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Spatial and temporal variability of in-stream water quality parameter influence on dissolved oxygen and nitrate within a regional stream network

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ABSTRACT

Maintaining elevated aqueous concentrations of dissolved oxygen (DO) and decreased concentrations of nitrate (NO_3) within stream environments is critical to sustaining aquatic life and the overall environmental health of a river system. Identifying system processes and system inputs that govern in-stream concentrations of DO and NO_3 is paramount to achieving satisfactory concentrations or implementing efficient remediation methods. As these processes and inputs often depend on a multitude of climatic, environmental, and anthropogenic factors, it is essential to determine the spatio-temporal variability in their control of DO and NO_3. In this study, a sensitivity analysis is applied to a regional-scale stream system of the Lower Arkansas River Basin in southeastern Colorado using a coupled QUAL2E-OTIS model to investigate the factors that govern DO and NO_3 in space and time. Using the revised Morris scheme, a total of 34 model input factors (boundary conditions, flow and mass inputs, model parameters) are included in the analysis. Besides identifying the model input factors that govern DO and NO_3 concentrations globally, the methodology also ascertains the influence of these factors according to location within the regional stream network and to season of the year. Results show that upstream solute concentrations, algal processes, channel roughness, groundwater discharge and solute mass loadings to the stream, and oxygen reaeration are the most influential processes and parameters in determining DO and NO_3 concentrations. Many processes (algal growth and respiration, chemical kinetic reactions) have a time-varying influence due to seasonal changes in water temperature and solar radiation. Other processes (groundwater discharge and solute mass loading) are of moderate influence in the Arkansas River but of very strong influence in the tributaries. These results not only identify parameters and processes that should be targeted during field data collection and model calibration, but also highlight the possibility of implementing efficient remediation strategies that target processes at different locations and at different times of the year.

1. Introduction

In-stream concentrations of dissolved oxygen (DO) C_{DO} (mg/L) and nitrate (NO_3) C_{NO_3} (mg/L) are of paramount importance due to their effects on aquatic life and the overall environmental health of a river system (Spalding and Exner, 1993; Melching and Flores, 1999; Ay and Kisi, 2012; Zahraeifard and Deng, 2012). Problems associated with inadequate C_{DO}, which can be brought about by consumption of introduced solid or dissolved organic matter (e.g., sewage waste) by decomposer organisms, include mortality of aquatic organisms and the overall decrease in stream esthetics (e.g., odor, taste). Problems associated with high C_{NO_3} include eutrophication, which induces DO depletion (i.e., hypoxia) due to increased biologic activity, and contamination of drinking water which can have serious negative health effects for infants due to methemoglobinemia (Fan and Steinberg, 1996).

As a means to assess the effect of environmental factors (e.g., point source, non-point source mass loadings) and remediation strategies on C_{DO} and C_{NO_3}, in-stream water quality models such as QUAL2E (Brown and Barnwell, 1987) and its successor QUAL2K (Chapra et al., 2008), QUASAR (Whitehead et al., 1997) and its successor Q^2 (Cox and Whitehead, 2005), and EPD-RIV1 (Martin and Wool, 2002) are widely used and applied to threatened river systems. These models simulate the transport and cycling of oxygen and nitrogen (N) in a one-dimensional (i.e., streams are assumed to be well-mixed vertically and laterally) stream network system, with advection, longitudinal dispersion, sources/sinks, and chemical reactions governing the fate and transport of each species.

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System sources/sinks include lateral inflow/outflow and associated species concentration, representing stream–aquifer interactions, and reaeration of DO from the atmosphere. Chemical reactions and cycling components include settling, algal growth and decay, algal uptake of N species and DO, DO sediment demand, organic matter consumption, hydrolysis of organic N, nitrification, and denitrification.

Although these models typically are used to describe baseline spatio-temporal water quality conditions in a river system and, once the model has been corroborated against observed data, to investigate changes in water quality due to viable management strategies, they also can be powerful tools in elucidating system processes, inputs, and system parameters that govern C_{DO} and C_{NO_3}. In general, such information for any hydrologic system can be useful in establishing optimal remediation schemes through targeting of identified influential processes; guiding effective field sampling strategies by focusing on influential system variables (e.g., water temperature, solar radiation) or inputs (e.g., groundwater inflow and associated solute concentrations); facilitating model parameter estimation and corroboration by focusing on the identified key parameters (Sincock et al., 2003); allowing for model simplification by elimination of non-influential parameters or processes (Saltelli et al., 2008); or identifying factors that may need more research to improve model confidence (Hall et al., 2009). Several studies (Chadderton et al., 1982; Sincock et al., 2003; Cox and Whitehead, 2005; Deflandre et al., 2006), for example, have investigated the factors that govern C_{DO}, with results depending on the studied river system.

An appealing approach in detecting influential factors from the multitude of model factors is sensitivity analysis (SA), which uses a stochastic set of model simulation runs to quantify the variation of model output variables in relation to changes in values of model input factors (forcing terms, initial conditions, model parameters). The use of SA for assessing key factors is a common approach for many hydrologic systems (Hall et al., 2005; White and Chaubey, 2005; Arabi et al., 2007), and has been used recently for in-stream water quality (Cox and Whitehead, 2005; Deflandre et al., 2006; Liu and Zou, 2012), particularly to assess governing factors for DO. For example, Deflandre et al. (2006) used the Fourier Amplitude Sensitivity Test (FAST), a method that quantitatively decomposes the variance of model output into fractions that are attributed to input factors, to analyze the influence of 12 parameters on DO in UK rivers.

Although the study of Deflandre et al. (2006) applied SA to two disparate streams (urban vs. rural), finding that DO is more sensitive to in-stream rate parameters in a rural stream as compared to an urban stream, a comprehensive analysis of spatio-temporal variability in model sensitivity has yet to be undertaken for in-stream water quality models, with all studies reporting global sensitivity indices for a given river system. Such an assessment can yield sensitivity indices for each factor along the length of the stream and during sequential time periods, thus providing valuable information regarding which factors dominate in-stream concentrations at different reaches of the stream and for different seasons of the year. Computing spatial- and temporal-variable sensitivity indices has been performed recently in a few hydrologic and hydraulic systems (Hall et al., 2009; Reusser et al., 2011; Marrel et al., 2011), with conclusions indicating that careful analysis of sensitivity in space and time is key to providing a more complete understanding of a particular hydrologic system.

In this study, a comprehensive sensitivity analysis is applied to a regional-scale stream system of the Arkansas River in southeastern Colorado using the QUAL2E model processes linked with the OTIS (One-Dimensional Transport with Inflow and Storage: Runkel, 1998) model to investigate the system factors that govern C_{DO} and C_{NO_3} in space and time. QUAL2E handles all water quality processes, whereas OTIS is used as the advection-dispersion solute transport engine. A total of 34 input factors (boundary conditions, flow and mass inputs, model parameters), many more than has been included in previous studies, are included in the SA, which is applied to the main channel of the Arkansas River as well as multiple tributaries that are fed principally by groundwater flow. As such, results provide detailed information regarding not only spatial and seasonal patterns of sensitivity, but also the occasion to compare and contrast between main channel and tributary systems. The SA method used is an improved variant of the Morris (1991) Elementary Effect (EE) method, enhanced by refining the sampling strategy and the computation of the sensitivity measure (Campolongo et al., 2007). Low computational cost is preserved, thus enabling a large number of factors to be included in the analysis. The SA approach not only provides a valuable examination of the system, but also serves as a preceding step to parameter estimation for the regional stream system, which will be undertaken in future work. As such, observed in-stream concentrations are used only to ensure reasonable model behavior for the sensitivity analysis simulations.

2. Methods

2.1. QUAL2E-OTIS water quality model

This study uses a coupled model approach, with QUAL2E used for in-stream water quality processes and the OTIS model used as the advection–dispersion solute transport engine, with the QUAL2E processes imbedded within the OTIS modeling code and simulated at every time step of the simulation. Whereas the stand-alone QUAL2E model can handle only steady stream flow applications, OTIS can be applied to unsteady flow applications, and hence the QUAL2E processes are included to provide an in-stream water quality model that can be applied to unsteady flow conditions. Whereas this study only is applied to steady flow conditions, thereby enabling an efficient sensitivity analysis methodology, future work will use the full capabilities of the QUAL2E-OTIS modeling framework. Fig. 1 shows the conceptual model of the resulting model framework and the in-stream processes simulated by QUAL2E, with QUAL2E handling the chemical reactions within the stream network.

The OTIS model characterizes the advective–dispersive transport of solutes in streams and rivers, with additional terms to account for lateral inflow/outflow and transient storage, although the latter feature is not used in this study. The advection–dispersion equation is solved using a Crank–Nicolson finite-difference solution, with the stream network divided into physically-uniform reaches and each reach divided into segments, with each segment representing a finite-difference cell. The original model can be applied to a single stream and account for multiple, non-interacting species (Runkel, 1998). For this study the modeling code was modified to enable the transport of solutes within a multi-stream network and to simulate the fate of multiple, interacting chemical species. For the former, the code was modified to simulate solute transport for any number of streams, with mass balance mixing calculations implemented at stream junctions; for the latter, the 4th-order Runge–Kutta method was implemented to solve the system of ordinary differential equations required for simulating the kinetics of interacting species (Chapra, 1997), and hence able to solve the QUAL2E mass-balance equations.

QUAL2E processes (Fig. 1) simulate the reactive behavior of DO, organic N, ammonia, nitrite (NO_2), NO_3, algae, and carbonaceous biological oxygen demand (CBOD) in a 1D stream network setting, with major reactions governing N cycling, DO fate, algal growth and respiration, and algal uptake of N and DO. C_{DO} increases due to atmospheric reaeration, which is dependent on C_{DO} and