Numerical simulation of flow and tracer transport in a disinfection contact tank

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Abstract: Chlorine is extensively used to disinfect drinking water supply. However, the design of chlorine contact tank is usually based on the volume displacement criterion, paying attention that detention time would be at least of half an hour. This criterion relies upon the assumption that plug-flow conditions hold along the tank. However, the existence and arrangement of baffles in the tank, and the tank inlet and outlet configurations can result in a much more complex flow pattern, where turbulent mixing, dead-zones and short-circuiting exist. This situation could result in an inefficient use of chlorine due to the formation of potentially carcinogenic compounds, which originate from residual chlorine in the tank. Further some bypassing allows some out-coming flow with less of the standard amount of contact with the chlorine dose. Therefore, understanding hydrodynamics and mass-transfer characteristics within a contact tank is very useful. The objective of the paper is to present the preliminary results of a numerical study undertaken to investigate hydrodynamics and turbulent transport and mixing inside a contact tank. Two-dimensional steady-state and time-variable numerical simulations were performed with Multiphysics 3.2a™ in a contact tank geometry, which is that experimentally studied by Shiono and Teixeira (Shiono and Teixeira, 2000). Tracer transport was analyzed in the case of a burst of concentration. Both velocity profiles and flow-through curves were generally in good agreement with experimental data. The model results pointed out the presence of recirculation areas near the baffles and the corners formed by the baffles and the tank walls. These areas introduced dead-zones in the tank deviating flow patterns from ideal plug-flow conditions.

Keywords: environmental fluid mechanics, turbulence, contact tank, numerical simulations, k-ε model, Multiphysics 3.2.

1. INTRODUCTION

Disinfection is a water treatment that it is applied in both drinking water and wastewater treatment systems with the purpose to inactivate microorganisms, some of which may be pathogenic, preventing transmission of waterborne diseases. If UV and ozone are often applied, chlorination is the most common method of disinfection currently used. This method involves addition of chlorine gas or salts to an aqueous stream moving in a contact tank, which should be designed to achieve the objective to bring as much water in contact with chlorine for as long as possible to obtain a certain level of disinfection. Typically disinfection systems are designed to provide efficient mixing of chlorine solution with raw water for a contact time of at least 30 minutes, with the concentration of free chlorine in the reactor effluent between 0.1 and 0.2 mg/L (Gyurek and Finch, 1998). Effective design of chlorine disinfection processes must integrate four major elements (Greene, 2002):

- chlorine and source water chemistry, since the process is affected by both physical and biological characteristics of water, such as suspended solids, temperature, pH, oxidisable substances;
- chlorine decay kinetics, since the loss of chlorine is characterized by an initial rapid loss period known as immediate demand, followed by a slow decay period. The first one could be expressed as:
  \[ \text{Cl}_{id} = \text{Cl}_{in} - \text{Cl}_0 \]  
  where \( \text{Cl}_{id} \), \( \text{Cl}_{in} \), and \( \text{Cl}_0 \) are immediate chlorine demand, applied chlorine dose and total initial chlorine residual. The slow decay process is typically modelled with a first-order kinetics;
- microbial inactivation kinetics, which is commonly expressed using a first-order rate (Chick-Watson model). However, disinfection systems rarely display first-order kinetics, so different models have been proposed, such as Hom kinetic model, Rational model, multiple target and series-event models (Gyurek and Finch, 1998);
- chlorine contact tank hydraulics, which is the focus of this paper.

As previously outlined, the main objective of the chlorine contact tank is to provide adequate
residence time for both the micro-organism and the disinfectant to achieve the desired degree of microbial inactivation. Achieving proper disinfection is generally quantified by the $C \times T$ rule, where $C$ is the minimum disinfectant residual measured at the tank outflow and $T$ is the minimum contact time. According this approach, the product $C \times T$ must exceed a value that depends on the type of disinfectant used, pH and temperature, as specified in regulatory documents, to obtain a defined level of inactivation for specified micro-organism, based on standardized inactivation rate estimates. The $C \times T$ rule often requires the use of $T_{10}$ as representative of the hydraulic residence time. $T_{10}$ is the residence time of earliest 10% of micro-organism to travel through the tank, as determined from a tracer Residence Time Distribution (RTD). In other words, $T_{10}$ is the RTD tenth percentile. In real contact tanks $T_{10}$ is shorter than the mean hydraulic detention time $T_{\text{mean}}$, which is calculated by dividing the tank volume by the water flow rate. Thus, one way to meet the disinfection criteria could be by increasing the chlorine dosage, but this also increases operational costs and may induce high concentrations of disinfection by-products (DBPS), that are not desirable (Hannoun et al., 1998). Therefore, the best way to optimize disinfection effectiveness is by increasing $T_{10}$ value and by reducing the required disinfectant dosage. The higher is the $T_{10}/T_{\text{mean}}$ ratio, the more effective is the contact tank. To achieve this goal compartment could be enlarged, resulting in additional storage volume, with higher construction and maintenance costs. A more cost-effective way to increase $T_{10}$ is to maximize the uniformity of flow patterns. The maximum $T_{10}$ is equal to $T_{\text{mean}}$, when all water particles entering the tank at a certain time flow in parallel through the tank and leave the basin at exactly the same time, i.e. plug-flow conditions. Thus, and also because most chemical reactions are more effectively completed in a plug-flow reactor (Wang et al., 2003), chlorine contact tanks are typically designed to approach plug-flow conditions. However, real contact tanks cannot achieve these conditions because of varying velocity gradients caused by flow disturbances (Hannoun et al., 1998). These are due first to boundary layers existing along the tank bottom and side walls. Water in boundary layer travels at below-average velocities, residing in the compartments longer that $T_{\text{mean}}$. On the other hand, water away from the wall travels at above-average velocities, with shorter residence time. If combined with sudden expansions in flow area, boundary layers can separate from the wall, resulting in recirculation zones where flow direction is the opposite of the main flow. To reduce the effect of boundary layer separation associated with flow expansions, baffle walls are commonly used, but they can also contribute to velocity gradients. In fact, since baffles force water around generally sharp turns, water particles on the outside of a turn must move faster that water on the inside. This gradient leads to different detention times and to stagnant water zones behind the turns. Finally, small inlets and outlets could produce velocity gradients since the velocity of water entering the tank through relatively small pipeline is significantly higher than the average velocity in the compartments. Similarly, a small outlet pipeline produces a velocity excess upstream of the outlet (Hannoun et al., 1998).

The overall effect of the aforementioned flow disturbances is longitudinal mixing, which produces non-uniform residence times as well as microbial and chlorine concentration gradients (Greene, 2002). Therefore, some part of the flow exits from the tank with less than the minimum amount of contact with the chlorine dose (short-circuiting), whereas other part of the flow has higher residence times due to dead zones existing in the tank. The ideal contact tank should be designed by reducing inlet and outlet velocities, by distributing the water uniformly throughout the compartment cross-section, by breaking up large scale eddies and by preventing short-circuiting. From the previous discussion it is evident how the disinfection effectiveness is strictly related to the contact tank hydraulic characteristics, that must be considered in details. Traditional approaches based on tracer studies and RTD models could provide useful information about hydraulics of existing contact tanks only. Also, they are quite time consuming and expensive to perform on full-scale tanks and are unable to reveal all the factors controlling tank hydrodynamics. Therefore, the application of computation fluid mechanics (CFD) methods to simulate turbulent flow patterns within the tank, in conjunctions with disinfectant decay and microbial inactivation models, is becoming in recent years the best approach to contact tank design (Hannoun et al., 1998; Greene, 2002; Wang et al., 2003).

The objective of the paper is to present the preliminary results of a numerical study undertaken to investigate hydrodynamics and turbulent transport and mixing inside a contact tank. Therefore, 2D steady-state and time-variable numerical simulations were performed with Multiphysics 3.2a™ in a contact tank geometry, which is that experimentally studied by Shiono and Teixeira (Shiono and Teixeira, 2000). Also, tracer transport was analyzed in the case of a burst of concentration.
2. NUMERICAL SIMULATIONS

Most of the available CFD studies on contact tanks are devoted to hydrodynamics only. Falconer and Liu [1987] have applied a 2D model to Elan contact tank comparing mean velocity distribution in the tank and flow through curves (FTC) predicted by the model with experimental data, while Stevenson [1995] applied Contank model to an existing contact tank. Hannoun and Boulos [1997] and later Hannoun et al. [1998] applied a CFD model which predicts flow field and FTCs in order to improve existing contact tanks through the addiction of baffles. Other studies were carried out in U.K. on Embsay contact tank comparing modeled hydraulic characteristics and FTCs with experimental data (Falconer and Ismail, 1997; Wang and Falconer, 1998a; 1998b). In some of these studies several combinations of different turbulent models and numerical schemes were tested against the measurements from a physical model of Embsay tank to identify the most suitable.

Turbulent stresses were modeled using a depth mean eddy viscosity model and the k-ε model. Numerical results demonstrated that k-ε model gave a good prediction of horizontal recirculation in the tank compartments, but also it predicted a smaller cross-sectional average velocity toward the end of the tank. On the contrary, prediction from depth mean eddy viscosity model did not exhibit any recirculation region (Wang and Falconer, 1998b). Finally, flow field and chlorine concentrations were modeled with good results in Elan contact tank using again different turbulent models and numerical schemes and comparing model prediction with experimental data (Wang et al., 2003). Notably, field data of Embsay tank gives a good prediction of horizontal recirculation region (Wang and Falconer, 1998a; 1998b). In some of these studies several combinations of different CFD models are based on the mass conservation equation and the Navier-Stokes equations of motion. Since the flow in the tank is turbulent, these equations must be averaged over a small time increment applying Reynolds decomposition, which results in the Reynolds-averaged Navier-Stokes equations (RANS). For a planar, incompressible flow these equations are:

\[
\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} - \frac{\partial \tau_{ux}}{\partial x} - \frac{\tau_{vy}}{\partial y} + \frac{\partial}{\partial y} \left( \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial x} \left( \frac{\partial \bar{v}}{\partial x} \right)
\]

\[
\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} - \frac{\partial \tau_{vy}}{\partial y} - \frac{\tau_{ux}}{\partial x} + \frac{\partial}{\partial x} \left( \frac{\partial \bar{v}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial \bar{u}}{\partial y} \right)
\]

\[
\frac{\partial \bar{p}}{\partial t} + \bar{u} \frac{\partial \bar{p}}{\partial x} + \bar{v} \frac{\partial \bar{p}}{\partial y} = \frac{\partial}{\partial y} \left( \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial x} \left( \frac{\partial \bar{v}}{\partial x} \right)
\]

where \( \rho \) and \( \mu \) are fluid density and viscosity, \( p \) is fluid pressure and \( u, v \) are velocity components in the \( x \) and \( y \) directions, respectively. The overbar indicates time-averaged quantities. Notably, in eq. (3) there is the turbulent kinetic energy \( \epsilon \), that if isotropic turbulence assumption holds could be estimated following the k-ε model approach as:

\[
v_t = \frac{C_\mu k'}{\epsilon'}
\]

where \( k' \) and \( \epsilon' \) are turbulent kinetic energy per mass unit and its dissipation rate, respectively, and \( C_\mu = 0.09 \). These parameters are estimated with the classical two equations of k-ε model:

\[
\frac{\partial k'}{\partial t} + \bar{V} \cdot \nabla k' = \frac{V_t}{\sigma_k} \nabla \cdot \nabla k' - \frac{\epsilon'}{\sigma_k} + 2 v_t \bar{D} \bar{D}
\]

\[
\frac{\partial \epsilon'}{\partial t} + \bar{V} \cdot \nabla \epsilon' = \frac{\epsilon'}{\sigma_\epsilon} \nabla \cdot \nabla \epsilon' + 2 v_t C_{1\epsilon} \frac{\epsilon'}{k'} \bar{D} \bar{D} - C_{2\epsilon} \frac{\epsilon'^2}{k'}
\]

where \( \bar{D} \) is deformation tensor, whereas \( C_\mu, \sigma_k, \sigma_\epsilon, C_{1\epsilon} \) and \( C_{2\epsilon} \) are constants, and their values are listed in Table 1.

**Table 1. Values of the constants of k-ε model**

<table>
<thead>
<tr>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\epsilon )</th>
<th>( C_{1\epsilon} )</th>
<th>( C_{2\epsilon} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.00</td>
<td>1.60</td>
<td>0.1256</td>
<td>1.92</td>
</tr>
</tbody>
</table>

Transport of solutes within the contact tank could be modelled using the 2D advection-diffusion equation:

\[
\frac{\partial C}{\partial t} + \bar{u} \frac{\partial C}{\partial x} + \bar{v} \frac{\partial C}{\partial y} = D_t \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)
\]

where molecular diffusion was neglected and only turbulent diffusion was considered with \( D_t \) as turbulent diffusivity and \( C \) as solute concentration. These equations were solved using Multiphysics 3.2a™ modeling package, which is a commercial...
multiphysics modeling environment (Multiphysics, 2005). Multiphysics 3.2a™ can solve for the same flow domain both motion equations and advection-diffusion equation. Particularly, both the $k$-$\varepsilon$ model application mode and the advection-diffusion application mode were used. They solve eqs. from (2) to (7) for the pressure $p$, the velocity vector components $\vec{u}$ and $\vec{v}$, $k$-$\varepsilon$ model parameters and solute concentration $C$ within the domain of the flow (Multiphysics, 2005). Fig.1 shows the geometry of the tank, which is the physical model in scale 1:8 of the contact tank of the Embsay Water Treatment Plant, located in UK, that was experimentally studied by Shiono and Texeira (Shiono and Texeira, 2000). The tank was 1.995 m long, 0.94 m wide and 0.6 m deep and it has 7 baffles and 8 compartments. The discharge entering the tank was 1.17 L/s, resulting in a mean water depth of 0.536 m and a mean cross-sectional velocity of 0.0104 m/s.

Figure 1. Plan view of simulated contact tank

The simulation was performed in two stages. First, steady-state turbulent flow within the tank was solved, using the $k$-$\varepsilon$ model. Second, mass-balance was solved on top of this field flow in the time-domain. Mass transport was described through advection-diffusion application mode, where the turbulent kinematic viscosity $\nu_t$ was used as turbulent diffusivity in the mass balance. Tracer transport was analyzed in the case of a burst of concentration of a solute.

For $k$-$\varepsilon$ model, inflow boundary condition was applied at the inlet, with uniform velocity profile and a fixed value for $k'$ and $\varepsilon'$ parameters, whereas neutral boundary condition was applied at the outlet. Finally, logarithmic law of the wall boundary condition was applied to the remaining boundaries, i.e. walls and baffles. For advection-diffusion equation, to simulate the burst of concentration a time-dependent flux boundary condition was applied:

$$\Phi_{\text{flux}}(t) = \Phi_{\text{flux,0}} \exp\left(1 - \frac{t}{2}\right)^2$$

where $\Phi_{\text{flux,0}}$ was a constant value which corresponds to that reported by Shiono and Texeira for their experiments [2000]. An insulation boundary condition was assumed at the walls and the baffles and, finally, advective flux boundary condition was applied to the outlet.

The $k$-$\varepsilon$ model application mode uses Lagrange $p2-p1$ elements to stabilize the pressure. Thus, second order Lagrange elements model the velocity components and $k'$ and $\varepsilon'$ parameters while linear elements model the pressure. The default element settings in this application mode always provide one order higher Lagrange elements for the velocity components than for the pressure. The advection-diffusion application mode applies only Lagrange quadratic element.

For the simulations water with density $\rho=1000$ Kg/m$^3$ and dynamic viscosity $\mu=1.00 \cdot 10^{-5}$, was selected as fluid. The mesh generation process was made assuming, among the others, as global maximum element size, maximum element size scaling factor, element growth rate and mesh curvature factor 0.04, 1, 1.3 and 0.3, respectively. Also, a finer maximum element size, namely 0.02 and 0.01, respectively, was set at both walls and baffles and at the internal edges of the tank, where errors tend to be large due to significant velocity/concentration gradients. Therefore, the used mesh had 14680 elements, 1468 boundary elements, with a minimum element quality of 0.4808. The number of degrees of freedom was 162220. About the solver settings, for steady-state analysis, stationary non-linear solver with Direct linear system solver was used, where the relative tolerance and the maximum number of iterations were set to $1.0 \cdot 10^{-6}$ and 45, respectively. For time-variable analysis, a time step of 1 second was selected extending the simulation until 1500 seconds. Streamline diffusion was introduced too.

3. ANALYSIS OF RESULTS

In the steady-state analysis, numerical simulations provided field velocity and pressure, kinematic viscosity $\nu_t$, $k'$ and $\varepsilon'$ values throughout the flow domain. First, numerical results pointed out velocity distribution within the tanks and, particularly, in the corners and behind the baffle turns. Fig.2a presents velocity field in the tank, with velocity values (the colour of the tank surface) and velocity vectors (arrows). It could be observed that in the first compartment remains uniform, while in the other compartment the effects of turns produces velocity variation in the cross-section. Also, low velocities (blue) were observed in the corners and in the inner side of the compartments, where recirculation and flow
reversal could be noted. Higher velocities (red) were calculated in the outer side of the compartments.

Figure 2a. Simulated flow field and velocity vectors in the contact tank

Notably, the analysis of experimental data demonstrated that the inlet configuration had a considerable impact on the characteristics of the flow through the tank (Texeira and Shiono, 1992). In fact, an appreciable 3D flow existed in the first three compartments, and a very significant part of the volume of these compartments was occupied by a recirculating and reversing flow field, as a consequence of the tank inlet design and the flow deflections by the tank walls. Also, the flow tended to be uniform over the water depth from Compartment 5 to about halfway along Compartment 8. Thus, the observations from this part of the tank could be applied to test a 2D model, which is actually not adequate to simulate the flow field in the whole tank (Wang and Falconer, 199b). Fig.2b presents velocity vectors in this part of the tank, i.e. Compartments from 5 to 7.

Figure 2b. Measured velocity vectors in the contact tank
It could be observed a good agreement with Multiphysics 3.2a™ 2D simulations since during the experiments rather large recirculating flow zones were identified behind the baffles, in Compartments 5-7. Also, small corner recirculating flow regions were observed in the transition region between the compartments. These separation regions produced dead-flow areas into the tank leading to a deviation from plug flow. These patterns are fairly reproduced by numerical results (Fig.3).

Fig.4 shows a comparison between longitudinal velocity along cross-section in the Compartment n.5 predicted by Multiphysics 3.2a™ and the field data, where $W$ is the width of the compartment. Negative values of the longitudinal velocity correspond to recirculation areas behind the baffle, but there is an overprediction of the velocities in the outer side of the compartment.

Figs.5a/5b presents results of the time-dependent analysis comparing in the case of a “burst” of concentration injection the experimental data measured in Compartments n.4 and n.5 with the corresponding numerical flow through curve (FTC) from Multiphysics 3.2a™. A good
agreement between experimental data and numerical predictions could be observed. The difference between model predictions and field data at the peak value in the Compartments n.4 and n.5 is of about 5.90% and 10%, respectively.

![Experimental data Multiphysics 3.2a](image)

**Figure 5b. FTC in Compartment n.5**

Further studies will be addressed to apply 3D model to the contact tank modeled in this paper.

### 4. CONCLUDING REMARKS

Recently, CFD models have been applied to investigate flow and solute transport in disinfection tanks. This paper presented preliminary results of a numerical study undertaken to investigate hydrodynamics and turbulent transport and mixing inside a contact tank. The configuration was previously experimentally studied by Shiono and Texeira [2000]. Flow field and mass-transport processes were simulated using $k$-$\varepsilon$ model and advection-diffusion equation with the software Multiphysics 3.2a™. Numerical results were in good agreements with the observed data for both flow field and tracer transport and mixing. Particularly, numerical results reproduced the recirculating flow regions that was experimentally observed behind the baffles and in the corners at the junctions between the baffles and the tank walls. Predicted flow through curves (FTC) for the case of a burst of a tracer concentration were in good agreement with the experimental data measured in each compartment. Since experimental works demonstrated that the flow could be considered as two-dimensional only in the compartments from n.5 to n.7, future studies should addressed to apply a 3D model to the tank.

### 5. REFERENCES


Multiphysics 3.2 User’s Guide, ComSol AB. Sweden, 2005


