (y/d=0) using different grid cells for x/d=2

The number of grid nodes generally depends on the flow configuration and the Reynolds number of the flow (Jones et al. 2002). For studying the grid dependency of the solution, the flow field was obtained with four different grid resolutions. The computational grids of 218,000, 276,400, 313,000 and 346,000 are used to study the grid sensitivity.

The grid dependency is analysed using the profiles of the turbulent kinetic energy at the jet centre plane (y/d = 0) at the location of x/d = 2 for jet injection angle 45° and crossflow Reynolds number 31917 are shown in Figure 4.3. From the results, it is observed that coarse mesh show much deviation as compared to the medium and finer mesh.

However, the predictions with medium and fine grid cells are close to each other. It was concluded to use the fine mesh of size 346,000 for all the cases analysed in the present work. All of the grid parameters including the length of the inlet and outlet pipe sections and the number of grid nodes were chosen after careful numerical experiments.
4.3 RESULTS AND DISCUSSION

In most practical situations, jets and plumes are either discharged vertically or at an angle to a crossflow. In such flow conditions, the jet and crossflow interaction and thermal or concentration spread are extremely important factors.

Accordingly, when the temperature or concentration field is strongly affected by the velocity field and can be regarded as a passive scalar, it is necessary to understand the mean and statistical characteristics of the thermal spread and mixing in such jets in crossflow (Manabendra et al. 2006).

The flow field and concentration profile within venturi-jet mixer for fully developed turbulent, incompressible and steady flow can be obtained with FLUENT solver. If the two components to be mixed have similar rheological properties and the grid resolution is chosen fine enough, the results predict the velocity, pressure and concentration fields within static mixing equipment with high accuracy.

Modern computers allow for simulations with highly resolved grids so that one is able to efficiently and accurately analyze every kind of static mixer using CFD (Fourcade et al. 2001, Liu 2006).

4.3.1 Mixing Performance

The detailed information of the concentration distribution is available for all experiments and simulations. The complexity of the flow inside the venturi-jet mixer makes the mixing analysis extremely difficult. Homogeneity measurements are essential for characterizing the performance of static mixers.
Several techniques are known for the determination of the mixing quality namely: conductivity measurements across the diameter, freezing in the mixture along the mixer tube by using epoxy resins, etc. All these methods aim to get a measurable value for the homogeneity.

Mixture parameter $S_o$, is the common technique, used both numerically and experimentally to analyze mixing. This parameter also provides information on the conveying performance of the mixer and is commonly used to determine if a material will be in the mixer too long for degradation to occur.

In this study, the mixing performance at different cross flow Reynolds number and jet injection angles are quantified by mixture parameter $S_o$. The mixture parameter was calculated from the data at different axial distances $x/d$ (5, 10, 15, 20, 25, 30, 35, 40, and 45) along downstream from the point of injection as (Kok and Vander Wall 1996):

$$S_o = \sqrt{\frac{\sum_{i=1}^{n}(c_i - \overline{c})^2}{(n-1)}}$$ (4.9)

where $\overline{c}$ is the averaged tracer concentration of the calculated region which is defined as $\overline{c} = \sum c_i / n$, $n$ denoting the total number of nodes in the region, and $c_i$ is the nodal tracer concentration. Ideally, in a non-mixing condition, the spatial variance is high and the mixture parameter is also high. For the fully mixed state, the mixer parameter is small.

Figure 4.4 shows the mixture parameter as a function of the inlet flow ratio of jet and crossflow for injection angles of 45°, 60°, 90°, 120° and 135°. In Figure 4.4 the results for the measurements are indicated with different symbols and simulations with different types of lines.
Figure 4.4 Mixing performance ($S_0/x \times 100$) for different injection angles

Figure 4.4 indicates that the mixing parameter decreases with an increasing mixture ratio and increasing injection angle. From Figure 4 it can be concluded that with injection angle greater than 90° cases have better mixing performance as mixture parameter is lower.

Also for all the cases presented the results show a very good comparison of the mixture parameter predicted by simulation and the measured value. This hints at a dependence on the momentum ratio of the jet and the cross flow ($u/v$) and also vortices can exist near the injection point due to the adverse pressure gradient in transverse mixers with right or obtuse injection angles (Xiaodong et al. 1999, Kok and Vander Wall 1996).

The improved mixing with a higher injection angle has the disadvantage of an increased pressure drop. This conclusion correlates with the experimental finding discussed in Chapter 3.

The integrals $\int_A u dA$ and $\int_A u dA$ can be directly related to the volume flow rates and tracer concentration through mass balances. Where $u$ is the
tracer velocity and \(c\) is the tracer concentration in the flow field. The mass conservation laws given by Equations (4.10) and (4.11) are also used to validate the computational results as proposed by Xiaodong et al. (1999).

\[
\int_A u dA = q_{cf} + q_j \quad \text{(4.10)}
\]

\[
\int_A u dA = c_1 q_{cf} + c_2 q_j \quad \text{(4.11)}
\]

where \(q_{cf}\) and \(q_j\) denote the flow rates of the crossflow and jet with tracer concentrations \(c_1\) and \(c_2\), respectively.

Figure 4.5 shows the plot of \(\int_A u dA\) for Re values 58002 and 104404 and the plot of \(\int_A u dA\) for Re values 69603 and 92803. The numerical results are compared with the data derived from the mass conservation laws in Equations (4.10) and (4.11) as shown in Figure 4.5(a-f).

In Figure 4.5, plot \(\int_A u dA\) represents the uniformity of the mixing and the plot \(\int_A u dA\) denotes the average tracer mass flow rate in the mixer from injection point to the exit of the mixer. It is clear from the plot \(\int_A u dA\) in Figure 4.5 that the tracer concentration decreases with increasing \(x/d\). Also Figure 4.5 shows, for mixer with greater than 90° injection the tracer concentration is less at all \(x/d\) distances considered indicating the better mixing than that of the mixers with acute angles. In this case, also it is observed that the velocity field controls the distribution of the concentration field.
Figure 4.5 Tracer mass conservation and mixing uniformity of various venturi-jet mixers (a) - (e): Notation same as (f)
4.3.2 Concentration Distribution

The alternate parameter which can be used to characterize the rate of turbulent mixing is the mixture fraction $f$. The mixture fraction is defined as the ratio of the local concentration of a tracer $c$ to its concentration $c_o$ at the exit of the jet in the mixer (Chornyi et al. 2008). Figure 4.6 shows the mixture fraction at five different planes in the downstream direction from jet injection for $\theta_o = 45^\circ$, $Re_{cf} = 44648$ and $\theta_o = 135^\circ$, $Re_{cf} = 57451$.

Figure 4.6 Mixture fraction for different planes downstream of the mixer at $x/d=5$, 10, 15, 20 and 25 for $\theta_o = 45^\circ$, $Re_{cf} = 44648$ and $\theta_o = 135^\circ$, $Re_{cf} = 57451$
It can be noticed that the mixed fluid compositions across the entire jet are within a narrow range of concentrations relative to the mean profile. So the shape of the mixture fraction (concentration distribution) is Gaussian profile immediately downstream of the injection. At all locations the shape is symmetric about n/d = 0 plane. It can be mentioned that mixture fraction tends to be weak with increasing x/d. Also it is noted that with increase in injection angle, the tracer concentration decrease at all the planes considered.

The mean concentration contours at various y–z planes at different downstream distances are shown in Figure 4.6, which shows that as the height (n/d) increases, concentration gets distributed over large region (Manabendra et al. 2006).

Figure 4.7 presents the tracer distribution of the mixers at x-z planes for \( \theta_0 \) 60°, 120° and Reynolds number 44684. Dispersion of the tracer concentration is controlled by the pair of vortices that forms in the x–z plane (Manabendra et al. 2006).

It is clearly shown in Figure 4.6 and Figure 4.7 that mixer performance with greater than 90° injection is better than that of the mixers with acute angles. This describes that the simulation results correlates well with the experimental findings.
4.3.3 Jet Trajectory

Jet trajectory is the locus of the local maximum tracer concentration of the jet and it coincides with the centreline of the jet. From the loci positions of the maximum values of the concentration the trajectory of the jet centreline can be obtained, this assumption is recommended by Smith (1996), Smith and Mungal (1998) and Hasselbrink (1996).

The jet trajectory indicates a qualitative representation of the jet flow, such as, the penetration, deflection of the jet and degree of streamline curvature (Manabendra et al. 2006). The flow field of a vertical jet in cross flow is observed to be influenced by the square root of fluid momentum ratio.
or a simplified effective velocity ratio $R = \frac{u}{v}$ for incompressible flow of jet and crossflow fluid with same density.

Abramovich (1963), Beer and Chigier (1974), and Schetz (1980) reviewed several publications concerning JICF and they concluded that, the flow field of the JICF depends primarily upon the velocity ratio. One of the important characteristics of jet in cross flow is the jet penetration and trajectory which directly affects the mixer dimensions and design. There are several theoretical and experimental research works available in the literature, which address the jet breakup and trajectory.

![Figure 4.8 Comparison of normalised jet trajectories from simulation results and correlation results for injection angles 45° and 120° and cross flow Reynolds number 31917 and 44648.](image)

The computed results of jet trajectories for 45° and 120° injection angles and Reynolds number values of 31917 and 44648 are compared with the correlation results for venturi-jet mixer. The upper part of the curved jet ($n/d < 0$) faces and mixes with the cross-flow. This half of the jet is referred to

\[
R = \left( \frac{\rho_j u^2}{\rho_d v^2} \right)^{1/2}
\]  

(4.12)
as the outer part and the other half \((n/d > 0)\) is referred to as inner part of the jet.

The amount of penetration of the jet into the crossflow and deflection of the jet depends upon the initial injection angle \(\theta_o\), momentum ratio, \(R\) and Reynolds number, \(Re\). The jet flow is almost unaffected by the cross-flow in the vicinity of discharge as the cross-flow is weak relative to the jet flow, but further downstream, the jet gets increasingly deflected due to a larger relative momentum of the cross-flow (Manabendra et al. 2007).

From Figure 4.8 it is also observed that higher the injection angle, higher is the depth of penetration of the jet and smaller is its deflection. In contrast, with increase in cross flow Reynolds number, the jet penetration decreases for both the cases shown in Figure 4.8. The simulated jet trajectories are in good agreement with and the correlation results.

### 4.3.4 Positioning of Jet in the Throat Region

The basic operating principle of the venturi-jet mixer is to convert pressure energy of motive fluid (crossflow) into kinetic energy. The low pressure and high velocity flow occurs at the throat portion. This causes the suction fluid (jet) to enter into the mixer and mix with the cross flow in the diverging portion. The remaining kinetic energy is then turned back into pressure across the diverging section.

To fix the location of jet in the mixer, pressure is used as the selection criteria. Pressure and velocity profile along the centreline of the venturi was determined from the simulation. Figure 4.9 shows the variation in the pressure and velocity along the centreline of venturi with crossflow velocity. The variation is closely related to the crossflow Reynolds number.
Figure 4.9 Pressure and velocity variation along the centreline of venturi

It is found from the result that the pressure is decreased and velocity is increased with increasing Re for the mixer. Also, it is observed that the low pressure created in the throat region is almost remains constant for a particular Reynolds number from inlet to the exit of the throat for all the cases considered. This reveals that jet can be placed at any position in the throat.

In the present work the jet is located at the centre of the throat for the accomplishment of jet with injection angles from 45° to 135°. Figure 4.10 displays the pressure field for injection angle 60° and crossflow Reynolds number values 38301 and 57451. In addition Figure 4.10 shows velocity field
for injection angle 120° and crossflow Reynolds number values 31917 and 51068.

**Figure 4.10 Pressure and velocity contour for various venturi-jet mixers**

### 4.3.5 Pumping Coefficient

The pumping coefficient $\phi$ is defined as the ratio of flow rate of jet, $m_j$ to the flow rate of the crossflow, $m_{cf}$ (Hui et al. 1999).

$$\phi = \frac{m_j}{m_{cf}}$$

(4.13)

The mass flow rate of the jet is determined from the numerical simulation for different crossflow Reynolds number and jet injection angles. It is observed that the jet flow increases with crossflow Reynolds number and
jet injection angle (not shown in Figure). The increase in jet flow with increase in crossflow Reynolds number may be ascribed to the increased momentum of the crossflow.

Figure 4.11  Pumping coefficient, $\Phi$ Vs crossflow Reynolds number, $Re_{cf}$ for different injection angles

Figure 4.11 presents the pumping coefficient as a function of the crossflow Reynolds number. The pumping coefficient is shown to decrease with increasing Reynolds number between 10% and 14%. The effect of the injection angle greater than 90° on the mixer compared to acute angle jet injection is generally to further augment pumping. Most of the comparable results show an increase between 17% and 25% over the jet with injection angle less than 90°.

4.3.6 Turbulent Intensity

The turbulence intensity, $I$, is defined as the ratio of the root-mean-square of the velocity fluctuations $u'$, to the mean flow velocity $U$. The root-mean-square of the turbulent velocity fluctuations can be computed as (Fluent User Guide 2005):

$$u' = \sqrt[3]{\frac{1}{3}(u_x'^2 + u_y'^2 + u_z'^2)}$$  (4.14)
Using turbulence kinetic energy $k$, equation (14) can be written as:

$$u^* = \sqrt{\frac{2}{3} k} \quad (4.15)$$

The mean flow velocity can be computed from the three mean velocity components $U_x$, $U_y$ and $U_z$ as:

$$U = \sqrt{U_x^2 + U_y^2 + U_z^2} \quad (4.16)$$

In the present work the turbulence intensity, $I$, and the hydraulic diameter are defined as turbulence parameters in the boundary conditions for k-$\varepsilon$ turbulence model. A turbulence intensity of 1% or less is generally considered low and turbulence intensities greater than 10% are considered high.

The turbulence intensity at the core of a fully-developed duct flow can be estimated from the following formula derived from an empirical correlation for pipe flows given in Equation (Fluent User Guide 2005).

$$I = 0.16 \text{Re}_{dh}^{-\frac{1}{6}} \quad (4.17)$$

where $\text{Re}_{dh}$ is the Reynolds number based on the hydraulic diameter of the mixer $d_h$.

Figure 4.12 presents the turbulent intensity contour of venturi-jet mixer for various injection angles 45°, 60°, 90°, 120° and 135° and crossflow Reynolds number of 57451.

Figure 4.12 clearly shows that turbulent intensity varies widely throughout the mixer. Along the downstream of injection, in particular, turbulent intensity reaches high values just after the jet injection.
With increasing injection angle, the turbulent intensity increases after the jet injection point and leads to better mixing performance. Also, turbulence intensity is increased with higher crossflow Reynolds number (not shown in Figure).

Figure 4.12 Contours of Turbulence intensity for Reynolds number 57451 and injection angles 45°, 60°, 90°, 120° and 135°