Modeling marine oily wastewater treatment by a probabilistic agent-based approach

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ABSTRACT

This study developed a novel probabilistic agent-based approach for modeling of marine oily wastewater treatment processes. It begins first by constructing a probability-based agent simulation model, followed by a global sensitivity analysis and a genetic algorithm-based calibration. The proposed modeling approach was tested through a case study of the removal of naphthalene from marine oily wastewater using UV irradiation. The removal of naphthalene was described by an agent-based simulation model using 8 types of agents and 11 reactions. Each reaction was governed by a probability parameter to determine its occurrence. The modeling results showed that the root mean square errors between modeled and observed removal rates were 8.73 and 11.03% for calibration and validation runs, respectively. Reaction competition was analyzed by comparing agent-based reaction probabilities, while agents' heterogeneity was visualized by plotting their real-time spatial distribution, showing a strong potential for reactor design and process optimization.

1. Introduction

Modeling of wastewater treatment processes has been of great importance due to the need for a full understanding of complex treatment systems and the optimization of their practical applications. Numerous modeling techniques, such as reaction kinetics and equilibrium (Mbamba et al., 2015; Eglal and Ramamurthy, 2015), computational fluid dynamics (Wols et al., 2015; Santoro et al., 2015) and artificial neural networks (Jing et al., 2015; Jing et al., 2016) have been extensively documented in the literature. An interesting note is that most of the existing techniques are designed to simulate bulk properties and rely much on the understanding of population-level dynamics rather than individual-level responses, such as heterogeneity among individuals, local interactions, and adaptive decision making (Schuler et al., 2011). The lack of individual-level information may result in an incomplete understanding of treatment processes, especially when competition and complex interactions among different components exist (Schuler, 2005, 2006; Hellweger and Bucci, 2009). For example, Hellweger (2007) argued that traditional lumped modeling approaches can introduce significant errors when simulating individual phytoplankton growth and trace metal transformation during eutrophication. Further, knowledge on the adsorption competition for photocatalytic

active sites (Wang et al., 2009) and heavy metal removal (Eglal and Ramamurthy, 2015), and microbial competition in biological wastewater treatment systems (Albuquerque et al., 2013) has not been made explicit by population-level techniques.

Recently, the importance of individual variations in wastewater treatment processes has favored the advancement of process-based models, particularly agent-based models (ABMs). These bottom-up models are particularly known for describing the behavior of individual system components from a micro point of view and yielding different predictions of bulk behaviors than conventional macro-scale approaches where population heterogeneity and intra-population variability are usually not appreciated. The core of ABMs emphasizes on the autonomous and adaptive nature of individuals such that each individual has its own characteristics/goals and can make its own decisions according to certain rules. By capturing the interactions of individuals with each other and with their surrounding environment, the behavior of the population can be simulated as a whole (Wilensky and Rand, 2015). Given most scientific knowledge exists at either individual- or population-level instead of both, ABMs can bridge this gap via exploring the effects of individual decisions on collective behavior and predicting how populations will change across time and space. Such an intuitive concept makes ABMs well-suited to model highly

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complex dynamics using only simpler rules and assumptions. Nonetheless, it is worth noted that the efficacy of agent-based modeling may be compromised by its underdeveloped theoretical framework and high computational demands (Esser et al., 2015). ABMs have been applied to a variety of problems such as human and animal migration, traffic control, stock trading, and land development (Bonabeau, 2002; Matthews et al., 2007; Hellweger and Kianirad, 2007; Crooks et al., 2008; Farmer and Foley, 2009; Schreinemachers and Berger, 2011; Filatova et al., 2013; Müller et al., 2013; Klabunde and Willekens, 2016). It has been recently argued that ABMs should have high potential for wastewater treatment modeling. The movement, behavior, and spatial distributions of different agents in wastewater, such as pollutants, reactive species, and microorganisms can be well simulated by ABMs. Subsequently, population-level behaviors (e.g., concentrations of pollutants) would emerge as a result of cumulative actions of agents (Schuler et al., 2011). In addition, ABMs do not have the same restrictions as population-level differential equations and can easily account for the numbers, distributions, and time delays of different molecules (Pogson et al., 2006). Xavier et al. (2007) applied agent-based simulation to describe the complex dynamics of four bacterial groups in an aerobic granular sludge sequencing batch reactor. Pereda and Zamarreno (2012) proposed a Matlab-based ABM for modeling activated sludge process in a batch reactor and obtained a better understanding of this phenomena. Bucci et al. (2012) developed an ABM to predict the heterogeneity of an enhanced biological phosphorus removal process. The biological variability in individual cell behavior and states was predicted by randomizing model parameters and state variables, respectively. However, to the best of our knowledge, the applications of ABMs in modeling wastewater treatment processes are still limited in the literature (Gernaey et al., 2004; Schuler et al., 2011). Most of the relevant studies have either used macro-scale behavior rules such as partial differential equations to approximate individual-level responses, or focused on simplified processes without considering reaction kinetics. In addition, the calibration of existing ABMs has mostly been done by trial and error attempts, which relies mainly on expert knowledge and may encounter problems when a large amount of experimental data is available.

Therefore, to help fill these gaps, the objective of this study was to establish a novel agent-based probabilistic approach for modeling of wastewater treatment processes by 1) developing a probability-based agent simulation model and 2) improving its performance through a global sensitivity analysis and a genetic algorithm-based calibration. The removal of naphthalene (NAP) from marine oily wastewater by UV induced photodegradation (experimental results adopted from Jing et al., 2014a) was modeled as a demonstrative example to examine the applicability and accuracy of the proposed modeling approach.

2. Methodology

2.1. Experimentation data

The original work of Jing et al. (2014a) was comprised of a factorial experimental design to study the removal of NAP from marine oily wastewater. In brief summary, photodegradation of NAP was carried out in a two-layer cylindrical reactor (Fig. S1 in Supplementary material). The outer body and inner section are made of aluminum and clear fused quartz, respectively, with eight 18.4 W low-pressure UV lamps (254 nm peak, full width half maximum of 15 nm, Atlantic Ultraviolet, Canada) evenly positioned between them. The inner quartz beaker (11.1 cm internal radius, 11.5 cm external radius, and 20 cm height) features a polycarbonate lid where a stainless steel paddle agitator, a 50 W heater, and a thermometer are mounted. The experimental system was constantly stirred in order to ensure a well-mixed solution. NAP (> 99%) and NAP D8 (> 99%, internal standard) were obtained from Aldrich, Canada. Dichloromethane and acetone were purchased from Honeywell Burdick and Jackson (USA) for stock solution preparation

and extraction. Seawater was obtained from a clean coastal site in St. John's, Canada and filtered through a 5 μm filter to remove organisms and debris. UV lamps were turned on once NAP stock solution was spiked into 6 L seawater to simulate the discharge of oily wastewater from offshore industries (Jing et al., 2015). Samples were taken half-hourly and sent for GC-MS analysis after pre-treatment. More details about the experiments are available in Jing et al. (2014a).

In this study, a probability-based agent simulation model was first developed to simulate the removal of NAP and then calibrated with data from 8 calibration runs (30 min interval from 0.5 to 4 h, excluding the start point; 8 samples per run, 64 data points in total). Data from another 4 validation runs (32 data points in total) were used to evaluate the performance of the calibrated model. Details about the calibration and validation runs can be found in Tables S1 and S2 in Supplementary material.

2.2. The agent-based simulation model

A probability-based agent simulation model for NAP removal was developed in the free software platform NetLogo 5.3.1 because it is an intuitive and well-documented programming tool with high flexibility and simplicity. NetLogo is a modified version of the Logo programming language and is particularly suitable for modeling complex systems which change over time. It employs a graphical environment to support numerous breeds of programmable agents to wander and interact in a grid of patches. All types of agents can interact with each other and perform multiple tasks concurrently by receiving pre-set instructions on their behaviors from the user. Detailed introduction to NetLogo can be found in Wilensky and Evanston (1999) and Wilensky and Rand (2015).

In this study, UV induced photodegradation of NAP in seawater can be described by the following simplified reaction scheme (Miller and Olejnik, 2001). It is assumed that radical reactions of chloride and nitrate are not involved given their insignificant contributions (Lair et al., 2008; Fang et al., 2017). NAP can absorb one photon (hv in Eq. 1) to transit to its excited state NAP* (Bayrakceken et al., 2012), which can further return to the ground state (Eq. 2) by dissipating energy via various ways such as internal conversion, energy transfer to other molecules, and emitting its characteristic fluorescence. Oxygen molecule (O_2), which is known to be an efficient quencher of excited state PAHs, in the ground triplet state can be excited into a reactive singlet state ($^1O_2$) by encountering a NAP* (Eq. 3). $^1O_2$ can then attack NAP and form products such as peroxides and hydroperoxides (Eq. 4) or return to the ground state by emitting energy (Eq. 5). In addition, humic substances (HS), which are the main components of natural organic matter in seawater, can also absorb one photon to transit to its excited state HS* (Eq. 6), return to the ground state (Eq. 7), react with O_2 to generate $^1O_2$ (Eq. 8), or be degraded by $^1O_2$ (Eq. 9) to form products. All photodegradation products are assumed to further react with $^1O_2$ and generate one or two products (Eqs. 10 and 11). It should be noted that Eqs. 6–11 are a lumped approximation of many photoreactions associated with HS and photochemical products.

$$\text{NAP} + hv \xrightarrow{p_1} NAP^* \tag{1}$$

$$NAP^* \xrightarrow{p_2} \text{NAP} + \text{energy} \tag{2}$$

$$\text{NAP}^* + \text{O}_2 \xrightarrow{p_3} NAP + {}^1O_2 \tag{3}$$

$$\text{NAP} + {}^1\text{O}_2 \xrightarrow{p_4} \text{Product} \tag{4}$$

$${}^1\text{O}_2 \xrightarrow{p_5} \text{O}_2 + \text{energy} \tag{5}$$

$$\text{HS} + hv \xrightarrow{p_6} \text{HS}^* \tag{6}$$

$$HS^* \xrightarrow{p_7} \text{HS} + \text{energy} \tag{7}$$