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Investigating the role of biofilms in trihalomethane formation in water distribution systems with a multicomponent model

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ABSTRACT

Biofilms are ubiquitous in the pipes of drinking water distribution systems (DWDSs), and recent experimental studies revealed that the chlorination of the microbial carbon associated with the biofilm contributes to the total disinfection by-products (DBPs) formation with distinct mechanisms from those formed from precursors derived from natural organic matter (NOM). A multiple species reactive-transport model was developed to explain the role of biofilms in DBPs formation by accounting for the simultaneous transport and interactions of disinfectants, organic compounds, and biomass. Using parameter values from experimental studies in the literature, the model equations were solved to predict chlorine decay and microbial regrowth dynamics in an actual DWDS, and trihalomethanes (THMs) formation in a pilot-scale distribution system simulator. The model's capability of reproducing the measured concentrations of free chlorine, suspended biomass, and THMs under different hydrodynamic and temperature conditions was demonstrated. The contribution of bacteria-derived precursors to the total THMs production was found to have a significant dependence on the system's hydraulics, seasonal variables, and the quality of the treated drinking water. Under system conditions that promoted fast bacterial re-growth, the transformation of non-microbial into microbial carbon DBP precursors by the biofilms showed a noticeable effect on the kinetics of THMs formation, especially when a high initial chlorine dose was applied. These conditions included elevated water temperature and high concentrations of nutrients in the influent water. The fraction of THMs formed from microbial sources was found to reach a peak of 12% of the total produced THMs under the investigated scenarios. The results demonstrated the importance of integrating bacterial regrowth dynamics in predictive DBPs formation models.

1. Introduction

Water quality reaching the consumer's tap is largely dictated by the physical, chemical, and biological processes that take place in the distribution system. While chlorine is routinely used by drinking water utilities to inhibit microbial regrowth in their distribution systems, it reacts with the residual natural organic matter (NOM) leading to the undesired formation of carcinogenic disinfection byproducts (DBPs). Moreover, the biodegradable fraction of NOM fed to the system supports the growth of biofilms (Gagnon and Huck, 2001), which play a major role in the accumulation and release of bacterial and pathogenic species, thus compromise the microbiological quality of the treated drinking water (Shen et al., 2016, 2015). Significant modeling efforts have been devoted over the past three decades to predict the formation of DBPs during water treatment (Brown et al., 2011; Chowdhury et al., 2009; Ged et al., 2015; Sadiq and Rodriguez, 2004); yet more research is still required to understand their formation and transport in the distribution system. Specifically, the role of biofilms has been generally overlooked in previous modeling studies despite their ubiquitous existence in drinking water distribution systems with considerable surface biomass concentrations (up to 10^4–10^7 CFU/cm^2) (Woolschlager et al., 2005).

Previous field studies found consistently higher levels of trihalomethanes (THMs) in the distribution network and at the points of use compared to finished water (Pieri et al., 2014; Toroz and Uyak, 2005). Experimental pilot-scale studies showed that the production of THMs in a simulated pipe environment was always higher than that observed for glass bottle tests, which was

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Nomenclature

C_i	concentration of species i (mg/L)
D_i	diffusion coefficient of species i (m^2/sec)
$f(r)$	radial flow distribution parameter
$k_{f,i}$	lumped mass transfer coefficient of species i (m/sec)
R_i	reaction involving species i (mg/L sec)
Re	Reynolds number (−)
r	radial coordinate (m)
r_f	radial location of the bulk/biofilm interface (m)
r_h	hydraulic mean radius (m)
r_0	pipe radius (m)
t	time (sec)
$\overline{u}$	average flow velocity in the pipe (m/sec)
x	axial coordinate (m)

Subscripts

b	bulk flow
i	one of the constituents
j	one of the wall zone reactions
k	one of the bulk flow reactions
L	longitudinal
r	radial
w	wall zone

accompanied by faster chlorine consumption rates in the pipe environment (Rossman et al., 2001). This observation was attributed to the existence of a reservoir of THMs precursor material attached to the pipe wall, which can be explained by the radial mass transfer of organic compounds to the biofilm, and the bio-sorption of NOM to the extracellular polymeric substance (EPS) (Wang et al., 2012a). On the other hand, biofilms were found to biodegrade haloacetic acids (HAAs), which influences their fate as their levels do not typically show a consistent increase with the residence time as in the case of THMs (Tung and Xie, 2009).

The microbial carbon content associated with the biofilm has been recently shown to act as a precursor for DBPs formation in the distribution system as a result of the chlorination of both pure bacterial cells (Wang et al., 2013a), or the EPS, which is largely composed of dissolved organic compounds such as polysaccharides, proteins and nucleic acids (Wang et al., 2012b; Z.Wang et al., 2013b). Hence, the detachment of biomass from the biofilm matrix by either active dispersal of planktonic cells (Xue and Seo, 2013) or passive dispersal due to fluid shear or grazing (Kaplan, 2010) can contribute to the total budget of DBPs precursors. Therefore, the question arises whether this contribution is significant enough to influence the dynamics of DBPs formation in the distribution system? Moreover, what would be the system conditions that might promote or depress this contribution? A multiple-species reactive transport model was developed to help answer these questions.

Numerous mathematical multispecies models have been developed in the literature to describe disinfectant decay and bacterial regrowth in the distribution system (Bois et al., 1997; Dukan et al., 1996; Lu et al., 1995; Munavalli and Kumar, 2004; Piriou et al., 1998; Zhang et al., 2004). A good review of these models and their limitations can be found in the literature (Chowdhury, 2012). One of the first-generation models was presented by Lu et al. (1995), which accounted for the simultaneous transport of substrates, disinfectants and microorganisms in the bulk phase and the biofilm under steady state conditions. However, their model did not account for substrate utilization and bacterial re-growth in the bulk phase, and assumed a simple first order reaction kinetics for chlorine decay. Munavalli and Kumar (2004) presented a dynamic multi-component model that considered a more realistic expression for chlorine decay with a parameter that depends on the concentration of the organic carbon, while Zhang et al. (2004) applied the alternating split-operator (ASO) algorithm to decouple the transport and reaction processes, which significantly simplified the numerical solution for the complex reaction mechanisms of the multi-component model. Yet, all these models were mainly concerned with simulating the biological processes in the distribution system, and none of them extended to include the formation and transport of DBPs. EPANET-MSX (Shang et al., 2008) is an advection based, public domain, generalized multi-species model that can be used to simulate the reaction and transport of any set of interacting chemical or biological species. However, like most of the other multi-species models, EPANET-MSX does not account for dispersion as a solute transport mechanism. Hence, it is not capable of providing accurate simulations for constituent transport in low flow pipes and dead-end zones. These zones are known to be responsible for most of the water quality degradation that takes place in the system due to extended residence times, and therefore require a special modeling approach such as the one we developed in our previous study (WU-DESIM) (Abokifa et al., 2016). With the increasing public awareness of the need for water conservation, the effect of these zones on water quality deterioration is expected to even magnify because of the generally lower flow rates (Nguyen et al., 2012).

In this study, a 1-D multi-component reactive-transport model (WU-MSRT – Washington University Multi-Species Reactive Transport) is developed to simulate the transport and consumption of disinfectants, transformation of the biodegradable fraction of NOM into biomass through bacterial regrowth in the biofilm, the release of biomass to the bulk fluid through detachment from the biofilm, and the formation of DBPs from precursors of both microbial and non-microbial origin. The model considers both advective and dispersive transport mechanisms, and hence is capable of efficiently simulating constituent transport under different flow conditions, ranging from the advection-dominated transport in the main trunk pipes to the dispersion-dominated transport in dead-ends. The model was applied to investigate the system conditions under which microbial carbon can significantly contribute to the overall DBPs budget in the finished drinking water including the effect of using booster re-chlorination to control bacterial regrowth in the system.

2. Methodology

2.1. Model development

2.1.1. Mathematical model

For a water parcel moving through a distribution pipe containing disinfectants, organic compounds, nutrients, biomass and disinfection byproducts, the biochemical reactions are considered to take place at two interconnected sites within the bulk flow and in the accumulated biofilm at the pipe wall. Solute transport can be appropriately modeled by a dynamic 2-D convection-diffusion equation in cylindrical coordinates to represent the mass balance on the concentration of each of the bulk phase constituents