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Designing a Dynamic Data-Driven Application System for Estimating Real-Time Load of Dissolved Organic Carbon in a River

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Abstract Understanding the dynamics of naturally occurring dissolved organic carbon (DOC) in a river is central to estimating surface water quality, aquatic carbon cycling, and global climate change. Currently, determination of DOC in surface water is primarily accomplished by manually collecting samples for laboratory analysis, which requires at least 24 h. In other words, no effort has been devoted to monitoring real-time variations of DOC in a river due to the lack of suitable and/or cost-effective wireless sensors. However, when considering human health, carbon footprints, effects of urbanization, industry, and agriculture on water supply, timely DOC information may be critical. We have developed here a new paradigm of a dynamic data-driven application system (DDDAS) for estimating the real-time load of DOC into a river. This DDDAS was validated with field measurements prior to its applications. Results show that the real-time load of DOC in the river varied over a range from −13,143 to 29,248 kg/h at the selected site. The negative loads occurred because of the back flow in the estuarine reach of the river. The cumulative load of DOC in the river for the selected site at the end of the simulation (178 h) was about 1.2 tons. Our results support the utility of the DDDAS developed in this study for estimating the real-time variation of DOC in a river ecosystem.

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1 Introduction

Naturally occurring dissolved organic carbon (DOC) is an important constituent of stream water quality. It contributes significantly to biological activities through the absorption of light and providing a substrate for microbial communities and to water chemistry through the complexation of metals and production of carcinogenic compounds with chlorine (Moore, 1989). DOC has been linked to acidification processes and to heterotrophic productivity and respiration in small streams, which are important in influencing rates of C cycling and CO_2 emissions (Dalzell et al. 2005). In addition, by forming organic complexes, DOC can influence nutrient availability and control the solubility and toxicity of contaminants. The occurrence of DOC in natural waters has been known for at least a century (Krogh, 1933). Because of the low pKa (3.5–5.5) of some DOC, its importance in freshwater systems has been widely recognized (Eshleman and Hemond, 1985). DOC is known to be a strong complexing agent for many toxic metals such as iron, copper, aluminum, zinc, and mercury (Eshleman and Hemond, 1985). DOC can also increase the weathering rate of minerals (Eshleman and Hemond, 1985, Drever, 1988) and increase the solubility and thus the mobility and transport of many metals and organic contaminants.

A variety of human activities and natural processes have resulted in elevated concentrations of DOC in streams. These include diverse inputs from throughfall, stemflow, inappropriate animal waste applications and disposal, forest clear cutting, agricultural practices, and different land use patterns (Moore 1989; Ouyang 2003). Furthermore, degradation, re-polymerization, and oxidation of litter and soil organic matter are also major sources of DOC (Dunnivant et al. 1992; Grant, 1997).

In the past, to determine surface water DOC and other water quality parameters in a stream, it has been necessary to collect samples and analyze them in a laboratory. This method often requires in excess of 24 h. However, when human health issues arise or other rapidly developing issues such as algal blooms are a concern, timely water quality information is required. Timely water quality information may also be less expensive, making it useful for many other reasons, including assessment of total maximum daily loads and the effects of urbanization, industry, 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 US streams (http://waterdata.usgs.gov/nwis/rt). These real-time water quality monitoring data normally include discharge, flow velocity, dissolved oxygen, pH, temperature, conductance, and chlorophyll. These data are valuable for monitoring of surface water quality. However, there is currently little real-time monitoring of DOC in surface waters due to the lack of suitable and/or cost-effective wireless sensors for this parameter. Knowledge of real-time DOC variations is critical to estimating surface water-quality status, carbon load, and CO_2 emission. To achieve this, a dynamic data-driven application system (DDDAS) was developed. This DDDAS utilizes the USGS real-time data for chlorophyll *a* (Chl *a*) and river discharge; a structural thinking, experiential learning laboratory with animation (STELLA; from ISEE Sytems) model for prediction of real-time variations of DOC based on the relationships between Chl *a* and DOC; a Visual Basic (VB) program for downloading the real-time data from the USGS website; and the Windows Scheduled Tasks wizard for automatic simulation (forecasting) control.

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

When a DDDAS is initiated, 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 insert them into the dynamic computation infrastructure for simulations. This DDDAS has the ability to dynamically employ simulations to guide the real-time measurements, and 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-

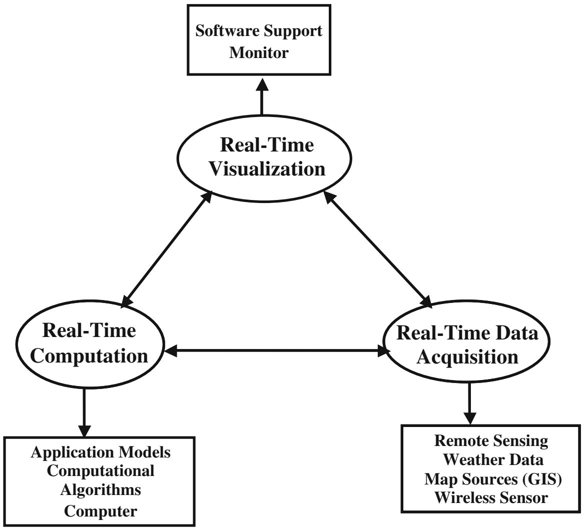


Fig. 1 A schematic diagram showing the basic concept of a dynamic data-driven application system

time measurements. This automatic steering of simulations and measurements with the ability to switch between the two infrastructures can be viewed through the dynamic visualization infrastructure. The dynamic visualization infrastructure is achieved through the software and hardware supports. Overall, the infrastructures are controlled and managed by the users. A specific example of a DDDAS applied to watershed contamination monitoring and predictions is found in NSF (National Science Foundation) (2000), Darema (2005), and Ouyang et al. (2007).

Chl *a* often is used to estimate algal biomass, with blooms being defined as Chl *a* concentration exceeding 40 μg L^{-1} (Stanley et al. 2003). During the last several decades, some 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). Canfield (1983) demonstrates that in Florida lakes, Chl *a* is significantly correlated with both TP and TN. Phosphorus is typically the limiting nutrient when the TP concentration is below 100 μg L^{-1}, whereas the N is the limiting nutrient when the TP is above 100 μg L^{-1}. However, very little effort has been devoted to investigating the correlation between Chl *a* and DOC. Legendre and Michaud (1999) used Chl *a* to estimate the particulate organic carbon (POC) available as food to large zooplankton population in the euphotic zone of oceans. These authors found that there is a good correlation between POC and Chl *a*.

STELLA is a user-friendly, 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 that depend 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; Peterson and Richmond 1996; Costanza et al. 2002; Aassine and El Jai 2002; Ouyang 2008; Ouyang et al. 2010a, b). A detailed description of the STELLA package can be found in Isee Systems (2006).

The goal of this study was to design a DDDAS for indirectly estimating the real-time load of DOC in the St. Johns River. The specific objectives were to: (1) evaluate the relationships between Chl *a* and DOC through regression using a long-term dataset from a regular (i.e., non-real-time) surface water-quality monitoring; (2) download the USGS real-time Chl *a* data from a monitoring station to a personal computer using a Windows-based VB program; (3) develop a STELLA model for predicting the real-time load of DOC in the river based on the real-time Chl *a* data and the relationships obtained from objective 1 as well as river discharge data; (4) create a batch file for linking the VB program and the STELLA model; (5) set up a Windows Scheduled Tasks wizard to guide the DDDAS on when to download the data, perform the STELLA simulation, display the simulations on the computer screen, and end the real-time forecasting for scheduling; (6) validate the DDDAS for estimating real-time variations of DOC using independent data; and (7) apply the DDDAS to forecast the real-time loads of DOC in the surface water ecosystem.

It should be noted that the USGS real-time monitoring station was close (<400 m distant) to the water-quality monitoring (or non-real-time) station used to develop relationship between Chl *a* and DOC and to validate this relationship. As stated above, most of the USGS real-time monitoring stations do not measure DOC in surface water ecosystems due to the lack of suitable and/or cost-effective wireless sensors. Therefore, it is impossible to directly estimate the real-time load of DOC based on the USGS real-time monitoring stations without independent water quality data.

2 Materials and Methods

A schematic diagram for the DDDAS in this study is presented in Fig. 2. This diagram shows the following five major components of the DDDAS: (1) a wireless sensor from a USGS real-time monitoring station; (2) a USGS real-time database website; (3) a STELLA

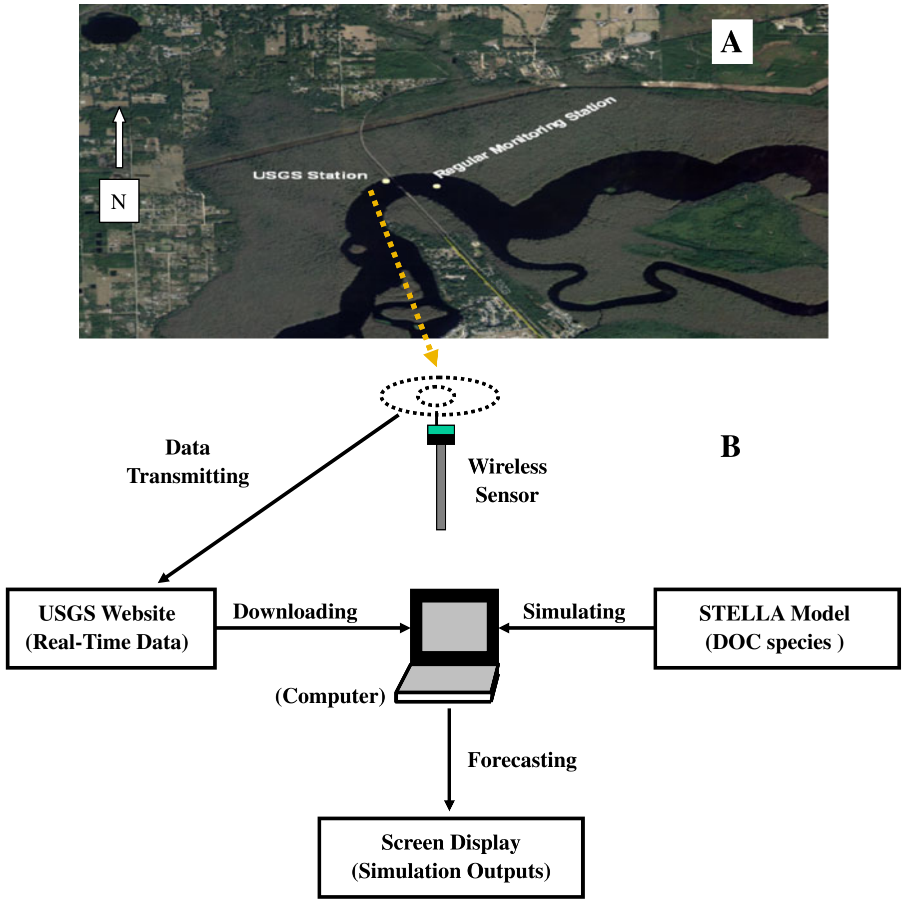


Fig. 2 **a** Location of the USGS real-time and regular monitoring stations near Satsuma, Putnam County, Florida, USA. The distance between the two stations is <400 m. **b** A schematic diagram showing a DDDAS framework for estimating real-time variations of DOC in a surface water ecosystem

model for simulating the real-time load of DOC in the river; (4) a computer for downloading the real-time data and performing simulations; and (5) a monitor for displaying simulation results. Details of these components are presented below.

2.1 Data Acquisition

The first step in developing the DDDAS is to select a study site (i.e., watershed) and a USGS monitoring station from the USGS website. This station should be close to a regular (non-real-time) monitoring station that has a long-term data set for DOC. In other words, both of these monitoring stations should be strongly autocorrelated. Once the real-time monitoring station is selected, a Windows-based computer program in Microsoft VB.NET is constructed for downloading the data to a personal computer. In this study, we selected USGS real-time monitoring station #02244040 (lat. 29°35′46″, long. 81°41′00″) located at the St. Johns River basin near Satsuma, Putnam County, Florida, USA (http://waterdata.usgs.gov/fl/nwis/uv /?site_no=02244040&PARAmeter_cd=00400,00095,00010). In close proximity to this real-time station, there is a regular water quality (i.e., non-real-time) monitoring station (29°35′43″, 81°40′45″) located <400 m to the upstream. This station is currently managed by the St. Johns River Water Management District (SJRWMD), Florida. All sampling activities for this station were conducted in accordance with the SJRWMD and US Environmental Protection Agency's standard operating procedures for the collection of water quality samples and field data. Both stations represent the same watershed drainage area. However, the USGS station measured the real-time data on river flow characteristics and some water quality parameters such as Chl *a* but not DOC, whereas the regular station collected most of the water quality parameters including DOC and Chl *a* but were not the real-time data and did not measure river discharge. The DOC data collected during 1993 to 2003 from the regular monitoring station were used to obtain the relationships (Fig. 3) between Chl *a* (mg/m^3) and DOC (mg/L)

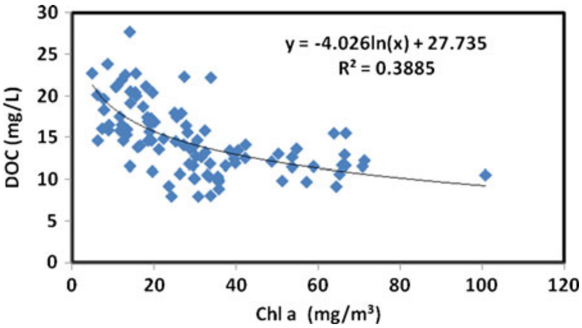


Fig. 3 Relationships of DOC and Chl *a* obtained from field measured data

resulting in the following equation:

$$\mathrm{DOC} = -4.026Ln(Chl\ a) + 27.735 \quad (1)$$

$$\left(R^2 = 0.3885p = 0.005\right)$$

This equation was used to predict the real-time variations of DOC contents based on the real-time variations of Chl *a* from the USGS monitoring station. The real-time load of DOC can then be calculated using the following equations:

$$\mathrm{Load_{DOC}} = 0.10194 * \mathrm{Discharge} * \ \mathrm{DOC} \quad (2)$$

where discharge is the river discharge rate (ft^3/s or 101940 L/h) at the real-time monitoring station and the Load denotes the mass of DOC loading from the station to down stream (kg/h).

2.2 STELLA Model

The first step in the modeling process was to develop a basic structure to capture the processes described above using STELLA. In Fig. 4, the rectangles are stocks that graphically represent the masses of nutrients. The flow symbols (represented by double lines with arrows and valves) represent the rates of nutrient discharge into or out of the stocks. The other variables are converters (represented by empty circles) that denote the rules or conditions controlling the stocks and flows through the connectors (represented by single lines with arrows). As shown in Fig. 2, the model first received the real-time Chl *a* and discharge data from the USGS station; then calculated DOC using Eq. (1); and finally estimated DOC load using Eq. (2).

After the basic STELLA structure was developed, the second step was to assign the initial values for stocks, equations for flows, and input values for converters. The STELLA modeling code showing the equations and input parameter values is given in Fig. 4. This code was automatically generated with STELLA once its structure was established. It should also be noted that the STELLA software has an "Interface" module that can display simulation outputs instantaneously.

2.3 DDDAS Framework

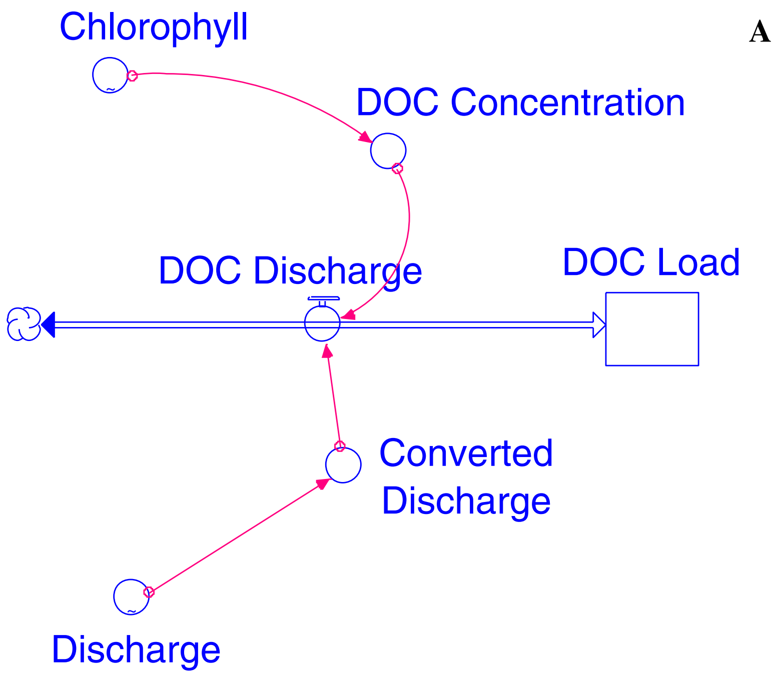
A batch file "RealTime.bat" was created by linking the following two executable files together: "USGS.exe" and "STELLA-DOC.exe". The "USGS.exe" was written with Microsoft VB.NET for instantly downloading the real-time data every 15 min from the USGS website. This dataset was saved in a Microsoft Excel file. The "STELLA-DOC.exe" was composed with the STELLA package for modeling DOC load and displaying the real-time predictions on a computer screen. The "STELLA-DOC.exe" file reads the Excel file to obtain the real-time inputs of Chl *a* and river discharge. A Microsoft Windows Scheduled Tasks wizard "RealTimeRun" in Windows XP was set up to include the "RealTime.bat" file and directed this batch file when to begin and end running of the "USGS.exe" and "STELLA-DOC.exe " files as well as the running time intervals.

In other words, the DDDAS developed in this study consisted of the following four files; (1) "USGS.exe", (2) "STELLA-DOC.exe", (3) "RealTime.bat", and (4) "RealTimeRun". To implement the DDDAS, users just need to click on the "RealTimeRun".

3 DDDAS Application

3.1 DDDAS Validation

Prior to using the DDDAS for estimating the real-time load of DOC in a river, its applicability must be validated. The validation is a process of comparing the DDDAS predictions with the field observations within a given time period. In this study, an attempt was made to validate the DDDAS predictions using an independent set of field observations collected from 2004 to 2009. Since no river discharge data were collected from the regular monitoring station, only the DOC data from the regular monitoring station



B

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DOC_Load(t) = DOC_Load(t - dt) + (DOC_Discharge) * dt
INIT DOC_Load = 0
INFLOWS:
   DOC_Discharge = Converted__Discharge*DOC_Concentration*0.000001
Converted__Discharge = Discharge*101940
DOC_Concentration = -4.026*LOGN(Cholrophyll)+27.735
Cholrophyll = GRAPH(TIME)
(0.00, 18.7), (0.25, 18.3), (0.5, 18.9), (0.75, 18.4), (1.00, 18.5), (1.25, 18.5), (1.50, 18.5), (1.75, 18.7), (2.00, 18.7), (2.25, 18.1), (2.50, 18.6),
(2.75, 17.9), (3.00, 18.4), (3.25, 17.9), (3.50, 18.4), (3.75, 18.8), (4.00, 17.9), (4.25, 18.8), (4.50, 18.3), (4.75, 17.8), (5.00, 17.9), (5.25,
17.5), (5.50, 18.7), (5.75, 18.0), (6.00, 17.9), (6.25, 17.5), (6.50, 18.6), (6.75, 19.0), (7.00, 17.8), (7.25, 18.2), (7.50, 18.1), (7.75, 18.1),
(8.00, 18.2), (8.25, 18.7), (8.50, 18.2), (8.75, 18.5), (9.00, 18.1), (9.25, 18.0), (9.50, 18.3), (9.75, 18.0), (10.0, 18.2), (10.3, 17.7), (10.5,
17.9), (10.8, 18.5), (11.0, 18.0), (11.3, 17.0), (11.5, 17.8), (11.8, 18.2), (12.0, 18.9), (12.3, 18.2), (12.5, 18.4), (12.8, 18.2), (13.0, 17.6)...
Discharge = GRAPH(TIME)
(0.00, 4290), (0.249, 5380), (0.497, 6740), (0.746, 8380), (0.994, 9460), (1.24, 11400), (1.49, 12600), (1.74, 12700), (1.99, 13000), (2.24,
13200), (2.49, 13200), (2.73, 14200), (2.98, 13400), (3.23, 14800), (3.48, 15700), (3.73, 15000), (3.98, 15800), (4.23, 16900), (4.47,
16300), (4.72, 13100), (4.97, 15100), (5.22, 14300), (5.47, 9950), (5.72, 12300), (5.97, 9990), (6.22, 7980), (6.46, 7600), (6.71, 4730),
(6.96, 3910), (7.21, 4060), (7.46, 2950), (7.71, 1840), (7.96, 1000), (8.20, 301), (8.45, -119), (8.70, -680), (8.95, -2220), (9.20, -2220),
(9.45, -3070), (9.70, -4190), (9.94, -5030), (10.2, -5170), (10.4, -4750), (10.7, -4330), (10.9, -4460), (11.2, -3480), (11.4, -2770), (11.7,
-955), (11.9, -397), (12.2, 853), (12.4, 2650), (12.7, 4020), (12.9, 6350)...
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Fig. 4 STELLA modeling map (**a**) for evaluating DOC load and its code (**b**) showing the equations and graphic input data from the USGS station

were used for validation of the DOC concentration prediction.

Comparison of the field measured and DDDAS predicted DOC contents as a time series plot is shown in Fig. 5. With a linear regression equation of $DOC_{predicted}=0.9427*DOC_{measured}$, $R^2=0.9313$, mean error=−0.86 mg/L, mean square error= 17.26 mg/L, and mean absolute error=3.39 mg/L, we concluded that a good agreement between the field measurements and the DDDAS predictions was obtained.

3.2 DDDAS Application

To obtain a better understanding of the real-time load of DOC in a river, a simulation scenario was performed in this study. This scenario investigated the real-time load of DOC in response to real-time variations of river discharge over a 1-week period. Input values for the real-time river discharge and Chl *a* contents every 15 min were downloaded from the USGS station (#02244040). The prediction began on October 27, 2010 and

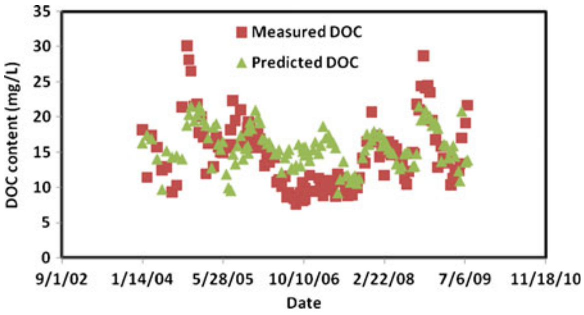

Fig. 5 Comparison of the DDDAS predictions with the field measurements for DOC

ended on November 2, 2010. It should be pointed out that USGS only provides the most current 60-day real-time data for this station with an interval of 15 min. A week of real-time data was selected in this scenario for efficiency and simplicity although it is easy to modify the DDDAS for a 60-day simulation period.

Real-time variation and the accumulation of DOC load in the river as predicted from the DDDAS are shown in Fig. 6. It should be emphasized that although this figure demonstrates the variations of DOC load for the entire simulation period (i.e., 7 days), in reality, the DDDAS was run every 15 min and the variations of DOC load at that particular time were displayed immediately on the computer screen. The users can then estimate the surface DOC status in a timely manner. The simulation ended at 2:09 pm on Monday, November 3, 2010.

Figure 6 shows that the load of DOC varied from positive to negative with a range from −13,143 to 29,248 kg/h DOC. The negative loads implied that the DOC flowed back to upstream, caused by the negative (back) flow of river (Fig. 6). The back flow of the river at the monitoring stations selected in this study was due to the tidal and ocean level influence as the stations were located within an estuarine system. The cumulative load of DOC increased as time elapsed and fluctuated due to the impacts of river discharge (Fig. 6). At the end of the simulation (178 h), the cumulative load of DOC for this station was about 1.2 tons.

4 Summary

In this study, we have developed a DDDAS for forecasting the real-time load of DOC in the St Johns River. The DDDAS was validated using independent field data with very good agreement between the predictions and the measurements.

A forecasting scenario was chosen to demonstrate the real-time load of DOC in an estuarine surface water ecosystem. Results showed that river discharge strongly affects the real-time load of DOC.

Our results revealed that the DDDAS developed in this study was feasible for estimating the real-time variation of DOC in the river. This approach may also be useful in predicting the real-time loads of other water quality parameters in surface water ecosystems.

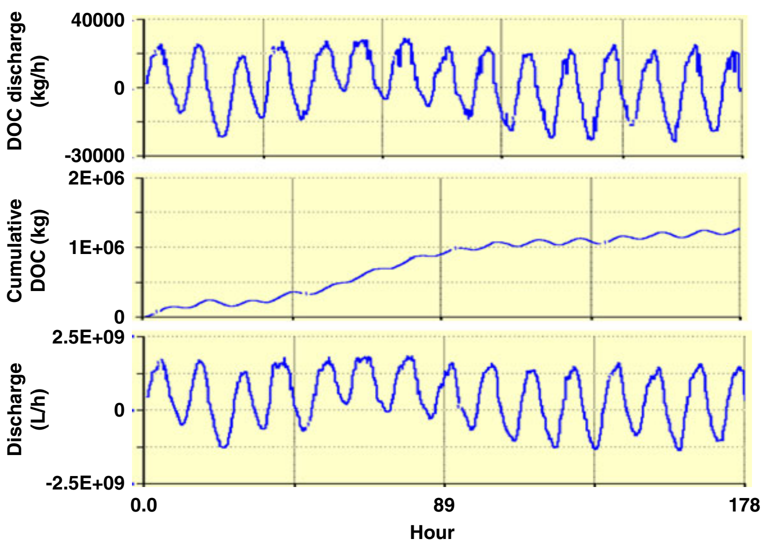

Fig. 6 Real-time and cumulative loads of DOC predicted from the DDDAS and real-time variations of river discharge obtained from the USGS monitoring station from October 27 through November 3, 2010. Note the tidal driver flow reversals in river flow

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