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The integrated disinfection design framework approach to reactor hydraulics characterization

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ABSTRACT

The integrated disinfection design framework (IDDF) is a new approach to determine disinfection requirements for drinking water treatment facilities. The framework may be applied to enhance or improve disinfection performance in lieu of using the surface water treatment rule (SWTR) Guidance Manual. The overall IDDF approach consists of four modules: hydraulic characterization, disinfectant demand/decay, inactivation kinetics, and disinfection by-product (DBP) formation. In this study, a review of the hydraulic characterization module is presented. The module was applied to two full-scale water treatment plant processes (1: a group of six filter beds, 2: a disinfection contactor). The data from the hydraulic characterization module, which consists of three methods to generate the residence time distribution (RTD) curve, was then used to demonstrate the microbial inactivation and DBP formation level that might be produced at the process effluent. Results suggest that the predicted microbial inactivation level is sensitive to the hydraulic characterization method. However, all three methods predict very similar DBP formation despite differences in the RTD data. Results also showed that the disinfectant dose applied to the contactor could be reduced by 35% and still maintain the same credit for *Giardia* inactivation specified by the USEPA CT tables. This reduction in disinfectant dose could result in a reduction in the total trihalomethane (TTHM) level by 10% and haloacetic acids (HAAs) by 20%.

Key words | CFD, disinfection, hydraulics, IDDF, model, tracer studies

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INTRODUCTION

Disinfection by-products (DBP) formation is a growing concern for many water treatment utilities. As a result of the tighter DBP limits proposed by the Stage 2 Disinfectant/Disinfectant By-Products (D/DBP) rule (USEPA 1998), most drinking water utilities will be challenged to achieve compliance while maximizing microbial inactivation. This balance between maximizing microbial inactivation and minimizing DBPs will require water treatment engineers to utilize tools that allow the investigation of alternative disinfection strategies without the need for conducting costly experimental treatability studies.

The integrated disinfection design framework (IDDF) concept was developed as an alternative tool for more accurate analysis of the disinfection process. The IDDF model was originally created with three components that collectively could be used to determine site-specific disinfection requirements (Bellamy *et al.* 2000):

1. Disinfection contactor hydraulics
2. Disinfectant demand and decay rate
3. Pathogen inactivation kinetics

Bellamy *et al.* (2000) utilized mathematical relationships for each of these disinfection components. By doing this, the integrated model could be solved with the following integral:

$$\log\left(\frac{N}{N_o}\right) = -\int_0^T \left(\frac{m}{nk^*}\right)^m kC_0^n \left(1-\exp\left\{\frac{-nk^*t}{m}\right\}\right)^m \frac{1}{\tau}\frac{1}{2\sqrt{\pi d\theta}}\exp\left(\frac{\{1-\theta\}^2}{4d\theta}\right)\mathrm{d}t \qquad (1)$$

where N = viable effluent microbial concentration, N_0 = influent microbial concentration, k, m, n = integral Hom model fitting parameters, k^* = disinfectant decay rate, τ = mean hydraulic residence time (HRT), $\theta = t/\tau$, C_0 = initial disinfectant concentration, and d = dispersion number in the plug flow dispersion (PFD) model. Used in this manner, the IDDF can predict the actual pathogen inactivation achieved with a given disinfectant dose.

Bellamy *et al.*'s approach is applicable if the hydraulic characterization of the disinfection contactor can be described exclusively by the open form of the PFD model used in Equation 1. However, when the T_{10}/HRT ratio (T_{10} is the time that 10% of the fluid parcels have reached the effluent) is less than about 0.5, a condition that is relatively common, PFD modelling may not be accurate. The definite integral approach of Equation 1 is also difficult to adapt to the use of other hydraulic modelling approaches such as N-tank in series or computational fluid dynamics (CFD).

Based on this assessment of the original IDDF concept, the following characteristics were identified as desirable to enhance this approach:

- the modelling approach should be understandable and accessible by a wide range of consultants and utility engineers,
- the modelling approach must be flexible enough to accept input from a range of alternative protocols (e.g. experimental tests, CFD), and
- the modelling approach must not utilize data that may be difficult to obtain.

The enhanced IDDF approach could then be proliferated and easily implemented at utilities to determine the site-specific disinfection performance.

HYDRAULIC CHARACTERISTICS

Hydraulic characterization of the continuous flow process is essential to understanding the level of treatment that can be achieved by that process. The goal of hydraulic characterization of a continuous flow process is to track the behaviour of different portions of the reacting fluid through the vessel. Most real systems have complicated hydraulic characteristics where reaction chambers have poor inlet/outlet configurations, dead zones, internal circulations, short-circuiting and/or bypassing of the reacting fluid.

These complicated hydraulic characteristics cause various portions of the reacting fluid to follow separate flow patterns through the vessel that will result in a wide distribution of fluid residence times. Deviations from ideal reactor configurations typically represent hydraulic inefficiencies and may result in unexpectedly poor reactor performance. Furthermore, these hydraulic inefficiencies may also lead to one or all of the following:

- Increased chemical costs
- Increased reaction by-products
- Higher capital costs

Various techniques can be used to quantify hydraulic characteristics of the reacting vessel. These techniques can be divided into two major categories: (1) experimental tracer tests, and (2) data interpretation models. This paper is devoted to describing these hydraulic techniques that have been incorporated into the overall IDDF protocol.

IDDF MODEL DESCRIPTION

The enhanced IDDF approach consists of four components or modules: hydraulic characterization, disinfectant demand/decay, inactivation kinetics, and disinfection by-product formation (Bellamy *et al.* 2000). A mechanistic or empirical formulation was developed for each of these components and serves as inputs to the IDDF model. Each module was also divided into three levels of complexity: Basic, Standard and Advanced (Bellamy *et al.* 2000). The goal of these levels was to provide users with varying skill sets and/or budget constraints to make use of the IDDF approach.

In terms of the hydraulic characterization module, the three levels are broken down into different methods for data input/collection techniques for generating the RTD data:

1. **Basic**: Literature T_{10}/HRT, dispersion coefficient (d) for input to the PFD model, number of tanks (N) for input to the complete mix tanks in series model.

Journal of Water Supply: Research and Technology—AQUA | 50.4 | 2001

2. **Standard**: Full-scale experimental tracer study using a neutrally buoyant tracer chemical.
3. **Advanced**: Disinfection contactor geometry and operating conditions for input to a computational fluid dynamics (CFD) model.

The PFD model assumes that mixing occurs in the flow direction caused by velocity gradients and that lateral or radial mixing is negligible. Environmental systems where PFD models work best include long narrow channels, packed beds, fluidized beds, and any system where a majority of the dispersion occurs in one dimension (Levenspiel 1972; Clark 1996). Other types of reactors could be modelled using this approach, such as mixing tanks or sinuous-baffled channel reactors. The PFD model is very simple to use and requires very little input data to generate the RTD function. The open form of PFD RTD function used in the basic approach is displayed in Equation 2.

$$f(\theta)=\frac{1}{2\sqrt{\pi\theta d}}\exp\left[-\frac{(1-\theta)^2}{4\theta d}\right] \tag{2}$$

The complete mixed tanks (*N*-tanks) in series model is based on setting up mixing tanks in series and allowing the fluid to flow from the effluent of one tank to the influent of the following tank. The pattern is repeated for *N* number of tanks. The *N*-tanks in series model is also very simple to use and requires little input data to generate the RTD function. The basic approach utilizes the gamma-extension to the *N*-tanks in series model and is displayed in Equation 3.

$$f(\theta)=\frac{N^N\theta^{(N-1)}}{\Gamma(N)}\,e^{-N\theta} \tag{3}$$

where $\Gamma(N)=\int_0^\infty \exp(-x)x^{N-1}dx$

The standard level (tracer study) makes use of experimental methods to determine the RTD curve. The experimental RTD curve is generated by injecting a neutrally buoyant, non-reactive tracer at the inlet to the process train and measuring the concentration of that tracer at the effluent as a function of time. The tracer concentration time-history curve is then converted to a dimensionless RTD curve. A summary of important issues when conducting an experimental tracer study is shown in Table 1.

The advanced level (numerical fluid mechanics modelling) involves a relatively new technology in the water treatment industry called CFD. CFD is the science of solving the governing equations of fluid flow through space and time. With CFD, a numerical description of the process flow geometry is developed by representing each location in space with a set of grid points. Fluid parameters such as velocities and turbulent quantities are then determined at each grid point. Once these fluid parameters have been determined, they are used as initial conditions for solving the convective-diffusion equation, which describes the movement of a neutrally buoyant tracer. The RTD curve is developed by monitoring a specific point at the effluent of the simulated process train as the convective-diffusion equation for tracer movement is being solved.

Several steps are required to develop a CFD model for determining the RTD function. Some of these steps may vary with different CFD software packages. It is important to review the specific CFD operating manual to determine any procedural differences. Table 2 summarizes the general steps required to develop the model and evaluate its performance.

The objectives of this study are (1) to demonstrate the use of the IDDF hydraulic characterization methods at full-scale water treatment facilities; (2) to assess the impact of hydraulic-characterization method selection on the predicted microbial inactivation and DBP formation level; and (3) to determine the potential reduction in disinfectant dose, TTHM, and HAAs using the entire RTD curve versus T_{10}. In this study, the basic level IDDF approach was used to characterize the hydraulics through a group of six filter beds. The standard and advanced levels were used to characterize the hydraulics through a disinfection contactor. The RTD curves produced by the basic and advanced IDDF approach were compared with experimental RTD curves to assess the accuracy and predictive capabilities of each approach. Finally, the RTD generated from the different hydraulic methods were used in conjunction with the IDDF microbial inactivation and DBP modules to predict the level of

Table 1 | Brief outline of important issues in an experimental tracer study

Issues	Comments
Tracer injection technique 1. Pulse input test 2. Step input test	Pulse input tests typically require less tracer chemical than Step input tests More mathematical manipulation is required with the Pulse input test to compute the RTD curve Step input tests provide an immediate repeatability check on the RTD data by monitoring the washout of the tracer when the influent tracer concentration flow is turned off
Tracer Chemical Type 1. Fluoride 2. Cations (calcium, magnesium, sodium, lithium, etc.) 3. Anions (chloride, sulfate, etc.) 4. Rhodamine WT	1. Fluoride is used already at many plants. This means that existing process equipment can be used to conduct the tracer study. However, probes for measuring fluoride are not accurate, and they are costly and difficult to measure fluoride at low concentrations 2. Cations can be fed as a dry form and measured accurately using atomic absorption. However, background levels must be well known, analyses are usually expensive to perform, and chemicals are expensive in the purity required for drinking water 3. Anions can be fed as a dry form and measured accurately with liquid chromatography. However, analyses by liquid chromatography are much longer than atomic absorption, background concentrations must be well known, analyses and chemicals are expensive 4. Rhodamine WT can be analysed with a fluorometer. Only a small concentration of this chemical is needed at the influent. However, chlorine tends to bleach the dye
Test duration and sampling frequency	Tracer tests should run for at least three theoretical hydraulic detention times in order to assure complete recovery of tracer mass. The mean time between tracer samples should not exceed 0.05 HRT below two detention times and 0.2 HRT above two detention times
Quality Assurance/Quality Control (QA/QC) checks	The tracer test can only be validated if certain QA/QC checks are performed. These checks include: • Tracer mass recovery: Valid for only Pulse input tests, it determines whether the total mass, injected at the process train influent, has been recovered at the effluent • Tracer hydraulic detention time: The computation of the hydraulic residence time using the tracer data should be within 5% of the theoretical residence time • For a step input tracer test, the tracer concentration in the effluent should be greater than 80% of the tracer influent concentration

microbial inactivation and DBP formation at the full-scale test sites.

CASE STUDY RESULTS AND DISCUSSION

Application of the basic level IDDF approach (direct-numerical non-ideal RTD models)

A hydraulic model of a real vessel or process train must reflect the principal hydraulic characteristics of the process that causes its behaviour to deviate from ideal conditions. For example, a pulse input tracer test was conducted through a group of six filters at Alameda County Water District. The tracer was injected in an open channel up-stream from the filters and then collected in the combined effluent channel. The process flow through the filter system was 13.7 MGD. The theoretical detention time for the six filters including the influent and effluent channel was 40 minutes. Figure 1 displays the experimental residence time density function (f(t/HRT)) from this tracer test. The theoretical detention time for the filter system was validated using the nonlinear least squares method (NLLS) (Haas *et al.* 1997). The NLLS method will

Table 2 | Operational procedure for developing a CFD model to determine the RTD curve

Procedure	Description
Develop detailed description of flow domain	The physical region should be large enough to account for any possible flow structures such as recirculation zones or flow over weirs. The mesh size should be fine enough to produce a grid independent solution and capture sharp gradients in velocity and turbulence in the flow
Select turbulence model	There are several turbulence models that can be selected. The most widely used and well documented on performance is the standard K-ε model. This model is recommended for use in the IDDF protocol
Identify and input boundary conditions	At the inlet boundary, normal velocity = process flow/inlet cross-sectional area, tangential velocity is zero. The inlet values of kinetic energy (Ke) and energy dissipation rate (ε) are often unknown. The advice is to take guidance from experimental data for similar flows (i.e. values of Ke and ε are well known for turbulent jet flows and can be found in popular turbulence books). The simplest method is to assume uniform values of Ke and ε computed from the following equations: $Ke=(IU)^2$ $\varepsilon=0.164\,\frac{Ke^{1.5}}{0.1H}$ I = turbulence intensity (typical range 0.01 to 0.05) U = normal inlet velocity H = characteristic inlet dimension (i.e. pipe diameter, sluice gate side dimension) For wall boundaries, velocities are set to zero and turbulence values are specified by using wall functions
Run Velocity/Turbulence model till convergence limit reached	Typically, the model is executed until the following convergence criterion is met: $\left\Vert \frac{V_i-V_{i-1}}{V_i} \right\Vert=0.001$ where V_i represents the solution vector at the ith iteration. The double bar represents the root mean square norm summed over all equations for the model
Reconfigure model to solve for time dependent tracer simulation	As in an experimental tracer study, the CFD tracer simulation can be run as either a pulse-input test or step-input test As in the experimental tracer study, >3 theoretical residence times is recommended for the overall simulation time
Perform RTD QA/QC	As in the experimental tracer study, quality assurance/quality control checks should be performed to validate the numerical solution. These checks include: 1. Comparison between numerically computed mean hydraulic detention time and the theoretical hydraulic detention time, 2. Total tracer simulation mass recovery (for pulse input test boundary conditions) Effluent tracer concentration is equal to the influent tracer concentration (for step input test boundary conditions), 3. Numerical solution does not change significantly with grid size or time step interval 4. Convergence limit has been reached

be discussed in the next section, which describes the case study with the standard-level hydraulic characterization method.

The data was fitted with the open form PFD model and the gamma extension N-tanks in series model (Equations 2 and 3). The parameters $N=4.05$ and

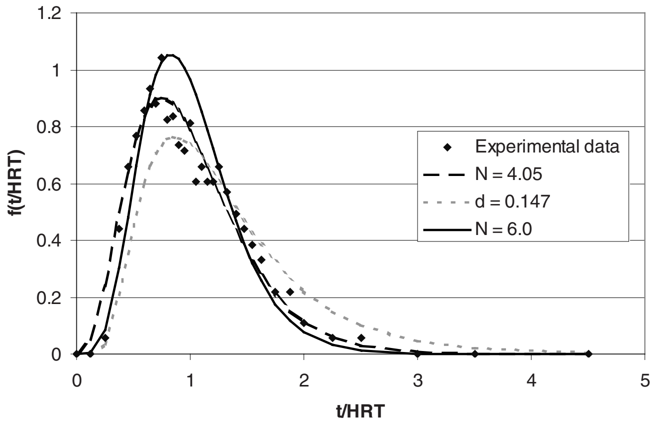

Figure 1 | Comparison between experimental and direct numerical model residence time density curves: complete mix tanks in series model (*N*) and PFD model (*d*).

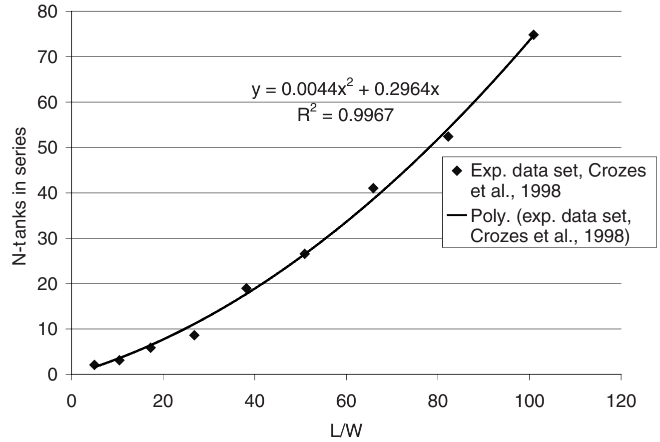

Figure 2 | Data conversion for reactor length to width ratio to *N* for *N*-tanks in series model.

Table 3 | Comparison between experimental and direct numerical T_{10}/HRT values

Experimental	Complete mixed tanks in series *N*=4.05	PFD *d*=0.147	
T_{10}/HRT	0.55	0.43	0.58
SQRT (SSE)		0.16	0.57

$d = 0.147$ were determined by minimizing the sum of the squares of the difference (SSE) between the data and the model residence time density (f(t)) function ($SSE = \Sigma(f(t)_{\mathrm{exp}} - f(t)_{\mathrm{model}})^2)$). The results are also displayed in Figure 1.

As shown in Figure 1, the *N*-tanks in series model provided a better fit to the experimental data than the PFD model. The PFD model was able to match the initial part of the experimental RTD curve (t/HRT = 0 to 0.2) and part of the curve between t/HRT = 1–1.7. The *N*-tank in series model was able to capture most of the curve beyond t/HRT = 0.5, however, it was not able to capture the initial tracer breakthrough.

Table 3 compares the values of T_{10}/HRT between the experimental data and the two direct numerical models. Based on Table 3, the PFD model was more effective at predicting the T_{10}/HRT value than the N-tanks in series model. However, the PFD's model prediction of the T_{10}/HRT value should be considered only a tiny victory because of its overall poor performance in capturing the filter system hydraulic characteristics (i.e. the entire RTD curve). In general, the T_{10}/HRT value only suggests that the six-filter system has an average hydraulic efficiency (USEPA 1991). The results in Figure 1 also suggest that the filter system hydraulics closely emulate a reactor that has properties of both a plug flow and complete mix tank reactor. Other researchers have shown similar results with single-parameter models and found that multi-parameter models better fit the experimental tracer data (Crozes *et al.* 1998).

However, in Crozes *et al.*'s study as well as in the present study, the best-fit value of *N* and *d* were based on experimental tracer data. The IDDF basic level would typically be used in lieu of experimental tracer tests. As a result, the user must select values of *N* or *d* that best describe the process hydraulics based on experience, rules of thumb, or published experimental results of similar reactor designs.

In the IDDF approach, the user can determine the *N* or *d* values based on the process length to width (L/W) ratio (Crozes *et al.* 1998) (Figure 2) or the desired T_{10}/HRT if the process has not been constructed (Bellamy *et al.* 2000). Crozes *et al.* developed the data set in Figure 2 from a series of tracer experiments in contactors with different L/W ratios. In Crozes *et al.* (1998), each tracer test RTD curve was then fitted with the N-tanks in series model to develop the relationship between N and L/W.

The filter system L/W ratio between the point of tracer injection and measurement was approximately 16. From Figure 2, this L/W value translates to $N = 6$. The resulting RTD curve with $N = 6$ is also shown in Figure 1. Unfortunately, the $N = 6$ RTD curve also does not perfectly fit the entire experimental RTD curve. However, it still may lead to a reasonable prediction of the effluent microbial inactivation and DBP formation compared with the best-fit N and d values. The predicted microbial inactivation and DBP formation using these N and d values will be explored later in this article.

It is clear from this simple example that single-parameter RTD models may not necessarily provide accurate representation of the entire contactor or process train hydraulic characteristic when using the process L/W ratio or the desired T_{10}/HRT to derive an N or d value. The user should be aware of their limitations as a predictor particularly when using L/W or T_{10}/HRT to produce N or d. However, this strategy is very simple to use and provides a quick approximation to the process hydraulics.

Application of the standard level IDDF approach (experimental tracer analysis of Marston WTP contactor)

A step-dose tracer study was conducted on the disinfection contact basin at the Marston WTP. Figure 3 displays a schematic of the Marston contactor. Fluoride was used as the tracer chemical because it is conservative, easily monitored and approved for use in potable water supplies. Fluoride was injected just downstream from the two sluice gates and prior to the perforated baffle. Fluoride was allowed to mix for one channel length to achieve complete mix across the channel cross-sectional area. Samples were collected through a sampling header at the beginning of the third channel to confirm the complete mix of the fluoride (SP1 in Figure 3). Effluent fluoride samples were collected through a sampling header in the middle of the 15th channel (SP2 in Figure 3).

Samples were collected at 1- to 2-minute intervals for one theoretical detention time and increased to 5-minute intervals for the remainder of the tracer tests. Fluoride measurements were made until the effluent concentration was at least 85% of the concentration at SP1. The flow from SP1 and SP2 discharged into a tap in the lab where the samples were measured with a fluoride ion selective probe. The experimental tracer tests were conducted at three target flow rates (20, 40, and 80 MGD). Based on the contactor volume, these flow rates correspond to a theoretical HRT of 257, 129, and 67 minutes, respectively. The resulting RTD curves from the tracer tests are displayed in Figure 4.

In Figure 4, the RTD curves are displayed as a function of dimensionless time that was normalized by the theoretical HRT for each respective flow rate. As shown in Figure 4, the Marston contactor has a high hydraulic

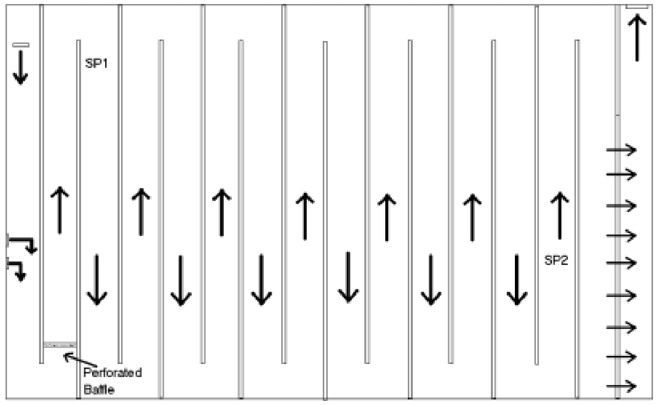

Figure 3 | Schematic of Marston WTP contactor.

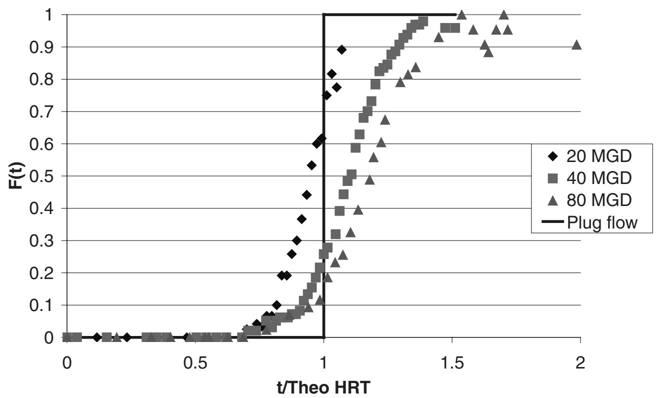

Figure 4 | Experimental RTD function for Marston contactor; time normalized with theoretical HRT.

 Journal of Water Supply: Research and Technology—AQUA | 50.4 | 2001

efficiency with T_{10}/HRT greater than 0.8. However, the results in Figure 4 also suggest that the contactor has a T_{10}/HRT greater than 0.95 for the 40 and 80 MGD flow rates. These results are questionable for the following two reasons:

1. For contactors with very high hydraulic efficiencies, the dimensionless RTD curve (F(t/HRT)) should collapse to the same curve regardless of flow rate.
2. T_{10}/HRT values greater than 0.95 should closely resemble a step-input response of an ideal plug flow reactor.

F(t/HRT) indicates all the possible exit times that a fluid parcel will achieve from travelling through the contactor. For high T_{10}/HRT values, the variation in times that a fluid parcel takes to exit the contactor is very small (i.e. the dimensionless variance is very close to zero). The reader should recall that the dimensionless variance is related to the amount of tracer dispersion through the contactor (Levenspiel 1972; Clark 1996). For a plug flow reactor where the dimensionless variance is ideally zero, F(t/HRT) has the same step shape curve regardless of the flow rate. As a result, F(t/HRT) curves produced for different flow rates through a plug flow reactor, should collapse to the same curve when plotted against dimensionless time. This may not be true for contactors with lower T_{10}/HRT values.

Low T_{10}/HRT factors suggest the existence of significant inefficiencies in the contactor hydraulics due to dead zones, bypassing, and/or mixing. These inefficiencies will affect the distribution of fluid parcel exit times and cause a change in the shape of the F(t/HRT) curve for different flow rates. Since there is little or no dispersion in highly efficient contactors, F(t/HRT) for high efficiency contactors should collapse to the same curve regardless of flow rate.

In the 40 and 80 MGD experimental F(t/HRT), the T_{10}/HRT factors are so close to 1 that the shape of F(t/HRT) should more resemble that of a plug flow reactor (Figure 4). In Figure 4, the 40 and 80 MGD F(t/HRT) still have some amount of dispersion as seen by the amount of time it takes the RTD function to reach a value of 1. The 40 and 80 MGD F(t/HRT) reach 1 at t/HRT values greater than 1.2.

The results in Figure 4 suggest that the dimensionless times for the 40 and 80 MGD F(t/HRT) may be incorrect and that these results may be caused by one of the following: (1) the true flow rate through the contactor may be less than 40 and 80 MGD, respectively; (2) there is an error in the volume used for the calculation of the theoretical HRT (this error in volume may also include not taking into account recording leads); and (3) the tracer is not an inert material and may have been adsorbed or been held back on the surfaces (Levenspiel 1972). The dimensionless times for the 40 and 80 MGD results can be easily checked by analysing the F(t/HRT) in Figure 4 using the NLLS method and computing the HRT from the experimental data (Haas *et al.* 1997).

The NLLS method consists of fitting a nonlinear function to the experimental residence time density data and minimizing the following objective function:

$$SSR=\sum_{i=1}^{N}(f(t_i)_{EXP}-f(t_i)_{NLF})^2 \tag{4}$$

where SSR = sum of the squares error; $f(t_i)_{\mathrm{exp}}$ = experimental residence time density data at time t_i; and $f(t_i)_{\mathrm{nlf}}$ = nonlinear residence time density function value at time t_i.

The nonlinear residence time density function used in the NLLS method is the Nauman/Buffham extension of the dispersion model and is described as:

$$f(t)=\sqrt{\frac{HRT}{2\pi t^3\sigma^2}}\exp\left[-\frac{(t-HRT)^2}{2HRTt\sigma^2}\right] \tag{5}$$

where σ^2 is the dimensionless variance. HRT and σ^2 are used as the fitting parameters. Haas *et al.* (1997) compared the NLLS method with the traditional method of moments to compute the experimental HRT and found the NLLS method to be more accurate. The NLLS analysis for the 20-MGD data set is displayed in Figure 5.

In Figure 5, the NLLS method determines the experimental HRT to be 252 minutes, which is well within the 5% deviation tolerance specified in the quality assurance/quality control (QA/QC) discussed in a previous article (Ducoste *et al.* 1999). Although F(t/HRT) did not reach 1 during the tracer test at the 20 MGD level, the NLLS method has been shown to accurately determine

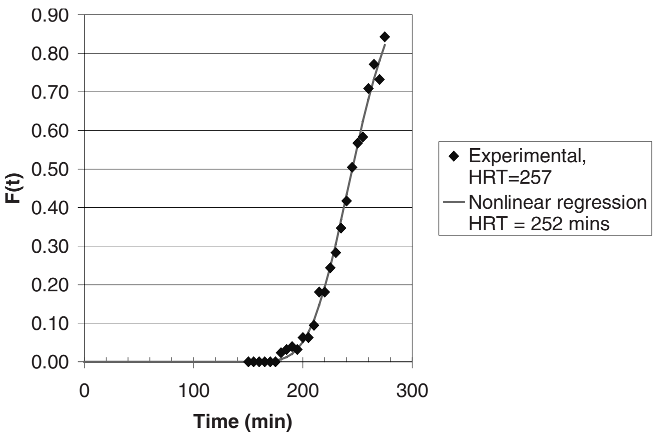

Figure 5 | Nonlinear least squares analysis of experimental tracer tests at 20 MGD.

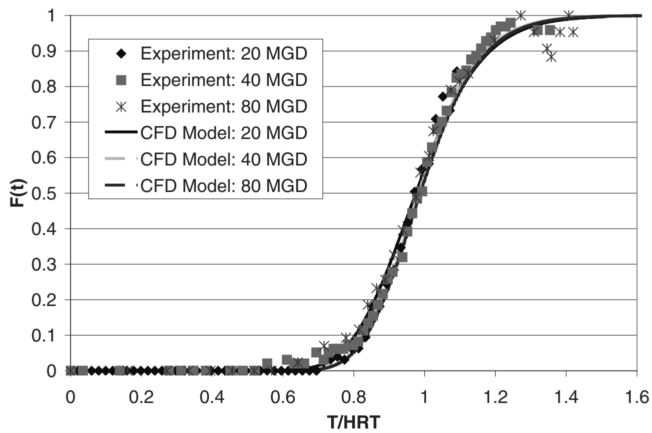

Figure 6 | Comparison between numerical and experimental RTD curves (experimental data sets were normalized with calculated HRT).

the experimental HRT value with a maximum F(t/HRT) = 0.75 (Haas *et al.* 1997). However, the NLLS analysis predicts that the experimental HRT is 144 and 81 minutes for the 40 and 80-MGD RTD functions, respectively. These values are higher than the theoretical values (40 MGD: 129 min and 80 MGD: 67 min).

While a non-conservative tracer could cause a significant deviation between the experimental and theoretical HRT, fluoride is considered a conservative tracer unless in the presence of significant alum floc concentrations. The presence of significant alum floc would not occur in the disinfection contactor. The volume used to compute the theoretical HRT was also correct since it was used to build the CFD models, which predict the correct HRT with these flow rates. The CFD results will be discussed in the next section. Based on these experimental HRT values, the actual flow rates may have been 36 and 66 MGD.

When the 40 and 80-MGD F(t/HRT) in Figure 4 were re-plotted with the experimentally determined HRT values, all three curves collapsed to one F(t/HRT) curve (Figure 6). Figure 6 demonstrates the importance of performing QA/QC checks to confirm or refute experimental tracer study results. The results in Figure 6 also show that T_{10}/HRT values greater than 0.8 may produce dimensionless F(t/HRT) whose shape is not a function of the flow rate. This concept was also confirmed using CFD modelling.

Application of the advanced IDDF approach (CFD analysis of Marston WTP contactor)

A numerical tracer analysis of the Marston WTP contactor was also done using CFD. Models were developed for the 20, 40, and 80 MGD flow rates. PHOENICS (CHAM, UK), a general purpose CFD software package based on the finite volume approach, was used in this study. Table 4 displays the model's boundary conditions. The grid spacing was approximately 0.6 m in each direction and was small enough to produce a grid independent solution without significantly affecting the computational cost. The time step interval used for the tracer transport simulation was 0.5% of the theoretical HRT. A small time step interval is also necessary to produce a grid independent solution (Ducoste & Brauer 1999). In the numerical tracer analyses, tracer was added continuously at the inlet (i.e. step input tracer test) (Teefy 1996). The tracer concentration was monitored at SP2 in Figure 3 until the effluent concentration was equal to the influent concentration.

Figure 6 also displays the CFD predicted dimensionless F(t/HRT) for the three flow rates in the Marston contactor. As shown in Figure 6, the CFD F(t/HRT) curves collapse to nearly the same curve regardless of the flow rate when plotted against dimensionless time. This prediction is consistent with results of tracer transport in contactors approaching the hydraulic characteristics of ideal plug-flow reactors. Furthermore, the CFD model

Table 4 | Momentum boundary conditions

Contact basin	Inlet (there is one inlet pipe and two sluice gates)				Walls and baffles
Marston	(1) 2.44 m pipe	20 MGD	40 MGD	80 MGD	Velocity = 0.0 (this represents the no slip condition)
	Normal velocity (m s^{-1})	0.094	0.188	0.376	
	Tangential velocity (m s^{-1})	0.0	0.0	0.0	
	(2) 1.83 × 0.77 m sluice gates	20 MGD	40 MGD	80 MGD	
	Normal velocity (m s^{-1})	0.155	0.311	0.622	
	Tangential velocity (m s^{-1})	0.0	0.0	0.0	
	At the three inlet locations	Kinetic energy = 0.0025 (Normal Velocity)^2			
		Energy dissipation rate = 1.64 (Kinetic energy)$^{3/2}$/(sluice gate width or pipe diameter)			

predictions accurately describe the amount of dispersion found experimentally in the Marston contactor. Subtle deviations of model predictions to experimental results may be due to an inaccurate description of the turbulence using the k-ε model, spatial grid refinements where high gradients in fluid flow properties exist, and inaccuracies in the numerical representation of the contactor geometry.

The experimental tracer results were also compared with single-parameter models (*N*-tanks in series and plug flow dispersion). Figure 7 displays the results of determining the single parameter model F(t/HRT) by deriving *N* and *d* from the contactor L/W ratio (Figure 2) (Crozes *et al.* 1998). For the Marston contactor (Figure 3), the L/W ratio is approximately 150. As shown in Figure 7, both single parameter models seem to predict much less tracer dispersion than the experimental results. This lower tracer dispersion may be caused by the inability of the single parameter model (using the L/W ratio to determine *N* or *d*) to capture the bypassing and/or mixing that occurs as the fluid turns 180 degrees around each baffle wall. The fluid bypassing and/or mixing enhances the dispersion of the tracer as it moves through the serpentine contactor. Although these by-pass/mixing zones are less pronounced in large L/W ratio contactors, these zones are still present. As a result, the curve in Figure 2 that relates the L/W ratio to *N* may not accurately describe the level of dispersion for L/W ratios beyond 100, the final data point used to develop that curve.

The results in Figure 7 indicate that the advanced level IDDF approach provides a higher degree of accuracy for

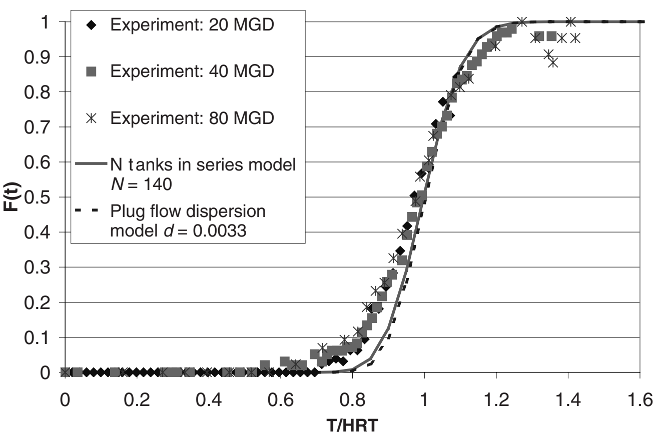

Figure 7 | Single parameter model predictions of the Marston RTD using contactor L/W ratio to compute *N* and *d* values (experimental data sets were nomalized with calculated HRT).

predicting the process hydraulics compared with the basic level approach. It also provides a comparable alternative to performing an experimental tracer analysis. However, whether the IDDF advanced level provides a significantly better prediction of the microbial inactivation or DBP formation level than the basic level to warrant its higher complexity or specialized user expertise will be explored in the following section.

Impact of hydraulic characterization method selection on microbial inactivation and DBP formation

In this study, the RTD data from both treatment plants using the different hydraulic characterization levels were used to calculate the expected microbial inactivation and DBP formation level. The expected microbial inactivation and DBP formation level in the contactor effluent can be computed using the segregated flow concept (Danckwerts 1958). The segregated flow concept treats each fluid parcel as a mini continuous stirred tank reactor (CSTR) that remains completely segregated from other fluid parcel CSTRs throughout its residence time. The extent of reaction in each fluid parcel CSTR depends only on its residence time. Under the segregated flow concept, the outlet microbial or DBP concentration can be determined as:

$$N_{out} = \int_0^\infty N_{batch}(t) f(t) dt \tag{6}$$

where N_{out} represents either the outlet microbial or DBP concentration, $N_{\text{batch}}(t)$ represents the microbial or DBP concentration of a batch after reaction time t, and $f(t)$ is the residence time density function. Table 5 displays the $N_{\text{batch}}(t)$ formulation for both microbial inactivation and DBP formation that is used in the IDDF model. The inactivation and DBP formation results are displayed in Tables 6 and 7, respectively.

Table 6 shows that the basic, standard, and advanced hydraulic characterization levels will predict roughly the same level of microbial inactivation in the Marston contactor effluent. The predicted inactivation using the basic level N-tanks in series model was also found to closely match the inactivation using the experimental tracer data for the Almeda County Water District (ACWD) filter system. Only the predicted inactivation using the PFD model for the ACWD filter system had more than a 15% deviation from the experimental tracer prediction.

Table 7 shows that all three hydraulic characterization levels predicted the same level of TTHM, HAA5, and HAA6 for the Marston contactor and the ACWD filter system. This result was true regardless of the flow rate in the Marston contactor. The lack of sensitivity to the different RTD methods is probably due to the amount of time allowed for DBP formation. As shown in Table 5, the DBP formation equations were developed for contact times between 2 and 168 hours. As a result, the relatively small differences in the RTD curve that occur on the order of minutes for all three characterization levels will not produce significant differences in DBP formation.

The results in Tables 6 and 7 seem to suggest that the IDDF basic level (N-tanks in series, PFD model) and the advanced level (CFD model) modules may predict similar levels of disinfection and DBP formation regardless of subtle differences in the RTD curve. These results are encouraging since experimental tracer tests cannot always be performed to determine the process hydraulic characteristics. Moreover, the relatively good agreement between the inactivation/DBP formation results produced using the single-parameter RTD models and the experimental RTD data is important since these models can be performed by most WTP professionals and require very little specialized expertise.

Although the inactivation/DBP formation model predictions using the basic level RTD data performed very well, more experimental tracer data need to be collected in contact basins that have significantly smaller L/W ratios and at multiple flow rates. Experimental tracer studies from researchers have shown that the shape of the dimensionless RTD curve (i.e. the amount of dispersion or mixing) can be a function of the flow rate for reactors with small L/W ratios (Shawwa & Smith 1998; Peplinski 2000). As a result, there is the potential for significant error to occur in predicting the inactivation level at multiple flow rates using the same L/W ratio to determine the amount of dispersion or mixing. Furthermore, the basic level hydraulic method does not provide a way to analyse the

Journal of Water Supply: Research and Technology—AQUA | 50.4 | 2001

Table 5 | Conditions used in the IDDF inactivation and DBP formation modules (Amy and Sohn 1999)

Inactivation module	
k_d (l min^{-1}) k (L/(mg-min)) t (min)	Integral Hom model: $Log\left(\frac{N}{N_0}\right) = -kmC_o^n \int_0^T \exp(-k_d tn)t^{m-1}dt$ k_d = disinfectant decay rate = 0.001 k = inactivation decay rate (*Giardia*) = 2.778 $pH^{-2.69}$ $Temp^{0.15}$ *m = inactivation constant* = 1.0 *n = inactivation constant* (*Giardia*) = 1.022 $Temp^{0.003}$ $pH^{-0.088}$ *CT range for k*: 56≤CT≤500 mg per l-min Model Temp: 20°C, actual temp used in simulation = 5°C pH = 7.5 C_0 = 1.4 mg l^{-1} free chlorine
DBP formation module (in coagulated water alum or iron treated)	TTHM = 3.296 $DOC^{0.801}$ $Cl_2^{0.261}$ $(Br^-)^{-0.223}$ $t^{0.264}$ HAA5 = 8.35 $DOC^{0.701}$ $Cl_2^{0.577}$ $(Br^-)^{-0.05}$ $t^{0.15}$ HAA6 = 5.22 $DOC^{0.585}$ $Cl_2^{0.565}$ $(Br^-)^{-0.031}$ $t^{0.153}$ DOC = dissolved organic carbon = 6 mg l^{-1}, model range: 1.0≤DOC≤7.77 Cl_2 = applied chlorine dose = 1.4 mg l^{-1}, model range: 1.1≤Cl_2≤14.2 Br = bromide concentration = 50 μg l^{-1}, model range: 36≤Br≤308 Model Temp: 20°C, actual temp used in simulation = 10°C pH = 7.5 Model reaction time range: 2 hr≤t≤168 hr pH and temperature correction HAAs = ($HAAs^+$pH = 7.5, Temp = 20°C)*$(c)^{(pH-7.5)}(e)^{(Temp-20)}$ c = 0.9216 (for HAA5) and 0.9320 (for HAA6) e = 1.022 (for HAA5) and 1.021 (for HAA6) TTHM = ($TTHM^+$pH = 7.5, Temp = 20°C)*$(c)^{(pH-7.5)}(e)^{(Temp-20)}$ c = 1.156 (for TTHM) e = 1.026 (for TTHM)

impact of perforated baffles or inlet/outlet hydraulic structures on the RTD curve. These design considerations will have to be addressed using the advanced level hydraulic characterization method where CFD has been shown to be sensitive to those design options.

Impact of using the entire RTD curve on microbial inactivation, TTHMs, and HAAs

As discussed in the previous section, the IDDF methodology utilizes the entire probability distribution of residence times to compute the effluent microbial inactivation and DBP formation level (Equation 6). This is a major departure from the USEPA CT method, which utilizes only one specific time from the RTD. In the case of the USEPA method, the T_{10} value may be conservative in its prediction of the true inactivation level at low inactivation levels. At low inactivation levels, the CT method requires a higher disinfectant dose and may further promote the formation of DBPs. However, when a high degree of inactivation is required, the T_{10} value may actually under-predict the disinfectant dose since the degree of inactivation is now driven by the contribution of organisms that have shorter residence times than the HRT. Although this factor was not explored in the present article, it may become an important issue as the drinking water community strives to achieve higher levels of inactivation.

A comparison between USEPA and IDDF prediction of the inactivation levels for the Marston contactor and ACWD filter system is also displayed in Table 6. The USEPA predicted inactivation levels were determined by multiplying the C_0 (initial residual free chlorine:

Journal of Water Supply: Research and Technology—AQUA | 50.4 | 2001

Table 6 | Predicted level of microbial inactivation for *Giardia* in Marston contactor and ACWD filter system using the IDDF model and USEPA CT tables

Data set	T_{10}/HRT	CT (mg/L-min)	USEPA log inactivation	IDDF log inactivation
Marston contactor				
20 MGD Exp.	0.81	293	3.31	4.45
20 MGD CFD	0.80			4.51
20 MGD $N = 140$	0.9			4.59
20 MGD $d = 0.0033$	0.9			4.63
36 MGD Exp.	0.83	167	1.89	2.70
36 MGD $N = 140$	0.9			2.75
36 MGD $d = 0.0033$	0.9			2.77
66 MGD Exp.	0.83	94	1.06	1.58
66 MGD $N = 140$	0.9			1.6
66 MGD $d = 0.0033$	0.9			1.61
40 MGD CFD	0.82	150	1.69	2.41
40 MGD $N = 140$	0.9			2.5
40 MGD $d = 0.0033$	0.9			2.52
80 MGD CFD	0.82	78	0.88	1.28
80 MGD $N = 140$	0.9			1.33
80 MGD $d = 0.0033$	0.9			1.34
ACWD filter system				
Exp.	0.46	26	0.29	0.72
$N = 4.05$	0.44	25		0.68
$N = 6.0$	0.52	29		0.72
$d = 0.147$	0.59	33		0.83

1.4 mg l^{-1} from Table 5) by the T_{10} value and using the USEPA CT tables for *Giardia*. In Table 6, the IDDF model predicts significantly more inactivation of *Giardia* than the level predicted using the USEPA CT tables. For the Marston contactor, the IDDF model predicts more than 35% higher inactivation for the same CT value. For the ACWD filter system, the IDDF model predicts 147% more inactivation for the same CT. However, the USEPA

Table 7 | Predicted level of DBP formation in Marston contactor and ACWD filter system

Data set	TTHM ($\mu g\ l^{-1}$)	HAA5 ($\mu g\ l^{-1}$)	HAA6 ($\mu g\ l^{-1}$)
Marston contactor			
20 MGD Exp.	38	25	18
20 MGD CFD	38	25	18
20 MGD $N = 140$	38	25	18
20 MGD $d = 0.0033$	38	25	18
36 MGD Exp.	34	25	17
66 MGD Exp.	30	24	17
40 MGD CFD	33	24	17
80 MGD CFD	28	23	16
ACWD filter system			
Exp.	25	22	15
$N = 4.05$	24	21	15
$N = 6.0$	24	21	15
$d = 0.147$	26	22	15

inactivation value for the ACWD filter system may be questionable since the calculated CT value is outside the range of the experimental data set on which the USEPA CT tables were based (USEPA 1991).

The IDDF results suggest that the treatment plant could reduce the disinfectant dose and still achieve the inactivation credit specified using the USEPA CT tables. This reduction in disinfectant dose would reduce the chemical costs as well as reduce the level of DBPs. The result of lowering the disinfectant dose on the inactivation and DBP formation levels for the Marston contactor is displayed in Table 8. In Table 8, the results show that the treatment plant can reduce the disinfectant dose by 35% and still meet the USEPA CT requirement. This reduction in disinfectant concentration will also lead to at least a 10% reduction in TTHMs and 20% reduction in HAA5 and HAA6. These results are important since they provide treatment plants with the possibility of reducing the cost of disinfection while meeting future stringent regulations in the D/DBP rules and still maintain adequate microbial inactivation.

GUIDANCE FOR USE OF THE IDDF HYDRAULIC CHARACTERIZATION MODULE

The IDDF can be used at various levels that require a wide range of resources. Before committing substantial resources to the development of the input parameters, a utility should judge the benefits of implementing the IDDF. Typically, the method used to calculate the contactor hydraulic efficiency will be based on whether the contactor already exists or is proposed as a new contactor (i.e. exists in a conceptual design).

All three levels of the hydraulic characterization methods (single parameter models, experimental tracer studies, CFD models) can be used to quantify the hydraulic efficiency of existing contactors. However, for new contactors, only single parameter and CFD models are applicable. Factors that influence hydraulic method selection include cost, accessibility of tools necessary to conduct test method, reliability of method, amount of time to complete test method, and employee expertise. These factors are important regardless of whether a hydraulic analysis is done on existing or new contactors. As a guide to determine which method is appropriate for a user's specific case, a simple decision flowchart is provided in Figure 8. Figure 8 should be used when there is uncertainty on the effort level required for quantifying the contactor hydraulic efficiency.

The decision flowchart initiates the user to think about the desired hydraulic efficiency (i.e. T_{10}/HRT) that the contactor should obtain. Through published empirical charts and figures, the user can determine the appropriate contactor L/W ratio that corresponds to the desired T_{10}/HRT ratio (Damron 1994; Crozes *et al.* 1998). If minimizing capital and operating costs or optimizing the contactor geometry to meet future stringent finished water quality regulations are not of primary concern, then there are no significant benefits to using the IDDF hydraulic characterization module and the user should terminate here. If,

Journal of Water Supply: Research and Technology—AQUA | 50.4 | 2001

Table 8 | Reduction in disinfectant dose and DBP formation for the same level of microbial inactivation predicted using the USEPA CT tables

Data set	CT	Disinfectant dose required using T_{10} (mg l^{-1})	Disinfectant dose required using IDDF (mg l^{-1})	Log (N/N_0)	Revised DBP formation levels (% reduction)		
					TTHM (μg l^{-1})	HAA5 (μg l^{-1})	HAA6 (μg l^{-1})
20 MGD Exp.	293	1.4	1.0	3.31	35 (9)	20 (19)	15 (19)
36 MGD Exp.	167	1.4	0.9	1.89	30 (11)	19 (22)	14 (21)
66 MGD Exp.	94	1.4	0.9	1.06	26 (11)	18 (23)	13 (23)
40 MGD CFD	150	1.4	0.9	1.69	29 (11)	19 (23)	13 (22)
80 MGD CFD	78	1.4	0.9	0.88	25 (11)	18 (23)	13 (22)

however, further hydraulic analysis of the contactor is needed to determine the overall RTD, then the user should move to the next stage that determines whether the analysis is accomplished on a new or existing contactor.

For new contactors, the decision flowchart asks the user whether a final design has been determined or if multiple configurations are being considered. If multiple baffle configurations are being considered, then the best course of action is to perform a CFD analysis. CFD analyses provide the best opportunity for evaluating the impact of the different baffle configurations on the contactor-effluent RTD. If a final baffle configuration has been selected, then the user has the option to use either a single-parameter RTD model or a CFD model to produce the contactor-effluent RTD. For greater accuracy, the user should select the CFD model.

In the case of an existing contactor, the user can approach the hydraulic analysis either through a current or future modified contactor-design demonstration or through implementation where regulatory approval is required. For demonstration purposes, the user should develop a CFD model, particularly when multiple design configurations are being considered for retrofit of an existing contactor. For existing contactors, users that have previously conducted or have the resources to conduct an experimental tracer test, should use these results as an RTD-function input to the IDDF model. Experimental tracer tests are the best alternative when resources to produce CFD models are not available. The user can also use single parameter models to generate the RTD function as the final alternative if neither CFD models nor experimental tracer tests can be conducted due to limited resources or personnel expertise.

In situations where regulatory approval is necessary, the only options available to determine the contactor hydraulic efficiency are experimental tracer studies or CFD models. Previously conducted tracer test results can be used to evaluate the hydraulic efficiency at the desired plant operating conditions. For contact basins with near-ideal hydraulic characteristics (i.e. $T_{10}/HRT \geq 0.8$), a normalized RTD curve can be used to predict the T_{10} value for any flow rate. However, for $T_{10}/HRT < 0.8$, old tracer data results should not be used if flow conditions during that tracer test are significantly different from current or future flow conditions. These situations require either new experimental tracer tests or simulated tracer tests using CFD. CFD simulated tracer tests would have a distinct cost advantage over experimental tracer tests when quantifying the contactor hydraulic efficiency for multiple flow conditions.

Overall, Figure 8 provides a simple hydraulic characterization module roadmap for selecting the level of analysis to determine the contactor hydraulic efficiency. The roadmap, however, does not include the cost component for each hydraulic characterization level. In the selection process, the user should weigh the costs (i.e.

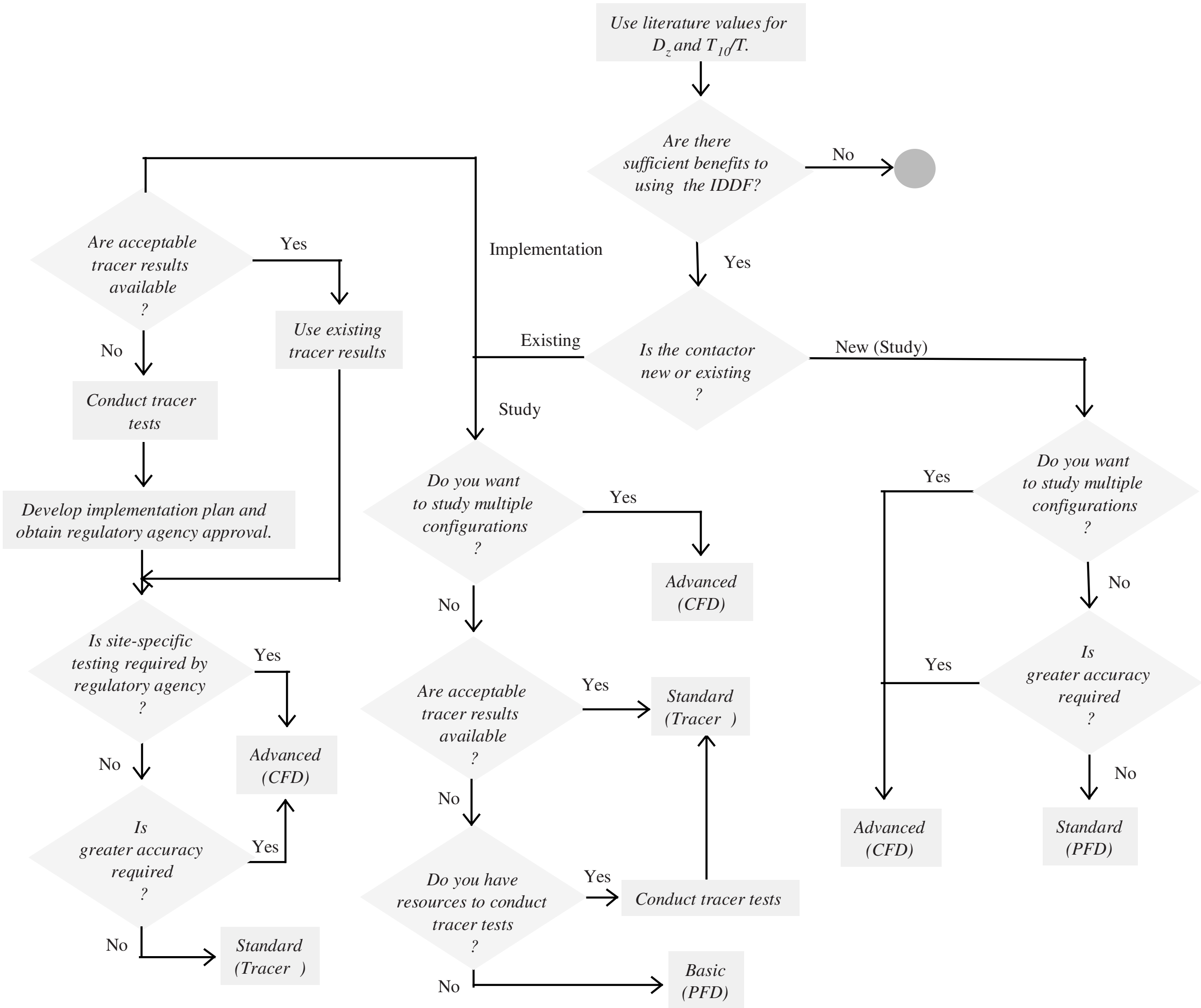

Figure 8 | Guidance for hydraulic characterization module alternative selection.

personnel-hours, chemical costs, analysis costs) associated with the chosen hydraulic characterization method.

CONCLUSIONS

- The IDDF approach is a tool that can be used to optimize the disinfection process to assure sufficient microbial inactivation while reducing DBP formation.
- The IDDF hydraulic characterization basic level RTD was found to match only part of the experimental RTD for the filter system. Within the basic level, the *N*-tanks in series model outperformed the PFD model. The predicted *Giardia* inactivation level using the *N*-tanks in series RTD

was within 6% of the inactivation level using the experimental RTD. The inactivation level using the PFD model RTD was within 17% of the experimental inactivation level.

- The IDDF hydraulic characterization advanced level (CFD modelling) was found to better predict the amount of dispersion in the disinfection contactor than the basic level (single-parameter RTD models) approach when *N* or *d* is determined using the contactor L/W ratio. Deviations in the RTD curve between the two levels, however, were not significant to cause major differences in the predicted *Giardia* inactivation level. Furthermore, no differences in the TTHM and HAAs were found when the RTD data were supplied from the basic or advanced levels. These results suggest that the basic level hydraulic characterization approach may be sufficient to produce the RTD data for contactors with high T_{10}/HRT ratios to predict the inactivation and DBP formation levels.
- The results of using the IDDF concept at the disinfection contactor site showed that the disinfectant dose could be reduced by 35% and still meet the USEPA CT requirement for *Giardia* inactivation. This reduction in disinfectant concentration could lead to a 10% reduction in TTHM and a 20% reduction in HAA5 and HAA6. These results suggest that treatment plants could reduce the cost of disinfection and the level of DBPs while still maintaining current levels of inactivation specified in the USEPA CT tables.

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