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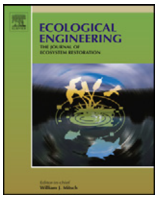

Estimation of real-time N load in surface water using dynamic data-driven application system

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ABSTRACT

Agricultural, industrial, and urban activities are the major sources for eutrophication of surface water ecosystems. Currently, determination of nutrients in surface water is primarily accomplished by manually collecting samples for laboratory analysis, which requires at least 24 h. In other words, little to no effort has been devoted to monitoring real-time variations of nutrients in surface water ecosystems due to the lack of suitable and/or cost-effective wireless sensors. However, when considering human health or instantaneous outbreaks such as algal blooms, timely water-quality information is very critical. In this study, we developed a new paradigm of a dynamic data-driven application system (DDDAS) for estimating the real-time loads of nitrogen (N) in a surface water ecosystem. This DDDAS consisted of the following components: (1) a Visual Basic (VB) program for downloading US Geological Survey real-time chlorophyll and discharge data from the internet; (2) a STELLA model for evaluating real-time N loads based on the relationship between chlorophyll and N as well as on river discharge; (3) a batch file for linking the VB program and STELLA model; and (4) a Microsoft Windows Scheduled Task wizard for executing the model and displaying outputs on a computer screen at selected schedules. The DDDAS was validated using field measurements with a very good agreement prior to its applications. Results show that the real-time loads of TN (total N) and NO_x (nitrate and nitrite) varied from positive to negative with the maximums of 1727 kg/h TN and 118 kg/h NO_x and the minimums of −2483 kg/h TN and −168 kg/h NO_x at the selected site. The negative loads occurred because of the back flow of the river in the estuarine environment. Our study suggests that the DDDAS developed in this study was feasible for estimating the real-time variations of TN and NO_x in the surface water ecosystem.

1. Introduction

Clean water is of vital importance for human societies and natural ecosystems. Agricultural, industrial, and urban activities are the major sources for contamination and eutrophication of rivers and lakes (Carpenter et al., 1998; David and Gentry, 2000; Dodds and Welch, 2000). The concentrations of biologically available nutrients in excess in surface water can lead to diverse problems such as toxic algal blooms, loss of oxygen, fish kills, loss of biodiversity, and loss of aquatic plant beds and coastal reefs. Nutrient enrichment in surface waters can also seriously degrade aquatic ecosystems and impair the use of water for drinking, industry, agriculture, and recreation and for other purposes. With an increased understanding of the importance of drinking water quality to public health and raw water quality to terrestrial life, there is a greater need to assess surface water quality.

In the past, to determine surface water quality in a stream, it is necessary to manually collect samples and send them to a laboratory for analysis. These analytical methods require at least 24 h or longer. However, when the human health or other instantaneous outbreaks such as algal blooms are concern, timely water-quality information is required. Timely water-quality information also is useful for other many reasons, including assessment of total maximum daily loads and the effects of urbanization and agriculture on a water supply. In response to the need for timely and continuous water-quality information, the US Geological Survey (USGS) has begun using an innovative, continuous, real-time monitoring approach for many nation's streams (http://waterdata.usgs.gov/nwis/rt). These real-time monitoring water quality data normally include discharge, flow velocity, dis-

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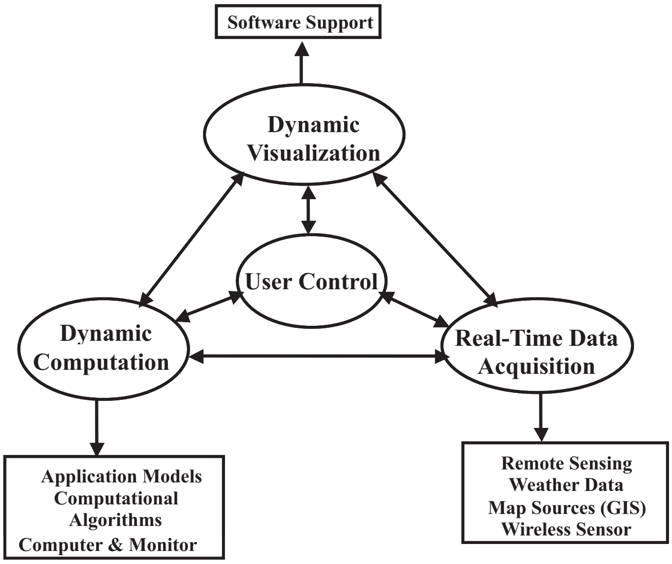

Fig. 1. A schematic diagram showing the basic concept of a dynamic data-driven application system redrawn after NSF (2000).

solved oxygen, pH, temperature, conductance, and chlorophyll. These data are valuable for monitoring surface water-quality indicators. However, there is currently very little activity to monitor the real-time variations of nutrients in surface waters due to the lack of suitable and/or cost-effective wireless sensors. Knowledge of real-time nutrient variations is critical to estimate surface water-quality status. Therefore, a need exists to develop a new paradigm for this purpose. To this end, a dynamic data-driven application system (DDDAS), which utilized the US Geological Survey (USGS) real-time chlorophyll *a* (Chl *a*) and river discharge data, a STELLA (Structural Thinking, Experiential Learning Laboratory with Animation) model for evaluation real-time variations of nitrogen (N), a VB.NET program, and the Windows interfaces, was developed in this study.

The DDDAS was probably first conceived by the US National Science Foundation around March 2000. Fig. 1 shows a basic concept of a DDDAS, which consists of the following four symbiotic components: user control, dynamic computation, real-time data acquisition, and dynamic visualization. A similar concept can also be found in NSF (2000), Douglas et al. (2004), Darema (2005) and Ouyang et al. (2007). Users control and interact with dynamic computation, real-time data acquisition, and dynamic visualization. Dynamic computation includes application models, computational algorithms, and all of the computing machines and their connections (e.g., computers and monitors). Real-time data acquisition involves the instantaneous data collections from remote sensing, climatic monitoring, GIS map sources, and wireless sensor measurements. Dynamic visualization includes supporting software and hardware for interactive visualization, which help users to control the system and make decisions.

When a DDDAS is launching, the dynamic computation infrastructure will start to run the application models and/or computational algorithms. Meanwhile, the real-time data acquisition infrastructure will start to collect the real-world data and inject them into the dynamic computation infrastructure for simulations. This DDDAS will have the ability to dynamically employ simulations to guide the real-time measurements, to determine when, where, and how it is best to gather additional data. In reverse, the DDDAS can also dynamically steer the simulations based on the real-time measurements. Such automatic steering of simulations and measurements with ability to switch between the two infrastructures can be envisioned through the dynamic visualization infrastructure. The dynamic visualization infrastructure will be achieved through the software and hardware supports. Overall, all of the infrastructures are controlled and managed by the users. A specific example of a DDDAS applied to watershed contamination monitoring and predictions can be found in Ouyang et al. (2007).

Chl *a* is often used to estimate algal biomass, with blooms being predicted to occur when the Chl *a* concentration exceeds 40 $\mu g\,L^{-1}$ (Stanley et al., 2003). During the last several decades, numerous studies have demonstrated a strong correlation among Chl *a*, total phosphorus (TP), and total nitrogen (TN) concentrations in north-temperate lake waters from around the world (Aizaki et al., 1981; Ahlgren, 1980; Sakamoto, 1966) and in Florida lakes (Huber et al., 1982; Canfield, 1983). Large- and small-scale experiments further suggested that P is a primary factor controlling algal growth, especially in northern lakes. Therefore, simple empirical TP–Chl *a* regression models (Dillion and Rigler, 1974; Jones and Bachmann, 1976) have been used to predict changes in Chl *a* concentrations in response to changes in TP concentrations. However, lakes surrounded by rich phosphate deposits and P-containing soils may be N limited. Existing equations using the P and Chl *a* correlation may inadequately estimate algal biomass under such circumstances. Canfield (1983) demonstrated that in Florida lakes, Chl *a* is significantly correlated with both TP and TN. The P is the limiting nutrient when the TP concentration is below 100 $\mu g\,L^{-1}$, whereas the N is the limiting nutrient when the TP is above 100 $\mu g\,L^{-1}$.

STELLA is a user-friendly and commercial software package for building a dynamic modeling system. It uses an iconographic interface to facilitate construction of dynamic system models. The key features of STELLA consist of the following four tools: (1) stocks, which are the state variables for accumulations. They collect whatever flows into and out of them; (2) flows, which are the exchange variables and control the arrival or the exchanges of information between the state variables; (3) converters, which are the auxiliary variables. These variables can be represented by constant values or by values depending on other variables, curves or functions of various categories; and (4) connectors, which are to connect among modeling features, variables, and elements. STELLA offers a practical way to dynamically visualize and communicate how complex systems and ideas really work (Isee Systems, 2006). STELLA has been widely used in biological, ecological, and environmental sciences (Hannon and Ruth, 1994; Costanza et al., 2002; Aassine and El Jai, 2002; Ouyang, 2008). An elaborate description of the STELLA package can be found in Isee Systems (2006).

The purpose of this study was to develop a DDDAS for indirectly estimating the real-time loads of N in a surface water ecosystem. Our specific objectives were to: (1) obtain the relationships between Chl *a* and total N (TN) as well as between Chl *a* and total Kjehldahl N (TKN) through linear regressions, using a long-term dataset from a regular (i.e., non real-time) surface water-quality monitoring station; (2) download the USGS real-time Chl *a* data from a monitoring station to a personal computer using a Windows-based VB.NET program; (3) develop a STELLA model for predicting the real-time loads of TN and NO_x (nitrate and nitrite) species in the surface water ecosystem based on the real-time Chl *a* data and the relationships obtained from Objective 1 as well as based on the river discharge data; (4) create a batch file for linking the VB.NET program and the STELLA model; (5) set up a Windows Scheduled Task wizard for implementing the DDDAS at given schedules; (6) validate the DDDAS for estimating real-time variations of N species using another independent dataset from the regular monitoring station; and (7) apply the DDDAS to forecast the real-time loads of N species in the surface water ecosystem.

It should be pointed out that the real-time monitoring station selected in this study was very close (<400 meters in distance) to the regular monitoring station in order to minimize the sample