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EFFECT OF THREE-DIMENSIONAL MIXING CONDITIONS ON WATER TREATMENT REACTION PROCESSES

ATHANASIOS ANGELOUDIS[(1)], THORSTEN STOESSER[(2)], CARLO GUALTIERI[(3)] & ROGER FALCONER[(4)]

[(1)] *Hydro-environmental Research Centre, Cardiff University, Cardiff, UK, angeloudisa@cf.ac.uk*
[(2)] *Hydro-environmental Research Centre, Cardiff University, Cardiff, UK, stoesser@cf.ac.uk*
[(3)] *Civil, Construction and Environmental Engineering Department, University of Napoli "Federico II", Napoli, Italy, carlo.gualtieri@unina.it*
[(4)] *Hydro-environmental Research Centre, Cardiff University, Cardiff, UK, falconerra@cf.ac.uk*

ABSTRACT

The performance of water disinfection facilities traditionally relies on Hydraulic Efficiency Indicators (HEIs), extracted from experimentally derived Residence Time Distribution (RTD) curves. This approach has often been undertaken numerically through computational fluid dynamics (CFD) models, which can be calibrated to predict accurately RTDs, enabling the assessment of disinfection facilities prior to the construction of disinfection tanks. However, a significant drawback of the conventional efficiency methodology prescribed for disinfection tanks is associated with the respective indicators, as they are predominantly linked to the internal flow characteristics developed in the reactor, rather than the disinfection chemistry which should be optimized. In this study three-dimensional numerical models were refined to simulate the processes of chlorine decay, pathogen inactivation and the by-product formation in disinfection contact tanks (CTs). The main objective of this study was to examine the effect of three-dimensional mixing on the reaction processes which were modelled through finite-rate kinetic models. Comparisons have been made between pathogen inactivation and disinfection by-product accumulation results produced by a RANS approach against the findings of a Segregated Flow Analysis (SFA) of conservative tracer transport. CFD Results confirm that three-dimensional mixing does have an effect on the reaction processes, which, however, is not apparent through the SFA approach.

Keywords: Contact Tanks; Water Disinfection; CFD; By-Products.; Pathogen Inactivation

1. INTRODUCTION

Water disinfection is a process designed for the inactivation of pathogenic micro-organisms in order to prevent the transmission of waterborne diseases. It normally occurs through the exposure of the water in the tank to disinfectant concentration doses for sufficient time to inactivate pathogenic microorganisms, in appropriately designed contact tanks (CTs). Serpentine contact tank units in particular suggest plug flow to be the optimal hydrodynamic condition at which disinfection performance is maximized (Rauen et al., 2012; Zhang et al., 2014). On the other hand, previous studies (e.g. Teixeira, 1993) indicate that the flow in CTs exhibits a residence time distribution (RTD) which is often significantly different from that dictated by plug flow. This digression is attributed to complex hydrodynamic processes, such as short-circuiting and recirculation zone formation (Kim et al., 2013a). The occurrence of internal recirculation and short-circuiting has been associated with a detrimental effect on the overall CT efficiency, since the exposure of pathogens with the disinfectant is either too short (insufficient treatment) or too long, which can result in the production of excessive disinfection by-products.

The US EPA's Surface Water Treatment Rule promulgated the Ct concept for the performance assessment of disinfection facilities, according to which the water has to remain in contact with a certain concentration of disinfectant (C), for a sufficiently long enough time t, so as to provide the desirable level of inactivation for different water quality conditions and disinfectants (Rauen et al., 2012). Pathogen inactivation is deemed to be achieved once the Ct product exceeds reference values (AWWA, 1990) derived empirically. The use of T as the contact time for the Ct product calculation is not recommended, since this does not take into consideration the hydraulic efficiency of the tank. Instead, guidelines recommend the use of the hydraulic efficiency indicator (HEI) t_{10}, which corresponds to the time elapsed in a tracer experiment for the passage of 10% of the injected tracer mass through the outlet monitoring section (Johnson et al., 1998).

A novel experimental technique for the assessment of pathogen inactivation was outlined by Asraf-Snir and Gitis (2011) which involved fluorescent labelling of microorganisms and injecting them as tracers in a bench-scale reactor, operating

with a constant feed of chlorine. It was argued that the residence time of a solute within a reactor is affected by the size of the solute particles. Some of the aspects of their investigation are of particular interest, firstly because it is the only reported application of reactive tracer experiment methodology to serpentine CTs and secondly due to some experimental considerations that serve as an example of how CFD, and specifically RANS approaches, can more practically be used as an optimization tool for disinfection processes. Namely, the hypothesis that the solute particle size is determinant to the outlet RTD shape is largely dependent on the hydrodynamic conditions established in the reactor. This applies under specific circumstances where molecular diffusion is comparable or larger than turbulent diffusion, a condition which is encountered in laminar flows. This was the case in the study of Asraf-Snir and Gitis (2011) as based on the specifications of flow and scale of their laboratory model, the Reynolds number was low (<100). In contrast, the flow developed in field scale models is characterized by a turbulent flow regime, where the effect of particle size on solute transport can be considered negligible compared to turbulent diffusion. This is an example of how the small scale of laboratory models can be problematic when reproducing the conditions encountered in larger scale.

Even if the dynamic similitude is retained and the Reynolds number is within an acceptable range (e.g. ≥ 3795; Teixeira and Rauen, 2013), an inevitable consequence of the reactor scale difference is that the tank retention time would be distorted. On the other hand, disinfection kinetics is heavily dependent on contact time (or theoretical retention time) while the hydrodynamics developed at the particular geometry are crucial for the reactant mixing. By adjusting the flow rate to match the contact time, the hydrodynamic flow structure is modified and the dynamic similitude between small-scale and field-scale model is lost. As a result, the disinfection under a specific contact time can only accurately be examined at full-scale conditions since only then the scaling effects associated with the hydrodynamics, surface roughness and contact time are absent. This is an advantage of developing a CFD methodology to simulate the disinfection efficiency directly at field-scale CTs, a practice which can be more flexible and inexpensive than conducting experimental investigations at such facilities.

Computational Fluid Dynamics (CFD) techniques have been extensively implemented to simulate flow conditions and mixing processes during the operation of CT facilities (Rauen et al., 2012; Gualtieri, 2006) with a view to predict hydraulic efficiency indicators (HEIs) for proposed CT designs (Kim et al., 2013a; Stamou, 2008). Unfortunately, HEIs cannot indicate disinfection specific parameters, such as optimum disinfectant dosage, pathogen survival levels or by-product formation potential, i.e. invaluable information for the operation of CTs which are often determined using empirical formulations, such as the Ct concept. Such parameters could be potentially deduced through the integration of disinfection kinetics into computational models, a practice which has only recently been reported in the literature (Angeloudis et al., 2014a,b,c; Wols et al., 2010; Zhang et al., 2000).

In this paper a 3D numerical model was refined for the representation of reactive tracer transport and disinfection processes in a small-scale contact tank model. Reactive simulations are discussed below featuring instantaneous injections of microorganisms and by-product precursors, applied in a geometry featuring turbulent flow regime and assuming molecular diffusion is negligible. The results were in turn compared with a refined Segregated Flow Analysis (SFA) approach which, however, does not take into account the effects of three-dimensional mixing within the reactor.

2. RESEARCH METHODOLOGY

2.1 Contact Tank Model and Experimental Data

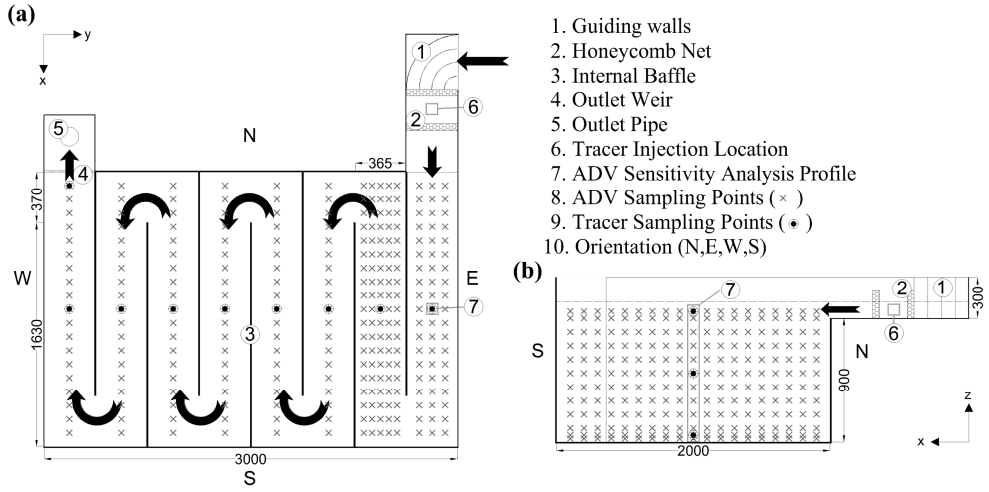

Figure 1. Contact Tank Configuration

All experimental data were acquired using a scaled disinfection tank, located in the Hydraulics Laboratory at Cardiff University (CT-1). It exhibited standard features of a baffled CT, i.e. the tank was separated into eight compartments through which the flow meandered due to the baffles being arranged in an alternating fashion (Angeloudis, 2014; Angeloudis *et al.*; 2014c). A constant flow rate of 4.72 l/s was set when collecting velocity measurements, which corresponded to a bulk velocity U_b of 12.5 mm/s and a tank theoretical retention time ($T=V/Q$) of 1265 s. Pulse tracer experiments involved Rhodamine WT injections at the inlet, while submersible sensors monitored fluorescence levels at designated locations for the production of normalized RTD curves. Figure 1 illustrates the laboratory model's main geometric features and also indicatively depicts velocity measurements and tracer sampling locations for the CT-1 configuration.

2.2 Computational Fluid Dynamics Models and Reactive Tracer Experiments

Reynolds Averaged Navier Stokes (RANS) simulations of the hydrodynamics were performed implementing a finite-volume approach on a structured orthogonal grid. A Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) was applied to couple the pressure to the velocity field and the standard k-ε turbulence closure was included to compute the Reynolds Stresses. Once the steady state flow field was obtained, the transport of scalar quantities were simulated by solving the three-dimensional Reynolds-averaged advection-diffusion equation. Details of the numerical methods, computational model setup, grid independency and validation of the CFD approach are not repeated here and the interested reader is referred to previously published work (Kim et al., 2013b, Angeloudis, 2014; Angeloudis et al., 2014a,b,c).

Reactive simulations were conducted for a chlorine disinfection scenario where, as soon as chlorine was introduced, it reacted with both organic and inorganic substances, leading to a process of decay. This decay rate is normally described through a first-order kinetic model. However, preceding studies (e.g. Brown et al., 2011) have illustrated that the initial introduction of chlorine in CTs is subject to contact with fast-reacting compounds. This is associated with a period of more rapid chlorine consumption, typically within the first 5 minutes of chlorination, and has been reported to correspond to a 37-53% decrease from the initial dosage concentration (Brown et al., 2010). In order to account for these effects, a semi-empirical parallel decay model was adopted as a source term for the solute transport of chlorine, given as:

$$\frac{\partial C_{Cl}}{\partial t} = -k_{FR} C_{FR}\, C_{Cl} - k_b C_{Cl} \qquad [1]$$

where C_{Cl} = the chlorine concentration (= 2.0 mg/l) and k_b = the disinfectant bulk decay rate (=2.77×10^{-4}s^{-1}). C_{FR} (=1 mg/l) is the concentration of fast reacting compounds and k_{FR} (4×10^{-3}s^{-1}) is the consumption rate of chlorine due to these compounds, respectively. C_{FR} itself was modelled to follow rapid first-order decay and became negligible after 5 min of contact time, minimizing the influence of fast reactants for the remainder of the process. The inactivation rate within the current investigation was represented in the pathogen transport model through the Hom model (Hom, 1972):

$$\frac{dN}{dt} = -mk' C^n t^{m-1} N \qquad [2]$$

where N = the microorganism population, n = a coefficient of dilution and m = an empirical constant. For *G.Lamblia* protozoa, *k'* was given a value of 8.04×10^{-4} (mg Cl/l)$^{-n}$(sec)$^{-m}$ for m = 1.20 and n = 0.96, in accordance with the investigations of Haas *et al*. (1995).

Recent concerns over the formation of potentially carcinogenic by-products during chlorination have led to the development of a wide range of mathematical models to predict the formation of by-products (Sadiq and Rodriguez, 2004). The accumulation of Total Trihalomethanes (TTHMs) has been considered in this study, by including an appropriate model for simulating the transport and formation of TTHMs through the CT system (Singer, 1994), as given by:

$$\mathrm{TTHM} = 0.00306[(\mathrm{TOC})(\mathrm{UV}_{254})]^{0.44}(\mathrm{C}_{\mathrm{Cl}})^{0.409}(\mathrm{Te})^{0.665}(\mathrm{pH}-2.6)^{0.715}(\mathrm{Br}+1)^{0.036}(\mathrm{t})^{0.265} \qquad [3]$$

where TTHM = the total trihalomethane concentration in μg/l, TOC = the total organic carbon concentration in mg/l (=4.0 mg/l), UV_{254} = the ultraviolet absorbance at 254 nm in cm^{-1} (=0.06cm^{-1}), Te = the temperature in °C (=25 ^{o}C) , Br = the bromide ion concentration in mg/l (=0.036 mg/l) and t = the contact time at the particular location.

The geometry and boundary conditions of the CFD simulations were chosen assuming a scenario of the CT disinfection being accommodated with a mean retention time T of 35 min, i.e. a realistic estimate for chlorination at water treatment works. This translated to a flow rate Q of 2.86 l/s. In turn an instantaneous injection of G. Lamblia was modelled to obtain an estimate of the pathogen inactivation. Similarly, a 4.0 mg/l instantaneous injection of TOC was conducted to model the accumulation of TTHM as an indication of the by-product accumulation.

2.3 Segregated Flow Analysis

Segregated Flow Analysis (SFA) is an integral component of the Integrated Disinfection Design Framework (IDDF), applying a more comprehensive approach to assess the disinfection performance compared to the more traditional *Ct* concept (Ducoste et al., 2001). The principle assumes that the fluid is divided into discrete elements according to their residence time deduced from RTD analyses. There is no mixing or transfer of material between these elements as complete segregation is retained (Wols et al., 2010). The chlorine concentration and the progress in the reactive processes of inactivation and by-product accumulation was determined by subjecting the original conservative concentration to the kinetics of equations [1],[2] and [3] associated with the elements' residence time *t* . As an example, given the exposure time, the G. Lamblia survival ratio $N/N_0(t)$ is calculated as

$$\frac{\mathrm{N}}{\mathrm{N}_0}(\mathrm{t}) = \exp(-\mathrm{k}'(\mathrm{C}_0\exp(-\mathrm{k}_{\mathrm{FR}}\mathrm{C}_{\mathrm{FR}}\mathrm{C}_{\mathrm{Cl}} - \mathrm{k}_{\mathrm{b}}\mathrm{C}_{\mathrm{cl}})^{\mathrm{n}}\mathrm{t}^{\mathrm{m}}) \qquad [4]$$

In turn, assuming segregated flow, the total survival ratio during a reactive tracer experiment represented by the function E(t) is expressed as

$$\frac{\mathrm{N}}{\mathrm{N}_0} = \int \frac{\mathrm{N}(\mathrm{t})}{\mathrm{N}_0}\mathrm{E}(\mathrm{t})\mathrm{dt} \qquad [5]$$

As with the pathogen inactivation (equations 4 and 5), a similar approach can be adopted for any other reactants. However, the treatment of accumulating by-products needs further attention. In contrast to the pathogens where the source is located at the inlet and the population is inactivated over time according to the original pathogen concentration N_0, by-products are produced from within the computational domain and their concentration is therefore related to the tank flow-rate Q and the tank volume. This is due to the presence of disinfectant and TOC concentrations acting as precursors for the formation of TTHMs along the entire flow volume upstream of the sampling point in each case.

3. RESULTS AND DISCUSSION

The suitability of the numerical model to reproduce scalar transport in the CT geometries was assessed through comparisons against hydrodynamic readings and tracer concentration data, obtained experimentally from the CT-1 laboratory model. Figure 2 serves as testament of the numerical model performance for the hydrodynamics and scalar transport. The numerical modelling strategy was therefore found to be successful in predicting the overall shape of the RTDs, particularly in the latter compartments (4-8), while also discerning to a reasonable extent the multiple concentration peak behavior induced by tracer reappearance at the sampling points of compartments 1 to 3.

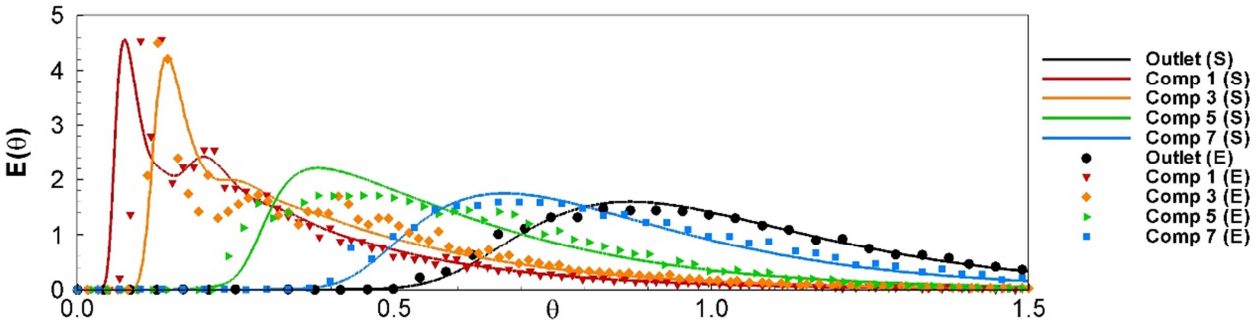

Figure 2. Comparison of RTD of conservative tracer transport obtained experimentally and computationally

A hydraulic efficiency analysis of the particular design (CT-1) was conducted in an associated investigation (Angeloudis et al., 2014c) which showed close agreement between the predicted and experimentally obtained quantities, such as t_{10} and the mixing indices σ^2 and Mo. The HEIs Mo and σ^2 are defined as: $Mo = t_{90}/t_{10}$ and $\sigma^2 = \sigma_t^2/t_g^2$ where σ_t^2 is the variance of the RTD curve (Markse and Boyle, 1973). The latter indicate the amount of mixing in the disinfection tank and are included for completeness in Table 1.

A distinguished advantage of a CFD approach is that it enables an appreciation of the complex three-dimensional mixing profile developed within the CT geometry. As a result, it can be observed that the first compartment was dominated by a large recirculation zone and significant two-dimensionality in the longitudinal plane. This flow pattern is a result of the inlet configuration which caused the flow to enter the first chamber by means of a high momentum jet. The conditions of compartment 1, resulted in subsequent recirculation zones occurring in compartments downstream which combined with the expected recirculation zones around baffle lees demonstrate the complexity of the tank hydrodynamics. A representation of the overall tank flow pattern is indicated in Figure 3 by means of streamtraces colored according to the velocity magnitude. High flow accelerations were apparent upon entry and the exit of the tank, which however diminish between the 4th until the 8th compartment where two-dimensional flow is established. The assessment of the initial three-dimensionality in terms of its impact on the process performance is arguable. While it is known that internal flow recirculations are treated as dead-zones and therefore as an inefficient use of the reactor volume, the inflow enters with the disinfectant concentration from a fraction of the tank cross-section flow depth. Before the process progresses further, this disinfectant should be evenly distributed and therefore vertical recirculations like the one in compartment 1 (Figure 3) act as the medium for that purpose. On the other hand, complete mixing for prolonged time leads to tailing effects and the short-circuiting peaks of Figure 2. The tailing effects can lead to by-product precursors being detained longer thus exacerbating by-product formation, while short-circuiting due to the induced local accelerations pose concern over inefficient exposure of pathogens downstream.

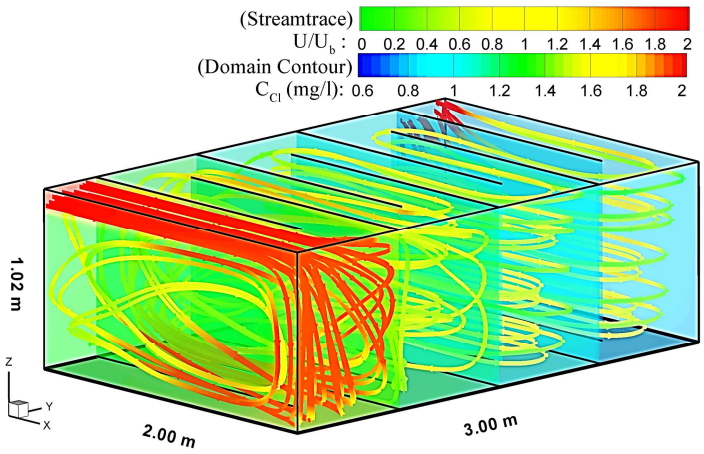

Figure 3. Three-dimensional flow pattern developed in the reactor and chlorine distribution assuming steady state conditions. Deviations from plug flow are apparent close to the inlet, outlet and in compartment transitional zones, leading to recirculation zones and uneven cross-sectional velocity profiles.

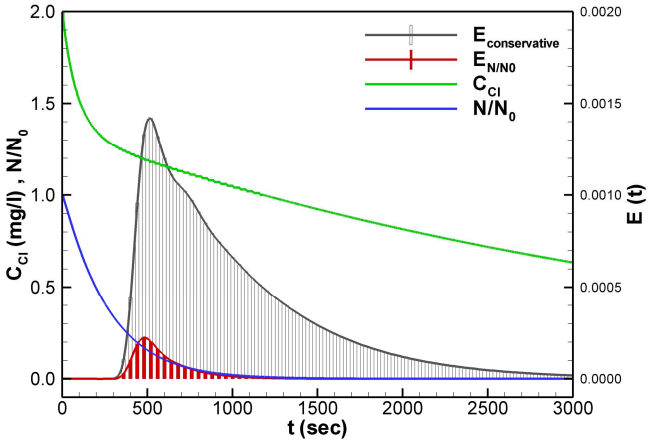

Figure 4. Chlorine concentration (C_{Cl}) in mg/l and the corresponding survival ratio (N/N_0) with respect to time. Given these values and the conservative tracer curve, the G.Lamblia reactive tracer curve could be obtained as indicated in the figure. The particular RTD curves were obtained numerically at the sampling point of compartment 4.

The chlorine transport in the CT numerical model suggests that due to the mixing in compartment 1-3 combined with the rapid early decay due to fast reactions, the initial 2 mg/ are distributed quickly and the average disinfectant concentration drops to a level of 1.2-1.4 mg/l within the first 2 compartments. It then gradually decays to approximately 0.8 mg/l at the outlet. However, there is a spatial variation of the chlorine distribution which cannot be acknowledged through the Segregated Flow Analysis. Instead, for SFA the chlorine concentration and in extension the pathogen survival ratio is directly connected to the time parameter as shown in Figure 4. A conservative tracer RTD curve (E) is included as an example of how the reactive tracer curve is calculated by multiplying $E(t) \times N/N_0$ with respect to time.

Taking into account the chlorine reactions with microorganisms, the *G.Lamblia* concentration injected was not conserved; this was reflected by an area below the normalized RTD curve unequal to unity (Figures 4, 5a-b). The disinfection efficiency was quantified for each of the CT compartments by comparing the areas between reactive and conservative tracer RTDs as indicated in Table 1. The percentage of tracer (*G.Lamblia*) loss following injection was calculated by subtracting the normalized area of the microorganism RTD from unity (i.e. the conservative tracer RTD curve area). Table 1 indicates the hydraulic efficiency indicator as calculated according to conservative tracer transport, along with the *G.Lamblia* inactivation SFA and CFD predictions. A clear pattern emerges, as the deviation between the two methods is pronounced in the compartments near the inlet region where three-dimensional mixing is prevalent, as suggested by the mixing indicators σ^2 and Mo. However, as the contact tank flow converges to more uniform cross-sectional flow conditions in the latter compartments, the inactivation predictions from the two methods seem to converge, with SFA appearing to underestimate the inactivation by as little as 0.15% at the outlet. A similar pattern is encountered in the by-product accumulation findings as seen in Figure 5(c).

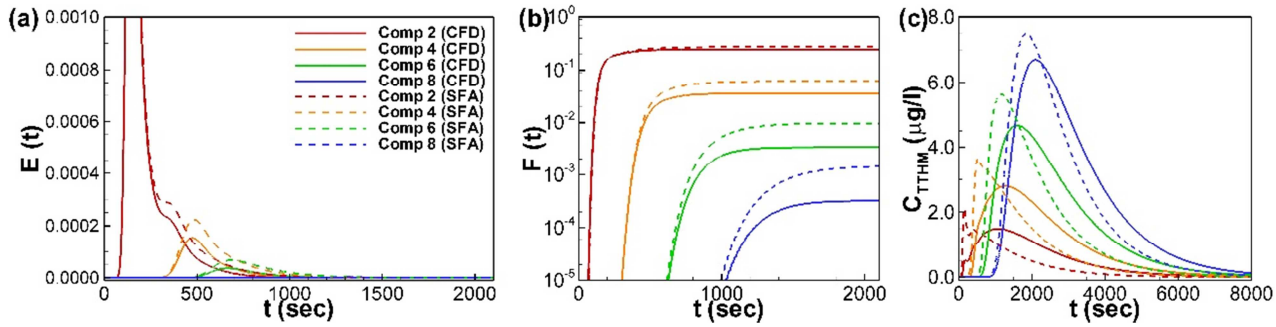

Figure 5. Comparison of Reactive Tracer results produced by the CFD methodology with the SFA analysis of Conservative RTDs

Table 1. Hydraulic Efficiency Indicators and *G.Lamblia* Disinfection Efficiency from the SFA and CFD approaches

	HEI				G. Lamblia Disinfection Efficiency		Deviation SFA-CFD (%)
	$t_{10}(\theta)$	$t_{90}(\theta)$	Mo	σ^2	SFA	CFD	
Comp. 1	0.259	2.036	7.854	0.636	75.61%	54.83%	37.90%
Comp. 2	0.245	2.170	8.839	0.802	79.89%	75.28%	6.12%
Comp. 3	0.368	1.932	5.240	0.493	86.03%	89.59%	-3.97%
Comp. 4	0.482	1.735	3.593	0.309	94.81%	96.39%	-1.63%
Comp. 5	0.560	1.601	2.855	0.207	97.85%	98.88%	-1.04%
Comp. 6	0.612	1.509	2.465	0.149	99.03%	99.66%	-0.64%
Comp. 7	0.651	1.445	2.220	0.115	99.62%	99.90%	-0.28%
Comp. 8	0.680	1.399	2.056	0.095	99.72%	99.97%	-0.24%
Outlet	0.721	1.440	1.995	0.092	99.83%	99.98%	-0.15%

Considering the given output from the computational model, some of the shortcomings of the SFA become apparent. For example, the RTD curve derived in compartment 1 is located in the centre of a recirculation zone. This implies that monitoring at that particular sampling point would be subject to the reappearance of tracer and therefore the whole RTD would be into question, and the SFA results as well. The same issue arises for the compartment 2 conservative tracer curve. Another issue would be associated with the estimation of chlorine only on a temporal basis, neglecting the established spatial distribution in the contact tank due to mixing. For instance, if we examine conditions of extensive tailing beyond the theoretical retention time, the SFA chlorine concentration is underestimated. This is because it actually reaches a steady state within the CT geometry due to its spatial distribution dictated mainly by the inlet flow and baffling conditions. Another approach would be to assume a constant disinfectant concentration at each sampling point, which however is equally flawed considering that the disinfectant concentration at that particular sampling point will be heavily connected to the upstream mixing conditions influenced by the individual geometry of the contact tank as well as the exposure time. Concurrently, for the by-product accumulation curve (Figure 5c), the actual distribution of TOC and chlorine upstream becomes crucial. For example, TOC and C_{Cl} concentrations can be transported to low-velocity recirculation zones due to turbulence diffusion, initially reducing the by-product formation along the main flow path and increasing it on the tailing part of the conservative RTD curve as predicted by the numerical simulations.

4. CONCLUSIONS

A CFD model was employed to solve the Reynolds Averaged Navier-Stokes (RANS) equations, to predict the mixing and disinfection characteristics of a standard 8-compartment contact tank. The validity of the numerical model data were assessed by comparing solute transport processes to experimental data. The analysis was then extended to investigate disinfection processes, through direct modelling of pathogen transport and by-product formation.

This was undertaken by simulating reactive tracer experiments featuring *G.Lamblia* population and Total Organic Carbon concentrations respectively. The simulation results were compared with the more theoretical predictions of Segregated Flow Analysis for each of the tracer monitoring points. The deviation between the two methodologies was clearly more pronounced in compartments where three-dimensional mixing was prevalent, but converged near the outlet in the presence of more consistent flow conditions. The results suggest that for contact tank units which are characterized by a satisfactory hydraulic performance, a SFA analysis may be sufficient to provide disinfection parameters, such as chlorine dosage and expected by-product accumulation, with the additional advantage of being computationally efficient.

However, the analysis of reactive tracer transport is currently at a preliminary stage and would benefit with more in-depth comparisons against experimental data, or more refined computational analysis that acknowledge the unsteady nature of the flow in the reactor (e.g. Large Eddy Simulations). With regard to the further development and practical application of the numerical approach discussed, there is a need to inform continuously the numerical methodology with more sophisticated kinetic models, which should be compared with experimental studies focused on how the water chemistry is altered during disinfection.

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