Computational Fluid Dynamics (CFD) applied to design and optimization of drinking water treatment facilities

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Abstract

This paper describes some examples of the use of CFD approach for the improvement of drinking water treatment facilities performance. It is shown, through the present study, that this simulation tool can be used successfully to make reasonable predictions for water hydrodynamics and disinfection efficiency over a range of different contactor geometries and flow conditions. The multiple advantages of this method explain its current use in full-scale facilities operation and process optimisation schedule as a reliable design and refinement tool. The data obtained by the numerical model provides a detailed knowledge about the fundamental flow features which are of extreme importance for the understanding of the phenomena of mixing and mass transfer. CFD model generation is less time consuming, more easily adjustable and more flexible than its equivalent physical model.

1 Introduction

Successful design and operation of reliable water treatment facilities has always been, and continues to be, a major concern to public health and water treatment professionals. Growing public concern, in addition to stricter legislation pertaining to the quality of drinking water, has led to more stringent contaminant regulations, which are affecting the treatment technologies (1). It was therefore necessary to optimise the existent contactors in order to meet the primary goals of adequate microbial disinfection, control of taste-and-odour compounds, and reduced disinfection by-products formation. Significant improvements of water treatment systems performance and process design optimisation can be undertaken in conditions of better understanding of the phenomena occurring in these systems. The last implies the use of more precise and more complex tools for scientific analysis such as, for example, the Computational Fluid Dynamics (CFD) hydraulics modelling approach which can replace classical tracer studies.

2 Objective

The main objective of this study is to ensure the final water quality by meeting the necessary CT_{10} value at the end of treatment. The improvement of the hydrodynamics in a group of three chlorination contactors is presented as an example. The main idea is to optimise water flow pattern in the entire system by proposing an internal baffling and imposing the flow in each contactor so that maximum contact time is achieved.
Different shapes of contact chambers are used today and very few rules exist to determine the relationship between contactor's geometry and its efficiency. Tracer studies and numerical modelling are the methods used nowadays to characterise hydrodynamics in these systems.

3 Material and Methods

The system studied was composed of three contactors situated in series. The entire volume is of 7000 m3. Figure 1 (view above) shows water flow in the system. Water, filtered on GAC (granulated activated carbon) arrives in reservoir R1 where it is chlorinated and then transferred to R2 and R3. The complexity of the system lies in the fact that multiple inlets and outlets exist so water leaving the system has different contact times and in the final mixture the contribution of each contactor must be quantified.

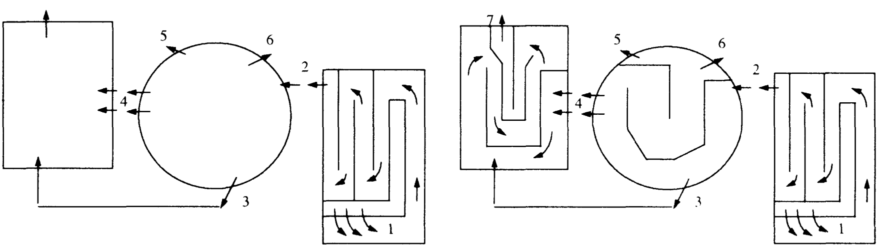

Figure 1a. Initial configuration *Figure 1b*. Modified chain

In order to characterise the hydrodynamics of a given contactor, tracer studies are the most common technique. But the use of CFD modelling and simulation is becoming very current in the recent couple of years. The basis of this approach is the theory of turbulent motion which consists in resolving a highly non-linear system of partial differential equations of fluid motion, the Navier-Stokes equations, in each point of the fully three dimensional flow by numerical

methods such as the finite volumes or the finite elements (2). Usually, the studied flows are steady, three-dimensional, single- or two-phase, turbulent, incompressible and newtonian. The different stages of CFD model elaboration can be described as following : numerical mesh construction, boundary conditions specification, transport equations solution, results post-treatment.
The output data obtained provides a detailed description of water flow inside the contactor (velocity vector field, nature and intensity of turbulence, pressure field, tracer concentration field, residual chlorine concentration field, residual micro-organisms concentration field). The information thus acquired, enables a better understanding and interpreting of hydrodynamic phenomena.
The software used to perform simulations (ESTET) was developed by EDF Hydraulics Research Laboratory (France) on the basis of the finite volumes method of discretisation for the solution of partial differential equations system. This software operates on Hewlett Packard or Silicon Graphics Unix workstations.

4 Model Geometry and Boundary Conditions

An appropriate set of assumptions was made concerning contactor flow conditions. It was assumed that the flow was three-dimensional, fully-turbulent, incompressible, steady, isothermal with constant properties. Turbulence was taken into account by using a standard k-ε model solving two additional transport equations - one for the turbulent kinetic energy k and one for the dissipation ε of this energy. The boundary conditions used are resumed in the table 1 herebelow.

B. C.	INLET JET 1	FREE SURFACE	WALL	OUTLET 2,3,4	OUTLET 5,6
VELOCITY	Ux = 0	$\frac{\partial U_X}{\partial z} = 0$	Ux = 0	Ux = free	Uz = free
	Uy = 0	$\frac{\partial U_Y}{\partial z} = 0$	Uy = 0	$\frac{\partial U_X}{\partial z} = 0$	$\frac{\partial U_Z}{\partial x} = 0$
	Uz = const.	Uz = 0	Uz = 0	$\frac{\partial U_Y}{\partial z} = 0$	$\frac{\partial U_Y}{\partial x} = 0$
TURBULENCE	$k = 0.003U_X^2$	$\frac{\partial \varepsilon}{\partial z} = 0$	$\frac{\partial k}{\partial n} = 0$	$\frac{\partial \varepsilon}{\partial z} = 0$	$\frac{\partial \varepsilon}{\partial n} = 0$
	$\varepsilon = 6\frac{k^{1.5}}{D}$	$\frac{\partial k}{\partial z} = 0$	$\varepsilon = \frac{0.16k^{1.5}}{0.41y}$	$\frac{\partial k}{\partial z} = 0$	$\frac{\partial k}{\partial n} = 0$

Table 1. Boundary conditions for the numerical simulations

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After the numerical mesh construction and boundary conditions specification, the finite volume model was run to obtain converged flow solution. The flow solution provided a detailed representation of the velocity, turbulent characteristics and pressure field.
Most of disinfection reactions tend to be of first order and proceed at a rate which is proportional to the micro-organisms concentration and can be expressed by Chick-Watson's law. US EPA used data obtained in batch conditions to define the so-called CT_{10} rule for drinking water disinfection efficiency estimation. It was already demonstrated (3) that this concept is meaningless in practice without data on the hydraulic behaviour of the system.
In order to estimate the T_{10} contact time, a hydrodynamic study must be performed providing tracer analysis data or numerical simulation results. In a complex system like the one considered (several reactors communicating by multiple inlets and outlets) experiences are extremely difficult to be carried out and to be exploited. That 's why a CFD model has been elaborated to describe the flow in the entire system. The overall T_{10} is then estimated as an average by applying the concept of « parallel streaks flow » (4). According to this concept the flow of the fluid can be represented as a multitude of streaks which can be classified in an increasing order of their residence time. The fluid enters simultaneously in each streak and leaves progressively at different times increasing from the bottom to the top. Each part of fluid leaving the system is considered separately as a streak transversed by a fraction of flow rate $dQ=q(t_s)dt_s$ with a uniform velocity $u(t_s)$. Thus, the length of each streak is proportional to its residence time ($L(t_s) = u^*t_s$) as it is shown on figure 2.

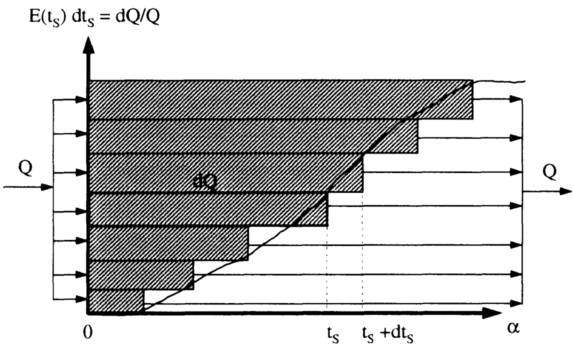

Figure 2. Schematic representation of the « parallel streaks flow » concept

Through an elementary streak the reaction evolves in a plug flow manner and the concentrations change as a function of the age of the fluid. The equation of mixing is given by :

$$C_{out} = \int_{streaks} C_{in}(t_S)\frac{dQ}{Q}$$

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5 Results and Discussion

The experimental work was carried out on two successive levels : velocity vector field calculation and Residence Time Distribution curve simulation.

5.1. Contactor R1

Operating conditions : Water flow rate = 2100 m^3/h
Volume = 2870 m^3
HRT = 82 min

The first reactor R1 is well-optimised and has a nearly perfect plug flow. The model identified from tracer study data was 25 CSTR in series and a T_{10}/τ ratio of 0.73 (fig. 3). It provides 40 % of the entire water contact time.

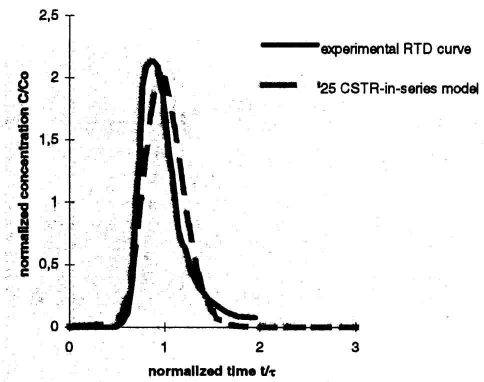

Figure 3. Residence Time Distribution curve for contactor R1

5.2. Contactor R2

Operating conditions : Water flow rate = 4800 m3/h
Volume = 1320 m3
Diameter = 29 m
Water height = 2 m
Mean hydraulic residence time = 17 min

The second reactor R2 has only one inlet through which it receives water coming from the first one but it has five outlets - three communicating with the third reservoir and two sending water directly to distribution. The total volume of this reactor is 2000 m^3 but because of the existing short-circuits phenomena an important part of water in this contactor has very low contact time (fig. 1a). In order to avoid bad performance and improve flow pattern simulation of baffling has been realised (fig. 1b).

The five outlets are operating under the following conditions (see figure 1b) :
Point 2 : inlet (water coming from R1)
Point 3 : outlet supplying 770 m^3/h to R3 (16 % of total flow rate)
Point 4 : outlet supplying 530 m^3/h to R3 (11 % of total flow rate)
Point 4 : outlet supplying 530 m^3/h to R3 (11 % of total flow rate)
Point 5 : outlet supplying 2160 m^3/h to distribution (45 % of total flow rate)
Point 6 : outlet supplying 810 m^3/h to distribution (17 % of total flow rate)

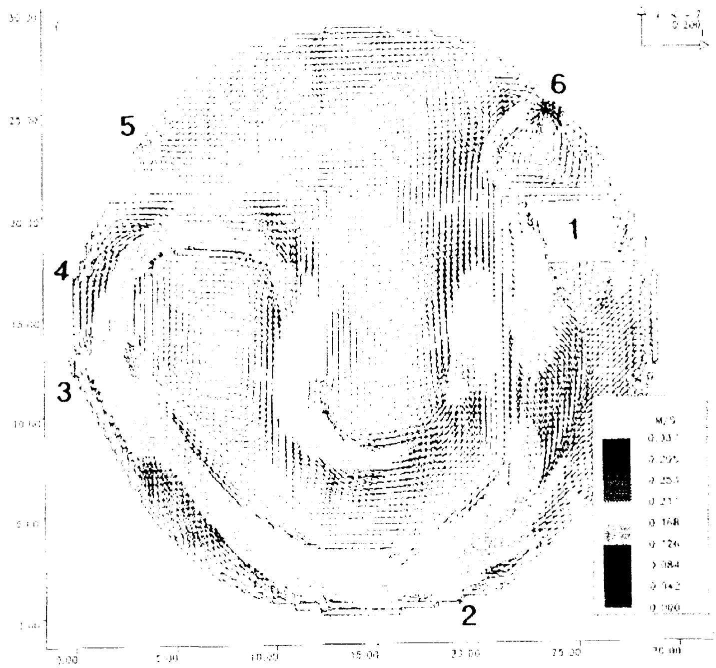

Figure 4. Vector velocity field in a horizontal plane of the reservoir R2

The numerical mesh of this 3D model was composed of 111 100 nodes in cartesian co-ordinates. Figure 4 shows the simulated velocity vector field on a horizontal cross section of the reservoir near the bottom in order to allow the visualisation of all singularities of the flow (points of inlet and outlet). Different flow patterns can be noticed - plug flow in the narrow parts along the baffles and recirculation zones near the inlet and the outlets where mixing takes place. The reservoir is supplied in water by a big pipe (cross section = 9 m^2) situated at the bottom and orientated towards the surface (point 1). Water enters

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in at about 0.15 m/s with a fountain-like flow which allows good vertical mixing. In the zone immediately next to the inlet complete mixing is attained very rapidly. Then the flow is guided in the peripheral zone of the tank by the main baffle which creates a plug flow pattern. Three of the outlet pipes are situated in this zone (2, 3, 4) and 1830 m^3/h is thus evacuated towards the next reservoir at this stage (nearly 40% of the total flow rate). The pumps 5 and 6 pump water out towards the distribution network. The most important velocities can be noticed in the region of the pump 6 (0.33 m/s), elsewhere inside the contactor the mean velocity is comprised between 0.05 and 0.2 m/s.
The proposed baffling allows the optimisation of the hydrodynamics in dependence to the fixed objectives and without any over-cost in baffling (in terms of civil engineering).

In a second stage a tracer has been injected according to the step method in the reservoir and its convection by the mean flow has been simulated as a function of time. Figure 5 shows the concentration field 1000 seconds after the tracer step input. Following tracer concentration evolution in time in the nodes specifying each outlet, it was possible to determine the mean residence time of each fluid fraction leaving the system (by the application of the « parallel streaks flow » concept) in order to estimate an average T_{10} for the entire system. A bundle of RTD curves (one for each outlet) was obtained which is presented on figure 6.

Figure 5. Tracer concentration field 1000 sec after the step input

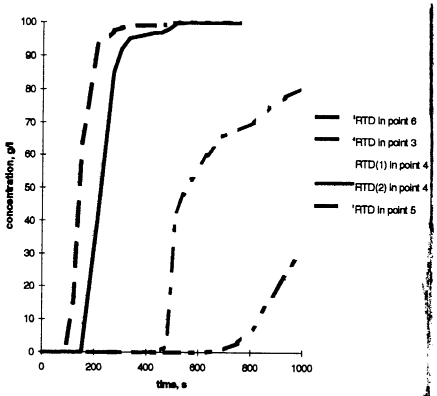

Figure 6. RTD Curves predicted by the CFD model for R2

5.3. Contactor R3

Operating conditions : Water flow rate = 1830 m3/h
Volume = 2000 m3
Length = 28.2 m
Width = 23.7 m
Water height = 3 m
HRT = 65 min

The third reservoir R3 has only one outlet connected directly to the distribution pipe but has three separate inlets by which it is supplied in water coming from R2. The total flow rate is divided between the different inlet in the following manner :

Point 1 : first inlet supplying 530 m3/h (29 % of total flow rate)
Point 2 : second inlet supplying 530 m3/h (29 % of total flow rate)
Point 3 : third inlet supplying 770 m3/h (42 % of total flow rate)
Point 4 : outlet pump evacuating 1830 m3/h towards the distribution network

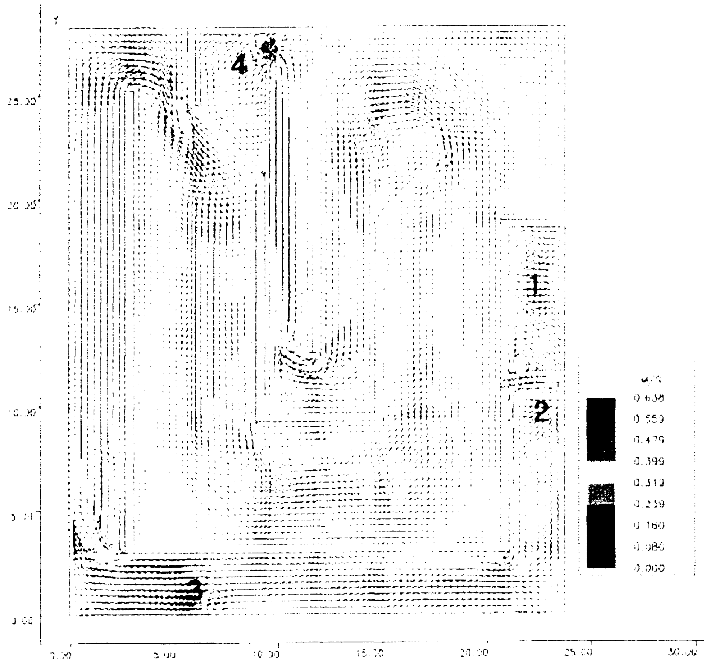

Figure 7. Velocity vector field in a horizontal plane near the bottom

Except from the nodes of the inlets and the outlet where the highest velocities are obtained (0.6 m/s), the entire fluid volume in the contactor is concerned by

relatively low velocities comprised between 0.08 and 0.16 m/s (fig. 6). The flow is conditioned by the internal baffles which impose quite successfully a plug flow pattern in the system. Small recirculation zones can be observed though, in the corners of the reservoir and behind each baffle.
The tracer concentration field in the contactor is represented on figure 8 1900 sec after the step input.
Between the group of first two inlets (1 and 2) and the inlet 3 the water has a plug flow character and the corresponding volume represents less than 10 % of the entire reservoir. That's why the three inlets have been considered as one for the RTD curve simulation and T_{10} determination. Thus, the calculated T10/t ratio for the entire contactor R3 was 0.65 which shows that the hydrodynamics has been well optimised. The hydraulic behaviour of the system can be compared to the performances of a 10 CSTR-in-series model as it is suggested on figure 9.

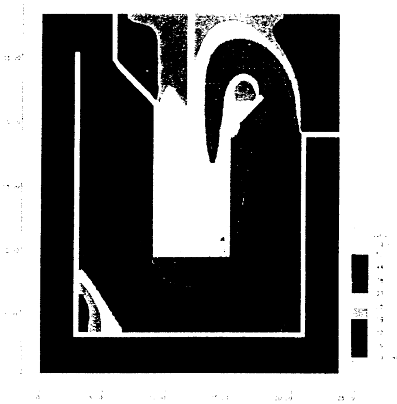

Figure 8. Concentration field in a horizontal plane about 1m below the free surface

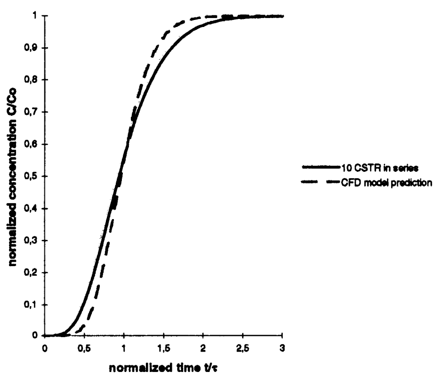

Figure 9. RTD curve for the contactor R3

Simulation results have been compared to the experimental measures and a good correlation between the numerical model predictions and the reality was found (5,6).

6 Conclusion

The study presented here was orientated towards improvement of water quality and increasing the performances of chlorine contactors by using the CFD approach.
CFD simulation tools are achieving increasing popularity due to the development of faster computers and high accuracy of numerical techniques.

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This work shows that data obtained by CFD approach provides more comprehensive and detailed information about the nature and the particularities of the flow which is of extreme importance in the design improvement procedure. That's why further application of these models to other water treatment processes such as ozonation and filtration is now in course of study. Some predictions for the local efficiency of the disinfection process were realised as well. Further application of this method can be used to study the impact on water quality of storage tanks (long residence times, loss of disinfection residuals) and distribution system network (growth and propagation of micro-organisms).

Key Words

Chlorination tank, Hydrodynamics, Modelling, Tracer studies, CFD, Optimising Flow Pattern, CT Concept, Disinfection Efficiency

GLOSSARY

C	current tracer concentration, *mg/l*
Co	intial tracer concentration for the step input or homogeneous tracer concentration for the pulse input at the inlet (quantity of tracer injected divided by contactor volume), *mg/l*
t	time, *mn*
$\mathbf{T_{10}}$	contact time (time necessary for 10% of tracer injected to be recovered at the outlet), *mn*
τ	hydraulic residence time HRT (contactor volume/flow rate), *mn*
Ux, Uy, Uz	three dimensional velocity components, *m/s*
k	turbulent kinetic energy, m^2/s^2
ε	turbulent kinetic energy dissipation, m^2/s^3

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