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Research article

Oxygen uptake prediction in rivers and streams: A stochastic approach

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Dissolved oxygen fluctuations in a river over a short period of time were assumed to be caused by the microbial growth dynamics, and a stochastic model was built for oxygen uptake. As a case study, biochemical oxygen demand (BOD) was measured in water from the Ura River, Oita River, and Otozu River flowing through the urban district of Oita, Japan. Water samples were taken from each river and partitioned into BOD bottles. BOD was measured in five of these bottles on each of nine days. The experimental results show that the average daily BOD decreased exponentially as expressed by the Streeter-Phelps equation. A wide range of the measured five daily BOD-values was expressed by the difference between the maximum and minimum BOD-values on each day for each river. After the first few days the range became smaller. The proposed stochastic model describes the observed experimental fluctuation of BOD over time. Eighty to ninety percent of the experimental BOD plots are within the 80% probability range given by the model. The uncertainty of BOD prediction can be expressed by the error which is the non-dimensional ratio of the range to the median. Modeled and experimental results reveal that the error is about 0.5–1 (50–100% of expected value) after a few days. This suggests that the BOD predicted by deterministic water quality models can include uncertainty, i.e. the actual BOD can be a quarter or double of the simulated value, for the time scale of a few days. For a longer period, e.g. more than a week, the error can become even more significant.

1. Introduction

Dissolved Oxygen (DO) in natural water bodies has a strong impact on fish, microorganisms, and other aquatic organisms, as well as aquatic chemical processes, and therefore, is one of the most important indicators of water quality. DO is related to the oxygen demand of the water. BOD (Biochemical Oxygen Demand) can be exerted by substances which are mainly dead organic matter, and was included in the classical stream water quality model by Streeter and Phelps (1925). As highlighted by Kannel et al. (2011), water quality models (e.g. QUAL, WASP, QUASAR, MIKE and EFDC) have been developed for water quality prediction and environmental assessment (Grenney et al., 1978; Ambrose et al., 1988; Danish Hydraulic Institute, 1996; Whitehead et al., 1997; EPA, 1999). In those mathematical simulation models, re-aeration (O'Connor, 1960), photosynthesis (Gulliver and Stefan, 1984), nitrification (Henze et al., 1999), oxygen uptake by sediments (SOD) (Higashino et al., 2004), and other processes, are taken into account in order to quantify the DO balance in the water. These processes are modeled separately from the oxygen demand by organic matter (BOD).

The classical river DO model (Streeter and Phelps, 1925) was formulated for a well-mixed turbulent river. Mixing by turbulence is often assumed in water quality models (e.g. Warm, 1987; EPA, 2010). Some water quality models have a strong linkage to fluid flow models, i.e. water quality is simulated for a given flow field (e.g. Hansen et al., 2012) in surface and/or subsurface flow. While the Monod equation is often used for the kinetics of microbial processes, e.g. nitrification, de-nitrification, the first-order decay equation is still valid when describing the degradation of organic matter (e.g. Warm, 1987; EPA, 2010). Equations including a lot of parameters can be assembled to simulate more complex biochemical kinetics in water quality models of natural and man-made water systems.

Although water quality models have been available for some time, prediction of accuracy is still in question. Simulated DO rarely matches field data at the hourly time scale, even when daily or weekly trends are well simulated (e.g. Demetracopoulos and Stefan, 1983). This can also be due to uncertainty in the water quality

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measurements. Studies of randomness in e.g. BOD dynamics began in the 1970's. First-order analysis, Monte-Carlo methods, and stochastic differential equations have been used to describe the uncertainty in BOD degradation. The randomness seen in water quality data has been incorporated into several water quality models. For instance, SIMCAT is a water quality model that includes the stochastic approach, describing the water quality throughout a catchment by Monte Carlo simulation to predict the behavior of the summary statistics, e.g. averages and percentile ranges (Warm, 1987; Cox, 2003; Crabtree et al., 2006; Nader and Etemad-Shahidi, 2012; Shao et al., 2013; Noutsopoulos and Kyprianou, 2014). Using a stochastic differential equation is the most recent approach, and has been applied to the BOD timeseries (Leduc et al., 1986, 1988) for raw sewage influent, or DO and BOD in a stream (Padgett et al., 1977; Finney et al., 1982; Zielinski, 1988; Tumeo and Orlob, 1989; Stijnen and Heemink, 2003; Revelli and Ridolfi, 2004; Boano et al., 2006; Liu and Zou, 2012). With the exception of BOD dynamics, a stochastic approach has been attempted to improve water quality prediction precision (e.g. Wang et al., 2009; Daly et al., 2014; Cox et al., 2015; Ghodsi et al., 2016). Stochastic approach has been used also for the water resources management (Nematian, 2016) and natural resources, e.g. food and water, management (Lin and Chen, 2016).

This study focuses on microbial processes, and assumes that the difficulties in predicting water quality and the uncertainty in measured water quality data are caused by spatial and temporal diversity in microbial growth and activities in a river cross-section. This is different from previous studies on stochastic BOD (e.g. Padgett et al., 1977; Finney et al., 1982; Leduc et al., 1988; Revelli and Ridolfi, 2004; Boano et al., 2006) that considered the uncertainty caused by the random first-order decay coefficient, random initial conditions, or random point inputs. Both random initial conditions and random inputs are difficult to be incorporated into e.g. the water quality projection for a river since the river may have many tributaries. Also, surface runoff from different landscapes, e.g. mountains, forests or cities, may need to be taken into account. It is difficult to give stochastic variables appropriately.

DO, organic matter, and other substrate concentrations can be homogeneous in a river cross-section because the river is well mixed due to turbulence. The distribution of microbes, however, may be heterogeneous in a river cross-section. Even if spatial distribution is uniform, microbial growth and activities may differ over time. These uncertainties can cause fluctuations and time variation of water quality.

The objective of this study is to develop a concept for the inclusion of uncertainty due to microbial activity in water quality prediction. For this purpose, oxygen uptake in river water was investigated theoretically and experimentally as a case study on the Ura River, Oita River, and Otozu River flowing through the urban district of Oita, a Japanese city with a population of about 0.5 million inhabitants. Those rivers are slightly polluted. Stochastic features of BOD in those rivers, considered as organic matter in this paper, were measured. A stochastic differential equation was introduced instead of the classical deterministic approach, in order to describe degradation of fluctuating BOD over time in the laboratory and along the stream. Although stochastic BOD decay has been studied in some previous works (e.g. Padgett et al., 1977; Finney et al., 1982; Leduc et al., 1986; Zielinski, 1988; Tumeo and Orlob, 1989; Stijnen and Heemink, 2003; Revelli and Ridolfi, 2004; Boano et al., 2006; Liu and Zou, 2012), a different point of view is herein proposed for useful and practical improvements. We assume that the oxygen uptake rate is composed of the rate constant plus fluctuations caused by microbial processes. This enables simulation of the BOD range and prediction error to quantify the potential difference between predicted and actual BOD for given conditions and time scales.

2. Model of dissolved oxygen uptake in water

2.1. Classical theory

The oxygen balance in water is important for microorganisms and fish. In rivers and streams it has been studied for more than a century. A classical model of dissolved oxygen (DO) in a polluted river is the very well-known Streeter-Phelps equation (1925), which is a solution to the linear first order differential equation.

$$\frac{dL}{dt} = -k_1 L \tag{1}$$

in which L is the biochemical oxygen demand (BOD) of organic matter remaining at time t in the water, k_1 is a constant coefficient, defining the rate at which the oxygen uptake proceeds, and t is travel time of the water. The analytical solution of Eq. (1) is

$$L = L_0 e^{-k_1 t} \tag{2}$$

in which L_0 is the initial oxygen demand of organic matter in the water, which is called the ultimate BOD (BOD at time t = infinity). The Streeter-Phelps equation assumes a stream that is perfectly mixed in a cross-section and at steady state flow.

The DO balance in the river is expressed by the equation.

$$\frac{dD}{dt} = k_1 L - k_2 D \tag{3}$$

in which D is the saturation deficit, ($D = C_{sat} - C$, where C_{sat} is the potential DO concentration in the river at saturation, C is the actual DO concentration), and k_2 is the re-aeration rate at the river surface. Eq. (3) can be solved analytically as

$$D = \frac{k_1 L_0}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) + D_0 e^{-k_2 t} \tag{4}$$

in which D_0 is the initial oxygen deficit.

2.2. Model of oxygen uptake using a stochastic differential equation

Measured BOD and DO in rivers have a stochastic fluctuating component which is not considered in the classical fully deterministic theory. Harmel et al. (2006) pointed out that the uncertainty in water quality data falls into four categories: stream flow measurement, sample collection, sample preservation/storage, and laboratory analysis. We assume that the fluctuation of the oxygen uptake rate with time is caused by microbial processes. In previous studies, the BOD fluctuation was considered to be due to the random initial conditions and a random rate coefficient k_1 in Eq. (1) (Padgett et al., 1977; Finney et al., 1982; Leduc et al., 1988). Revelli and Ridolfi (2004) successfully modeled BOD by assuming a deterministic decay coefficient and random input.

To describe the growth of microbes, Eq. (5) may be applied to oxygen consuming microorganisms when organic matter and oxygen are abundant.

$$\frac{dN}{dt} = \mu N \tag{5}$$

in which N(t) is the momentary (instantaneous) number of organisms and μ is a first order growth rate coefficient taken to be a constant value. Eq. (5) gives an exponential growth of microbes. However, the rate μ may be variable over time due to intermittent