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A variable reaction rate model for chlorine decay in drinking water due to the reaction with dissolved organic matter

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ABSTRACT

A second order kinetic model for simulating chlorine decay in bulk water due to the reaction with dissolved organic matter (DOM) was developed. It takes into account the decreasing reactivity of dissolved organic matter using a variable reaction rate coefficient (VRRC) which decreases with an increasing conversion. The concentration of reducing species is surrogated by the maximum chlorine demand. Temperature dependency, respectively, is described by the Arrhenius-relationship. The accuracy and adequacy of the proposed model to describe chlorine decay in bulk water were evaluated and shown for very different waters and different conditions such as water mixing or rechlorination by applying statistical tests. It is thus very well suited for application in water quality modeling for distribution systems.

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1. Introduction

Chlorine is widely used for the disinfection of drinking water due to its relatively low cost and ability to maintain a disinfectant residual throughout water distribution systems (WDS). However, due to the reaction of chlorine with dissolved organic matter and bromide ion, potentially harmful disinfection by-products (DBPs) can be produced, such as trihalomethanes (THMs) and haloacetic acids (HAAs), which may have adverse effects on human health (Nieuwenhuijsen et al., 2000; Richardson et al., 2007). Furthermore, a high dose of chlorine at the entry of WDS to maintain a desired level of chlorine residual at the system endpoints, will generate taste or odor complaints from upstream consumers and may require booster doses (rechlorination) at intermediate locations to reduce the initial dose. Accordingly, the chlorine dose and residual should be kept low to limit DBPs formation. Meanwhile, it is required to maintain sufficient chlorine residual to protect against contamination and to limit bacterial regrowth.

To optimize the chlorine dose at the WDS entry and limit DBPs formation, or to properly place booster stations in WDS, an accurate and widely applicable kinetic model for chlorine decay is needed (Clark, 1998; Kastl et al., 1999, 2003; Kiéné

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Nomenclature

c_{Cl} (t)	Chlorine concentration at time t [mg L^{-1}]
c_{Ri} (t)	Concentration of ith chlorine-reactive site R_i at time t
c_R (t)	Concentration of all chlorine-reactive sites at time t [mg L^{-1}]
Cl	Chlorine
DBPs	Disinfection by-products
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
FO	First order
F	Frequency factor
ICCs	Initial chlorine concentrations
k_i	Reaction rate constant for the ith reactive-site [L mg^{-1} h^{-1}]
k_{ov} (t)	Overall variable reaction rate coefficient at time t [L mg^{-1} h^{-1}]
k_{ov} (0)	Initial overall variable reaction rate coefficient [L mg^{-1} h^{-1}]
$k_{ov,mix}$	Overall variable reaction rate coefficient for mixing [L mg^{-1} h^{-1}]
P_i	Disinfection by-product of a specific reaction
P	The collection of all disinfection by-products
R_i	The ith chlorine-reactive site with $i = 1, \ldots, n$
R	The collection of all chlorine-reactive sites
SO	Second order
THMs	Trihalomethanes
VRRC	Variable reaction rate coefficient
WDS	Water distribution systems
X	Fractional conversion
2R	Two-reactant
$\Delta c_{Cl,max}$	Total (or maximum) chlorine demand [mg L^{-1}]
Δc_{Cl} (t)	Consumed chlorine at time t [mg L^{-1}]

et al., 1998; Ohar and Ostfeld, 2014). In practice, the kinetic model of chlorine decay is required to be compatible with hydraulic models, such as EPANET (Rossman, 2000; Rossman et al., 1994; Shang et al., 2007). Even for unchlorinated WDS, which are often found in European countries such as The Netherlands, Denmark and Germany, chlorine decay models are needed as well. For these WDS, it is important to know how chlorine depletes in case of application after an accidental contamination.

It is generally agreed that the chlorine decay model ideally should describe two mechanisms: homogenous decay due to the reaction between chlorine and reactants in bulk water (bulk decay) and wall decay due to the reaction between chlorine and pipe materials, and biofilm etc. Fisher et al. (2011) emphasized the need for an accurate model of bulk decay prior to any attempt to characterize the wall decay, and pointed out that separating chlorine decay into bulk and wall decay minimizes the effort required for calibration. Therefore, this study is focused on the bulk reaction.

Chlorine bulk decay models have been developed as first order (FO) and as second order (SO) models. The latter considers two reactants in water: chlorine and chlorine-reactive species (Clark, 1998; Kastl et al., 1999). The FO models are shown to be highly unsuited for modeling, while the SO models show potential capability to simulate chlorine profiles in WDS (Fisher et al., 2011; Jegatheesan et al., 2006). Kastl et al. (1999) proposed an SO model, which is based on the assumption that chlorine reacts with two classes of reactants, namely notional fast and slow reducing agents with individual fast and slow rate coefficientsover the reaction period, respectively. Hereafter, this is termed the two-reactant (2R) model (Fisher et al., 2011; Jabari Kohpaei and Sathasivan, 2011). In this 2R model, the so-called fast or slow notional reducing agents are used to represent the complex mixture of (unknown) reactants, and the respective fast or slow reaction rate coefficient is an alternative interpretation of the collection of corresponding reactants. It is assumed that the fast and slow reaction rate coefficients remain constant during the respective reaction periods. However, chlorine disappears in bulk water due to concurrent reactions with a multitude of aqueous constituents with individual reactivities, and should not be simply treated as a fast or slow reducing agent (Deborde and von Gunten, 2008; Qualls and Johnson, 1983). In fact, the reactivity and concentration of all chlorine-reactive species decrease with reaction time. Therefore, to better predict chlorine bulk decay and minimize recalibration, an overall variable reaction rate coefficient (VRRC) should be introduced to replace separated fast and slow reaction rate coefficients, which is related to the reaction progress and is an alternative interpretation of the collective individual rate constants. Furthermore, to simplify the calibration process, the fast and slow reducing agents which were estimated by the 2R model should be replaced by a sum of the chlorine-reactive reactants.

Jonkergouw et al. (2008) proposed a variable rate coefficient model with an empirical equation for concentration-weighted rate coefficient calculation. However, the model efficiency in accordance with its complexity is being questioned and some of the parameters are not readily interpretable. Specifically, systematically lower calibrated initial chlorine concentrations (ICCs), rather than those experimentally determined, were used in order to improve the data fit during model validation. Supposedly, the authors had to use such a method due to the straightforward approach they chose which assumed the initial concentration of all reactants to be equal to the total or dissolved organic carbon concentration of a water sample multiplied by 5 or 10 (arbitrarily chosen). Although the accuracy of the model was evaluated at different temperatures, the model parameters were derived for different temperatures, rather than using invariant parameters for the entire data set (Fisher et al., 2011, 2012).

Consequently, the objectives of this work were to (1) develop an SO model for chlorine decay due to the reaction with dissolved organic matter which takes into account the decreasing reactivity of the reactants in water, (2) derive an overall variable reaction rate coefficient k_{ov}, which is described as a function of chlorine consumed, to reflect the decreasing reactivity of reactants (therefore, the model is referred to as VRRC model in this work), (3) show the applicability of the model to chlorination of several water samples collected from different sources and with different organic matter contents, and (4) show the applicability of the model to chlorination of identical water samples at a wide range of

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