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Modelling flow and concentration field in rectangular water tanks

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Abstract: Water storage tanks are usually designed with two objectives, i.e. to provide a specified maximum storage volume and to fix a certain total head over the water supply network. Only more recently, some attention has been paid to the water quality inside the storage tank since this can significantly affect the quality in the distribution systems. Sometimes conceptual models were proposed in the literature, but computational fluid dynamics (CFD) methods can be considered as the best analysis and predictive tool in storage tanks water quality studies.
In this paper, FLUENT®, a commercial CFD code, was applied to model flow and concentration field of a tracer within a 3D rectangular water tank. In the numerical study an approach based on the Reynolds Averaged Navier-Stokes (RANS) equations was applied, where the closure problem was solved by using the concept of turbulent viscosity. Particularly, the classical two-equation k-ε model was used. The transport of a tracer inside the tank was also simulated using advection-diffusion equation. Some indicators of mixing efficiency within a drinking water storage tank were presented and discussed. Finally, numerical results demonstrated that about 82% of the tank volume was under complete mixing conditions.

Keywords: environmental hydraulics, CFD, water quality modelling, rectangular water tanks, mixing indicators

1. INTRODUCTION.

Nowadays the use of the numerical methods in hydraulic network modelling is common. Nevertheless, the study and monitoring of water quality along the distribution network is an issue that is still under development. This is partially due to the difficulty to determine the effect of water quality on the networks. The presence of different points of injection and leakages, which can deteriorate suddenly the water quality, or the progressive age of mains make the problem more complex. In a hydraulic modelling framework, the tanks are complex systems, because the inherent complexity in terms of connections (inlets, outlets, control valves, etc.). If the study considers the evolution of the water quality, the problem is even more complex, because the tanks behave like chemical and biological reactors.
Several authors, such as Yeung [2001], Mahmood et al. [2005], Patwardhan, [2001] and Marek et al., [2007], have developed algorithms to address the issue of water quality in tanks. The objective was to make a three-dimensional model of fluid dynamics consistent with one-dimensional simulation of pipeline networks.
In this paper, FLUENT®, a commercial CFD code, was applied to model fluid motion and concentration field of a tracer within a 3D rectangular water tank. Also, the numerical study was used to define the parameters that represent the evolution of concentrations inside the tank considering different patterns of interchange flows. In the presented study a conservative substance was considered, ignoring the effects of chemical reaction. The study demonstrated that a CFD model is a useful tool to support the hydraulic modelling if

element complexity does not allow a complete mixing approach.

1.1 CFD models applied to water storage tanks

Few modelling studies of water quality in storage tanks are available in the literature. Chlorine decay inside the tank was assumed and related to conceptual transport models. These models consider the tank as an ideal reactor in two ways. On one hand the continuous flow stirred tank reactor (CSTR) consists of an intensively mixed volume in which there is a uniform concentration distribution. On the other hand the plug-flow reactor (PFR), where transport is only due to advection in the flow direction and complete transverse mixing is assumed, Gujer, [2008]. Mau et al. [1995]) developed an explicit model for simulating water quality in storages defining up to three different behaviours within the tank. Rossman [2000] includes four different models for tanks in the water quality solver of EPANET. The fraction of completely mixed conditions within the tank is a required parameter when studying water quality models in EPANET. However, the hydraulic processes in a storage tank are complex, so they cannot be properly described by these basic conditions. Water quality inside the tank as well as the water quality leaving the tank are largely affected by the tank flow patterns, which, in turn, depend on the tank internal arrangements. Modeling studies may be grouped as (Van der Walt, [2002]):

- black box models, in which a statistical or empirical relationship between inputs and outputs from the tank are established with no considerations for the actual flow conditions in the tank. Black box models are often used in pipe network analysis where the storage tank is part of a larger system. The above conceptual models are commonly used and complete mixing is mostly assumed in storage tanks. Actually, complete mixing, if easy to model, is appropriate for all tank configurations. Rossman and Grayman [1999] concluded that complete mixing holds only for cylindrical tanks with height/diameter ratios lower than 1 and operating under fill and draw conditions. In most cases, storage tank geometry results in large grey zones between complete mixing and plug flow conditions. Also, in complete mixing assumption, the dimensionless variables defined to characterize tank performance are based on total volumes and average flow rates;
- opaque box models, which divide a storage tank into zones or compartments that resemble reality better. Each zone represents prominent features of the storage tank such as mixing, plug flow or zones of short-circuiting. These models are also termed compartment models or system models (Grayman et al., [1996]). However, they require a priori assumptions on the flow in the compartments and their parameters cannot be measured in the field but must be derived by best-fit analysis on a set of field-measured inflow and outflow tracer concentrations (Grayman et al., [1996]). Thus, they can only be applied once the tank is built so cannot be used as a design tool. Finally, they need to be used with care if the operating conditions, on which the model was based, changed;
- glass box models, which have the objective to describe as completely and accurately as possible the flow patterns in a storage tank. These models do not need any a priori assumption on the flow characteristics as they are based on computational fluid dynamics (CFD) techniques, which can obtain sufficient spatial and temporal detail of the hydraulics by using mass and momentum conservation principles. Also, CFD can easy link flow field in the storage tank with the concentration field of a tracer by using the advection-diffusion equation. Thus, glass box models are real predictive models and can be applied to design tank. Finally, they can be easy adapted to different operational conditions.

From the previous discussion it is evident that the application of CFD methods to simulate turbulent flow patterns within the storage tank must be considered as the best approach in the analysis and design of storage tank if drinking water quality issues are of concern. Few CFD studies are available in the literature for drinking water storage tanks. Grayman et al. [1996] applied a CFD model to the Ed Heck cylindrical tank in Azusa, California, USA, pointing out significant non symmetric patterns across the tank cross section. They did not include thermal effects on the flow patterns that could explain some discrepancies between modeled and observed results (Grayman et al., [1996]). Hannoun and Boulos [1997] applied CFD techniques to the design and optimization of two proposed identical rectangular clearwells at the Mohawk water treatment plant in Tulsa, Oklahoma, USA. Both the clearwells were baffled, but in the second one a diffusion wall was added downstream of each turn. Each diffusion wall had 0.15 m sides square openings uniformly spaced in both the vertical and horizontal directions. Diffusion walls were aimed to provide a more uniform flow downstream of each turn. Simulations provided the ratio T_{10}/T, where T_{10} is the residence time of earliest 10% of the fluid to travel through the clearwell and T is the average residence time of the clearwell. This ratio is believed to be an important parameter in water and wastewater tank unit analysis (Gualtieri and Pulci Doria, [2007]; Texeira and Siqueira, [2008]) and is in widespread use for compliance with regulations (Hannoun and Boulos, [1997]). Model results demonstrated that the diffusion walls increased T10/T ratio of 10%, from 0.63 to 0.70 (Hannoun and Boulos, [1997]). Yeung [2001] applied a CFD model to study the behaviour of a range of service storage tanks with a rectangular plan form. Detailed analysis of flow distribution and water age suggested that tanks with horizontal inlets were better mixed than those with vertical top water level inlets. With increasing length to width ratio, the flow characteristics of tanks with vertical inlets increasingly resembled plug flow conditions (Yeung, [2001]). Mahmood et al. [2005] applied a CFD model to different types of storage tanks existing in the Virginia Beach drinking water distribution system. They used field measurements to validate CFD model and demonstrated that CFD methods are an effective tool in predicting mixing features in storage tanks and in providing useful insights in the design of location and orientation of inlet/outlet pipes and of internal arrangements of the tank. CFD studies were also carried out on the flow and entrainment processes in a jet-mixed tank (Patwardhan, [2002]; Marek et al., [2007]). Patwardhan validated CFD results by using experimental data. Marek et al. applied 3D unsteady Reynolds-averaged Navier-Stokes equations (RANS) to investigate several variations of jet velocity, nozzle diameter and nozzle angle in a jet-mixed tank. The CFD model was validated on the basis of previous literature experimental data and its results were compared with those obtained by Patwardhan (Marek et al., [2007]). Gualtieri [2009] investigated hydrodynamics and turbulent mixing inside a circular storage tank by applying two-dimensional steady-state and time-variable numerical simulations. Four internal configurations of baffles were compared using the Morrill Index (MI) as the main hydraulic performance indicator. Martinez-Solano et al. [2009] developed also a two dimensional model for simulating behavior of interchange in flows. CFD techniques were here used to analyze mixing inside tanks.

2. NUMERICAL MODEL OF RECTANGULAR WATER TANK.

2.1 Geometry and equations

A rectangular tank geometry was used to study the dispersion and mixing of tracer injected inside the volume of clear water. The tank had a volume of 1500 m^3 with dimensions 20×25 m and a water depth of 3 m. Figure 1 shows an overview of the simulated tank. The inflow to and outflow from the tank were around 50 L/s. Since the volume was 1500 m^3, these flowrates lead to a theoretical retention time of 8 hours, which is very small compared to those typically used in water tanks. Both inlet and outlet pipes had a diameter of 250 mm while the tracer was injected through a third pipe with a diameter of 40 mm. The incoming velocities were of 1 m/s in both main flow and tracer pipes. To get the velocity profiles completely established, in the simulations a length of 4 m was adopted for all the pipes.

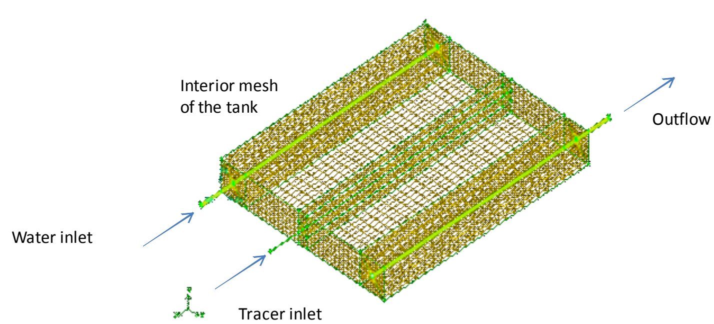

Figure 1. 3D geometry and mesh of the rectangular tank.

As previously outlined, CFD methods are considered the best analysis and predictive tool in storage tanks water quality studies. CFD models are based on the mass conservation equation and the Navier-Stokes equations of motion. Since the flow is turbulent, these equations must be averaged over a small time increment applying the Reynolds decomposition, where flow quantities are decomposed in a temporal mean and a fluctuating component. The application of this decomposition results in the RANS equations; where the turbulence effect appears as a number of terms representing the interaction between the fluctuating velocities. These terms are the Reynolds stresses. These equations provide the simplest level of modeling a turbulent flow. They introduce the closure problem, which can be solved, in analogy with the viscous stresses in laminar flow, by using a turbulent viscosity concept. For an incompressible 3D flow, the RANS equations are [FLUENT, 2005]:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial}{\partial x_j}\left(\rho \overline{u}_i \overline{u}_j\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{u}_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{u'_i u'_j}\right) \tag{2}$$

where ρ and μ are fluid density and dynamic viscosity, p is fluid pressure and u_i and u_j are velocity components in the i and j directions, respectively. The overbar and the prime indicates, rescpetively, time-averaged and fluctuating quantities. In the study FLUENT®, a commercial CFD software based on a finite volume method, was used, where RANS closure problem was solved by using the classical two-equations k-ε model (Launder and Spalding, [1972]). The standard k-ε model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ε). In this model, the flow was assumed to be fully turbulent and isotropic.

The transport of a tracer inside the tank was modelled using the 3D advection-diffusion equation [FLUENT, 2005]:

$$\overline{u}_i \frac{\partial \overline{C}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D_{t\text{-}i}\frac{\partial \overline{C}}{\partial x_i}\right) \tag{3}$$

where $D_{t\text{-}i}$ is the turbulent diffusion coefficient in the i direction and the effects of molecular viscosity were neglected. The tracer mass fraction was considered in the histogram calculated by the code. Turbulent diffusivity was derived from turbulent viscosity following Reynolds analogy. Their ratio is the turbulent Schmidt number Sc_t, which was assumed to be equal to 0.7.

2.2 Description of the mesh

The mesh was prepared using Gambit®. A roughness of 0.1 mm was adopted for the inner walls of the tank and the water level inside the tank was assumed to be constant. The mesh for the volume was prepared using a structured scheme with hexahedral cells with dimensions 0.33×0.33×0.5 m. The structured mesh was the most convenient in this sort of model. Several cell sizes were tested, combining simulation time, number of iterations needed and accuracy of the solution and finally a mesh with 19059 cells was used. A detail of the mesh in the proximity of the main flow inlet is shown in Figure 2.

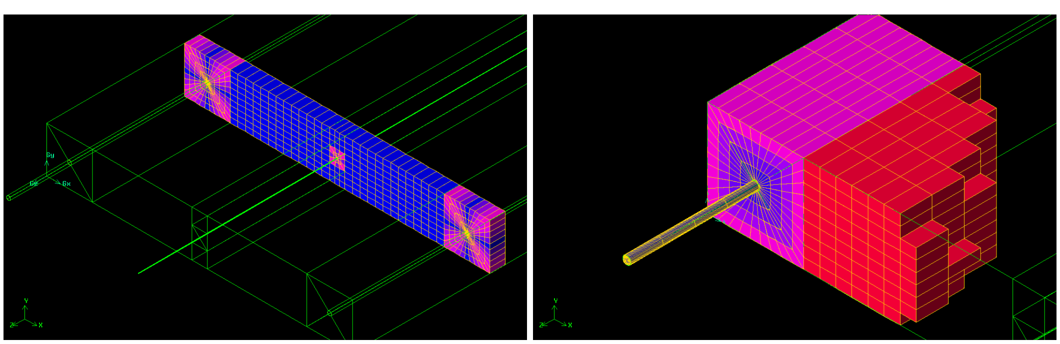

Figure 2. Detail of the mesh in this particular representation

The characteristics of the generated mesh are listed in Table 1.

Table 1. Mesh characteristics

Minimum face area (m²)	5.12×10^{-5}
Maximum face area (m²)	0.05
Number of cells	19059

2.3 Selecting the boundary conditions.

For the inlet pipes, a velocity inlet boundary condition was used. For the tank walls a no-slip wall condition with roughness of 0.1 mm was used. However, for the outlet and the free surface some possibilities were studied. For the free surface, a symmetry boundary condition was used first. This solution forced a higher number of iterations and smaller convergence criteria in order to satisfy continuity equation. This is due to the high difference between the area of the inlet and outlet surfaces on one hand, and the free surface on the other hand. Finally, a zero shear stress wall boundary condition demonstrated to behave better than the previously tested conditions and therefore it was used for the free surface of the tank. The outlet was first defined as a pressure outlet, but some problems were encountered with the continuity equation and the energy balance. Finally, the continuity in the flow was ensured with an outflow boundary condition. Figure 3 shows the boundary conditions adopted. To analyze the concentration along the mesh a conservative species transport model was selected, considering thus as indicator, the mass fraction of one of the fluid considered as the tracer along the cells. Mass fraction represents the fraction of volume in the cells occupied by the tracer in relation to that occupied by the water and it is considered as a percentage.

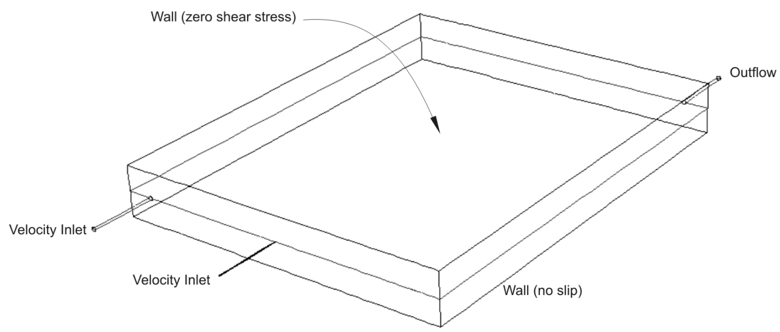

Figure 3. Boundary conditions defined for the rectangular tank

For the simulations, inlet turbulence parameters, such as inlet kinetic energy k and inlet turbulence intensity must be assigned. The turbulence intensity, I_T is defined as the ratio of the root-mean-square of the velocity fluctuations (u'), to the mean flow velocity, (u_{avg}). The turbulent length scale L_T is a physical quantity related to the size of the large eddies that contain the energy in turbulent flows. Also it is a measure of the size of the turbulent eddies that are not resolved. For fully developed turbulent flow these parameters can be obtained as [FLUENT, 2005]:

$$I_T = \frac{u'}{\bar{u}} = 0.016 \cdot Re^{-1/8}; \qquad L_T = C_\mu \frac{k^{3/2}}{\varepsilon} \tag{4}$$

where Re is the inflow Reynolds number. Usually, turbulence intensity ranges from 1% (low turbulence flow) to 10% (high turbulence flow). Table 2 lists some details of the turbulence boundary conditions at the inlets, where L_T, I_T and D_H are the turbulent length scale, the turbulence intensity and pipeline diameter, respectively.

Table 2. Detail on boundary conditions

Boundary condition	Inlet Turbulence Conditions
Inlet water	I_T=3.42% D_H= 0.125 m
Inlet tracer	I_T=3.92% – D_H= 0.02 m

Figure 4 shows the convergence process. A convergence criterion of 10^{-4} and 10^{-3} was assumed for continuity and turbulence parameters, respectively. The final number of iterations was 1387.

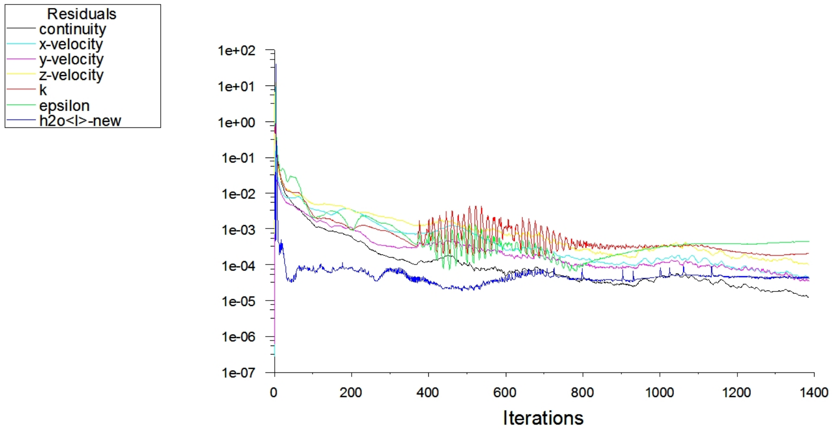

Figure 4. Residuals for iterations in the modelling

3. ANALYSYS OF RESULTS. DISCUSSION

Since the objective of this study was to simulate mixing processes within the tank, mixing parameters were considered. There are several parameters in the literature allowing to evaluate mixing processes (Teixeira and Siqueira, [2008]). They can be classified in two main groups: Eulerian and Lagrangian parameters (Sturman and Wiggins, [2009]).
The parameters in the first group, i.e. Eulerian parameters, are related to the effort made to get mixing and are mainly based in hydrodynamic variables. This is an indirect parameter to evaluate mixing inside the tank. Power input to the tank is the main variable. Examples of parameters in the first group are the power number, the turbulence intensity (mainly used for mechanical mixers), the detention time, and the velocity gradient as described in Metcalf & Eddy [1995]. The two latter are used for both mechanical and static mixers.
The second group (Lagrangian parameters) directly evaluates the level of mixing itself. Obviously, in this case the main variable is the concentration or its distribution within the tank. Some examples of these parameters are the concentration histogram, the cumulative distribution or the standard deviation. These parameters provide better information on mixing, but are more difficult to obtain. This paper focused on the histogram as a way for evaluating mixing.

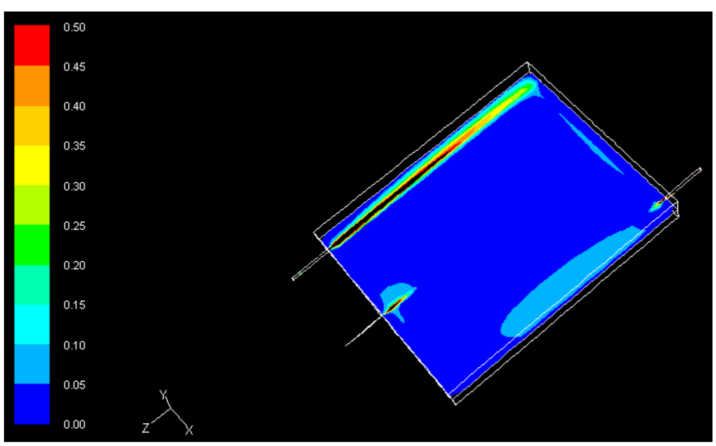

Figure 5. Detail of velocity magnitudes (in m/s) at mid-depth of the tank.

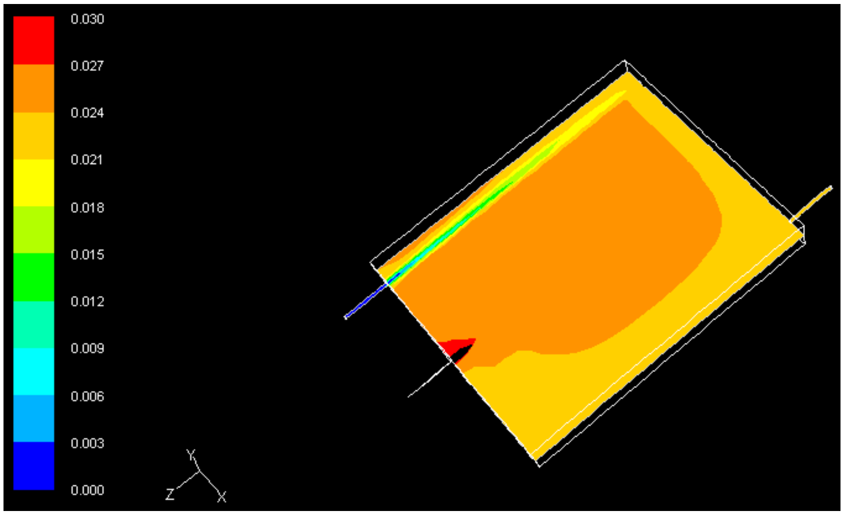

Figure 6. Illustration of the tracer mass fraction at mid-depth of the tank.

In this study, some parameters representing the mixture in the tank were analyzed. Figure 4 shows flow field in the central plane of the tank. Velocity variation due to the inlet pipes can be noted. Figure 5 presents the tracer distribution in the central plane of the tank. A good correlation between velocity and concentration gradients can be observed. In fact, in static mixers the turbulence is assumed to promote the mixing and depends on the velocity among many other factors. Mixing is high when the difference between concentrations is small. So, a good method of quantifying the tracer distribution is to use a histogram of the concentration.

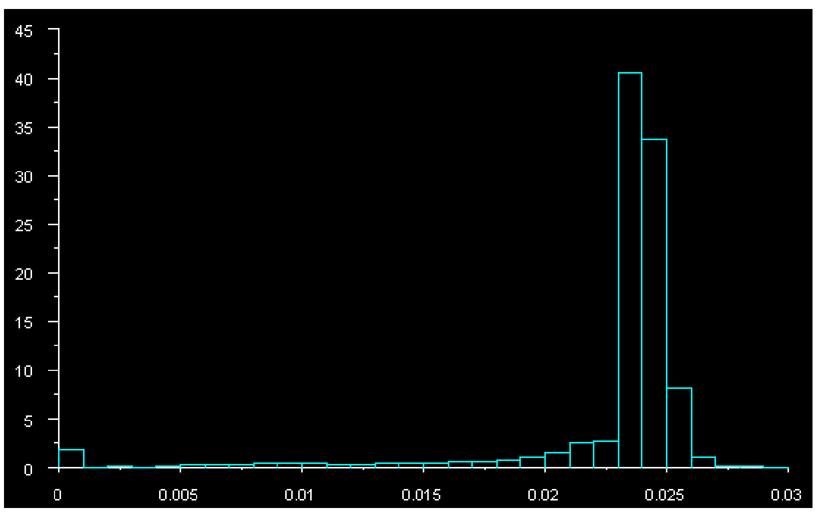

Figure 7. Histogram of mass fraction

Figure 7 shows the histogram of mass fraction in the tank. It can be observed that the mixing was relatively strong, with most of the cells with a concentration very near to the expected average concentration of 2.50%. A classic Lagrangian measure for quantifying mixing is the variance of the concentration (Sturman and Wiggins, [2009]). In this case, the variance is $2.88 \cdot 10^{-3}$ for the calculated average concentration of 0.025 (2.5%). Another metric was proposed: the fraction of completely mixing in the tank. The completely mixed fraction of the tank may be defined as that in which the concentration reaches the value of mean ± 10%, based on experiences in CFD modelling for this type of systems. This percentage may be considered as arbitrary, but has been used as a way to compare different tank settings (Martínez-Solano et al. [2006]). The completely mixed fraction of a completely mixed tank will be of 100%. On the contrary, in a tank with a tracer uniformly

distributed and with the same average value this fraction will be of 20%. Therefore, it can be stated that the mix in this tank is closer to a completely mixed tank rather than an uniformly distributed tank.
Under this approach a first histogram was yielded, to determine the percentage of the volume of the tank which was under the mixed situation. Thus, when representing the value of the accumulated concentration (Figure 8), it was noted that virtually most of the volume enclosed in the tank containing a concentration around 2.5%. This value was used in presenting the results. As considered, a deviation of ±10% around this value provides the concentration range to consider complete mixing, which in this case comprise between 2.25 and 2.75% of concentration. Figure 8 represents the mass fraction (x-axis) vs. the number of cells in which this value is present in the model results.

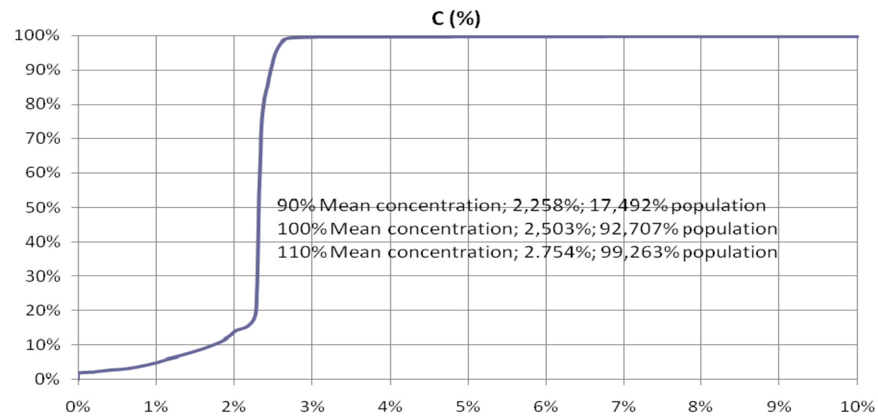

Figure 8. Cumulative histogram of mass fraction

From simulation results, it was possible to determine the percentage of the volume of the tank which was under the complete mixing condition. From the graph in Figure 8, about 81% of the tank volume was under complete mixing.
Another aspect that might be taken into account is the power needed to get a good mixing. Rushton and Oldshue [1953] defined the power needed to get a mixing in a static mixer as:

$$P = \Delta p \cdot Q \qquad (5)$$

where P is the power, expressed in W, Δp is the pressure drop through the mixer (in Pa) and Q is the flow rate that crosses the mixer (in m^3/s). In our problem, the flow was set in 50 L/s and the pressure drop calculated by the model is 13277 Pa. With this data, the power consumed by the tank was around 687 W. Since there is a need to relate power and tank size, Metcalf & Eddy [1995] proposed the use of the velocity gradient as a method to quantify the performance of mixers in water engineering. The velocity gradient can be calculated as:

$$G = \sqrt{\frac{P}{\mu \forall}} \qquad (6)$$

where $\forall$ is the volume of the mixer. In this case, the velocity gradient was 21.4 s^{-1}. This value is very small and close to those in flocculators in water and wastewater treatment plants.

Table 3. Typical values of detention time and velocity gradient in different wastewater treatment processes (adapted from Metcalf & Eddy, Inc., [1995])

Process	Detention Time	Velocity Gradient (s^{-1})
Typical rapid mixing	5 – 20 s	250 – 1500
Rapid mixing in contact filtration	< 1 – 5 s	1500 – 7500
Typical flocculation processes	10 – 30 min	20 – 80
Flocculation in direct filtration	2 – 10 min	20 – 100
Flocculation in contact filtration	2 – 5 min	30 – 150

Water distribution tank (this study)	8 hr	21.4

Table 3 lists typical values of detention time and velocity gradient in different water and wastewater treatment processes (Metcalf & Eddy, Inc., 1995).

4. CONCLUSION. FUTURE RESEARCH

The paper proposed a protocol for the mixing analysis inside a drinking water tank with different behaviour of interchange. This protocol was based on CFD simulations, which provided flow and concentration field inside the tank. In turn, these results were applied to determine the level of mixing in the tank by using some parameters, such as velocity gradient, concentration histogram and concentration cumulative distribution. The analysis of flow and concentration fields pointed out a good correlation between velocity and concentration gradients. Second, the histogram of mass fraction in the tank showed that with most of the cells had a concentration very near to the expected average value. Third, numerical data demonstrated that about 82% of the tank volume was under complete mixing conditions. Finally, the velocity gradient inside the tank was quite small and in the range of those typical in flocculators of water treatment plants.

Future research will be addressed twofold. First, to allow an objective estimation the level of mixing in tanks, some correlations must be done between the parameters presented in the paper and other traditional parameters. Second, this protocol must be applied as complementary tool to EPANET, which is the most widely applied software in water quality studies for water distribution networks.

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