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Object-oriented modeling approach to surface water quality management

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Abstract

The lack of sufficient water quality data in many places hinders the efforts of surface water quality modeling, and therefore affects the process of water quality management. In this paper, the potential of an object-oriented simulation environment for surface water quality management, based on the concepts of system dynamics (OO-SD), is discussed. The characteristics, along with a brief explanation, of the OO-SD approach are provided. A case study on the use of the OO-SD modeling approach for surface water quality management in southeastern Kentucky, USA, is described to highlight key features of the approach. In a later section, advantages and present shortcomings of the OO-SD approach to model hydrologic systems are discussed. The potential use of the proposed approach, especially in data-poor conditions, and the challenges that lie ahead of hydrologists to fully exploit such a modeling approach are identified.

Keywords: Water quality management; Object-oriented modeling; Data-poor conditions; STELLA

1. Introduction

Watershed modeling lies at the center of water resources planning and management. The reliance on hydrologic models is increasing to cope with emerging problems and to exploit new data sources. Studying complex hydrologic problems and synthesizing different kinds of information have been made possible using models. The watershed models are of different types and are intended to serve different purposes. They can be classified according to the processes that they describe to be either lumped or distributed. They can be also deterministic, stochastic, or mixed. Based on time scale, models can be classified into event-based, continuous-time, and large time-scale models. Models may use analytical, numerical, and analog solution techniques. Hydrologists classify models into data-driven models and mechanistic models. Data-driven models, sometimes called black-box models, are usually inferred from the raw or processed data and the formulation may not be conceptually supported by the mechanism of the phenomenon under consideration. There are abundant examples of data-driven models employed to hydrologic systems for different purposes. Regression models (e.g., Hirsch, 1982), linear time series models, nonlinear time series analysis (e.g., Porporato and Ridolfi, 1997), and artificial neural networks (Govindraju and Rao, 2000) have been used for a variety of purposes, such as forecasting, rainfall runoff modeling, estimation of missing hydrologic data, and modeling of water quality parameters in streams.

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Although mechanistic models, sometimes called process-based models, are usually data-intensive and frequently over-parameterized, they have been found to be useful in a wide variety of applications related to surface water quality. The number of available mechanistic models is larger than practical to be listed in this brief study. One of the frequently used models is the HSPF (Donigian et al., 1995), which covers wide areas of applications including point and nonpoint source pollution analyses. QUAL2E (Brown and Barnwell, 1987) is also used for modeling the fate and transport of pollutants in streams. However, models have yet to become common planning or decision-making tools (Adenso-Diaz et al., 2005), especially in the area of water quality management. Towards achieving this goal, Singh (1995) has correctly observed that most mechanistic models need to be packaged at the level of a user who is not necessarily a hydrologist, and should be integrated with, or at least have the capability for integrating with, social (Beck, 2005), economic, and management modules. Furthermore, modelers or users of these models should address the issue of the applicability of the models in data-poor conditions, especially when multitudes of field parameters, which are necessary for mechanistic model calibration, are not measured.

In this paper, an example of a simple object-oriented modeling approach to surface water quality management is presented. The aim of the presented model is to provide a pragmatic modeling approach to surface water quality modeling for management purposes, especially in the case of data-poor conditions.

2. The dilemma of water quality modeling

Both data-driven or empirical and mechanistic approaches have been used in the past for water quality modeling studies (Chapra, 1994). In many situations when availability of water quality data is limited, the empirical approach becomes essential to characterize the pollutant loadings. Many examples of the application of empirical models (e.g., Reckhow and Chapra, 1983; Jian and Yu, 1998) are available in the literature. Although mechanistic modeling environments (Newham et al., 2004) attempt to overcome the limitations associated with other modeling approaches, their data requirements can be overwhelming. A number of physical and process-based parameter values are often required for such modeling and the reliability of the results is questionable in the absence of large data sets. An example of a good modeling approach is one recommended by Chapra (2003), namely "an adaptive approach starting with simpler models at the initial phases and then progressing to more complex frameworks as additional data are collected". Simonovic (1992) suggested that systems analysis has its own place in the field of water resources management and that simulation is an essential tool for developing a quantitative basis for water management decisions. There is, however, a strong need to explore simulation tools that can represent the complex systems in a realistic way and that enable water resources managers and operators to be involved in model development and thereby to increase their confidence in the modeling process.

A modeling approach with at least seven specific characteristics is needed. These characteristics are: (i) the watersheds, or any hydrologic system, are to be described and simulated in a simple fashion; (ii) the model should start simple, relying on the available data (similar to data-driven models), yet also be expandable in order to benefit from more data as these become available; (iii) the model should be adequately dynamic to cope with the nature of hydrologic systems; (iv) the model should have the ability to simulate both linear and nonlinear processes; (v) the model needs to provide a way to represent the feedback mechanism in order to handle counter-intuitive processes; (vi) the model should have the ability to model human intervention and any shocks that might be encountered in the system; and (vii) the model should have the ability to test different policy or management scenarios for better decision-making. Although embodying all these characteristics in one modeling approach might appear difficult, the emergence of system dynamics modeling within an object-oriented simulation environment has made this approach possible. In this paper, an object-oriented simulation environment that adopts the system dynamics modeling approach (OO-SD) is utilized. A case study is provided to explore some of the capabilities of the technique in surface water quality management. Finally, the potential opportunities and challenges of the OO-SD technique's use in hydrologic modeling are discussed.

3. Object-oriented modeling based on the system dynamics approach (OO-SD)

Object-oriented (OO) modeling is a way of thinking about problems using models organized around real-world concepts (Rumbaugh et al., 1991). It is a way to organize software as a collection of discrete objects that incorporate both data structure and system behavior (Simonovic et al., 1997). Data are organized into discrete, recognizable entities called objects. These objects could be concrete (such as a river reach) or conceptual (such as a policy decision). Numerous tools can be used for the implementation of an object-oriented modeling approach, and the STELLA (HPS Inc, 2001) is used for the work presented in this paper. STELLA employs the object-oriented simulation environment as an appropriate approach for the implementation of systems thinking (system dynamics (SD)).

Stocks and *flows* are the building blocks (objects) of the OO-SD model. A simple illustration of stocks and flows is the accumulation of interest in a bank account (Ford, 1999) or inflow of water into a reservoir. Fig. 1 shows a simple model to keep track of the inflow in a reservoir. The double line represents the flow of water from a source, represented by a cloud, into the reservoir (stock). The cloud can be viewed as a stock that is outside the system boundary. The single lines in Fig. 1 connect the rainfall and runoff coefficients to the inflow. These are called *connectors*, which show the flow of information inside the model. *Converters* (such as rainfall and runoff coefficients) can represent any process as a function of time or any input value or parameter.

The OO-SD simulation approach relies on understanding complex interrelationships existing between different elements within a system. This is achieved by developing a model that can simulate and quantify the behavior of the system. Simulation of the model over time is considered essential to understanding the dynamics of the system. Understanding of the system and its boundaries, identifying the key variables, representation of the physical processes or variables through mathematical relationships, mapping the structure of the model, and simulating the model for understanding its behavior are some of the major steps that are carried out in the development of an SD model. It is interesting to note that the central building blocks (objects) of the principles of the SD approach, named hereafter as the OO-SD approach, are well suited for modeling any physical system (Ford, 1999).

The governing equations in an OO-SD model are represented by finite difference expressions used for modeling different elements in a system, and are solved using standard numerical schemes. For example, in the case of a stock, a continuity equation for mass balance is developed considering the inflows and the outflows, whereas a converter carries a functional relationship between different variables that can be represented in a mathematical or a graphical form.

4. OO-SD in water resources

Although the OO-SD approach has found a wide variety of applications in the fields of social studies, economics, industrial engineering, and urban planning to the point that a portion of a scientific journal (*System Dynamics Review*) is dedicated to publishing its applications in different fields, the area of water resources has not benefited enough from this modeling approach. A few published articles on the use of OO-SD in water resources or hydrologic modeling can be found.

Matthias and Frederick (1994) have used the OO-SD approach to model sea-level rise in a coastal area. Fletcher (1998) has used it as a decision support tool for the management of scarce water resources. Simonovic and Fahmy (1999); Simonovic et al. (1997); and Palmer et al. (1993) have used the OO-SD approach for long-term water resources planning and policy analysis for the Nile River basin in Egypt. A conceptualization of hydrological models using this approach has been briefly outlined by Lee (1993), who indicated that the OO-SD modeling approach is a candidate as an excellent tool for teaching hydrological modeling. A real application of what Lee has indicated in 1993 has been materialized by Li and Simonovic (2002), who adopted OO-SD for predicting floods in prairie watersheds (Red River). Cassell et al. (1998) have modeled phosphorous dynamics to understand how complex watersheds process phosphorous, and to develop management perspectives to achieve goals of environmental quality as well as resource sustainability. Other useful applications of OO-SD to ecological systems (Jamu and Piedrahita, 2002; Moffatt and Hanley, 2001; Voinov et al., 2004) can be found.

In this paper, a simple OO-SD-based model for surface water quality management in Kentucky is proposed to exemplify the utility of the OO-SD approach to surface water quality modeling. The case study addresses, in a simple and pragmatic way, the commonly complicated issue of fate and transport of pathogens in streams. The application presented in this paper benefits largely from the OO approach. However, it does not fully utilize all the characteristics of system dynamics; limited

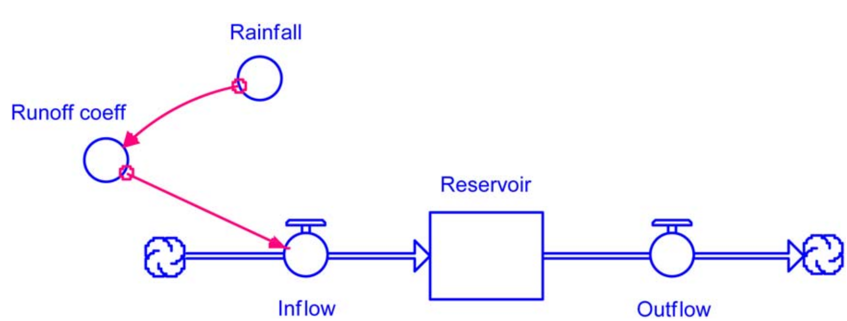


Fig. 1. Basic components (object structure) of a system dynamics model.

feedback loops and counter-intuitive behaviors are involved in the case study presented in this paper.

5. Development of a pathogen transport model in southeastern Kentucky

A significant number of streams in southeastern Kentucky, USA, do not meet their designated uses due to pathogens, nutrients, and pH impairment. The impairment due to fecal coliform contamination is most likely caused by ineffective wastewater systems such as bypass from wastewater treatment plants, improperly operated privately owned package plants, straight pipes discharging raw sewage directly into a receiving stream, failing septic systems, illegal dumps, and mining operations (Kentucky Water Resources Research Institute (KWRRI), 2000). In this region alone it has been estimated that there are over 32,000 straight pipes and failing septic systems that discharge raw sewage directly into the streams.

An area of seven watersheds (sub-basins) in southeastern Kentucky is used as a case study region for this paper (Fig. 2). All the watersheds lie within the North Fork of the Kentucky River basin, which has an eight-digit identification number of 05100201. The identification number corresponds to a hydrologic unit code (HUC) designated by the US Geological Survey (USGS) as part of their national watershed classification scheme. These 8-digit HUCs are broken down further to smaller 11-digit HUCs, adding three more digits for identification purposes. The water flows from six headwater sub-basins (11-digit HUCs), namely 05100201-010, -020, -040, -050, -060, and -070, toward sub-basin 030. The land-use is predominantly deciduous forest type in all the sub-basins. The land-use percentages for deciduous forest type for sub-basins (HUC-11) 05100201-010, -020, -030, -040, -050, -060, and -070 are 98.08%, 97.76%, 96.15%, 99.29%, 98.79%, 99.21% and 96.21% respectively. The sub-basin areas and lengths of main channels are (337 km^2, 16 km), (144 km^2, 12 km), (162 km^2, 14.4 km), (167 km^2, 12 km), (128 km^2, 6.4 km), (68 km^2, 3.2 km), and (220 km^2, 16 km), respectively.

Continuous records of streamflow data are available only in sub-basins 010 and 030. Streamflows at the remaining basins are estimated in proportion to respective contributing drainage areas. Similarly, monthly samples are collected and analyzed for fecal coliform concentrations only in watersheds 010 and 030, as part of the Personal Responsibility In Desirable Environment (PRIDE) project. The fecal coliform concentrations in this area were found to range from 10 to 78,000 count/100 ml.

The OO-SD modeling approach is used in this study to combine both process-based and data-driven techniques to handle the issue of pathogen transport and fate in the study area. No hydrodynamic conceptual model is used to route the streamflows but rather the fecal loads at the 11-digit HUC sub-basins are linked to the streamflows. A significant correlation found between the fecal coliform load and the streamflows (Eq. (1)) in a recent study (Elshorbagy et al., 2004) supports such an idea. The fecal contamination is attributed to straight pipe(s) and failing septic systems (SF) in the area. Therefore, the regression equation linking flows to fecal load at HUC-11, 05100201-010, can be normalized using

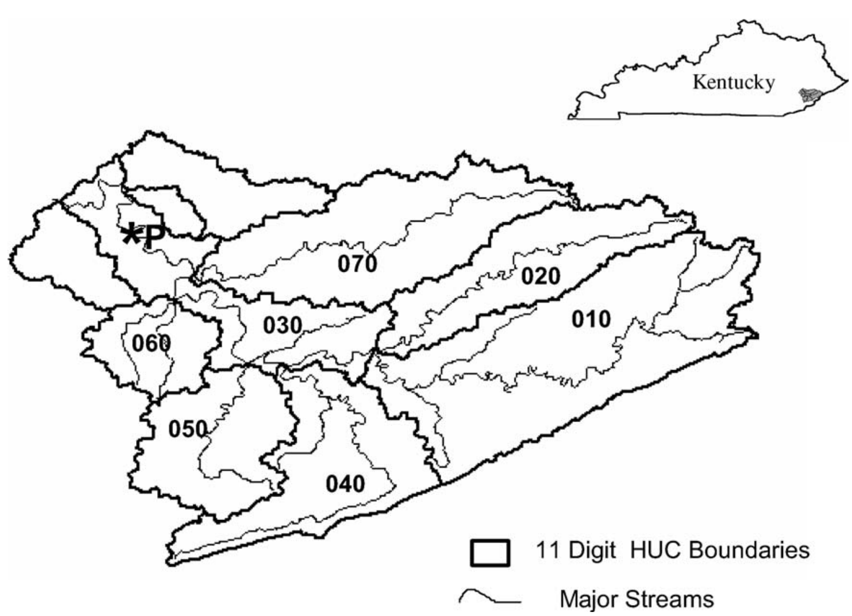


Fig. 2. Map of the case study region in the North Fork basin of Eastern Kentucky.

the total number of SF. This regression equation is found to be as follows:

$$L = 3060443.8 \times Q^{1.44} \quad (1)$$

where L is the fecal load (count/day) per one SF and Q is the streamflow (ft^3/s). The fecal coliform load is estimated by multiplying the concentration (count/100 ml) by the streamflow (Q). The regression coefficient of determination (R^2) is found to be equal to 0.75 (Elshorbagy et al., 2004). Available pathogen data collected through the PRIDE sampling effort suggest a similar form of load–flow relationship provided by Eq. (1) in two watersheds. Also, the SF density (SF per area of the watershed) is approximately equal for all the watersheds. The reason for using the load instead of the concentration in Eq. (1) is to allow for apportioning the total load on the SF by dividing the load by the number of SF, which can be used in the model as a policy variable. The functional form of the flow–fecal coliform load relation is assumed in this study to be similar in all the headwater HUC-11 sub-basins. The high number and the density of SF in the area may justify why the fate and transport of the pathogen loading behave in a way similar to a nonpoint source pollution. There is a possibility of having a slightly different power (different from 1.438 in Eq. (1)) in the regression equation for each 11-digit HUC. In this way, both the power of the regression and the number of SF can be treated as decision variables (i.e., changed for the purpose of generating future scenarios) in the proposed model. However, the power of the regression equation is kept unchanged in this study since Eq. (1) is derived based on load per one SF, and there is not sufficient evidence to support such a change of the power of the regression equation.

Fecal coliform load is modeled as a substance that declines (decays) as a first-order process (Thomann and Mueller, 1987):

$$L_t = L_0 \times e^{-kt} \quad (2)$$

where L_t and L_0 are the fecal coliform load at downstream and upstream points (count/day), respectively, k is the decay rate (per day), and t is the travel time (days) that is estimated from the traveling distance and velocity of streamflow. Mean velocity is considered so that travel time is kept constant. Factors such as sunlight, water temperature, and salinity are not explicitly considered in the model. The effect of all these factors are implicitly considered and are lumped into one decay factor, k. However, inclusion of individual factors or relationships linking these factors to pathogen survival rate in the modeling approach is straightforward if data are available. Because streamflow is an exogenous variable and not hydraulically simulated in our model, it remains constant within each sub-basin. In this case, the decay factor k, which is intuitively linked to the concentration (Thomann and Mueller, 1987), can be linked to the streamflow. Streamflow (Q) is the same on both sides of Eq. (2), and therefore eliminated. The OO-SD model built for the study area is shown in Fig. 3a, where *Flow* objects represent the fecal loading rate and *Converters* represent the flow-fecal load functional relationships. Stocks handle the pollutant decay, where only surviving pathogens become outflow from the *Stock* object. Measured fecal coliform concentrations at HUC-11 05100201-030 are used to validate the proposed model. Fig. 3a shows the sub-model of one HUC-11 sub-basin. Six similar sub-models are built and cascaded to form the entire model (Fig. 3b). Years 1999 and 2000 are used for model calibration and validation, respectively (Fig. 4). Only 9 months of data are available for the validation year. The calibration process is carried out using mean squared error as a criterion for model performance. The decay rate, k, of 0.5 (per day) was obtained from the model calibration process. To overcome the problem of lack of data (only monthly fecal coliform concentration samples are available at a few locations), the functional relationship between fecal coliform loads and streamflow is used to generate daily loads based on daily flows. In this way, empirical, or data-driven, model capabilities are embedded in the OO-SD model along with mechanistic relationships, such as the decay of pathogens.

The model is run, simulating the daily fate and transport of the fecal coliform loadings through the different sub-basins from the headwaters down to the downstream point (P). The object structure shown in Fig. 3 represents only one sub-basin. The units 010, 020, 040, 050, 060, and 070 are parallel units that discharge to the downstream unit 030. After propagating the total daily pathogen loads (decay considered), along with the daily cumulative flows, the daily loads at point P and other outlets of the sub-basins are calculated by the model. Based on limited available observations on streamflow velocities in the region, an average value of 1.0 day was considered as a travel time between each sub-basin and the downstream point P. This allows for modeling the fate and the transport of the fecal coliform between the upstream sub-basins and the downstream point P. Total load at P is equivalent to the sum of loads coming from all upstream sub-basins. Accordingly, daily fecal coliform concentrations are computed, at each sub-basin outlet as well as at P, by dividing the daily pathogen load by the streamflow at each outlet. The number of days with concentrations higher than the pre-specified standards is counted in the model and marked as impaired days. This is achieved through a virtual time stock created in the model to accumulate the number of days when the impairment conditions exist. Such a stock cannot be considered as a component of the model structure but rather a calculation unit. The results are summarized in the first row of Table 1 as the

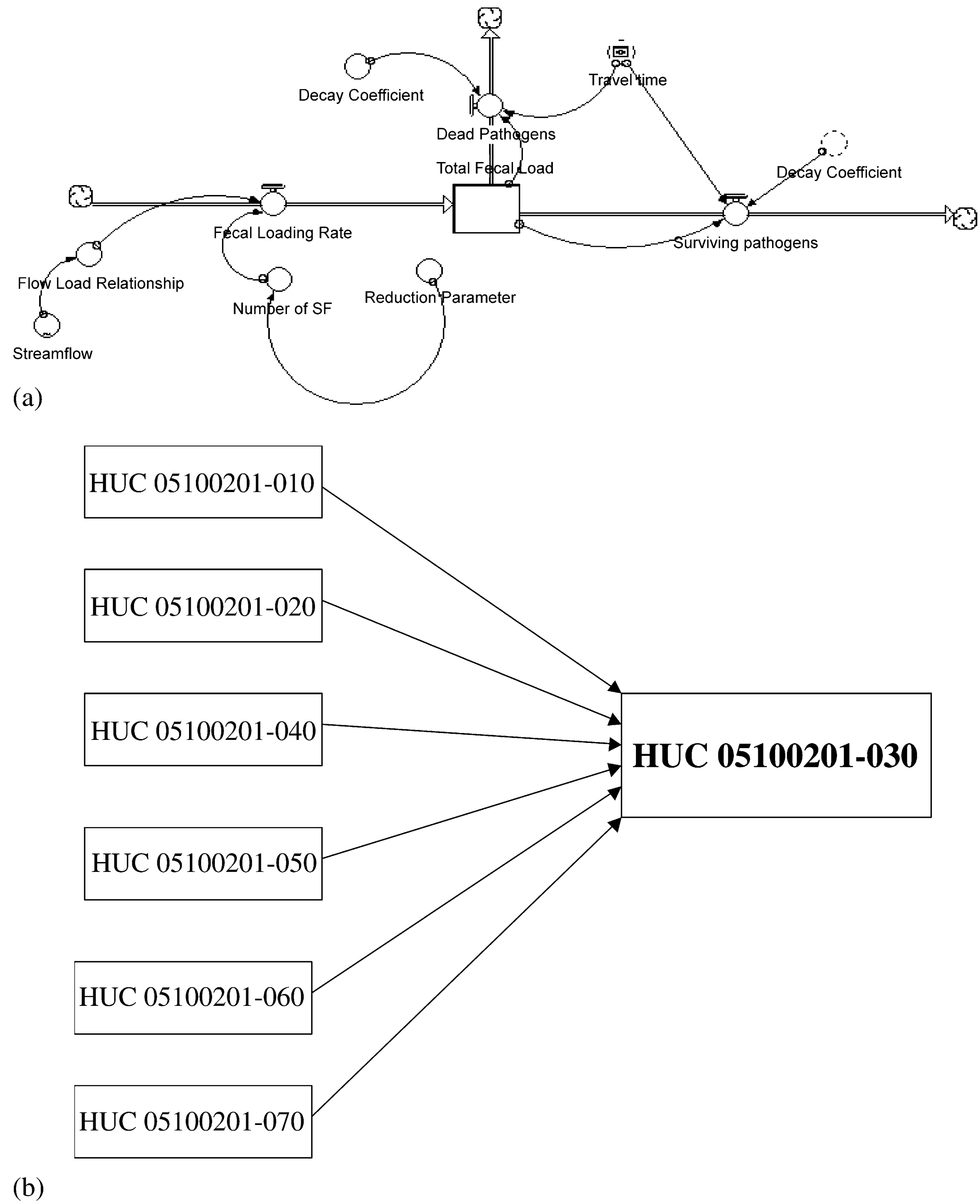
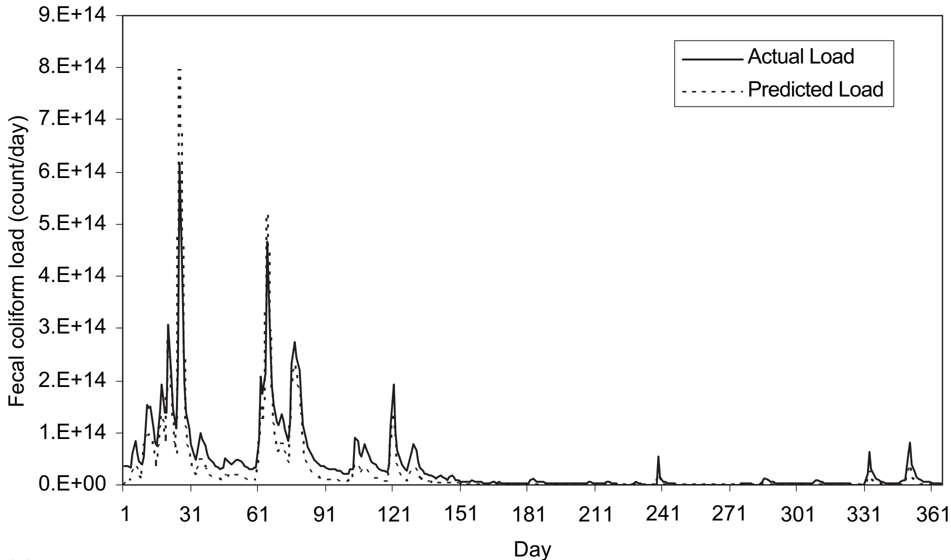


Fig. 3. Structure of the object-oriented model. (a) Model of one sub-basin (e.g., 05100201-020), (b) schematic of the entire watershed representing the study area.

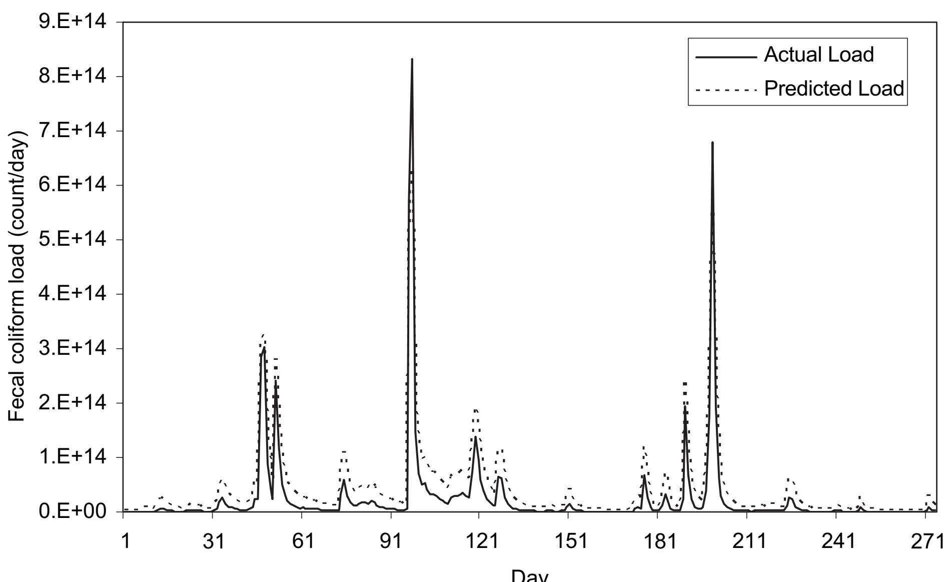
base scenario B, which is based on the data for year 1999. Finally, average annual loads at each point (outlet) are also computed based on the daily loads.

6. Scenario generation, results, and analysis

Four scenarios were designed in order to help assess the effects of streamflows and the number of straight pipes and failing septic systems (SF) on a downstream point under consideration (point P, Fig. 2). Streamflow and the number of SF are the variables, which are handled as potential candidates to shape future scenarios in the process of scenario generation. The scenarios are as follows: (1) a year of low flows with 30% decrease in the number of SF; (2) the same year of low flows used in scenario 1 but with 30% increase in the number of SF; (3)



(a)



(b)

Fig. 4. Model performance in (a) calibration and (b) validation.

a year of high flows with 30% decrease in the number of SF; and (4) the same year of high flows used in scenario 3 with 30% increase in the number of SF. These scenarios are by no means exhaustive but they help address the effects of both natural conditions (wet and dry years) and human intervention (changing the number of SF in the basins) on the fecal coliform concentrations in the streams.

The scenarios are evaluated using two criteria: the average annual fecal coliform load and the number of days within which the stream will be impaired. As explained in the previous section, the model is set up to output those two criteria as the outputs of the run. Due to the large variation of fecal coliform concentrations throughout the year, the average annual load of the pollutant might not be representative of the stream health. The average annual load could be high but concentrated in less number of days, which suggests that the stream is not impaired most of the year, and

Table 1
Average annual fecal load and number of impaired days

Scenario	Average annual flows (ft^3/s)	Average annual fecal load (count/day)	Number of impaired days
(B)	974.7	2.24×10^{14}	230
(1)	503.4	2.25×10^{13}	269
(2)	503.4	4.17×10^{13}	325
(3)	974.7	1.57×10^{14}	214
(4)	974.7	2.91×10^{14}	250

vice versa. Therefore, assuming a water quality standard of 400 count/100 ml, the number of impaired days and the average annual load are estimated in each scenario.

The distribution of the fecal coliform concentrations at point P is shown in Fig. 5. It should be noted that the two criteria used in this paper for scenario evaluation may lead to different conclusions. Although the average annual load in scenarios 3 and 4 is higher than that of scenarios 1 and 2 (Table 1), respectively, the number of impaired days is fewer. This is probably due to the fact that high flows cause more dilution and, therefore, lower concentrations.

The proposed modeling approach can help in the process of allocating funds to different sub-basins based on relative contribution of each sub-basin to the downstream pollution problem, which is one of the major objectives of the on-going PRIDE project (Kentucky Water Resources Research Institute (KWRRI), 2000). The output of the model proposed in this study, based on the data of the verification year (2000), is shown in Fig. 6. One can observe that the 11-digit HUC 05100201-070 has the maximum pollution share and thus would be a candidate for the highest attention and allocation of resources. In addition to its utility in general analysis, the proposed OO-SD model can also be used to set or evaluate different management strategies (scenarios).

7. Discussion

The OO-SD modeling approach is easily implemented within the STELLA simulation environment, which actually packages the modeling capabilities of traditional models with decision-analysis tools. Fig. 7 presents a portion of the interface of the model developed in this study. Sliders make it easy for analysts or decision-makers to change the values of decision variables and see the effects on the model outputs

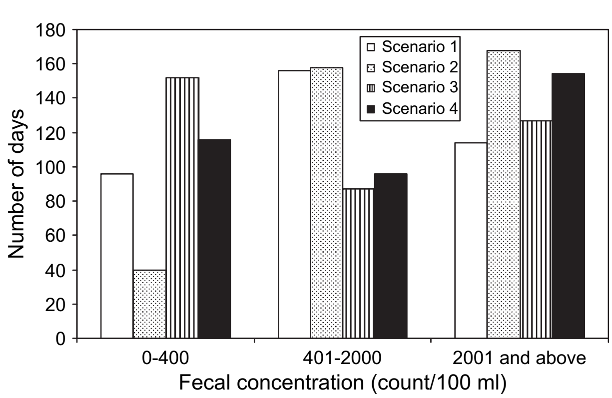


Fig. 5. Number of impaired days under different management scenarios.

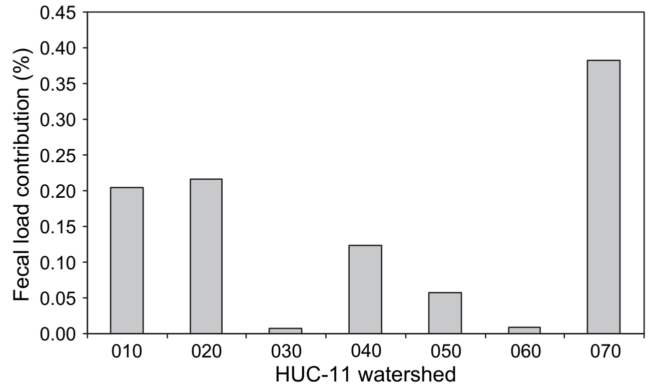


Fig. 6. Pollution share of individual HUC-11 sub-basins.

promptly in forms of graphs, tables, and final values. Furthermore, it is possible to combine the advantages of both empirical and mechanistic models in one approach as is shown in the case study presented in this paper. A regression model is incorporated with the conceptual exponential decay model of pathogens to help model the process at hand, overcoming problems of data gaps. Yet the OO-SD modeling approach maintains the flexibility of changing the parameters of the model and any decision variable in order to generate future scenarios.

OO-SD models are easily expandable. The way in which the OO-SD model is constructed facilitates the task of starting with a simple model that can utilize available data (quantitative and qualitative). When additional data (e.g., water salinity) become available, the model can be expanded by adding additional building objects and/or connections. Similarly, the whole structure of the model can be modified to represent a different or an updated understanding of the system. This feature could be highly valuable in watershed management, where incoming new data is a continuous process over time.

The OO-SD technique does, however, contain some current shortcomings. These shortcomings should be viewed as future challenges whose solutions may require collaboration between researchers from the system dynamics community and hydrologic modelers. Although, as the name indicates, OO-SD is efficient in handling the dynamic behavior of a system, it is not perceived to be representative of spatial variability within the system. There could be a way to overcome such a negative aspect by creating an object (e.g., a converter) to establish a relationship between the state variable and space (e.g., concentration of water quality parameter vs. distance). A more efficient way could be through developing a link between SD and GIS (Ford, 1999).

OO-SD is intended to be a simulation technique. Therefore, it does not contain capabilities of optimization. To maximize the utilities of OO-SD in hydrologic modeling, optimization capabilities can be either built

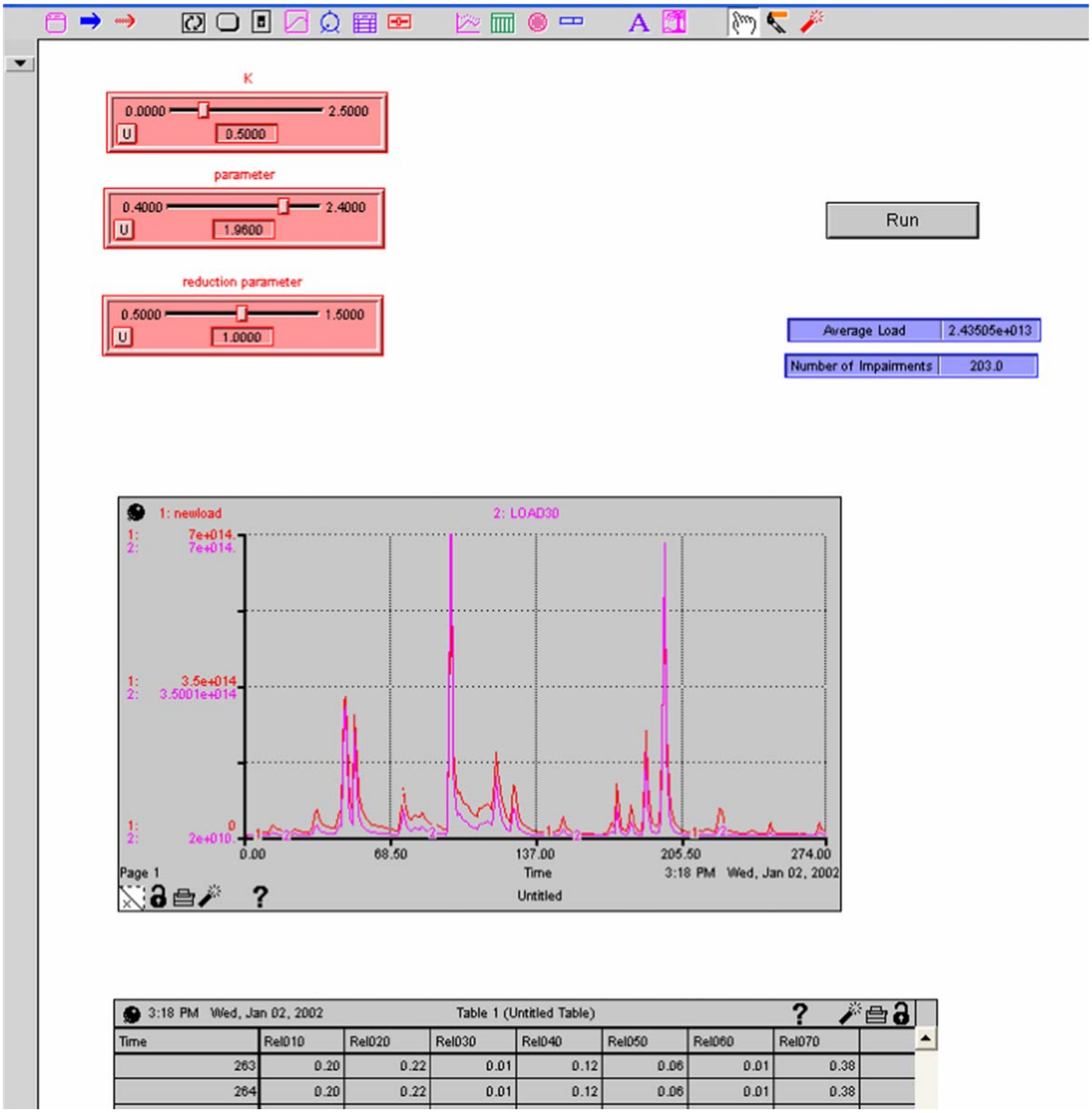


Fig. 7. Interface of the watershed management model developed within STELLA.

in a Software such as STELLA or achieved through coupling STELLA and a spreadsheet (e.g., Excel). This may improve the performance of an OO-SD model in applications such as reservoir operation, and also in the calibration of the OO-SD model itself.

8. Conclusions

Object-oriented simulation, based on the concepts of system dynamics (OO-SD) is not presented in this paper as a replacement for traditional hydrologic models but rather as a feasible alternative in data-poor conditions, and as a potential candidate when involvement of decision-makers is crucial for the modeling exercise. There have been a few endeavors in water resource literature on the use of OO-SD but its full capabilities have not yet been fully utilized for hydrologic modeling. In this paper, the utility of this modeling approach for surface water quality management has been exemplified through its application to watersheds in southeastern Kentucky. Different sub-basins have been prioritized based on their relative contribution of pollutant loads to a downstream point of interest. Sub-basin -070 have been identified as the major pollutant contribution to the downstream point of interest. The impacts of various management scenarios on the number of impaired days have been assessed. Although the proposed modeling approach can be successful in packaging a variety of features needed for hydrologic modeling, there are current shortcomings, such as spatial analysis and optimization, which form future challenges for hydrologists to work on.

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