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Influences of model structure and calibration data size on predicting chlorine residuals in water storage tanks

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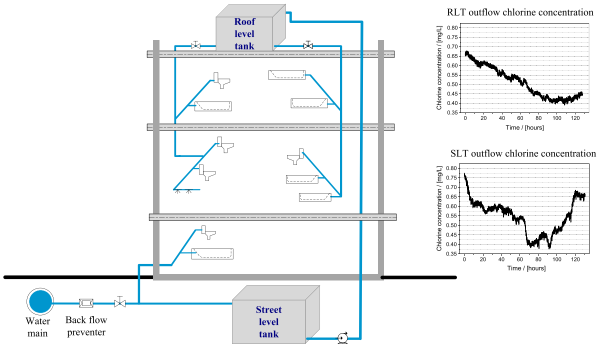
HIGHLIGHTS

- Six combinations of different hydraulic and water quality modules were evaluated.
- Hydraulic modelling process of MC provided better estimates than CSTR.
- Water quality modelling process of VRRC provided better predictions than FO and SO.
- Accuracies of six models increased with an increasing calibration dataset size.
- MC-VRRC required minimum calibration data to obtain reasonable predictions.

GRAPHICAL ABSTRACT



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ABSTRACT

This study evaluated the influences of model structure and calibration data size on the modelling performance for the prediction of chlorine residuals in household drinking water storage tanks. The tank models, which consisted of two modules, i.e., hydraulic mixing and water quality modelling processes, were evaluated under identical calibration conditions. The hydraulic mixing modelling processes investigated included the continuously stirred tank reactor (CSTR) and multi-compartment (MC) methods, and the water quality modelling processes included first order (FO), single-reactant second order (SRSO), and variable reaction rate coefficients (VRRC) second order chlorine decay kinetics. Different combinations of these hydraulic mixing and water quality methods formed six tank models. Results show that by applying the same calibration datasets, the tank models that included the MC method for modelling the hydraulic mixing provided better predictions compared to the CSTR method. In terms of water quality modelling, VRRC kinetics showed better predictive abilities compared to FO and SRSO kinetics. It was also found that the overall tank model performance could be substantially improved when a proper method was chosen for the simulation of hydraulic mixing, i.e., the accuracy of the hydraulic mixing modelling plays a critical role in the accuracy of the tank model. Advances in water quality modelling improve the calibration process, i.e., the size of the datasets used for calibration could be reduced when a suitable kinetics method was applied. Although the accuracies of all six models increased with increasing calibration dataset size, the tank model that consisted of the MC and VRRC methods was the most suitable of the tank models as it could satisfactorily predict chlorine residuals in household tanks by using invariant parameters calibrated against the minimum dataset size.

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Nomenclature

CSTR	Continuously stirred tank reactor
MC	Multi-compartment
FO	First order
SRSO	Single-reactant second order
VRRC	Variable reaction rate coefficient
SLT	Street-level tank
RLT	Roof-level tank
ICCs	Initial chlorine concentrations
	$\Delta c_{Cl,\max}$ Total (or maximum) chlorine demand [mg/L]
c_{Cl} (t)	Chlorine concentration at time t [mg/L]
$c_{Cl,Ci}$ (t)	Chlorine concentration of compartment i (C_i) at time t [mg/L]
k_{FO}	First order reaction rate constant [1/min]
k_{SRSO}	Single-reactant second order reaction rate constant [L/mg/min]
k_{ov}	Overall (variable) reaction rate coefficient [L/mg/min]

1. Introduction

Household water storage tanks are commonly used to store drinking water in many countries and are regarded as one of the most cost-effective ways to store drinking water for residential and commercial consumption as well as for other water-related uses (Al-Bahry et al., 2011; Al-Omari et al., 2008; Kilvington et al., 2004; Oswald et al., 2007). Household tanks are classified according to their installation location as a street-level tank (SLT) or a roof-level tank (RLT). SLTs are usually installed underground, whereas RLTs are located on top of buildings. SLTs and RLTs are usually connected by pumps, i.e., the outflow of the SLT is the inflow of the RLT. Both have the ability to satisfy water demand fluctuations, avoid water supply shortages, equalize operating pressures, and store extra volume for an early stage of fire extinguishing.

Improper design and operation of these storage tanks may cause water quality problems because they can act like chemical and biological reactors with a prolonged residence time, such as overnight stagnation (Lautenschlager et al., 2010) or even 1–2 days retention (Momba and Kaleni, 2002). More explicitly, the water quality deterioration in storage tanks is attributed to (1) the physical factor, e.g., sedimentation caused by insufficient mixing (Grayman et al., 1996); (2) the microbiological factor, e.g., biofilm formation (van der Merwe et al., 2013), proliferation of opportunistic and pathogenic bacteria as well as free-living amoebae (Eshcol et al., 2009; Kilvington et al., 2004; Stockman et al., 2011; Winck et al., 2011), and taste and odor compounds released by organisms (Zhou et al., 2017); and (3) the chemical factor, e.g., disinfectant depletion (Sathasivan et al., 2010; Zhang et al., 2011). Among these factors, concerns about the maintenance of sufficient chlorine residuals have been addressed by regulatory requirements for a concentration of 0.2 mg/L at the point of delivery (WHO, 2008), which protects the drinking water from recontamination during storage. Specifically, negative relationships were found in storage tanks between residual chlorine concentrations and the presence of *Pseudomonas Aeruginosa* (Ribas et al., 2000). Hence, to maintain tank water quality during storage and avoid shortages of chlorine residuals, a suitable tank model is required for quantitative simulation of the residual chlorine concentrations (Grayman et al., 1996).

In terms of the modelling approach, an integrated environmental modelling framework usually consists of hydraulic and water quality modelling processes/modules (Gu et al., 2017; Kun et al., 2015). Generally, the simulation of water quality, such as chlorine residuals, relies not only on the adequacy of chlorine decay simulation but also on the accuracy of the hydraulic modelling that describes flows and flow velocities (Pasha and Lansey, 2010; Waeytens et al., 2017). The output of the hydraulic modelling is then a prerequisite for the water quality simulation (Grayman et al., 2004; Lansey and Mays, 2000). The hydraulic modelling process has been developed from the physical scale to the mathematical approaches. The physical approach simulates the hydraulic conditions, such as water age, by conducting tracer tests (Clark et al., 1996). However, this approach may lead to a substantial inaccuracy due to the difficulties in measuring tracer movement. With advances in computational resources, numerical modelling has gained in popularity with the approaches taken falling into two general categories: system and computational fluid dynamics (CFD) (Grayman et al., 1996). The system approach divides a storage tank into different compartments, in which each compartment is completely mixed and water flows between the different compartments (Grayman, 1999; Lemke, 2012; Mau et al., 1995). When one compartment is used as a surrogate for the whole tank, it is described as a continuously stirred tank reactor (CSTR) method. In the CSTR method, water entering the tank instantaneously and completely mixes with the chlorine in the tank, resulting in a uniform mixture at all times. When two or more compartments are considered, it is referred to as a multi-compartment (MC) method. Specifically, the MC method separates the total volume of the tank into several compartments, and a complete mixing state is assumed within each compartment. Both CSTR and MC methods belong to the system approach and have reached the application level. The CFD approach is usually used with the assistance of computational software (Hua et al., 2017; Waeytens et al., 2015; Xavier and Janzen, 2017). It provides a more accurate hydraulic simulation but requires more computational effort than the system approach. Thus, considering the different approaches' benefits and costs, the selection of a proper hydraulic modelling strategy should be case-dependent (Grayman et al., 1996; Zhang et al., 2014).

In terms of the water quality modelling process, chlorine decay simulations have been developed from first order (FO) to second order (SO) models. The SO models have been further developed from a single-reactant second order (SRSO) with a reaction rate constant, to a two-reactant second model (2RSO) model with two reaction coefficients, i.e., fast and slow reaction coefficients, and then a second order model with a variable reaction rate coefficient (VRRC) (Clark and Sivaganesan, 1998; Clark and Sivaganesan, 2002; Fisher et al., 2011; Fisher et al., 2017a; Hallam et al., 2003; Hua et al., 2015; Jonkergouw et al., 2009). Some of those models have been successfully combined with variables, such as temperature, pH, water mixing, and pipe wall reactions. However, the developed chlorine decay models are commonly used for the simulation of chlorine residuals in drinking water distribution pipe systems and the service reservoirs (Kennedy et al., 1993; Mau et al., 1995; Rossman et al., 1994; Sathasivan et al., 2010; Zhang et al., 2011). In other words, the model application for the prediction of chlorine residuals in household storage tank is still limited.

Compared with the storage facilities in distribution systems, the volume capacity of household tanks is much smaller. In addition, the inflow and outflow for household storage tanks are neither continuous nor simultaneous. Especially for RLTs, the inflow is usually controlled by the pump that elevates the water from the SLT while the outflow is controlled by the terminal tap water usage. This indicates a complicated operation scheme and variable water level in household tanks, which make the overall modelling process more challenging. Therefore, considering the intermittent inflow/outflow and the variable inflow/outflow rates, which may consume substantial computing capacity in the CFD approach, the system approach was selected for the mixing simulation in this study.

Collectively, the focus of this study was to predict the fluctuation of the residual chlorine concentrations in storage tanks (RLT and SLT) by a suitable integrated tank model which consists of hydraulic mixing and water quality modules (modelling processes). The hydraulic mixing condition in the tanks was simulated using the system approach including CSTR and MC methods. Water quality, i.e., reaction kinetics of