Use of computational fluid dynamics to assess the disinfection performance of a combined sewer overflow treatment chamber

D.A. Egarr[1]*, M.G. Faram[2], I. Guymer[3], T. O'Doherty[1], N.Syred[1]

[1] *Cardiff University, Queen's Buildings, The Parade, PO Box 925, Cardiff, CF24 0YF*
[2] *Hydro International plc, Shearwater House, Clevedon Hall Estate, Victoria Road, Clevedon, N. Somerset, BS21 7RD*
[3] *School of Engineering, University of Warwick, Coventry, CV4 7AL*
**Corresponding author, e-mail EgarrDA1@Cardiff.ac.uk*

ABSTRACT

The fluid residence time characterisation of a 3.4m diameter Hydrodynamic Vortex Separator (HDVS) has been carried out over a range of flowrates. Computational Fluid Dynamic (CFD) modelling has also been undertaken for the same conditions and validated against the experimental results, for which reasonable correspondence has been found. Using the results from the CFD modelling and batch inactivation results from the disinfection of secondary treated wastewater, it is shown that the theoretical performance of a HDVS as a contact vessel for disinfection can be predicted.

KEYWORDS

Combined sewer overflows (CSOs), Computational Fluid Dynamics (CFD), disinfection, hydrodynamic vortex separator (HDVS), residence time, wastewater treatment

INTRODUCTION

The oldest and most traditional urban drainage systems in developed Europe are combined sewers, whereby storm and surface water, as well as foul sewage, is transported to wastewater treatment facilities in the same pipeline. A problem with this system is that during wet weather, the quantity of water entering the sewer network can exceed the design limit, requiring the provision of emergency relief points, or 'Combined Sewer Overflows' (CSOs), which pass polluting water and organic material into adjacent watercourses, such as rivers and streams. A form of CSO is a Hydrodynamic Vortex Separator (HDVS) primarily used for solid-liquid separation. The use of HDVSs as disinfection vessels has been reported by Boner *et al.* (1993). However, a detailed understanding of such systems in this context has not yet been obtained. This paper is concerned with the development of tools for predicting HDVS disinfection performance using Computational Fluid dynamics (CFD). Such tools will enable systems to be designed with better efficiency with regard to the consumption of chemicals. Validation against outputs from an experimental RTD analysis is undertaken prior to predicting the disinfection performance of a HDVS.

THEORY

Residence time

The flow characteristic of any system, including a HDVS, will lie somewhere between plug flow (pure advection with no dispersion) and completely mixed. In a complete plug flow operating condition, the response to a pulse injection is such that all elements being tracked leave the device at the same residence time. In a completely mixed or Continuously Stirred Tank Reactor (CSTR), the elements of fluid being tracked will leave the device over a range of residence times. Between these two limits, both advection and dispersion processes occur, producing typical residence time distributions. Levenspiel (1962) discusses this in detail. Fluid residence time is a key quantity that can be used to determine the effectiveness of a process. For example, the residence time will determine the strength and quantity of disinfectant that is required if a system is to be used to disinfect a flow.

Disinfection

Since the early 1900's, a number of rate equations have been proposed to describe the inactivation of micro-organisms (Chick, 1908: Hom, 1972: Haas and Joffe, 1994). In predicting the survival of micro-organisms during disinfection in a continuous flow reactor, Severin *et al.* (1984), report: "In the scale up of inactivation data from batch data to a flow-through reactor with complete mixing, it was found that the use of simple mixed, second order kinetics leads to severe errors due to the effects of initial resistance on survival under the completely mixed, flow-through reactor regime. The errors encountered are so severe as to completely miss the prediction that the relative resistance of organisms can change due to the mixing condition". Li, (2004), reports: "It has been realized that a plug flow reactor is the most efficient reactor in disinfection facilities and a CSTR is probably the poorest possible configuration for efficient disinfection". The series event kinetic model (Severin *et al.*, 1984) is given by

$$\frac{N_t}{N_0} = e^{-kct} \sum_{i=0}^{j-1} \frac{(kct)^i}{i!} \qquad (1)$$

Where: N_t = Number of organisms at time t $\quad$ N_0 = Initial number of organisms

k = Kinetic rate constant, $m^3/s.kg$ $\quad$ c = Disinfectant concentration, kg/m^3

j = Lethal number of reactions

The series event kinetic model has also been developed for predicting the performance of a continuous flow system and is given by (Severin *et al.*, 1984):

$$\frac{N_t}{N_0} = \left(\frac{1}{1+kc\tau'}\right)^N \sum_{i=0}^{j-1} \left[\frac{i+N-1}{N-1}\right] \left(\frac{kc\tau'}{1+kc\tau'}\right)^i \qquad (2)$$

Where: t' = Residence time in one CSTR, s $\quad$ N = Number of CSTRs

The number of Continuously Stirred Tank Reactors (CSTRs) that is representative of the continuous flow system is attained by fitting the Tanks In Series Model (TISM) (Levenspiel, 1962) to a residence time distribution determined using a pulse injection of tracer through the continuous flow system. The TISM assumes that a series of CSTRs, of equal volume, are connected in series.

The mean residence time of a single CSTR is therefore given by $\frac{\bar{t}}{N}$ where $\bar{t}$ is the mean residence time of the temporal concentration distribution. The TISM with 1 CSTR is equivalent to a completely mixed flow regime. As the number of tanks increases, the flow regime approaches plug flow. It can be seen that as the number of CSTRs in Equation 2 increases, the survival rate decreases, which supports Li (2004) in that a plug flow reactor is more efficient than a CSTR.

Pretorius and Pretorius (1999) carried out batch inactivation studies using monochloramine as a disinfectant on "secondary treated effluent from a typical biological nutrient removal wastewater treatment plant, treating mainly domestic sewage". This should give a more realistic indication of the effectiveness of monochloramine than using pure culture bacteria and distilled water. It was found that the kinetic rate equation proposed by Severin *et al.* (1984) Equation 1, generally gave the best fit, with j equal to 2. To verify that the results from the batch inactivation studies were applicable to a continuous flow system, disinfection was carried out using two bench scale chlorine contact tanks and compared with predicted survival using Equation 2. Comparing the predicted and measured data, an R_t^2 value (Young *et al.*, 1980) of 0.94 was acquired, which represents a good fit.

METHODS

HDVS Test Rig

A 3.4m diameter HDVS was fed from a header tank using a 0.178 m internal diameter pipe, marked 'A' in Figure 1.

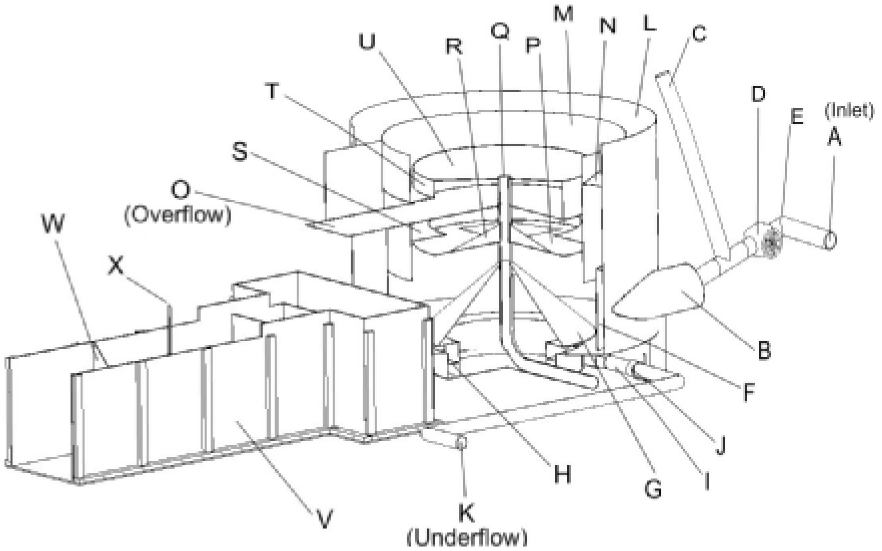

Figure 1. HDVS test Rig.

Due to limited space within the laboratory, the 0.178 m pipe was attached to the tangential inlet of the HDVS, 'B', with a sudden expansion and was angled downwards at 14°. 3.2 diameters upstream of the HDVS inlet was a stand-pipe, 'C', 3.5 diameters upstream of the standpipe a butterfly valve, 'D' and 2.25 diameters further upstream a 90° bend, 'E'. On entry to the HDVS the fluid strikes a deflector plate, 'F'. The HDVS has several internal components, including the cone, 'G' and a helix, 'H', below the cone that entrains the fluid into the underflow 'I'. The underflow discharge was controlled using a second butterfly valve, 'J', and the fluid discharged into a channel at 'K'. The valve at 'J' therefore allowed the HDVS to operate at any required flow split which is expressed as a percentage of the inflow, Q_i i.e. $100.Q_b/Q_i$ where Q_b is the base flow or underflow. Whilst the fluid is within the device it may swirl between the outer wall of the separator, 'L' and the dip-plate, 'M', to which a downward motion to the fluid is applied by a Venturi plate, 'N' and which also guides the fluid under the overflow, 'O'. Prior to the fluid passing over the overflow it must pass between a baffle, 'P', which is attached to the central underflow, 'Q' and which is supported by stiffeners ‘R’ and a second baffle attached to the dip-plate, ‘S’. From here the fluid passes over the weir, ‘T’ and through the screen, ‘U’ onto the overflow, where it discharges into a second channel, ‘V’. This second channel included a 90° V-Notch weir, ‘W’ and ruler, ‘X’, used to determine the flowrate from measurements of flow depth. In a usual installation of this type of system, a self priming siphon is attached to the overflow to produce a backwash, the purpose being to wash floatable material trapped on the mesh into the central underflow. However, for testing within the laboratory, the siphon was omitted. For all the flowrates investigated, the discharge through the underflow, Q_b, was 0.020 m^3/s.

For the residence time testing, Rhodamine WT fluorescent tracer was used along with three SCUFAs (Self-Contained Underwater Fluorescence Apparatus) produced by Turner Designs. Rhodamine WT is a tracer that fluoresces under the light produced by a green LED built into the SCUFA and the amount of fluoresced light from the dye is proportional to the concentration up to the limit of linearity. Rhodamine WT was injected into the flow at the header tank as a pulse input over a time period of 15 to 25 seconds. The header tank was chosen as the position to inject the tracer to maximise mixing prior to the inflow to the HDVS. A SCUFA was placed in the inlet through the standpipe so that a trace for the inflow could be recorded. One other SCUFA was placed at the centre of the overflow and another at the underflow. For each flowrate, the residence time distribution was measured three times, the average outputs of which are presented in this paper, with the exception of the lowest flowrate, where only one repeat was possible. The experimental residence time distributions were then analysed using the ADE (Advection Dispersion Equation) (Rutherford, 1994) and ADZ (Aggregated Dead Zone) models (Young and Wallis, 1986) and the parameters in the models optimised using a procedure by Guymer (2002). These models were chosen as they consider the shape of the inlet distribution of the tracer, unlike the TISM.

CFD – Grid setup and boundary conditions

The CFD code FLUENT was used to model the HDVS. The inlet pipe to the HDVS in Figure 1 was offset slightly in order to prevent over-skewed cells at the point the inlet pipe is joined to the HDVS vessel wall as this would result in appreciable error and possible convergence problems during computation of the flow field. The walls forming the dip plate, baffle plates and cone etc were modelled as having zero thickness, due to the very fine cells that would result from modelling the actual thickness of these components. The height of the water at the overflow was based on measurements taken during experimental testing and thus, a different grid was required for each flowrate. When the discharge at the overflow was below 0.119 m^3/s, the shallow fluid depth at the overflow made accurate representation difficult. In these conditions, the outlet was positioned at the top of the weir, ‘T’, Figure 1. A frictionless wall was used to represent the free surface, a method used by Green *et al.* (2002). The overflow was specified as a pressure outlet for which all the flow quantities excluding pressure are extrapolated from the interior. The underflow was specified as a negative velocity inlet to acquire the desired flowsplit. However, the point at which the flow leaves the underflow, ‘K’ in Figure 1, is very close to a 90° bend. The profile for the velocity from the underflow was therefore predicted by modelling the underflow between ‘I’ and ‘K’ in Figure 1 separately, with a flowrate of 0.020 m^3/s and then exporting the components of the velocity at the outlet of the underflow, as well as the turbulent quantities, to the full model of the HDVS. The valves at ‘D’ and ‘J’ in Figure 1 create a disturbance to the flow, so the effects of these were included by representing the valve as a zero thickness face, orientated at an appropriate angle in each model. A combination of the arrangement of internals within the HDVS such as the baffles, stiffeners and Venturi plate in the upper region and the deflector plate and cone which overhangs the base of the main vessel and which also incorporates a very narrow gap for the passage of fluid into the underflow, meant that a purely tetrahedral mesh was chosen over a hexahedral. The mesh comprised approximately 766,000 cells. A check for grid dependency was made by increasing the number of cells in the main vessel by approximately 300,000 which revealed the results to be grid independent. A steady state solution was achieved for all the models using the Reynolds Stress Model which closes the Reynolds averaged Navier-Stokes equation by solving transport equations for the Reynolds stresses. FLUENT's default 'segregated solver' was used as this has been traditionally used for incompressible to mildly compressible flows (Fluent Inc., 2003). The method for determining the mean residence time is one that was developed for evaluating the mean residence time in Heating, Ventilation and Air Conditioning (HVAC) systems, Roos (1999) and Bertak *et al.* (2001). This has been shown to be applicable to the prediction of mean residence time of wastewater treatment components by Egarr *et al.* (2005) who also give details for the prediction of the residence time distribution and hence the flow regime.

RESULTS

CFD Validation

The average experimental R_t^2 value for the ADE model fit to the experimental data was 0.916 and 0.964 for the ADZ model. An example of the fit by the ADZ model to the overflow temporal concentration distribution is shown in Figure 2. The sampling frequency of the SCUFA is 1Hz. The R_t^2 value of the fit by the ADZ model in Figure 2 is 0.968 which is therefore representative of the average fit by the ADZ model which is generally quite good.

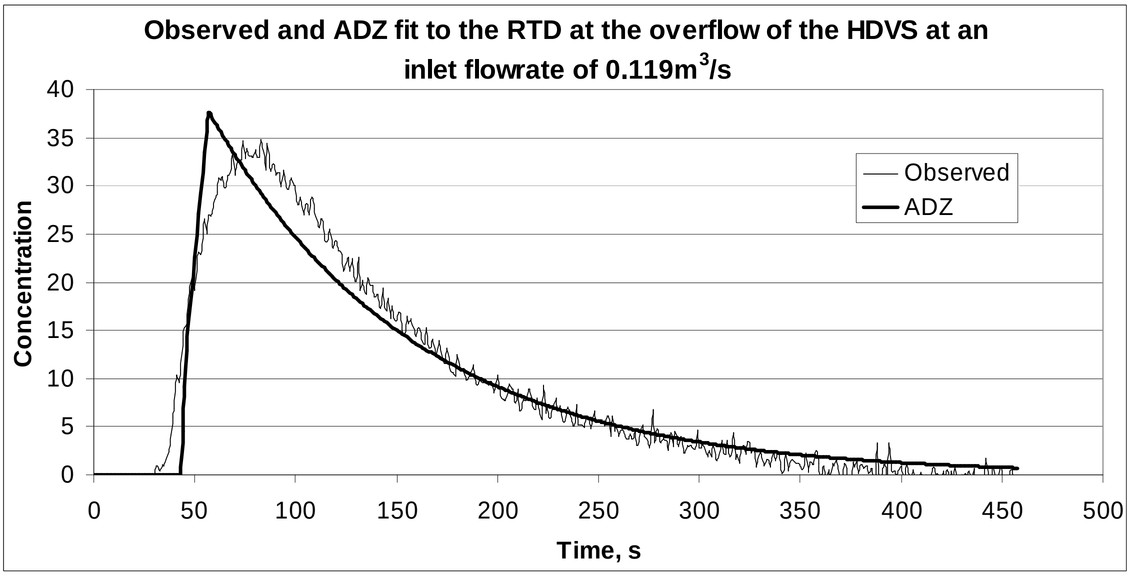

Figure 2. Comparison of the observed and ADZ fit to the RTD at the overflow of the HDVS

As the ADZ model gave the best fit compared to the ADE, then the CFD will only be validated against the derived parameters from the ADZ model. Table 1 compares the mean residence times for the overflow and underflow. It was not possible to analyse the data for the overflow at an inlet flowrate of 0.027 m^3/s, due to noise in the data and the long residence time, that would mean monitoring the overflow for a period longer than practically possible. From Table 1, the CFD predicted mean residence time appears to compare well for the overflow. However, there is a greater discrepancy at the underflow, particularly at lower flowrates. The second parameter to be validated in the ADZ model is the dispersive fraction which has an affect on the shape of the temporal concentration distribution. Since the ADZ concentration prediction is dependent on the inlet trace an inlet distribution of tracer that was of a Gaussian form was chosen initially. The ADZ model was then fitted to the predicted outlet concentration curves and the travel time and time delay optimised, which gave an R_t^2 value of 0.931 for both the underflow and overflow. To optimise the inlet distribution, a second inlet trace was used that took the form of the overflow concentration curve which was reduced to a period of 40 seconds and adjusted to give a peak value of 1000 kg/m^3. Using this inlet profile the ADZ model was refitted to the outlet concentration curves and after optimisation, the R_t^2 values were 0.958 and 0.967 for the overflow and underflow respectively. The average R_t^2 value for the ADZ models that were fitted to the experimental data was 0.964 and the second inlet profile was therefore considered acceptable. This was then used to produce concentration versus time curves to which the ADZ model was fitted for all the flowrates for which experimental data was recorded. Table 1 shows a reasonable comparison between the computed Dispersive Fraction for the experimental and CFD data.

Table 1. CFD and ADZ mean residence time and dispersive fraction comparison.

	Mean residence time, s				Dispersive fraction			
	Overflow		Underflow		Overflow		Underflow	
Flowrate, m^3/s	ADZ	CFD	ADZ	CFD	ADZ	CFD	ADZ	CFD
0.187	87	92	92	71	0.707	0.626	0.683	0.603
0.150	107	115	124	86	0.685	0.626	0.694	0.622
0.119	154	145	149	111	0.753	0.649	0.816	0.632
0.077	214	211	213	163	0.713	0.679	0.803	0.652
0.027	-	-	586	440	-	-	0.720	0.724

Disinfection

Having established that CFD gives reasonable prediction of residence times, a pulse input of tracer at the inlet to the HDVS in the CFD models was used to produce a RTD to which the TISM was fitted and the parameters (i.e. mean residence time and the number of tanks) optimised. This is required to determine the number of CSTRs that characterise the RTD and hence, apply Equation 2 to predict the disinfection performance. The average R_t^2 for the TISM fit to the CFD generated RTD curves for all the flowrates was 0.977 whereby a good fit by the TISM was made for each RTD. Thus, Equation 2, which relies on a good fit of the TISM in order to predict survival rates, is an appropriate model for this system. Pretorius and Pretorius (1999), determined the kinetic rate constant and the lethal number of injections required in Equation 2. Hence, with mean residence time predictions, the number of CSTRs acquired by fitting the TISM to each of the RTDs, kinetic rate constants and lethal number of injections, the survival at the outlet of the HDVS can be predicted for a number of flowrates and a range of monochloramine concentrations. This is shown in Figure 3 for a pH of 7 at 25°C. The performance of the HDVS as a disinfection vessel assumes that a step input of monochloramine has been introduced into the HDVS at the inlet where it is completely mixed and that the disinfectant is uniformly dispersed within the HDVS. Decay of the disinfectant due to the nature of the wastewater is assumed to be taken into account by the kinetic rate constants determined by Pretorius and Pretorius (1999). With mean residence times at the overflow of the HDVS predicted using CFD, at a number of flowrates, a function that describes the mean residence time in one CSTR at the overflow has been found and used in conjunction with Equation 2 to give a model, specific to the 3.4 m diameter separator operating with an underflow of 0.020 m^3/s, that predicts the micro-organism survival at the overflow and is given by

$$\frac{N}{N_0} = \left(\frac{1}{1+2.9363kcQ^{-1.1422}}\right)^4 \left[1+\left(\frac{4}{3}\right)\frac{2.9363kcQ^{-1.1422}}{1+2.9363kcQ^{-1.1422}}\right] \qquad (3)$$

Thus, for a given rate constant and disinfectant concentration, Equation 3 may be used to predict the disinfection performance as a function of the inlet flowrate of fluid. Alternatively, the disinfection performance may be established as a function of the concentration of disinfectant for a given inlet flowrate of fluid and rate constant. Figure 3 shows the prediction made by Equation 3 for an inlet flowrate of 0.119 m^3/s, which confirms that Equation 3 is a useful design tool for predicting the required conditions for a given survival of micro-organisms. The design flowrates for these systems are often based on the characteristics of the wastewater, and hence, the settling velocity of particulates (Andoh and Smisson, 1996).

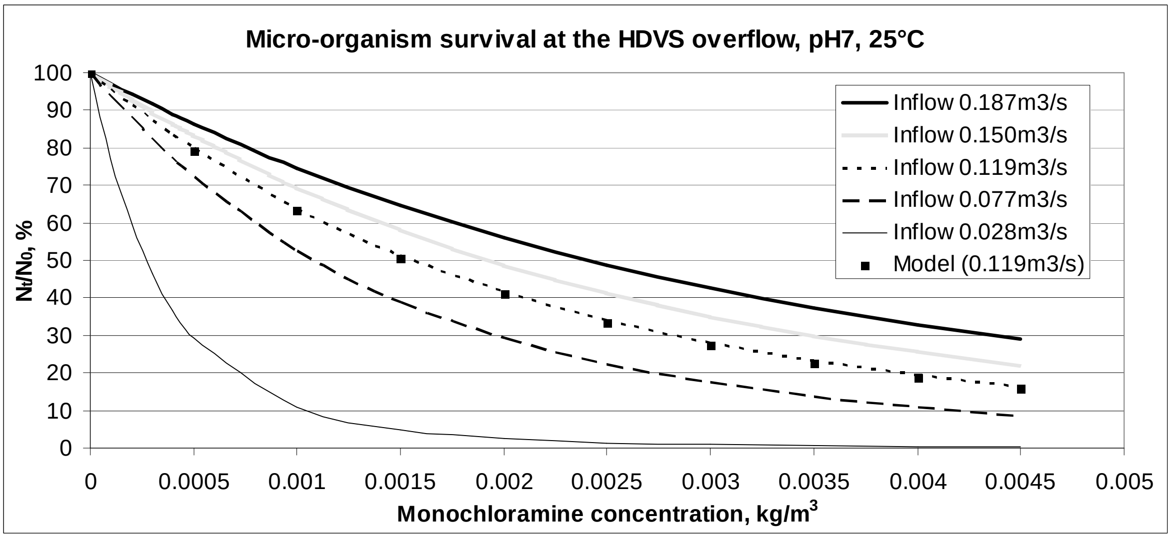

Figure 3. Micro-organism survival at the HDVS overflow at pH7 and 25°C.

Figure 3 shows that at any particular flowrate, as the concentration of monochloramine increases, the survival decreases. For all the flowrates, the number of CSTRs that were found to describe the RTD of the HDVS was 4. As the flowrate decreases, so does the survival. This can therefore be attributed solely to a higher contact time rather than a change in flow regime. Hence, Figure 3 shows that higher kill rates can be achieved by different changes: the concentration of the disinfectant can be increased, the flowrate reduced, a larger HDVS or a series of HDVSs employed to increase the mean residence time of the fluid. Although the diameter of the HDVS studied in this work was 3.4 m, HDVSs with diameters as large as 16 m have been installed in practice. Further work would be desirable in undertaking an experimental disinfection study on a HDVS for which the results could be used for a more complete validation of CFD models. Batch inactivation studies at different temperatures would take into account regional climate variations and inactivation studies for effluent from different parts of the world may reveal that the rate constant is influenced by the site from which the effluent is obtained. This could be due to a more acidic fluid due to acid rain in urban areas, or the presence of different strains of micro-organisms.

CONCLUSIONS

- The CFD predictions compare reasonably well with the derived ADZ model parameters.
- Using CFD in conjunction with experimentally derived kinetic rate constants, the theoretical disinfection performance of a HDVS has been determined.
- A model has been proposed for the theoretical prediction of the disinfection performance of a HDVS, and hence, the economical use of disinfectant.
- A scaling law for residence time in various sizes of HDVS would allow a more robust model to be developed for predicting disinfection performance.

ACKNOWLEDGEMENTS

The authors would like to acknowledge EPSRC and Hydro International for funding. Particular thanks must go to Mr John Blanksby (now at the University of Sheffield) for inputs relating to the setting up of the facility and for allowing access for this project.

REFERENCES

Andoh, R.Y.G., Smisson, R.P.M. (1996). The practical use of wastewater characterization in design, Wat. Sci. Tech., Vol. 33, No. 9, pp127-134.

Bertak, M., Cermak, M., Clarke, J.A., Denev, J., Drkal, F., Lain, M., MacDonald, I.A., Majer, M., Stankov, P. (2001). Experimental and numerical study of local mean age of air, Seventh International IBPSA Conference, 13-15 August, pp773-780.

Boner, M.C., Hides, S.P., Turner, B.G. (1993). High Rate Treatment of Combined Sewer Overflows in Columbus, Georgia, Proceedings on the Sixth International Conference on Urban Storm Drainage, 12-17 September, pp1671-1676.

Chick, H.E. (1908). An investigation of the laws of disinfection, J. Hyg., 8, pp92-158.

Egarr, D.A., Faram, M.G., O'Doherty, T., Phipps, D.A., Syred, N. (2005). Computational fluid dynamic prediction of the residence time distribution of a prototype hydrodynamic vortex separator operating with a base flow component, Proceedings of the Institute of Mechanical Engineers, Journal of Process Mechanical Engineering, Vol. 219, No. E1, pp53-67.

Fluent Inc. (2003). FLUENT 6.1 Documentation (Fluent Inc., Lebanon, NH).

Guymer, I. (2002). A National Database of Travel Time, Dispersion and Methodologies for the Protection of River Abstractions, Environment Agency R & D Technical Report, ISBN 1 85705 821 6.

Haas, C.N., Joffe, J. (1994). Disinfection under dynamic conditions; modification of Hom's model for decay, Environ. Sci. Technol., Vol. 28, No. 7, pp.1367-1369.

Green, D.J., Haas, C.N., Farouk, B. (2002). Numerical simulation of chlorine disinfection processes, Water, Science and Technology: Water Supply, 2 (3), pp167-173.

Hom, L.W. (1972). Kinetics of chlorine disinfection of an ecosystem, J. of the Sanitary Eng. Div. ASCE 98 (SA1), pp183-194.

Li, L. (2004). Effects of Initial Microbial Density on Disinfection Efficiency in a Continuous Flow System and Validation of Disinfection Batch Kinetics in a Continuous Flow System, Ph.D. Thesis, Drexel University.

Levenspiel, O. (1962). Chemical Engineering, John Wiley and Sons.

Pretorius, P.C., Pretorius, W.A. (1999). Disinfection of purified sewage effluent with monochloramine, Water SA, Volume 25, No. 4, pp463-471, ISSN 0378-4738.

Roos, A. (1999). On the Effectiveness of Ventilation, PhD Thesis, Eindhoven University of Technology, Eindhoven, The Netherlands.

Rutherford, J.C. (1994). River Mixing, John Wiley and Sons.

Severin, B.F., Suidan, M.T., Engelbrecht, R.S. (1984). Series event kinetic model for chemical disinfection, J. Environ. Eng., 110 (2), pp430-439.

Young, P., Jakeman, A., McMurtrie, R. (1980). An instrument variable method for model order identification, Automatica, Vol. 16, pp281-294.

Young, P.C., Wallis, S.G. (1986). The aggregated dead zone (ADZ) model for dispersion in rivers, Proc. of the conference on water quality modelling in the inland natural environment, Bournemouth, pp421-433.