An enhanced tanks-in-series model for interpretation of tracer tests

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ABSTRACT

Imperfect hydraulic behaviour of water treatment units, expressed by stagnation space and bypassing, may substantially reduce treatment efficiency. Computational fluid dynamics (CFD) and residence-time distribution (RTD) based tracer test models may be used to identify such problems; the RTD models are more appropriate for operating treatment units. A three-parameter tank-in-series RTD model for interpretation of tracer tests is presented in this paper, where the parameters are the number of tanks, the portion of dead-space and the portion of bypassing. Expressions for the first three moments of the proposed RTD function are derived. An optimization procedure, implemented in MS Excel, is then used to obtain the number of tanks, and the fractions of dead-space and bypassing minimizing the difference between tracer test data and unit's residence-time distribution function. The uniqueness of the solution is discussed, and comparison with simpler one and two-parameter models is provided. Results were compared with experimental data obtained from real drinking water treatment plants located in the cities of Nuevo Laredo and Río Bravo, Tamaulipas; and Piedras Negras, Coahuila, Mexico.

Key words | dead-space and bypassing, multi-parameter models, residence time analysis, tanks-in-series, tracer test, water treatment plants

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NOTATION

A	constant in the quadratic Equation (26)
$C(t)$	concentration evolution at the treatment unit exit
$E(t)$	normalized residence-time distribution function
i	index representing current concentration, tank number or time value
$i\ max$	number of measured concentration values
M	fraction of unit's volume effectively used in treatment process (with no stagnation space)
$(1-M)$	fraction of stagnation space in unit's volume
n	fraction of flow rate effectively used in treatment process
$(1-n)$	fraction of flow rate involved in bypassing
N	number of reactors in series
Q	volumetric flow rate
t	time
V	treatment unit volume
$\Gamma(\ )$	Gamma function
$\delta(\ )$	Dirac delta function
$\epsilon(\ )$	error function
μ	average residence time
μ_2'	second central moment (variance)
μ_3'	third central moment
θ	dimensionless residence time
$\langle\theta^r\rangle$	rth moment of RTD function
θ_{eff}	effective dimensionless residence time
τ	global mean residence time
τ_{eff}	effective mean residence time

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INTRODUCTION

Many water treatment plants in Mexico (and maybe around the globe) operate with lower treatment efficiency, compared with their design or expected efficiency. The insufficient hydraulic efficiency of some treatment units, such as mixing tanks, flocculation and sedimentation units and others, is among the most important factors that affect the overall plant performance. Treatment units are often designed under the premise of idealized flow conditions, such as completely stirred reactor, perfect plug flow reactor, and so on. The real flow pattern inside the treatment unit normally is very different; in particular, important efficiency-reducing *stagnation space* and *bypassing* frequently occur.

In a continuous flow treatment unit, stagnation space is a liquid volume that is not constantly renewed by the inflow to the unit. Bypassing is expressed by preferential flow paths where liquid volumes leave the unit before the expected residence time, and before the expected mixing with the rest of the liquid volume. In order to define measures to improve the unit efficiency, it is important to identify if such undesirable effects take place inside the unit and what is their extent. Two types of numerical model have been used to study the flow distribution inside the treatment units in order to identify such hydraulic problems: computational fluid dynamics (CFD) models and flow tracing residence-time distribution (RTD) models.

The CFD models are based on discretizing the flow region, specifying boundary conditions and solving numerically coupled nonlinear partial differential equations to simulate the movement of water. If properly implemented, they are able to provide detailed information in space and time about the flow inside the treatment unit. Although CFD modelling has been widely used in chemical, nuclear and mechanical engineering, its use in the water industry is a relatively recent development (Haestad Methods *et al.* 2003, p. 379). Harwood and Wicks (2001) presented an overview of the CFD application in the water industry. More recent CFD applications to water treatment are presented by Huang *et al.* (2002), Craig *et al.* (2002) and Greene *et al.* (2002, 2004). There exist many CFD commercial packages (for example Fluent, www.fluent.com/). Some research-oriented authors (and software vendors) state that CFD models represent the cutting edge for flow modelling in water treatment. However, such tools also have disadvantages and limitations to be applied for practical work. Results depend on the choice of governing equations, boundary conditions and discretization level. Certain parameters are assumed, so CFD models must be validated experimentally before being totally trusted.

Commercial CFD packages are normally expensive, but the most serious limitation of the CFD models is the need for a knowledgeable person, with a high level of skill and understanding of fluid mechanics and numerical modelling, to properly implement the model. As an example, for modelling turbulent flows the commercial package Fluent offers the Reynolds Stress Model, standard k-ε and RNG modification of k-ε model, the turbulent viscosity transport model of Spalart and Allmaras, large eddy simulation, detached eddy simulation, and several different models for approximation of boundary conditions at wall. It is not an easy task, even for a person familiar with fluid mechanics, to decide which of these models is the best for a specific problem.

The application of the flow tracing residence-time distribution (RTD) models consists in addition of a substance (tracer) to the incoming flow and measurement of its concentration at the outflow of the treatment unit (Levenspiel 1999) as a function of time until nearly zero or constant tracer concentration is reached, depending on the type of tracer addition method. Since every fluid element-carrying tracer will take a different period of time to reach the unit outlet, the obtained concentration curve represents *the residence-time distribution* of the unit, and is a characteristic of the mixing that occurs inside it. The obtained residence-time distribution curve can be used to reveal the hidden hydraulic behaviour of water treatment units (flocculation, sedimentation and mixing tanks). Known techniques include simplified methods such as that proposed by Rebhun & Argaman (1965), which consists of correlation of the experimental curve with some basic hydraulic characteristics, as well as fitting to the experimental data of an equation (mathematical model) that describes the hydraulic performance of the treatment units in terms of stagnant (dead) spaces, bypassing, and similarity with basic flow types, such as plug flow and stirred reactors, expressed by a certain number of reactors in series (Levenspiel 1999, Fogler 1992).

Compared with CFD models, RTD models are much simpler, and less expensive, to apply in operating treatment plants, provided a suitable equation (model) and curve fitting tools are available. A distinctive advantage of the RTD models over the CFD models is that the study can be carried out even when the exact interior geometry of the treatment unit is not completely known. Any CFD model would require the exact flow region geometry to be specified beforehand. In operating treatment units, unexpected sludge accumulation, broken interior distribution pipes or channelling devices, or other not directly visible problems may cause the imperfect flow behaviour. CFD models may not be useful in such cases. This way, CFD models can be used in the design of new treatment units, but are less applicable for analysing the flow problems in operating units.

Several basic RTD models are available in chemical reaction engineering textbooks, such as Levenspiel (1999) and Fogler (1992). As a rule, those are very approximate models that attempt to capture all of the imperfect flow behaviour in one parameter, such as the number of reactors in series or dispersion coefficient. Wang *et al.* (1998) reported a two-parameter approach with respect to calculation of disinfection efficiency of drinking water ozonation contactors. In this paper, a three-parameter residence-time distribution model for several tanks in series with dead space and bypassing is proposed. The model is applied to water treatment plants in Mexico, using instantaneous tracer addition, in which a known amount of tracer is added in a very short time. The direct measurement of tracer concentration at the unit flow exit provides the residence-time distribution data, against which the mathematical model function is fitted through an error minimization procedure to obtain the hidden hydraulic behaviour of the unit in terms of the number of tanks in series, and portions of stagnation space and bypassing flow. The proposed model is compared with one and two-parameter models.

METHODS

Background

The following background equations and definitions are used in the proposed model (Levenspiel 1999):

Considering a volume V and a constant flowrate Q, the theoretical mean residence time τ is given by:

$$\tau = \frac{V}{Q} \tag{1}$$

The average residence time μ after an instantaneous (pulse) tracer input is defined as:

$$\mu = \frac{\int_0^\infty tC(t)dt}{\int_0^\infty C(t)dt} \approx \frac{\sum tC(t)\Delta t}{\sum C(t)\Delta t} \tag{2}$$

where t denotes time, and $C(t)$ is the system response to the applied stimulation (the measured concentration evolution at the treatment unit exit).

The normalized residence-time distribution function $E(t)$ is:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} \tag{3}$$

$$\int_0^\infty E(t)dt = 1 \tag{4}$$

where, using the measured data, the denominator in Equation (3) is approximated as:

$$\int_0^\infty C(t)dt = \sum_{i=1}^{i_{\max}-1} \left[\frac{C(t_{i+1}) + C(t_i)}{2}\right](t_{i+1} - t_i) \tag{5}$$

representing the area beneath the measured residence-time distribution curve.

For the sake of generalization, the residence time (t) and the distribution function, $E(t)$, are made dimensionless as follows (Fernandez-Sempere *et al.* 1995):

$$\theta = \frac{t}{\tau} \tag{6}$$

$$E(\theta) = \tau E(t) \tag{7}$$

Model of perfectly mixed reactors in series with stagnation space and bypassing

The purpose of this model is to define a residence-time distribution function that correlates more closely with the experimental data, considering a number of tanks in series and possible dead spaces and bypassing at each tank. The model considers the pulse injection method because it is mathematically simpler, as well as easier to apply during the actual verification at water treatment plants.

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Figure 1 shows the basic assumptions and variables of the problem. The flow through the treatment unit is represented as flow through a series of N equal size continuous flow stirred tank reactors (CFSTRs), allowing for dead-spaces $(1-M)$ and bypassing $(1-n)$ at each CFSTR.

Applying material balance principles and Laplace transform solution techniques, the residence time distribution function for the model shown in Figure 1, for an instantaneous (Dirac function type) tracer addition at the unit's inlet, is given by Equation (8) below. The full mathematical development is contained in Martin-Dominguez *et al.* (1999).

$$E(\theta)=\frac{Nn}{M}\sum_{i=1}^{N}\frac{N!e^{\frac{-nN\theta}{M}}\left(\frac{Nn\theta}{M}\right)^{i-1}(1-n)^{N-i}n^{i}}{(N-i)!i!(i-1)!}+(1-n)\delta\left(\frac{Nn\theta}{M}\right) \qquad (8)$$

In Tzatchkov *et al.* (2005), Equation (8) is obtained from an entirely different probabilistic approach. In its flow path through the N tanks, from the treatment unit inlet to the treatment unit outlet, a fluid particle will visit some tanks, but will bypass others. The probability that a particle visits an individual tank is exactly n, and the residence time for the series of N tanks equals the sum of the residence times for each of the possible series of 1, 2, …, N tanks visited (expressed by the term $e^{-nN\theta/M}(Nn\theta/M)^{i-1}/(i-1)!$), weighted by the probability of the corresponding number of tanks being visited (given by the rest of the terms in the summation).

A simpler model, where bypassing is allowed only over the whole series of reactors, is shown in Figure 2. The residence time distribution function for this case can be obtained as a combination of the known reactor-in-series model (Levenspiel 1999), with a Dirac delta function representing the bypassing. The result is:

$$E(\theta)=\frac{n^{N+1}}{M}\frac{N^{N}}{(N-1)!}\left(\frac{n\theta}{M}\right)^{N-1}\exp\left(-\frac{Nn\theta}{M}\right)+(1-n)\delta\left(\frac{Nn\theta}{M}\right) \qquad (9)$$

It can be proved by direct substitution that Equation (9) represents the last term (corresponding to $i=N$) in the summation given by Equation (8). According to the probabilistic treatment given by Tzatchkov *et al.* (2005), this term considers that bypassing may take place

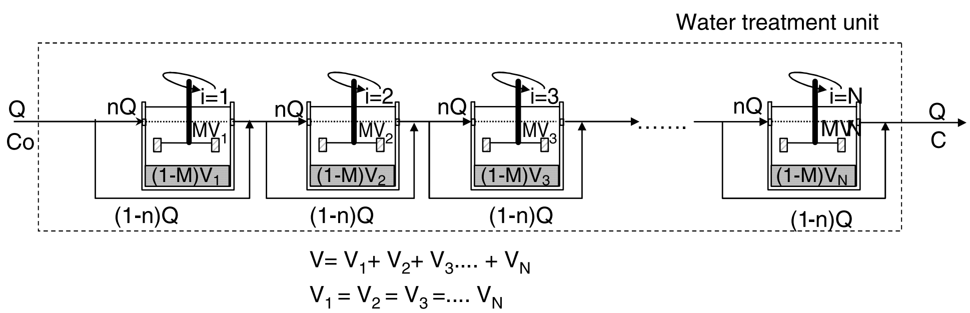

Figure 1 | Reactors in series with stagnation spaces and bypassing at each reactor.

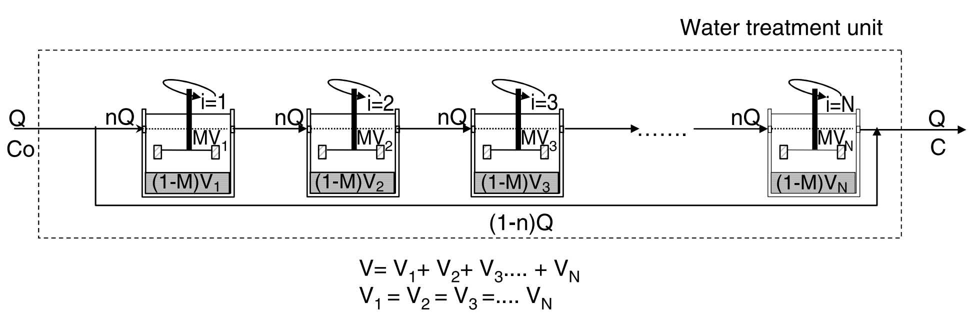

Figure 2 | Reactors in series with stagnation spaces and bypassing over the group of reactors.

simultaneously in all reactors in Figure 1. This way Equation (9) can be considered as a particular case of the more general Equation (8) that takes into account the probability of bypassing that may take place in any number of reactors. Which of these two models to use depends on the specific problem. If global bypassing is suspected, Equation (9) may be used, otherwise the more versatile Equation (8) is recommended. Unless otherwise stated, the rest of this paper deals with the model given by Equation (8).

For reasons explained as follows, the quantity $(n/M)\ \theta$ can be named *effective dimensionless residence time* θ_{eff}. By definition, the unit volume not affected by stagnation space is MV, and the rate of flow not affected by bypassing is nQ. Then, instead of the theoretical residence time τ given by Equation (1), the effective residence time τ_{eff} is

$$\tau_{eff} = \frac{MV}{nQ} = \frac{M\tau}{n} \tag{10}$$

Substituting τ from Equation (10) in Equation (6) and rearranging, the following definition for θ_{eff} is obtained:

$$\theta_{eff} = \frac{t}{\tau_{eff}} = \frac{n}{M}\theta \tag{11}$$

Substituting Equation (11) in Equation (8), and applying a transformation similar to that represented by Equations (6) and (7), the residence-time distribution function is obtained in the following form:

$$E(\theta_{eff}) = \frac{Nn}{M}\sum_{i=1}^{N}\frac{N!e^{-N\theta_{eff}}N^{i-1}\theta_{eff}^{i-1}(1-n)^{N-i}n^{i}}{(N-i)!i!(i-1)!} + (1-n)\delta(\theta_{eff}) \tag{12}$$

For $n=1$ (no bypassing) the numerator of all terms in the summation in Equation (12) equals zero, except for the last term (for $i=N$) where $(1-n)=0$ to power zero equals one. The residence-time distribution function for a series of completely-mixed reactors affected by dead-space only (no bypassing) is thus obtained as:

$$E(\theta_{eff}) = \frac{N^N}{M}\frac{\theta_{eff}^{N-1}e^{-N\theta_{eff}}}{(N-1)!} \tag{13}$$

For $M=1$ (no dead-space) Equation (13) converts to the well-known residence-time distribution function for a series of completely stirred reactors (Levenspiel 1999). For $N=1$ Equation (12) converts to the well-known residence-time distribution function for one completely stirred reactor (Cholette and Cloutier 1959), affected by dead-space and bypassing:

$$E(\theta_{eff}) = \frac{n^2}{M}e^{-\theta_{eff}} + (1-n)\delta(\theta_{eff}) \tag{14}$$

Finally, for $N=\infty$ Equation (12) converts to the Dirac delta function divided by M, just the same (for $M=1$) as the well known residence-time distribution function for an infinite series of completely mixed reactors (Levenspiel 1999). This way, most of the known residence-time distribution functions for series of completely stirred reactors are particular cases of Equation (12).

Moments, mean, variance and skewness of the proposed RTD function

From statistics, the rth moment of the RTD is

$$\langle\theta^r\rangle = \int_0^\infty \theta^r E(\theta)d\theta = \int_0^\infty \left(\frac{M\theta_{eff}}{n}\right)^r \sum_{i=1}^{N}\left[\frac{Nn}{M}\frac{N!(1-n)^{N-i}n^i e^{-N\theta_{eff}}N^{i-1}\theta_{eff}^{i-1}}{(N-i)!i!(i-1)!} + (1-n)\delta(\theta)\right]\frac{M}{n}d\theta_{eff} \tag{15}$$

where, according to Equation (11), θ and $d\theta$ are substituted by:

$$\theta = \frac{M}{n}\theta_{eff},\quad d\theta = \frac{M}{n}d\theta_{eff} \tag{16}$$

Assuming that the order of integration and summation can be switched, and considering that the Dirac delta function at the origin does not contribute to the moments, i.e., $\int_0^\infty \theta^r\delta(\theta)d\theta = 0^r = 0$:

$$\begin{aligned}\langle\theta^r\rangle &= \left(\frac{M}{Nn}\right)^r\sum_{i=1}^{N}\frac{N!(1-n)^{N-i}n^i}{(N-i)!i!(i-1)!}\int_0^\infty e^{-N\theta_{eff}}(N\theta_{eff})^{i+r-1}d(N\theta_{eff}) \\ &= \left(\frac{M}{Nn}\right)^r\sum_{i=1}^{N}\frac{N!}{(N-i)!i!(i-1)!}\Gamma(i+r)\end{aligned} \tag{17}$$

where $d(N\theta_{eff}) = Nd\theta_{eff}$, and $\Gamma(i)=(i-1)!$ is the Gamma function (i is an integer; note: $\Gamma(i+1) = i\,\Gamma(i)$). For $r=1$, 2 and 3, Equation (17) gives

$$r = 1: \langle\theta\rangle = \frac{M}{Nn}\sum_{i=1}^{N} i \frac{N!(1-n)^{N-i}n^i}{(N-i)!i!(i-1)!} = M \tag{18}$$

$$\begin{aligned} r = 2: \langle\theta^2\rangle &= \left(\frac{M}{Nn}\right)^2 \sum_{i=1}^{N} (i^2 + i) \frac{N!(1-n)^{N-i}n^i}{(N-i)!i!(i-1)!} \\ &= \frac{M^2}{Nn} + M^2 + \frac{M^2(1-n)}{Nn} \end{aligned} \tag{19}$$

$$\begin{aligned} r = 3: \langle\theta^3\rangle &= \left(\frac{M}{Nn}\right)^3 \sum_{i=1}^{N} (i+2)(i^2 + i) \frac{N!(1-n)^{N-i}n^i}{(N-i)!i!(i-1)!} \\ &= M^3 Nn[2 + 3N + N^2 - 2(1-n)(1-N^2) \\ &\quad + (1-n)^2(2 - 3N + N^2)] \end{aligned} \tag{20}$$

Using known relations from statistics, from Equations (18) to (20) the second central moment μ_2' (equal to the variance) and the third central moment μ_3' (relative to the skewness) of the RTD given by Equation (8) are obtained as:

$$\mu_2' = Var[\theta] = \langle\theta^2\rangle - \langle\theta\rangle^2 = \frac{M^2}{N}\frac{2-n}{n} \tag{21}$$

$$\begin{aligned} \mu_3' &= 2\langle\theta\rangle^3 - 3\langle\theta\rangle\langle\theta^2\rangle + \langle\theta^3\rangle \\ &= \frac{2M^3}{N^2}\frac{(1-n)^2 + (1-n) + 1}{n^2} \end{aligned} \tag{22}$$

In the absence of bypassing and dead space ($n = 1$; $M = 1$), the moments in (18), (19) and (22) reduce to the standard base case results tabulated in Levenspiel (1999). The mean and variance of the RTD are 1 and $1/N$ respectively.

The results in Equations (18), (21) and (22) could be used to estimate roughly N, M and n from field data. A more refined procedure to obtain them is presented in the next section.

Optimization procedure to obtain model's parameters

The parameters to be obtained from Equation (8) are M, n and N. They can be obtained as follows:

1. Tracer is introduced at the unit inlet, and its concentration is measured at discrete times t_i at the unit exit. The obtained concentration evolution curve is $C(t)$. Using Equations (3), (5) and (7) the $C(t)$ series data is converted to $E(\theta)$ series data.
2. For each t_i (respectively θ_i) the difference (or *error*) between the measured $E(\theta_i)$ and that predicted by Equation (8) (where M, n and N are still unknown) is formulated.
3. The *error function* for the entire dataset is defined as:

$$\varepsilon(M, n, N) = \frac{\sqrt{\sum_{i=1}^{i_{\max}} [E(\theta_i)_{\text{experimental}} - E(\theta_i)_{\text{prediction}}]^2}}{(i_{\max} - 1)} \tag{23}$$

where i max is the number of measured concentrations.

4. The minimization of the function $\varepsilon(M, n, N)$ given by Equation (23), subject to the restrictions $0 \le M \le 1, 0 \le n \le 1$ and N (integer) >0 provides the sought M, n and N parameters.

A MS Excel VBA (Visual Basic for Applications) application was programmed in order to implement this procedure. The user introduces the measured data, the application obtains M, n and N using MS Excel built-in functions (the Solver tool) to perform the error function minimization, and plots the experimental and the model predicted $E(\theta)$ values. The application allows the user to introduce different starting values for M, n and N, in order to see if the obtained solution is sensitive to them. Some examples of the application of this procedure on real water treatment plants are presented later in this paper.

RESULTS AND DISCUSSION

Uniqueness of the solution

Since Equation (8) involves three parameters to be obtained (N, n and M), it is important to know if the solution it provides is unique, that is, if the same solution may be obtained by different combinations of N, n and M. The uniqueness of the solution can be analysed from Equations (18), (21) and (22). Equation (18) shows that the portion of active-space M is uniquely defined by the mean of the measured concentrations. This is in fact a well-known property of any RTD curve (Levenspiel 1999). The variance computed from Equation (21), however, is not unique; that is, after computing M from Equation (18), it is possible to obtain the same variance with different combinations of N and n. In order to analyse the uniqueness of the solution it is necessary to involve the third central moment given by Equation (22). The number of reactors N can be expressed directly from Equations (21) and (22) respectively, as follows:

$$N = \frac{M^2}{\mu_2'}\frac{2-n}{n} \quad (24)$$

$$N = \sqrt{\frac{2M^3}{\mu_3'}\frac{(1-n)^2+(1-n)+1}{n^2}} \quad (25)$$

Equating the right-hand sides of Equations (24) and (25), one equation with one unknown n (or $(1-n)$) is obtained. If this equation has only one physically valid root, then the solution is unique because only one value for N can be obtained from Equation (24). By simple algebraic transformations, Equations (24) and (25) can be reduced to the following quadratic equation for $(1-n)$:

$$(1-n)^2 - A(1-n) + 1 = 0 \quad (26)$$

where A $(A > 0)$ is a constant involving M, μ_2' and μ_3'. A known property of any quadratic equation of the type of Equation (26) is that the product of its two roots equals one. This in turn is possible only when one of the roots $(1-n)$ is less than 1 (physically meaningful root since $n > 0$ in that case) and the other is larger than 1 (physically not meaningful root since $n < 0$). This proves the uniqueness of the RTD function defined by Equation (8).

Figure 3 shows the $E(\theta)$ curve computed by Equation (8) for $M = 1$ (no dead-space) and different combinations of N and n, selected by pairs so that every two combinations $N - n$ in a pair provide the same variance computed by Equation (21). As is seen from this figure, for large numbers of tanks-in-series N Equation (8) provides almost the same $E(\theta)$ curve for different combinations between N and n. This means that, even when the fitting provided by the model represented by Equation (8) theoretically is unique, for large N it is *practically not unique*; that is, very similar fittings can be obtained with different combinations of parameters in that case. The same turns out not to be true for a small number of tanks, say for $N < 11$. For a large number of tanks, the $E(\theta)$ curve tends to be symmetric (for $n = 1$ and for $n < 1$). It is known that the third moment (the skewness) of the curve is a measure of its symmetry. The skewness is zero, or near zero, for symmetric curves. Figure 4 shows the third moment of the $E(\theta)$ curve computed by Equation (22) for $M = 1$ and different values of N and n. As an example, its values are less than 0.05 for $n = 1$ and $N > 6$, $n = 0.8$ and $N > 9$, and $n = 0.6$ and $N > 13$. These values, along with the shape of the curve, may be used as a rough guide for the appropriateness of the proposed three-parameter model. If the observed $E(\theta)$ curve is symmetric, corresponding to a large N, a two-parameter (N and M) model may be sufficient. If the curve is asymmetric, the application of the proposed three-parameter model provides more detailed information about the flow inside the treatment unit.

Figure 4 suggests that $n < 1$ becomes important to be considered for a high level of bypassing and completely

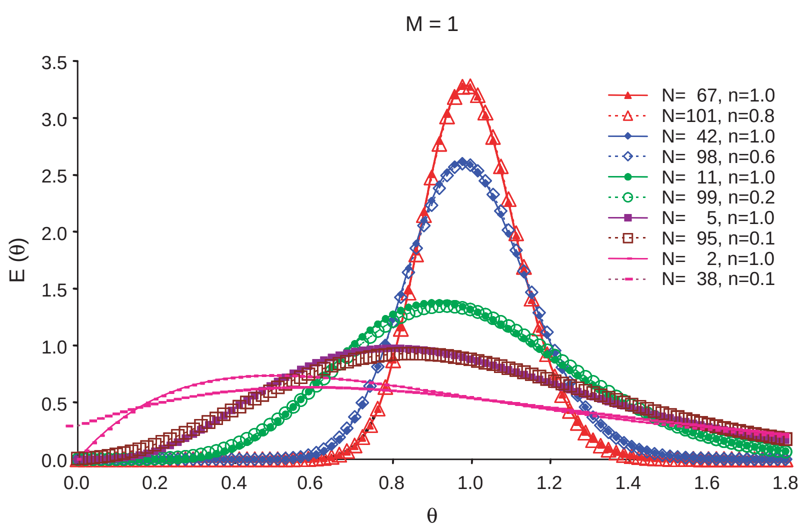

Figure 3 | $E(\theta)$ curves obtained by the proposed three-parameter model for pairs of combinations N-n with the same variance in each pair.

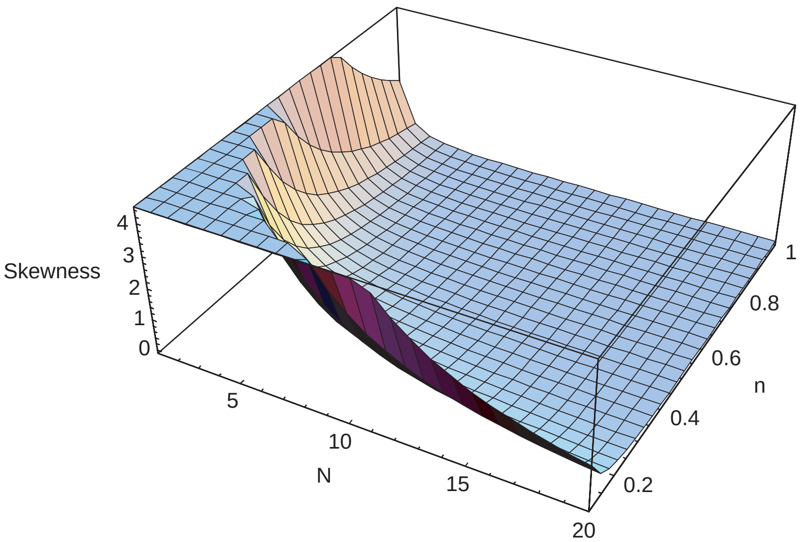

Figure 4 | Third moment (skewness) of the proposed three-parameter model curve for different *N* and *n*.

mixed conditions. Situations of this kind are possible, for example, in some mechanical flocculation units, where the completely mixed conditions are maintained by mechanical mixing devices but their imperfect behaviour causes bypassing. As Monk and Trussell (1991, pp. 408–409) say, 'Short-circuiting is an inherent problem in mechanical flocculation... As can be seen from Figure, a single compartment results in approximately 40 percent of the inflow into a compartment passing through in less than half the theoretical detention time'.

The simple Excel optimization (curve fitting) procedure, described in the previous section, does not guarantee a unique solution. The Excel Solver tool numerical solution requires starting values for M, N and n and may converge, in principle, to a local minimum of Equation (23). This turns out not to be a serious problem in practical applications. Equations (18), (21) and (22) (respectively (26)) provide good starting values for M, N and n, hopefully near the global minimum point of Equation (23). The Excel solution is fast and displays straightforwardly a chart with the obtained fitting, allowing the user to run the application with different starting values and evaluate visually the goodness of the solution in each run. As an additional help, the variance and the third moment (the skewness) of the solution are computed from the measured $E(\theta)$ series and by the theoretical Equations (21) and (22). Then, if more than one good fitting is obtained for different M, N and n, the best one is that with the least difference between the sample and the theoretical second and third moments. Further discussion of choices of n, N and M is given in the next section.

Otherwise, a global minimum seeking procedure for Equation (23) might be developed using known global optimization techniques. Considering that the objective of this work is to present a simple practical tool for interpretation of tracer tests, such optimization is beyond the scope of this paper.

Effect of model's parameters

Figure 5 shows the $E(\theta)$ function computed by Equation (8) for a relatively low number of N ($N = 10$), with and without dead-spaces ($M = 0.5$ and $M = 1$, respectively), and different portions of bypassing. Figure 6 shows the same function for a large number of N ($N = 100$), and $M = 0.2$, $M = 0.6$, and $M = 1$. The presence of dead-space shifts the $E(\theta)$ curve to the left and upwards. For a large number of N (corresponding to a plug-flow-like reactor), the maximum of $E(\theta)$ is located almost exactly at $\theta = M$. The same is not true for a small number of N, where the maximum is located to the left of $\theta = M$. The effect of N is the same as for the conventional one-parameter tank-in-series model (Levenspiel 1999); that is, for a small number of N complete-mixing conditions, and for a large number of N

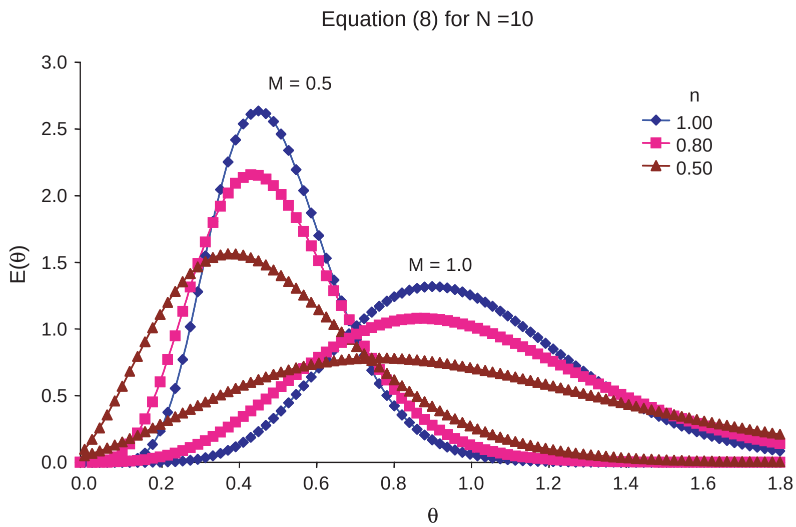

Figure 5 | Model's behaviour for a relatively small number of tanks in series (N=10) and different values of M and n.

plug flow conditions are approached. In either case, the presence of bypassing ($n < 1$) flattens the $E(\theta)$ curve.

Similar conclusions can also be drawn from an analysis of the expressions for the moments of the RTD function, Equations (18), (21) and (22). According to Equation (21), the presence of dead-space ($M < 1$) decreases the variance of the RTD curve (i.e. makes it narrower and taller). The number of tanks in series N acts in a similar way. The presence of bypassing ($n < 1$) counteracts the number of tanks in series N. Regarding the third moment (the skewness) of the RTD curve, the effects are similar, being a much higher skewness for small values of n. A higher (positive) value of the skewness of the curve means an asymmetric curve tail extending out towards more positive values of θ. In the conventional one-parameter tank-in-series model (Levenspiel 1999) the RTD tends to a symmetric curve for large values of N (its skewness tends to zero). This way it is unable to fit measured data with narrow and tall asymmetric curves. Such cases are indicative for simultaneous plug flow-like behaviour and bypassing, and can be identified with the proposed three-parameter model. The distinct difference between plug flow behaviour and bypassing in this context is that in the former the tracer resides (with minimal mixing) for the expected

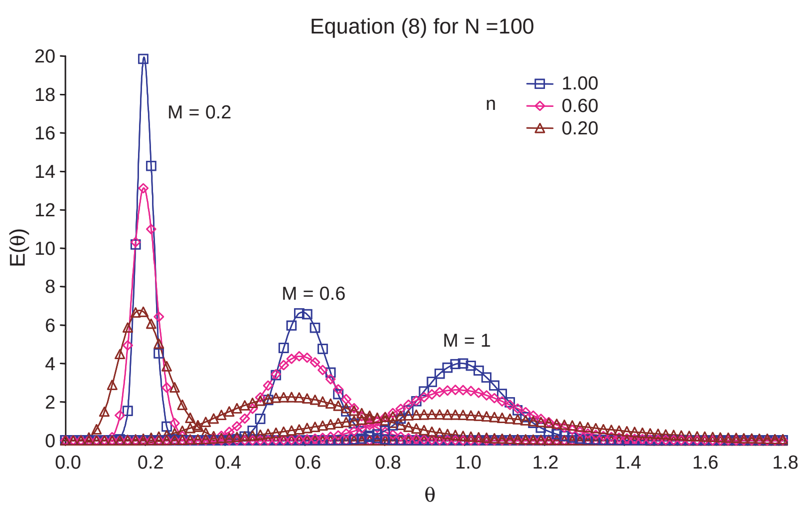

Figure 6 | Model's behaviour for a large number of tanks in series (N=100) and different values of M and n.

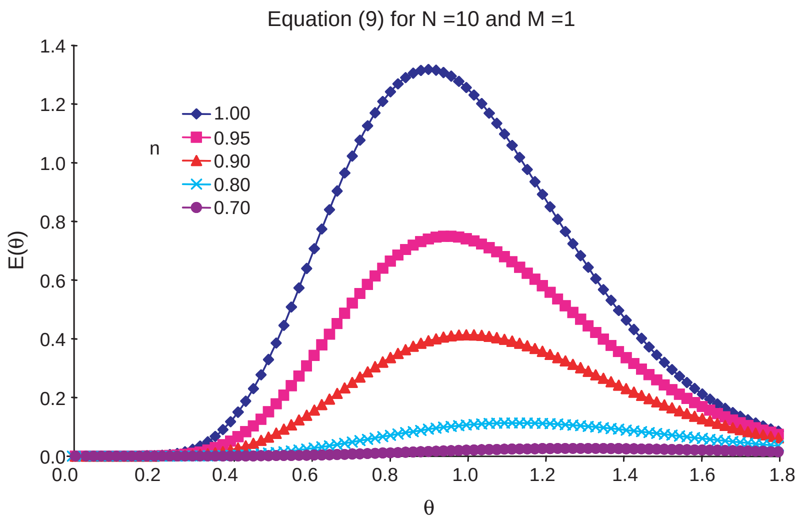

Figure 7 | Behaviour of the model shown in Fig. 2 (global bypassing) for $N=10$, $M=1$ and different values of n.

mean time inside the treatment unit, while in the latter the tracer residence time is (theoretically) zero. The case of plug flow-like behaviour with asymmetric tail is visible in Figure 6 for $M = 0.2$ and $n = 0.2$.

Figures 5 and 6 show that the centroid of the $E(\theta)$ curve moves to a lesser value for $n < 1$ compared with $n = 1$. This is natural, since n expresses *internal bypassing* in the model given by Equation (8), that is, a possible bypassing at each tank. Because of that internal bypassing tracer particles pass through the unit faster, resulting in a smaller overall residence time. Figure 7 shows the behaviour of the model represented by Figure 2 (global bypassing) for different values of n. The trend is qualitatively different here. The centroid of the $E(\theta)$ curve moves to a larger value for $n < 1$ compared with $n = 1$. The global (external) bypassing reduces the flow passing through the treatment unit, resulting in a higher value of the effective residence time, as defined by Equation (10).

Bypassing is undesirable for most water treatment systems, and if detected corrective measures should be taken to avoid it. CFD models may be useful in such cases, obtaining the detailed flow distribution inside the unit and thus defining abnormally high velocity flow paths and the reason for them. Otherwise, a careful examination of the inlet and outlet devices, and the unit's interior geometry may help to identify the bypassing problem and find a solution for it.

Experimental measurements

In order to assess the validity of the above-mentioned model, an experimental programme was carried out at several drinking water treatment plants along the northern border of Mexico (Martin-Dominguez 1999).

For the experiments, common salt was used as a tracer, previously dissolved in water to obtain liquid brine, which was poured in at the units' inflow ports.

The amount of salt used in each unit was calculated in order to obtain an initial tracer concentration of 20 to 30 mg l^{-1} once the total amount of salt had dissolved into the unit's volume. Tracer injection was performed in places where there was a higher chance of having a homogeneous mixing with the inflow before it entered the treatment unit. For flocculation tanks, the tracer was injected either at the rapid mixing tanks or at the inflow channels. For sedimentation tanks, the channels from the flocculation tanks were selected.

The total dissolved solid concentration was measured at the outlet of the studied units using a conductivity meter and began simultaneously with the injection of the tracer at the inflow of the unit.

Measurements were performed at the outflow of each chamber in hydraulic flocculation tanks, and in several internal locations of sedimentation tanks. The time intervals between readings were fixed between 1 and 3 minutes, depending on the residence time of each unit.

Table 1 | Characteristics of studied units

	Treatment plant/City		
	Nuevo Laredo, Tam.	Rio Bravo, Tam.	Piedras Negras, Coah.
Unit type	Mechanical flocculation with four chambers	High rate sedimentation	Vertical hydraulic flocculation
Test location	Exit third chamber	Exit	Exit first chamber
Volumetric flow ($l\ s^{-1}$)	158	145.5	166.0
Unit volume (m^3)	172.8	507	102

Table 2 | Unit with predominant complete mixing behaviour

Nuevo Laredo, Tam.	
Flocculation tank (exit third chamber)	
τ	18.22 min
μ	14.67 min

The proposed model was applied to drinking water treatment units with diverse hydraulic behaviours, such as presumed well mixed, plug flow, stagnation space and bypassing, as detailed in Table 1. For comparative purposes, the results are overlaid with a two-parameter (N and M only) model that neglects bypassing (i.e. for $n = 1$), as explained in the next section.

EXPERIMENTAL RESULTS AND COMPARISON WITH MODEL

In the following, $(1 - M)$ is the volume fraction of stagnation space; $(1 - n)$ is the flow fraction involved in bypassing, and N the number of reactors in series that best describes the units' behaviour. The obtained results show that the mechanical flocculation tank (Table 2 and Figure 8) presents a behaviour, at the exit of the third chamber where the actual measurements were done, close to that of a perfect mixed reactor with 6% bypass problems, and 7% of stagnation space. The model predicted three reactors in series, which correctly fits reality. The best fitting obtained by a two-parameter (N and M only) model that neglects bypassing (i.e. for $n = 1$), is shown in the same Figure. Although the bypassing portion is not high in this case, it is

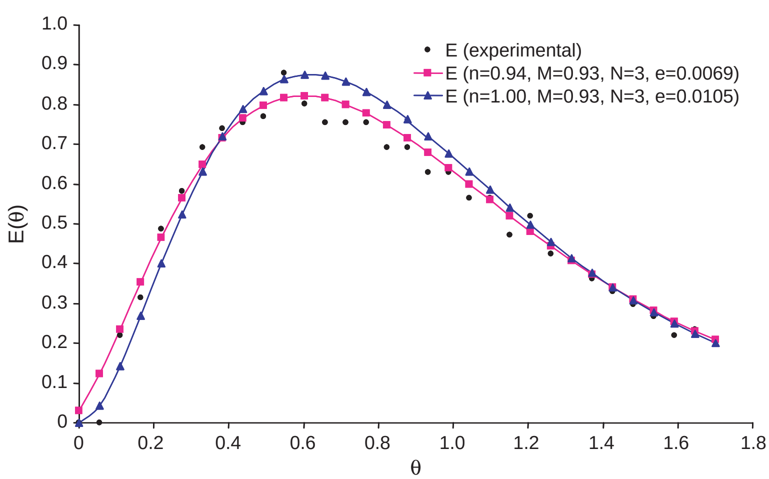

Figure 8 | Unit with predominant complete mixing behaviour (Nuevo Laredo, Tam.).

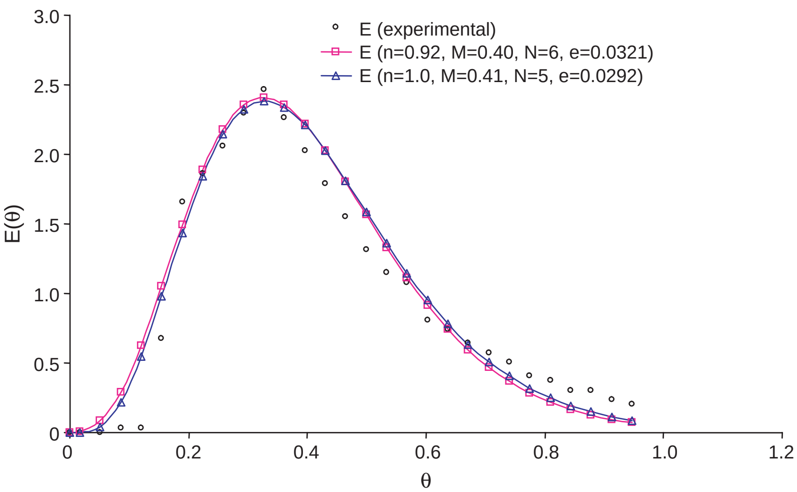

Figure 9 | Unit with predominant complete mixing behaviour (Rio Bravo, Tam.).

seen that the proposed three-parameter model fits the observed data better.

The model's prediction for the high rate sedimentation tank resulted in a high fraction of stagnation space (Table 3 and Figure 9). For this case the simpler two-parameter model produces almost the same fit.

The hydraulic flocculation tank presented a clear plug-flow behaviour (Table 4, Figure 10), which is normally expected for this kind of unit, practically without stagnation space or bypassing. Although simpler one and two-parameter models could be applied as well, the proposed three-parameter model converges directly to the same result (1% dead-space and 1% bypassing).

CONCLUSIONS AND FUTURE WORK

A three-parameter RTD model for a series of tanks with dead-space and bypassing is developed, making possible the analysis of the hidden hydraulic behaviour of water treatment units. In particular the fraction of stagnation space, bypassing and the theoretical number of tanks in series can be obtained by an optimization procedure that minimizes the error between tracer test data and model's residence-time distribution function. The applicability of the proposed model compared with simpler one- and two-parameter models is analysed. For symmetric RTD curves and a large number of reactors-in-series, the simpler one and two-parameter models may be sufficient. For a small number of reactors-in-series ($N < 11$) the RTD is asymmetric and the proposed model may provide a better fit. This way hydraulic problems inside operating water treatment units can be identified and corrective measures defined, such as modifying the inlet and/or outlet

Table 3 | Unit with predominant complete mixing behaviour

Rio Bravo, Tam.	
High rate sedimentation	
τ	58.08 min
μ	25.2 min

Table 4 | Unit with predominant plug flow behaviour

Piedras Negras, Coah.			
South flocculation tank (exit)			
τ			10.24 min
μ			10.08 min
Fraction			
M	n	N	ε
0.99	1	76	0.0145

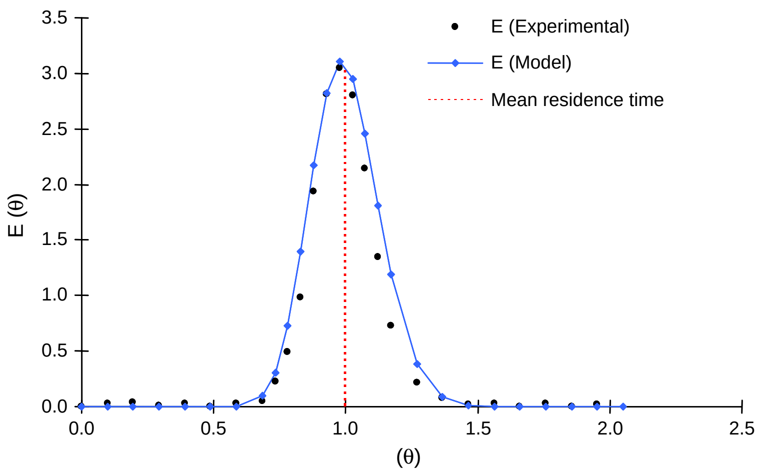

Figure 10 | Unit with predominant plug flow behaviour (Piedras Negras, Coah.).

structures in order to better distribute flow, additional flow channelling inside the unit (where applicable), and so on. Sometimes hydraulic problems are due to indirectly perceptible sludge accumulation inside the unit, so the model may also be useful to identify the need for maintenance measures.

The model was applied to predict the stagnation space fraction, bypass fraction and hydraulic behaviour of three water treatment units in Mexico: a high rate sedimentation tank, a baffled hydraulic flocculation tank and a series of four-chamber mechanical flocculation tanks. The obtained results show that the model matches the experimental data, and the hydraulic predictions are qualitatively coherent with the observed behaviour in each studied unit.

The model could be further validated if scaled transparent units are used to produce and observe the stagnation space and bypass conditions, against which the model's predictions could be compared.

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REFERENCES

Cholette, A. and Cloutier, L. 1959 Mixing efficiency determinations for continuous flow systems. *Can. J. Chem. Engng*, June 1959, **37**(3), 105–112.

Craig, K., De Traversay, C., Bowen, B., Essemiani, K., Levecq, C. and Naylor, R. 2002 Hydraulic study and optimization of water treatment processes using numerical simulation. *Wat. Sci. Technol.: Wat. Suppl.* **2**(5-6), 135–142.

Fernandez-Sempere, J., Font-Montesinos, R. and Espejo-Alcaraz, O. 1995 Residence time distribution for unsteady state systems. *Chem. Engng*, **50**(2), 223–230.

Fogler, H. S. 1992 *Elements of Chemical Reaction Engineering* (2nd edition), Prentice Hall International Series, New Jersey.

Greene, D. J., Haas, C. N. and Farouk, B. 2002. Numerical simulation of chlorine disinfection processes. *Wat. Sci. Technol.: Wat. Suppl.*, **2**(3), 167–173.

Greene, D. J., Farouk, B. and Haas, C. N. 2004 CFD design approach for chlorine disinfection processes. *J. Am. Wat. Wks Assoc.*, **96**(8), 138–150.

Haestad Methods,, Walski, T. M., Chase, D. V., Savic, D. A., Grayman, W., Beckwith, S. and Koelle, E. 2003 *Advanced Water Distribution Modeling and Management*. Haestad Press, Waterbury, Connecticut.

Harwood, R. and Wicks, J. 2001 Computational fluid dynamics and the water industry: An overview with case studies. *Water Software Systems: Theory and Applications*, B. Ulanicki, B. Coulbeck and J. Rance (Eds), Research Studies Press Ltd, Baldock, UK, pp. 245–255.

Huang, T., Brouckaert, C. J., Docrat, M. and Pryor, M. 2002 A computational fluid dynamic and experimental study of an ozone contactor. *Wat. Sci. Technol.*, **46**(9), 87–93.

Levenspiel, O. 1999 *Chemical Reactions Engineering* (3rd edition). John Wiley & Sons, New York.

Martin-Dominguez, A., Tzatchkov, V. G. and Mercado-Escalante, J. R. 1999 *Modelacion del Flujo en Unidades de Tratamiento de*

Agua Potable. Research project TC-9906, Instituto Mexicano de Tecnología del Agua, Jiutepec, Mor., Mexico.

Monk, R. D. G. and Trussell, R. R. 1991 Design of mixers for water treatment plants: Rapid mixing and flocculators. A. Amirtharajah, M. M. Clark and R. R. Trussell (Eds.), *Mixing in Coagulation and Flocculation*, AWWARF, Denver, Colorado.

Rebhun, M. and Argaman, Y. 1965 Evaluation of hydraulic efficiency of sedimentation basins. *J. Sanitn Engng Div., ASCE*, **91**, 37–45.

Tzatchkov, V. G., Buchberger, S. G. & Martin-Dominguez, A 2005 Probabilistic approach to residence-time distribution in water treatment units. *ASCE EWRI World Water & Environmental Congress, Anchorage, Alaska, 15–19 May 2005*, pp. 1–12.

Wang, R.-Y., Park, H.-S., Kang, J.-W. and Oh, H.-J. 1998 The hydrodynamic parameter optimization in design of drinking-water ozonation contactors. *J. Wat. Suppl.: Res. & Technol. – AQUA*, **47**(3), 153–160.

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