ABSTRACT

Mixing processes in water storage tanks are an important factor for maintaining an adequate quality of drinking water. The flow and mixing in these tanks are often investigated with extensive experimental studies. However, much progress has been made in recent years in numerical simulation techniques, and with the growth in speed and capacity of modern supercomputers, computational fluid dynamics (CFD) simulations can now be a valuable addition to the laboratory experiments.

In this paper we present the results of three-dimensional URANS simulations of the flow and entrainment processes in a jet-mixed tank. Several variations of jet velocity, nozzle diameter and nozzle angle are investigated, and two differencing schemes with different accuracies to approximate the convective fluxes are applied. The predicted results are compared to experimental data as well as to other CFD results taken from the literature. The main objective of the work presented is to develop a CFD code that can be used as a flexible modelling tool for the design and optimization of water storage tanks including the effects of varying water depths and density stratification.

Keywords: CFD, URANS, jets, turbulent mixing processes, water storage tanks

1 INTRODUCTION

Good drinking water quality is essential to public health and the deterioration of the quality of the water in water storage tanks is an increasing concern for water utilities. An important issue is maintaining adequate water quality throughout the storage facilities and distribution system, which is not a trivial task. Problems that may occur in storage tanks include hydraulic short-circuiting, poor mixing and circulation, and excessive detention time (long water age). These can result in loss of disinfectant residual leading to microbiological activities and formation of disinfection byproducts so that water quality deteriorates. The residence times in water storage tanks depend generally on the geometry and operation of the tank. In particular the locations, configurations, and orientations of inlet and outlet pipes have a strong impact on the mixing processes. For good design and operation of water storage tanks it is essential to be able to predict precisely the residence times, for which detailed information on the hydrodynamics and the related turbulence properties are needed. Flow velocity measurements in water storage tanks are difficult to obtain. Water quality in the tank may only be monitored by withdrawing samples at a few locations in the tank, but sampling at a few locations only provides a limited picture of potential water quality deterioration.

Consequently, flow and mixing processes in water storage tanks have often been investigated by extensive experimental work. Previous laboratory studies of flows driven by
the momentum of the inflowing jets have used scale models of water storage tanks and were mainly focused on determining the residence time as a bulk parameter using different techniques of concentration measurements (Metzger & Westrich 1978, Maruyama et al. 1982, Rosmann & Grayman 1999). These measurements provided good information about the overall behaviour of the tank as a mixing reactor but not about the driving physical processes. The most recent developments in this field use optical measurement techniques, such as Laser-Induced-Fluorescence (LIF) and Particle-Image-Velocimetry (PIV), combined with increased computer power that provide much more information. Roberts et al. (2005) used a 3-D LIF system to measure the concentration of a tracer in different water storage tanks and presented guidelines on the design of the inlets and outlets in order to maximize jet-mixing.

In addition, much progress has been made in recent years regarding numerical simulation techniques. With the growth in speed and capacity of modern supercomputers, computational fluid dynamics (CFD) simulations can now be a valuable supplement to the laboratory experiments. CFD provides a wide variety of methods ranging from techniques with high-resolution in space and time that solve the flow field completely along with details of the whole range of turbulent fluctuations (Direct Numerical Simulation, DNS), to procedures that are based on time-averaged turbulent quantities (RANS) where only an average picture of the hydrodynamics is obtained. Despite the capacities of modern computers, DNS, due to its extremely high computational demand, is still used mainly for research purposes. Our objective is to develop a CFD code that can be employed as a flexible engineering tool for the design and optimization of water storage tanks. A three-dimensional URANS model is currently being enhanced and validated.

In this paper we present initial results of three-dimensional URANS-simulations of the flow and mixing processes in a jet-mixed water storage tank. Jet mixing is one of the simplest ways to achieve mixing whereby some water in the tank is withdrawn by a pump and returned as a high-velocity jet through a nozzle. The numerical results are validated on the basis of experimental studies carried out by Gaikwad (2001). Additionally they are compared to recently reported numerical simulations of the same experiments described by Patwardhan (2002).

2 NUMERICAL FRAMEWORK

The numerical model that is used in this study was developed originally at Bristol University and was validated on a large variety of open-channel flow situations (Stoesser, 2002). The program calculates hydrodynamics for a general three-dimensional geometry, discretized by the Finite Volume Method on curvilinear coordinates. The unsteady Reynolds averaged Navier-Stokes (URANS) equations are solved together with the unsteady continuity equation, written as:

\[
\frac{\partial U_i}{\partial t} + \frac{\partial U_i j}{\partial x_j} = \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \delta_i j - \rho u_i u_j \right) + \frac{1}{\rho} F_j
\]

\[
\frac{\partial U_i}{\partial t} + \frac{\partial U_i j}{\partial x_j} = 0
\]

where \(U\) is the velocity vector averaged over the (Reynolds-averaging) time \(t\), \(x\) is the spatial geometrical scale, \(\rho\) is the water density, \(P\) is the pressure, \(\delta\) is the Kronecker delta and \(u\) is the velocity fluctuation in time during the time step \(\Delta t\), when \(U\) is subtracted. \(F\) represents external forces (gravity, wind, etc.). The second term on the right side of the first equation is the Reynolds stress term, which must be solved with a turbulence model. Two different semi-empirical statistical approaches are implemented for this purpose: the two-equation standard
The *k*-\( \varepsilon \)* model (Rodi, 1980) and the two-equation *k*-\( \omega \)* model (Wilcox, 2000). The *k*-\( \varepsilon \)* model is widely used and has proved its accuracy and reliability in many practical applications such as open-channel flows with complex geometry. Although less common, the *k*-\( \omega \)* model has shown better results for certain applications, especially for flows with adverse pressure gradients (Wilcox, 2000).

The SIMPLE method is used for the pressure-velocity corrections and the convective and diffusive fluxes are approximated by applying the hybrid differencing scheme with first/second order accuracy (depending on the local Peclet number, e.g. Stoesser, 2002) or the HLPA differencing scheme with second order accuracy (Zhu, 1991). Time advancement is achieved by a second order, three-time-level implicit scheme. The resulting matrices are solved iteratively with the SIP method (Stone, 1968). Structured grids are used, as the SIP method offers high efficiency in solving the resulting sparse matrices. However, structured grids have considerable disadvantages concerning the discretization of complex geometries. Therefore, a multi-block algorithm was implemented, which splits the computational domain into multiple structured sub-domains with overlapping grid cells at their interfaces. In addition to the stability and efficiency of the equation solver this method allows parallel computations on network clusters (Domain Decomposition) thus permitting a large number of grid nodes. The parallelization was realized using the Message Passing Interface (MPI) standard.

In addition to solving the transport equations for the turbulent quantities *k*, \( \varepsilon \), and \( \omega \), mentioned above, the code provides computation of further advection-diffusion-equations for the unsteady transport of heat or dissolved material.

To solve the partial differential equations mentioned above, appropriate conditions must be specified at each boundary of the computational domain. At an inflow boundary a Dirichlet boundary condition is set, i.e. the values for velocity, *k*, \( \varepsilon \), \( \omega \), and tracer concentrations have to be prescribed. At an outflow boundary, neither the value of the flow variable nor the flux is known. Therefore, a zero variable gradient condition (Neumann boundary condition) is used. The water surface is treated as a rigid lid with a symmetry boundary condition, i.e. the normal flux and the gradients of all variables are specified to be zero. Impermeable walls are treated with the no-slip condition and velocities are set to zero at the walls. However, since the occurrence of steep gradients at this boundary would require a very high grid resolution near the wall, a log-law approach is employed in order to connect the wall shear stresses to the dependent variables.

For unsteady computations, in addition to the boundary conditions, initial conditions for each variable have to be specified at each node in the computational domain. In the computations reported here the initial conditions are obtained from a converged solution of a steady a priori simulation.

### 3 Setup and Boundary Conditions

The geometry and boundary conditions for the numerical simulations presented here were selected based on the laboratory experiments of Gaikwad (2001). Numerical simulations performed by Patwardhan (2002), who used a similar numerical scheme but a coarser grid, are also available and are included for additional comparison.

The simulated tank had a diameter of 0.5 m and was filled to a depth of 0.5 m. Water was used as the working fluid and sodium chloride solution was used as a tracer. The conductivity was monitored at four locations using a conductivity probe and a chart recorder. Figure 1 shows a sketch of the experimental setup including the measurement locations. The jet was oriented at angles of 30°, 45°, 60° and 90° to the horizontal, and data were collected over a wide range of nozzle diameters and jet velocities. The following were chosen for simulation: a nozzle diameter of 21 mm with a jet velocity of 2.1 m/s and nozzle angles of 45° and 90° and
a nozzle diameter of 8 mm with a jet velocity of 4.4 m/s also with nozzle angles of 45° and 90°. The resulting Reynolds numbers based on nozzle diameter and jet velocity are 44,100 and 35,200 respectively.

Fig. 1: Experimental setup for the measurement of mixing time (Patwardhan, 2002, modified)

The computation domain was discretized in space by employing 10 grid blocks, about 900,000 grid nodes overall were used. Figure 2 shows the grid geometry in side and plan views. The tank consists of eight blocks and two additional blocks were used to represent the inlet and outlet pipes. By including a certain part of the in- and outflow pipe disturbing influences of boundary conditions applied directly at the tank could be minimized.

Fig. 2: Three dimensional grid consisting of 10 blocks; Left: side view; Right: plan view
4 RESULTS AND DISCUSSION

4.1 FLOW FIELD

Figure 3 shows streamtraces (coloured by the velocity magnitude, where red and green indicate higher velocities and blue indicates low velocities) with a nozzle angle of 45° and a jet velocity of 4.4 m/s. It can be seen that the flow conditions in the tank are highly three dimensional and complex. When the jet impinges on the opposite wall the velocities are significantly reduced. The flow diverges in all directions and complex circulation patterns can be observed. With respect to mixing Figure 3 indicates that no short circuiting or stagnant zones are expected, leading to homogeneous and efficient distribution of fresh water in the tank.

Simulated distributions of flow velocities in the longitudinal central plane, i.e. y=0 (see Figure 1) are shown in Figure 4 for different nozzle angles, nozzle diameters and jet velocities. The flow velocities were normalized with the initial jet velocity.

Fig. 3: Simulated three dimensional flow field for a nozzle angle of 45°, a nozzle diameter of 8 mm, and a jet velocity of 4.4 m/s; Convection Scheme: Hybrid

Fig. 4: Calculated flow velocities (normalized with the jet velocity) and streamtraces in central plane y=0 (see Figure 1); Convection Scheme: Hybrid; Left: nozzle angle: 45°, nozzle diameter: 21 mm, jet velocity: 2.1 m/s; Middle: nozzle angle: 45°, nozzle diameter: 8 mm, jet velocity: 4.4 m/s; Right: nozzle angle: 90°, nozzle diameter: 8 mm, jet velocity: 4.4 m/s
It can be seen that the flow fields for the 45° nozzles are very similar. In both the 2.1 and 4.4 m/s cases, a large recirculation zone occurs above the jet, and a second, smaller circulation zone occurs below the jet in the central plane. The visualizations show slightly higher normalized velocities for the 2.1 m/s jet. The reason for this is the smaller nozzle diameter in the 4.4 m/s case, so the mass and momentum fluxes of the jet are slightly smaller. In contrast to the 45° nozzle, the 90° nozzle shows only one large circulation region, and mixing times were computed to be almost two times longer, indicating significantly reduced mixing efficiency.

The convection scheme can have an important effect on the results. Figure 5 shows a comparison of the flow velocities in the central plane y=0 (see Figure 1) obtained with the first/second order HYBRID scheme and with the second order HLPA differencing scheme. The absolute differences in normalized velocities are shown in Figure 5 right. It can be observed that the streamtraces are generally very similar but the HYBRID scheme overestimates diffusion near the entrance leading to a wider jet especially near the nozzle. This is where the scheme switches to a pure first order upwind scheme due to convection/diffusion ratios larger than two. The differences in mass and momentum transport lead to different predictions of tracer mixing. This is discussed further below.

4.2 MIXING PROCESSES

Unsteady simulations to predict the mixing of a passive tracer in the tank were carried out using the steady flow calculations described above for the initial condition. The initial tracer concentration was specified at the grid cells corresponding to the tracer input location in the experiments (see Figure 1). The predicted concentration distributions were normalized with the fully mixed concentration in order to compare them with the measured values.

Figure 6 shows the variation of the simulated concentration over time at probe locations 1 and 2 (see Figure 1) for the 45° jet with a velocity of 4.4 m/s as well as the corresponding experimental data and the CFD results from Patwardhan (2002).

It can be seen that the simulated curves at probe location 1 are in fairly good agreement to the experimental results. Between 10 and 15 seconds the concentrations are slightly overestimated and a higher peak is obtained in the simulations. In contrast to the results of Patwardhan (2002) the time where the tracer reaches the sampling probe, i.e. when the concentration distribution starts to increase, is predicted almost exactly. The differences between the results of the HYBRID and the HLPA schemes are very small at this location.
Fig. 6: Comparison of simulated concentration profiles (Convection Schemes Hybrid and HLPA) with experimental measurements and CFD results from Patwardhan (2002); nozzle angle: 45°, nozzle diameter: 8 mm, jet velocity: 4.4 m/s; Probe locations 1 and 2

The simulated concentration distribution at probe location 2 is less satisfactory. The peak tracer concentration is overestimated by a factor of two and the tracer reaches the sampling location 2 too soon. Both convection schemes deliver similar results, however, the HYBRID scheme, which uses second order central differences at that location, produces less diffusion than HLPA, hence slightly higher concentration peaks than for the HLPA scheme are observed. Nevertheless, a slight improvement over the results of Patwardhan can be claimed.

The calculated concentration variation over time at probe locations 1 and 2 for the 45° jet with a velocity of 2.1 m/s, as well as the corresponding experimental data and the CFD results from Patwardhan (2002) are shown in Figure 7.

Fig. 7: Comparison of simulated concentration profiles (Convection Schemes Hybrid and HLPA) with experimental measurements and CFD results from Patwardhan (2002); nozzle angle: 45°, nozzle diameter: 21 mm, jet velocity: 2.1 m/s; Probe locations 1 and 2

At probe location 1 only the HYBRID scheme accurately predicts the time (t = 10 s) for the tracer to reach the sampling location as well as the gradient of the concentration distribution. Interestingly, the calculation with the HLPA scheme shows a different behaviour, which is surprising because in all the other simulations and at all other locations the HYBRID and the HLPA scheme show nearly identical temporal tracer distributions. During the time period between 10 and 20 seconds a dip in the temporal distribution of the concentration is observed in the measurements, which is not reproduced in any of the simulations. Between 20 and 30 seconds the HYBRID scheme is again quite accurate. For that flow case at probe location 1 only the HYBRID scheme delivers somewhat acceptable results. The HLPA calculations as well as the CFD results from Patwardhan (2002) are not in agreement with the experimental data.
The results at probe location 2 are better. Both differencing schemes predict the time when the tracer reaches location 2 and the gradient of the profile is in very good agreement with the data. Again, the HYBRID scheme predicts more pronounced peaks. Overall, the match between measured and calculated is very satisfying and again improvements over the results of Patwardhan (2002) were obtained.

Figure 8 shows the predicted (HLPA scheme) concentration distribution for the jet velocity of 4.4 m/s and a nozzle angle of 45° at simulation times 10 s, 20 s, and 30 s in the longitudinal central plane y=0 (see Figure 1). The corresponding results for the perpendicular central plane x=0 (see Figure 1) are presented in Figure 9. This is the same case as given in detail for probe locations 1 and 2 in Figure 6.

The sequences show how the tracer is transported and entrained over time by the flow field (see also Figure 5). It can be seen that after 10 seconds mixing mainly occurs in the direction of the jet and near the water surface. The tracer has not yet reached the areas perpendicular to the jet. After 20 seconds, the tracer is mixed fairly well on the far side of the jet and now highest concentrations are seen on the near side. The entrainment of the tracer
into the jet can be seen quite clearly (Figure 9, middle). After 30 seconds the tracer is fully mixed (differences less than 5%) in both cross sections shown. This is in very good agreement to the data obtained from the measurements, where a mixing time of 30 seconds was found.

An apparent asymmetry that can be seen in Figure 9 needs to mentioned. The calculated concentration distribution in the central plane along x=0, i.e. perpendicular to the jet, is not symmetric although this would be expected from a RANS simulation in a symmetrical domain with a symmetrical in- and outflow. A detailed investigation showed that the non-symmetrical results could be traced back to the fact that the grid was not absolutely symmetric and small round-off errors caused the asymmetrical velocity and tracer distributions observed during the unsteady simulations.

5 CONCLUSIONS
A three-dimensional unsteady RANS CFD model was applied to predict flow and mixing in jet-mixed water tanks. The predicted mixing time and concentration profiles were compared to experimental measurements for different jet velocities and nozzle angles. The numerical model predicted the overall mixing time very well (not shown here in full detail), however apart from one probe location the predicted concentration profiles are generally not in good agreement with the experimental measurements. It was clearly shown that the convection scheme can have an effect on the tracer distribution and that improvements were accomplished in comparison to the CFD results from Patwardhan (2002). This improvement can be attributed mainly to the use of a finer grid. Finer grids or higher order turbulence modelling may improve the predictions further. This work is currently in progress.

Future work will be directed towards the correct prediction of buoyancy effects resulting from temperature differences in the storage facility and furthermore towards the simulation of the fluctuating water level during filling and draining operations.

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