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Robust empirical modeling of dissolved oxygen in small rivers and streams: Scaling by a single reference observation

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SUMMARY

A scaling-based, data-driven empirical model was developed for robust predictions of the diurnal cycle of stream dissolved oxygen (DO) by utilizing a single reference observation as the scaling parameter. The scaling concept was investigated by predicting hourly DO time-series of May to August from different streams representing four distinct US EPA Level III Ecoregions of Minnesota. Absence of any clear temporal trends or site-specific groupings of model parameters suggested a useful generalization and robustness of the scaled, dimensionless DO model over time and space. DO predicted using seasonal (May–August) averages of site-specific parameters simulated the observed diurnal DO cycles with high accuracy (root-mean-square error based coefficient of variation, CV(RMSE) = 0.07–0.11), superior linear correspondence (correlation coefficient, r = 0.87–0.96), and acceptable efficiency (Nash–Sutcliffe Efficiency, NSE = 0.58–0.74); the high accuracy predictions of hourly DO for different days with a single set of dimensionless parameters for the entire season underscore the temporal robustness of the scaled DO model. Nearly equivalent predictions were obtained using monthly averages of parameters, reaffirming the temporal robustness of the dimensionless model. Impressive predictions using parameters of independent sites, as well as a set of spatially averaged (i.e., quasi-regional) seasonal parameters, demonstrated spatiotemporally robust model performance. Model robustness was further demonstrated by deriving and quantifying analytical, dynamic sensitivity and uncertainty measures. The research is an example of useful scaling applications in ecohydrological engineering. The relatively robust, empirical DO model can be applied for simulating continuous (e.g., hourly) DO time-series from a single observation (or a set of limited observations) at different stream sites of comparable watershed sizes. The method can also be used to fill-in missing data in observed sub-daily time-series of periodic water quality variables. High resolution, continuous DO time-series will facilitate a dynamic assessment of the general health of streams and river ecosystems.

1. Introduction

Dissolved oxygen (DO) is a key determinant of water quality and an indicator of the general health of aquatic ecosystems. Natural processes (e.g., photosynthesis and respiration, atmospheric diffusion and reaeration) and regular anthropogenic interventions (e.g., pollution) generally result in a sharp diurnal cycle of DO in streams and rivers. Subject to the variations in hydro-climatic and biogeochemical drivers (e.g., stream flow, photosynthetically active radiation, land use, water temperature, nutrient availability, and organic waste), the DO cycle tends to vary at different stream sites or at the same site for different days. Lack of continuous DO data monitoring often leads to collecting grab samples at coarse spatial and temporal intervals, making the assessment of stream health by regulatory criteria (such the total maximum daily load, TMDL) arbitrary. A standard method is, therefore, necessary to generate fine-resolution, continuous DO concentration information from a limited number of observations for a more appropriate and dynamic assessment of the daily stream health. It is hypothesized that scaling the different diurnal DO cycles by corresponding single reference observations would lead to a general, dimensionless diurnal DO cycle for the same stream, as well as for different streams of comparable watershed sizes and geographic regions. The hypothesis is tested by developing a data-driven, empirical DO model to provide robust (in time and space) predictions of hourly DO for small rivers and streams.

Much research has focused on the analysis and prediction of DO in stream and river ecosystems. Dyar and Alhadeff (2005) used a standard harmonic analysis procedure to develop an empirical

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model to predict the annual DO cycle by leveraging correlations among daily DO, Julian day, latitude, and elevation of 31 Georgia streams. Van Orden and Uchrin (1993) also reported success with harmonic analysis to simulate the variability of DO deficit in streams. Gallegos et al. (1977) applied the Fourier transform to determine the short-term variation of aquatic oxygen exchanges. Examples of empirical DO models without involving harmonic analysis include Piasecki (2004), Rounds (2002), Adrian and Alshawabkeh (1997), Butcher and Covington (1995), and Erdmann (1979a,b).

Numerous mechanistic (i.e., process-based) models (e.g., QUAL2K (Chapra et al., 2008) and QUAL2E (Brown and Barnwell, 1987)) are available for simulation and prediction of river water quality variables, including DO. Marsili-Libelli and Giusti (2008) suggested relatively simple modeling as a feasible tool to describe water quality in small rivers. More recent research (e.g., Freni et al., 2010; Mannina and Viviani, 2010a,b; Mannina, 2010) used the conceptual linear reservoir modeling approach and/or an extension of the classical advection–dispersion equations (Chapra, 1997), emphasizing different modeling aspects (such as data monitoring, calibrations, and uncertainty analysis) and numerical schemes. Following varying levels of process complexity and model structure, mechanistic models generally involve a large matrix of parameters (making predictions highly uncertain) and require input data for many input variables that are often unavailable at appropriate spatiotemporal resolutions. In contrast, empirical models are data-driven and often less expensive because of their simple structures and reduced parameter sets. However, a common limitation with both empirical and mechanistic DO models is that the model parameters are mostly site-specific and, therefore, a new calibration is often needed for applications at a different site.

The concept of scaling has been touted as a key to develop robust modeling and prediction tools in many science and engineering disciplines. Examples of relevant scaling research can include that in ecology (Milne et al., 2002; Ruddell and Kumar, 2009; Warnaars et al., 2007; Hondzo and Warnaars, 2008; West et al., 2001), environmental engineering (O'Connor et al., 2006; Hondzo et al., 2005; Stein et al., 2001), and hydrology (Lima and Lall, 2010; Paola et al., 2006). Hondzo et al. (2005) derived a scaling based power law model of DO to analyze dissolved oxygen distribution at the sediment–water interface of a small lake. Abdul-Aziz et al. (2007a,b) formulated an extended stochastic harmonic analysis (ESHA) to develop scaling-based empirical and semi-empirical DO models; the main objective of both models was to convert DO measured at different clock times of the day to those at a reference time.

This paper extends the previous research (Abdul-Aziz et al., 2007a,b) to develop a scaling-based robust, empirical model for simulating the diurnal cycle of stream DO from a single reference observation. The key objective is to obtain robust predictions of high frequency (e.g., hourly), continuous DO with an appropriately scaled empirical model. The spatiotemporal robustness of the model parameters and predictions are demonstrated using hourly DO observations of different days and years for stream sites representing four distinct U.S. Environmental Protection Agency (US EPA) Level III Ecoregions of Minnesota.

2. Materials and methods

2.1. Conceptual framework of scaling

The concept of DO scaling is demonstrated schematically by assuming hypothetical diurnal cycles representing a single or multiple stream sites (Fig. 1a). As shown, the magnitudes of the DO cycle of different days $(1,2,\ldots,N)$ are different. Therefore, a potential classical harmonic model (Priestley, 1981) would require a unique set of parameter values to represent each diurnal DO cycle, resulting in N sets of parameters for N diurnal cycles. Based on the common availability of reliable data, a reference-time (t_{ref}) single observation (DO_{ref}) from each cycle can be selected as the scaling parameter to normalize the corresponding diurnal cycle. The scaling should ideally result in the collapse of DO cycles of different days into a general, dimensionless diurnal DO curve (DO^*) that has a value of unity (1.0) at the reference time for any day (Fig. 1b). The scaled model is assumed to be robust, because it represents the normalized DO cycles of any day and provides a single set of parameter values for N days. The dimensionless model is parameterized by applying an extended stochastic harmonic analysis (ESHA) (Abdul-Aziz et al., 2007a) using observed data of all available days. The predicted DO cycle of any day is then obtained by multiplying the unique dimensionless model (DO^*) by the corresponding reference observation (DO_{ref}).

The main advantage of ESHA over a classical harmonic analysis (Priestley, 1981) is that ESHA provides the appropriate parameter estimation framework for forcing the harmonic model through the normalized, single reference-time observation (i.e., 1.0) (Abdul-Aziz et al., 2007a). Therefore, ESHA exclusively allows the proper representation of the entire diurnal cycle of DO for different days at the same stream site (or at different sites) from the

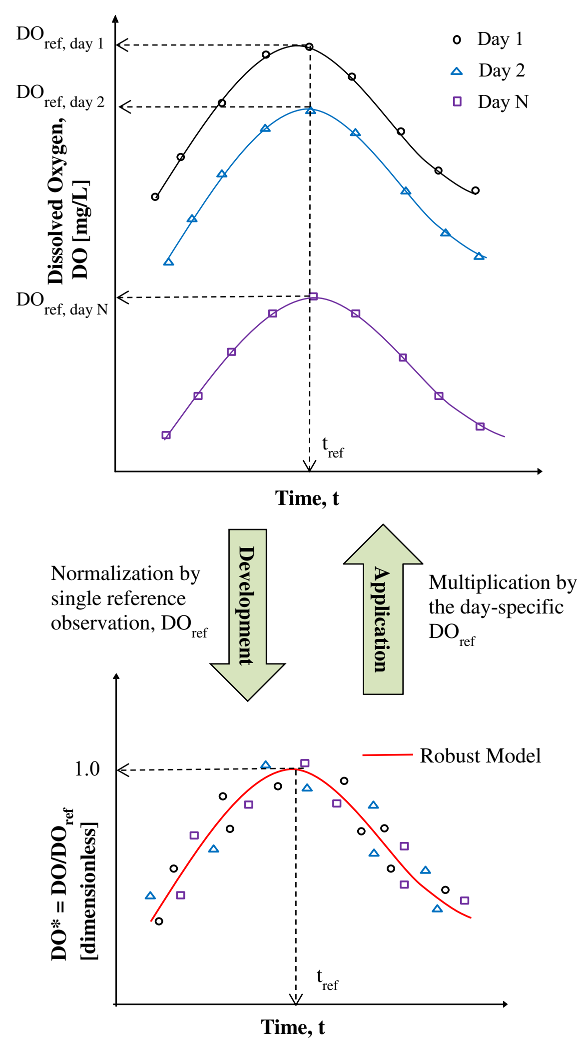

Fig. 1. Schematic showing the conceptual framework for development and application of the scaled model.