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Predicting the disinfection efficiency range in chlorine contact tanks through a CFD-based approach

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ABSTRACT

In this study three-dimensional computational fluid dynamics (CFD) models, incorporating appropriately selected kinetic models, were developed to simulate the processes of chlorine decay, pathogen inactivation and the formation of potentially carcinogenic byproducts in disinfection contact tanks (CTs). Currently, the performance of CT facilities largely relies on Hydraulic Efficiency Indicators (HEIs), extracted from experimentally derived Residence Time Distribution (RTD) curves. This approach has more recently been aided with the application of CFD models, which can be calibrated to predict accurately RTDs, enabling the assessment of disinfection facilities prior to their construction. However, as long as it depends on HEIs, the CT design process does not directly take into consideration the disinfection biochemistry which needs to be optimized. The main objective of this study is to address this issue by refining the modelling practices to simulate some reactive processes of interest, while acknowledging the uneven contact time stemming from the RTD curves. Initially, the hydraulic performances of seven CT design variations were reviewed through available experimental and computational data. In turn, the same design configurations were tested using numerical modelling techniques, featuring kinetic models that enable the quantification of disinfection operational parameters. Results highlight that the optimization of the hydrodynamic conditions facilitates a more uniform disinfectant contact time, which correspond to greater levels of pathogen inactivation and a more controlled by-product accumulation.

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1. Introduction

Disinfection is a process designed for the inactivation of pathogenic micro-organisms, thus preventing the transmission of waterborne diseases. Disinfection of water supply occurs through contact with suitable dose concentrations of disinfectant, and for sufficient time for micro-organisms to be inactivated, in appropriately designed contact tanks (CTs). Chlorine contact tank units suggest plug flow to be the optimal hydrodynamic condition at which disinfection performance is maximized (Stamou, 2002; Falconer and Tebbutt, 1986; Marske and Boyle, 1973). Under such flow conditions, disinfectant transport becomes ideal by remaining in the tank for a uniform duration, whilst achieving the desired disinfection.

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However, previous studies (e.g. Teixeira, 1993; Shiono and Teixeira, 2000) indicate that flow exhibits a residence time distribution (RTD) which can be significantly different from that dictated by plug flow. The shape of the tracer RTD curves can provide an insight into the hydrodynamic and mixing conditions, as explained by Levenspiel (1999). Digression from plug flow can be attributed to complex hydrodynamic processes, such as short-circuiting and recirculation zone formation (Kim et al., 2010). Short-circuiting occurs when particles pass through a reactor quicker than the theoretical hydraulic residence time (T). Recirculation zones not only promote short-circuiting (since they occupy a considerable part of the tank volume) but they also trap solutes and particles (or pathogens), which are then retained in the tank for a longer period than T. The occurrence of such flow patterns has a detrimental effect on the overall CT efficiency, because the exposure of pathogens with the disinfectant is either too short (insufficient treatment) or too long, which can result in excessive disinfection by-products.

Computational Fluid Dynamics (CFD) techniques have been implemented widely to simulate flow conditions and mixing processes during the operation of CT facilities (Rauen et al., 2012; Salzano and Gualtieri, 2014). Such computational models are normally set-up to firstly reproduce available tracer experimental results and subsequently predict hydraulic efficiency indicators (HEIs) for proposed CT designs (Kim et al., 2013a, 2013b; Zhang et al., 2013a; Amini et al., 2011; Gualtieri, 2007, 2006). Unfortunately, HEIs cannot indicate disinfection specific parameters, such as optimum disinfectant dosage, pathogen survival level or by-product formation potential, i.e. invaluable information for the operation of CTs which are often determined empirically. Such parameters could be potentially deduced through the integration of disinfection kinetics into computational models, a practice which was scarcely reported in the literature until recently (Angeloudis, 2014; Zhang et al., 2014; Wols et al., 2010; Wang et al., 2003; Zhang et al., 2000).

Results are presented herein of 3D numerical model simulations of tracer transport and disinfection processes in seven different design configurations of a small-scale contact tank model. The core objectives of this investigation were to:

- a) Review the hydraulic efficiency of each individual design computationally and compare the predictions against available experimental data,
- b) Study a range of inlet and baffle configurations for their capability in inactivating pathogens and producing byproducts under the same disinfection conditions, and
- c) Examine the by-product concentration and pathogen survival ratio range associated with each design, based on their RTD.

2. Research methodology

2.1. Contact tank configurations and experimental data

The contact tank configurations modelled were based on a small-scale disinfection tank, which was studied at Cardiff University, which was 3.0 m long, 2.0 m wide and 1.2 m deep

(Fig. 1). The baffling configuration inside the prototype was particularly flexible as shown by Fig. 1(a-b), where the internal baffle arrangement could be altered with relative ease. In addition, the physical model featured two inlet options, an open channel entry or a pipe inlet. The channel inlet was located in the northeast corner of the tank and consisted of an open channel of width $W_c = 0.365$ m and depth H_i of 0.30 m, which is approximately 1/4 of the tank depth. Honeycomb flow straighteners were located in the approach channel to promote uniformity as the flow entered the system. In line with the centre of the shallow approach channel, there was a 152 mm internal diameter plastic inlet pipe as indicated in the cross section of Fig. 1(c). A tracer injection mechanism was incorporated by Rauen (2005), which consisted of a diffuser, a control valve with a connection for a syringe and three injection needles placed around the inlet pipe. The water level, controlled via a rectangular sharp crested weir at the outlet, was measured to be at $H_t = 1.02$ m during experimentation (Angeloudis et al., 2014).

The seven designs of CT1-C, CT1-P, MS1-P, MS2-P, MS3-P, MS4-C and MS4-P (Fig. 1) were selected due to the availability of experimental data from previous studies, thus enabling the validation of hydrodynamic and solute transport simulations. CT1-C was an 8 compartment model which exhibited the standard features of a conventional baffled contact tank, i.e. it was separated into a certain number of compartments of equal volume where the flow meandered due to the baffles being arranged in an alternating fashion. CT1-P shared the same baffle configuration, but the flow entered the system by means of the pipe instead of the channel as indicated by Fig. 1(a and c). The MS3-P setup was a highly inefficient design paradigm as it featured no baffles to neutralize the inflow three-dimensionality towards plug flow conditions. The MS1-P and MS2-P were combinations between the MS3-P and CT1 baffle configurations to demonstrate how the gradual addition of baffles influenced the disinfection efficiency (Fig. 1(b)). In these three cases, only the pipe inlet was imposed. The MS4 (i.e. both MS4-C and MS4-P) configurations on the other hand were characterized by an optimized baffling configuration, which had been shown to outperform the hydraulic efficiency results of CT1 (i.e. CT1-C and CT1-P).

All experimental data were acquired in the investigations of either Rauen (2005) or Angeloudis et al. (2014), where an experimental campaign was launched for the investigation of hydrodynamics and tracer transport using Acoustic Doppler Velocimetry (ADV) and tracer dye injection techniques. Operative conditions established during laboratory experimentation for each design configuration are summarised in Table 1 for completeness. The hydrodynamic measurements of Rauen (2005) focused on the observation of some hydrodynamic aspects encountered in CT1, MS1-P, MS2-P, MS3-P and MS4, whereas the measurements of Angeloudis et al. (2014) aimed at the formation of a comprehensive data set for the CT1-C design to be used as a benchmark for numerical modelling studies. Of particular relevance to the present work were the pulse tracer experiments of both studies, which involved Rhodamine WT injections at the inlet, where submersible sensors monitored fluorescence levels at designated locations for the production of normalized RTD curves and the derivation of HEIs.

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