Mathematical Simulation Tools for Developing Dissolved Oxygen TMDLs

G. Vellidis, P. Barnes, D. D. Bosch, A. M. Cathey

Abstract. *In many regions of the U.S., low dissolved oxygen (DO) is a common freshwater impairment. States, territories, and tribes of the U.S. are required by federal law to develop Total Maximum Daily Loads (TMDLs) for waters not meeting established DO standards. Regulators and other professionals are increasingly relying on mathematical simulation models to develop these TMDLs. Because of the wide variety of potential applications and the number of models in existence, consistent and comprehensive model evaluations are needed to ensure that TMDL developers are able to select appropriate models for their application. The goal of this article is to provide a guide to mathematical simulation models available for developing DO TMDLs. For this work, a model is defined as easily available software that can be used to simulate DO dynamics in lotic systems. Four commonly used DO simulation models (QUAL2E, HSPF, EFDC, and WASP) are described in detail, while the characteristics of several others are summarized in tabular form. A case study is used to illustrate the process of developing a DO TMDL. DO models continue to become more sophisticated and thus better able to simulate the natural environment. Despite advancements, many DO models are still not capable of simulating some of the most complex drivers of DO dynamics, partly because the scientific community does not yet fully understand these processes, and continue to require user-estimated inputs for these processes. Because these processes are complex and difficult to quantify, model users are forced to rely on the few published data, which may or may not be applicable to their conditions. To overcome these limitations, future research must focus on understanding these processes and creating comprehensive and easily accessible databases of DO parameters.*

Keywords. *Case study, Dissolved oxygen, EFDC, HSPF, QUAL2E, Simulation models, TMDLs, WASP, Watersheds.*

States, territories, and tribes of the U.S. determine the designated use for each waterbody under their jurisdiction. Designated uses can be drinking water supply, contact recreation (swimming), aquatic life support (fishing), etc. States, territories, and tribes (hereafter referred to as states) are also responsible for establishing water quality standards for these designated uses. All states are required to regularly assess water bodies within their jurisdictions and develop Total Maximum Daily Loads (TMDLs) for waters not meeting established water quality standards in accordance with Section 303(d) of the Clean Water Act and the U.S. Environmental Protection Agency (EPA) Water Quality Planning and Management Regulations (40 CFR Part 130).

A TMDL is a calculation of the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards and an allocation of that amount to the pollutant's sources. Alternatively, a TMDL is the sum of the allowable loads of a single pollutant from all contributing point and nonpoint sources. The calculation must include a margin of safety to ensure that the waterbody can be used for the purposes the state has designated. The calculation must also account for seasonal variation in water quality (EPA, 2005a).

The amount of dissolved oxygen (DO) in water is one of the most commonly used indicators of lake, river, and stream health. Throughout the rest of this article, the terms rivers and streams will be used interchangeably to represent flowing freshwater. In most streams, aquatic fauna become stressed as DO drops below 4 or 5 mg L^{-1}. Under extended hypoxic (low DO) or anoxic (no DO) conditions, most higher forms of life are driven off or die. Noxious conditions, including floating sludges, bubbling, odorous gases, and slimy fungal growths, may prevail (Masters, 1998). Consequently, most state water quality standards require a daily DO concentration average of 5 mg L^{-1} and no less than 4 mg L^{-1} at all times for waters supporting warm water species of fish. Higher standards may exist for unique fisheries. For example, in Georgia, waters designated as trout streams must maintain a daily average of 6 mg L^{-1} and no less than 5 mg L^{-1} at all times. These standards have been adopted by states to ensure that adequate concentrations of DO are available to sustain desirable aquatic fauna.

Causes of Low DO

In many regions of the U.S., low DO is a common freshwater impairment. Clearly, low DO is not a pollutant.

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The authors are **George Vellidis, ASABE Member Engineer,** Professor, Department of Biological and Agricultural Engineering, University of Georgia, Tifton, Georgia; **Phil Barnes, ASABE Member Engineer,** Professor, Department of Biological and Agricultural Engineering, Kansas State University, Manhattan, Kansas; **David D. Bosch, ASABE Member Engineer,** Hydraulic Engineer, USDA-ARS Southeast Watershed Research Laboratory, Tifton, Georgia; and **Anna M. Cathey,** Engineer, Buck Engineering, Atlanta, Georgia. **Corresponding author:** George Vellidis, Department of Biological and Agricultural Engineering, University of Georgia, Tifton, GA 31793-0748; phone: 229-386-3377; fax: 229-386-3958; e-mail: yiorgos@uga.edu.

However, it is commonly presumed that DO concentrations below the standard are associated with increased biological activity resulting from N (nitrogen) and P (phosphorus) enrichment. This increased biological activity is generally excessive algal growth. When excessive algal blooms decay, DO is depleted due to the biochemical oxygen demand (BOD) of the decomposition process. BOD exerts an oxygen demand in the water column and contributes to biotic and abiotic oxygen demand in the sediments (Lee, 2003). As the organic matter decays, aerobic bacteria deplete the available oxygen within the lower water column at a faster rate than oxygen diffusion from surface waters (Rabalais, 2002). Therefore, hypoxic conditions will remain if oxygen consumption rates are greater than oxygen resupply.

Within the past 20 years, it has generally been recognized that established DO standards may not be universally applicable and that in certain ecosystems, natural conditions alone create DO concentrations below these standards (Ice and Sugden, 2003; Vellidis et al., 2003, Carey et al., 2005, 2006). As a result, in 1986, EPA proposed an alternative standard for these types of waters. The alternative standard states:

"Where natural conditions alone create dissolved oxygen concentrations less than 110% of the applicable criteria means or minima or both, the minimum acceptable concentration is 90% of the natural concentration" (EPA, 1986).

Although several states have included this alternative standard in their regulations, it is notoriously difficult to apply because little research has been done to determine natural levels of DO and research results that are available are ecosystem specific. Nevertheless, states have developed several acceptable methods for determining whether a stream is naturally low in DO. According to the Georgia Environmental Protection Division (Georgia EPD) guidelines, for example, natural conditions can be determined by examining historic data, comparisons to reference watersheds, application of mathematical models, or any other procedure deemed appropriate by the Georgia EPD Director (Georgia EPD, 1999).

Nationwide, there are many contemporary water quality data sets. However, a historical data set that could be used to interpret the natural levels of DO is generally not available. Such data would have to predate large-scale agriculture and urbanization as well as reflect the changes that a river or stream underwent as it experienced anthropogenic point and nonpoint impacts. Natural conditions can also be determined through comparisons with reference watersheds. Reference watersheds are watersheds that can be considered relatively free of anthropogenic impacts. A National Wildlife Refuge may be considered a reference watershed. Mathematical simulation models may also be used to understand the naturally occurring levels of DO in streams. The advantages of modeling include the ability to model any time or place and the ability to partition natural and anthropogenic influences on DO. As a result, regulators and researchers are increasingly relying on mathematical simulation models to develop TMDLs.

Because of the wide variety of potential applications and the number of models in existence, consistent and comprehensive model evaluations are needed to ensure that TMDL developers are able to select appropriate models for their application. New applications create additional concern because no model is designed to meet all the needs of researchers, regulatory agencies, planning organizations, consultants, and environmental groups (Parsons et al., 2001). If models are to be used effectively for TMDL planning and development, model users should be aware of the following: the original purpose of the model, the characteristics and operating principles of the model, the conditions under which the model will perform properly, data and calibration requirements, output produced by the model and, finally, the model's limitations. The goal of this article is to provide regulators, researchers, and other professionals engaged in the TMDL process a guide to mathematical simulation models available for developing DO TMDLs. For this work, a model is defined as easily available software that can be used to simulate DO dynamics in lotic systems.

Dissolved Oxygen Sinks and Sources

DO concentration in freshwater is a function of oxygen sources and sinks. DO is removed through biochemical oxygen demand (BOD), chemical oxygen demand (COD), sediment oxygen demand (SOD), and through respiration by plants and other organisms living in the water. DO is added through reaeration or photosynthesis. Algal photosynthesis and respiration often dominate photosynthesis and respiration in freshwater systems and are often combined and reported as net photosynthesis (Joyce et al., 1985). In addition, DO concentrations in the main stream can be increased or decreased by DO concentrations in water entering through tributaries or subsurface flow. Mathematically, the flux of DO in a stream or river was described by Cox (2003a) as:

$$\frac{dM}{dt} = M_i - M_o + (P - R) + C_R - BOD - COD - SOD - C_D \pm \Delta S \qquad (1)$$

where

t = time
M_i = mass flux of DO entering the waterbody
M_o = mass flux leaving
P = DO added through photosynthesis
R = DO utilized by respiration
C_R = aeration and reaeration (represented by the reaeration coefficient)
BOD = biochemical oxygen demand
COD = chemical oxygen demand
SOD = sediment oxygen demand
C_D = degassing of oxygen due to temperature
ΔS = changes in the waterbody due to transport from external sources.

In the summer, rising temperatures reduce the solubility of oxygen, while lower flows reduce reaeration (Masters, 1998). Although solubility is not a problem in the winter, ice may reduce availability of atmospheric oxygen. A comprehensive in-stream water quality model that simulates DO dynamics should address each of these six processes listed above as well as compensate for the effects of temperature (Bennet and Rathburn, 1972). Because it is important for DO model users to understand these processes, they are briefly described in the next few paragraphs. A much more detailed description of these processes, including the governing differential equations, was presented by Cox (2003a). A more applied description of the governing equations is provided by Cathey (2005) and Cathey et al. (2006). Figure 1 depicts a schematic of the major processes influencing the concentration of DO in lotic systems.

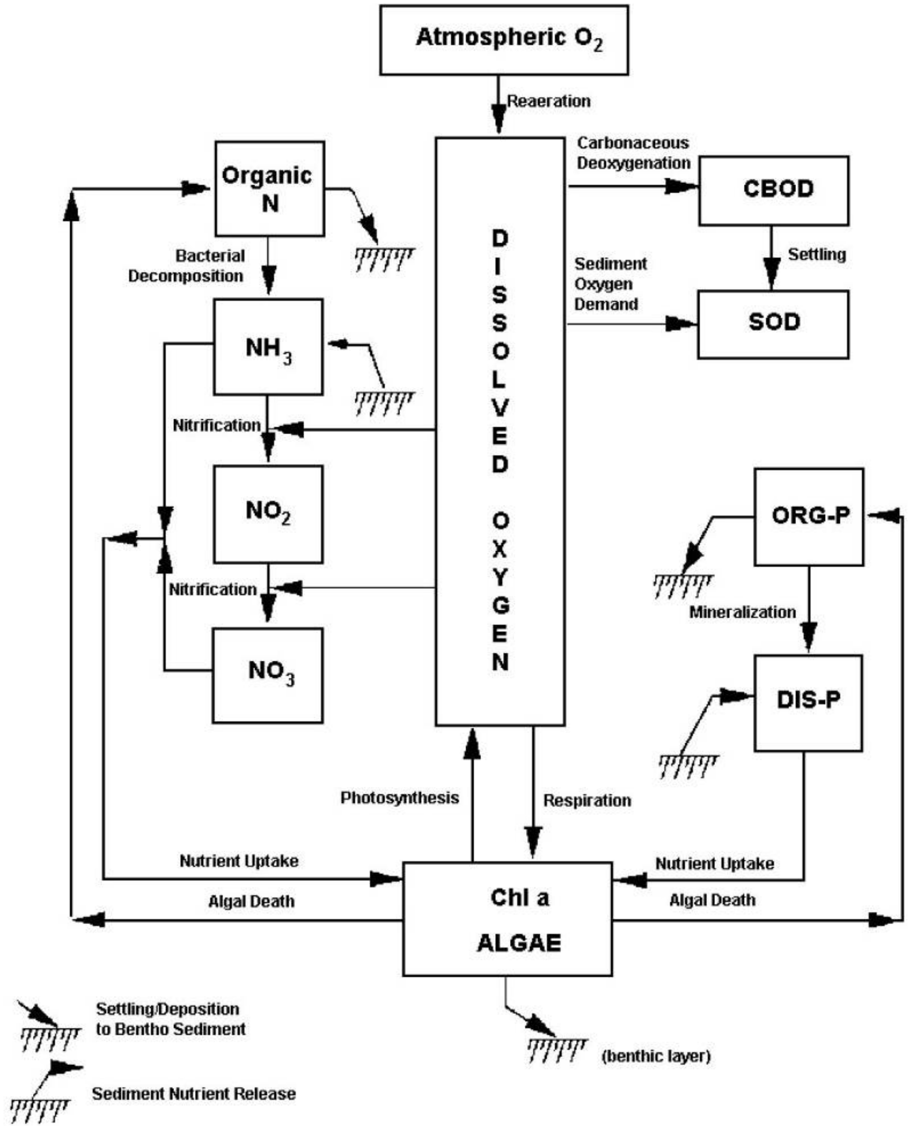

Figure 1. Schematic of the major processes influencing DO in rivers (EPA, 1997).

Biochemical Oxygen Demand (BOD)

When biodegradable organic matter is released into a body of water, microorganisms, especially bacteria, feed on the organic matter, breaking it down into simpler organic and inorganic substances (Masters, 1998). The total amount of oxygen required to oxidize organic matter suspended in the water column is called the biochemical oxygen demand (BOD). BOD is reported in terms of mass of oxygen consumed per unit volume, usually mg L^{-1}. BOD is composed of two more specific oxygen sinks: carbonaceous biochemical oxygen demand (CBOD) and nitrogenous biochemical oxygen demand (NBOD). CBOD is the oxygen demand created by microorganisms that obtain their energy from oxidizing organic carbon. NBOD is the oxygen demand created by microorganisms that obtain their energy from oxidizing nitrogen. The total amount of oxygen required for biodegradation is an important measure of the impact that a waste will have on the receiving body of water (Masters, 1998). The five-day BOD, or BOD_5, is the total amount of oxygen consumed by microorganisms during the first five days of biodegradation and is an indicator of the potential impact of organic matter/wastes added to a waterbody. Because NBOD usually does not become measurable until after day five, BOD_5 is an indicator of ultimate CBOD, which is the amount of oxygen required for complete biodegradation of carbonaceous organic matter added to a waterbody. Ultimate CBOD can be measured experimentally or estimated from BOD_5 using a simple exponential relationship (Cathey et al., 2005). Although its value as an indicator of ultimate BOD (BOD_u) is debated, the BOD_5 test has, nevertheless, become a standard water quality measurement parameter.

BOD may come from natural sources like leaf litterfall or from anthropogenic point or nonpoint sources like wastewater treatment plant discharges or agricultural runoff. Detritus (non-living particulate organic matter), whatever its origin, is an important source of BOD. BOD may also be also influenced by incoming water from tributaries. In streams, biochemical oxygen demanding substances can either be suspended in the water column, settle to the bottom, or be resuspended from the sediment.

Chemical Oxygen Demand (COD)

COD is the amount of oxygen required for the chemical oxidation of organic or inorganic compounds in water and is usually an important sink of DO in rivers that receive industrial effluents such as iron sulfite and aldehyde, which are readily oxidized (Cox, 2003a). In the presence of DO, oxidation takes place rapidly, so the oxygen demand is observed close to the pollutant source and can be quite significant. COD is generally not an important parameter in rivers or streams that do not receive industrial effluents. But because COD measurements are easier to conduct and often more repeatable than BOD measurements, some regulatory agencies allow measurement of COD as a surrogate for BOD provided that a linear relationship between the two can be developed for the stream in question.

Sediment Oxygen Demand (SOD)

Sediment or benthic oxygen demand is the rate at which DO is removed from the overlying water column by biochemical processes in the stream bed sediments (Hatcher, 1986) and is reported as mass of oxygen consumed per unit area and time, usually g m^{-2} d^{-1}. SOD results primarily from the decomposition of organic matter, which is deposited and incorporated into the channel bed (Cox, 2003a). Sources of organic matter may be allochthonous (external) such as leaf litter or autochthonous (internal) such as the settling of already suspended biodegradable organic matter (Bowman and Delfino, 1980; Matlock et al., 2003; Cox 2003a, Crompton et al., 2005). SOD serves as a critical sink of DO and can be defined as two separate processes (Wu, 1990; Seiki et al., 1994). The first process is biological respiration by organisms (primarily decomposers) within the sediment matrix. The second process is the chemical oxidation of reduced matter found within the matrix. Factors affecting SOD include temperature, the oxygen concentration at the interface between the sediment matrix and the water, characteristics of the sediment matrix, the velocity of the water over the sediments, water chemistry, and the biological community (Bowie et al., 1985). A comprehensive review of measured SOD values as well as techniques for experimentally measuring SOD are provided by Crompton (2005) and Crompton et al. (2006). Cathey et al. (2006) describes the parameterization of SOD for a DO model application.

Net Oxygen Production from Photosynthesis

Phytoplankton, periphyton, and attached and unattached aquatic plants all respire and photosynthesize. During respiration, they consume oxygen, while during photosynthesis they produce oxygen. Consequently, primary production can be both a source and a sink of DO in streams. Aquatic plants respire continuously, consuming oxygen. But, during the day, when there is a source of light, they are also able to photosynthesize and produce oxygen. Because phytoplankton biomass can fluctuate much more rapidly than the biomass of macrophytes, phytoplankton can have a large impact on the DO of an aquatic ecosystem and exaggerate the diurnal DO curve observed in most aquatic systems (Guasch et al., 1998). It is therefore common to assume that net oxygen production from photosynthesis is represented by phytoplankton. However, periphyton and macrophyte respiration could be an important DO sink in certain lotic systems. Net oxygen production can be determined experimentally (Odum, 1956; Vollenweider et al., 1969) or mathematically (DiToro, 1975; Thomann and Mueller, 1987). A detailed description of the governing equations is provided by Cathey (2005) and Cathey et al. (2006).

Reaeration

Reaeration represents the physical flux of oxygen between the water surface and the atmosphere. The rate of reaeration is proportional to the DO deficit and a volumetric reaeration coefficient (O'Connor and Dobbins, 1958; Churchill et al., 1962). The volumetric reaeration coefficient represents the rate at which oxygen enters a body of water from the atmosphere. Depth, velocity, internal mixing, wind mixing, temperature, surface films, waterfalls, dams, and other physical obstacles affect the reaeration coefficient in streams (Thomann and Mueller, 1987).

There are many accepted methods for estimating the volumetric reaeration coefficient (Churchill et al., 1962; O'Connor and Dobbins, 1958; Owens et al., 1964; Thackston and Krenkel, 1969; Tsivoglou and Neal, 1976). The three most often used are the Tsivoglou equation (Tsivoglou and Neal, 1976), the O'Connor Dobbins equation (O'Connor and Dobbins, 1958), and experimental techniques such as the gas tracer injection method (Tsivoglou and Wallace, 1972). A detailed description of the governing equations is provided by Cathey (2005) and Cathey et al. (2006).

Dissolved Oxygen Simulation Models

Practically all in-stream DO models are based on the original or a modified form of the Streeter-Phelps equation (Streeter and Phelps, 1925). The original equation (eq. 2) was developed to predict the effects of waste discharges into a river and describes the DO sag curve (fig. 2):

$$D = D_0 e^{-k_a \frac{x}{u}} + \frac{k_d L_0}{k_a - k_d}\left(e^{-k_d \frac{x}{u}} - e^{-k_a \frac{x}{u}}\right) \qquad (2)$$

where

D = DO deficit (DO saturation minus the actual level of DO) (mg L^{-1})
D_0 = DO deficit at $x = 0$ (mg L^{-1})
k_a = first-order reaeration rate coefficient (d^{-1})
x = distance (m)
u = average velocity (m s^{-1})
k_d = first-order deoxygenation rate constant (d^{-1})
L_0 = ultimate CBOD (mg L^{-1}).

The DO sag curve predicts the difference between the DO concentration and the saturation value of DO (DO deficit) in a volume of water over time or distance following the introduction of organic matter (fig. 2b). When a biochemical oxygen demanding substance such as sewage enters a river, the organic material provides a source of energy for aerobic decomposer microorganisms living in the water column. This energy surplus leads to population growth in the decomposers and DO consumption through their respiration. As their population increases, they consume more organic material and more oxygen, leading to the critical point downstream at which DO reaches its minimum value and river conditions are at their worst. At this critical point, following the laws of supply and demand, the microbial population peaks and then begins to decline as the food supply becomes limiting.

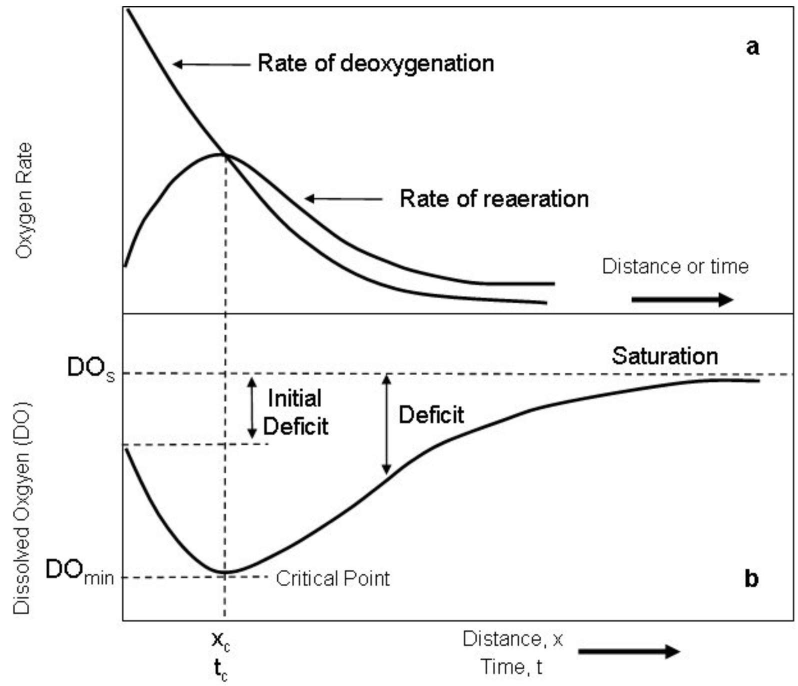

Figure 2. (a) Deoxygenation and reaeration responses to the organic material, and (b) the DO sag curve, which is characteristic of change of DO concentration in a river after the introduction of organic material.

As oxygen is consumed by the decomposers, the river is also reaerated by the physical flux of oxygen from the air into the water. While the oxygen demand is greater than the reaeration rate, DO concentration decreases (fig. 2a). When oxygen demand becomes less than the reaeration rate (beyond the critical point), DO concentration increases until it reaches atmospheric equilibrium (fig. 2b). This characteristic change of DO concentration in a river after the introduction of organic material is called the DO sag curve (fig. 2b).

There are many mathematical models that simulate DO dynamics in streams. Most were developed to simulate parameters associated with National Pollution Discharge Elimination System (NPDES) permits (or equivalent permitting) such as BOD, ammonium, and DO concentrations downstream from point discharges. Some models were developed specifically to simulate DO, while others are broader in-stream water quality models that include DO as one of several simulated parameters. A few watershed-scale transport models also include in-stream water quality modules that address DO.

Some models are specific to one river catchment, while others have been used widely and applied globally. In general, people have developed catchment-specific models because they found that widely used models were not well suited to their conditions or because the data required to parameterize widely used models were not readily available. It is also generally true that catchment-specific models are more difficult to apply elsewhere because they were not developed for broad dissemination and thus lack easy-to-use interfaces, adequate documentation, and adequate distribution networks. A summary of several widely used models for simulating DO concentrations in rivers and streams is presented in tables 1 and 2. The summary tables were adapted from the United States Geological Survey (USGS) Surface and Water Quality Models Information Clearinghouse (http://smig.usgs.gov). Intended users of these models are engineers, scientists, and regulatory agencies with some degree of modeling experience.

The following sections describe a subset of the models presented in tables 1 and 2 that are commonly used within the U.S. for simulating DO and that have also been used for DO TMDL development. Cox (2003b) provides a parallel description of models used in the U.K. for simulating DO in lowland rivers. A comprehensive review of agricultural nonpoint-source water quality models was published by Parsons et al. (2001).

QUAL2E (Enhanced Stream Water Quality Model)

QUAL2E is one of two models most often used for developing DO TMDLs within the U.S. This is likely because the model is intended as a tool for developing TMDLs (USGS, 2005). QUAL2E is a mechanistic, deterministic, one-dimensional, steady-state model that simulates flow and water quality in streams and rivers that can be assumed to be well-mixed. It is not suited for unsteady flows or for domains receiving variable inputs of water quality constituents. However, the model allows diurnal variations in meteorological forcing functions so that water temperature and algal photosynthesis can be simulated. The model also allows branched networks to be simulated. It simulates the major nutrient cycles, algal production, SOD and CBOD, atmospheric reaeration, and their effects on DO (Birgand, 2001). QUAL2E-UNCAS is an enhanced version of QUAL2E that allows uncertainty analyses of the steady-state water quality simulations. QUAL2K is an updated version of QUAL2E that includes several new modeling elements. Both are described in subsequent paragraphs. Brown and Barnwell (1987), Birgand (2001), and Cox (2003b) provide detailed evaluations of QUAL2E and its sister models.

Model Operation

All three QUAL models use a finite difference solution to the one-dimensional advective-dispersive mass transport and reaction equation. The conceptual representation of a stream

Table 1. Model characteristics and status of currently available water quality models that explicitly simulate DO. This information was adapted from the USGS Surface and Water Quality Models Information Clearinghouse (http://smig.usgs.gov).

Model Name	Dimensions[a]	Domains	GUI[b]	Status
Transport-Only Models				
BLTM	1-D	Rivers, estuaries	No	Public domain; supported by USGS
CE-QUAL-ICM	1, 2, 3-D	Rivers, lakes, estuaries, reservoirs, and coastal areas	Yes	Public domain; limited support from USCE-WES[c]
CE-QUAL-R1	1-D (v)	Lakes, reservoirs	No	Public domain; limited support from USCE-WES; no updates anticipated
CE-QUAL-RIV1	1-D (l)	Rivers, channel networks	No	Public domain; limited support from USCE-WES
Flow and Constituent Transport Models				
CE-QUAL-W2	2-D (v)	Rivers, reservoirs, estuaries	Yes	Public domain; limited support from USCE-WES; J. E. Edinger Associates, Inc., and Advanced Technology Systems, Inc., provide support services
EFDC/HEM3D	1, 2, 3-D	Rivers, lakes, estuaries, reservoirs, and coastal areas	Yes	Public domain; supported and maintained by Tetra Tech
HSPF	Watershed	Watersheds, channel networks	Yes	Public domain; supported by USGS
MIKE 11	1-D (l)	Rivers, estuaries, channel networks	Yes	Commercial software package; support provided by DHI and other service centers world wide
MIKE 21	2-D (h)	Estuaries, coastal areas	Yes	Commercial software package; support provided by DHI and other service centers world wide
MIKE 3	3-D	Rivers, lakes, estuaries, reservoirs, and coastal areas	Yes	Commercial software package; support provided by DHI and other service centers world wide
QUAL2E/QUAL2K	1-D (l)	Rivers, channel networks	Yes	Public domain; QUAL2K supported by EPA
SWAT	Watershed	Watersheds, channel networks	Yes	Public domain; supported by USDA-ARS[d]
WASP/DYNHYD	1, 2, 3-D	Rivers, lakes, estuaries, reservoirs, and coastal areas	Yes	Public domain; WASP6 and WASP7 supported by EPA

[a] (h) = horizontal, (l) = longitudinal, (v) = vertical.
[b] GUI = Graphical user interface.
[c] USCE-WES = United States Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi.
[d] USDA-ARS = United States Department of Agriculture – Agricultural Research Service.

Table 2. List of constituents relevant to DO simulated by each of the models listed in table 1. The constituent list was adapted from the USGS Surface and Water Quality Models Information Clearinghouse (http://smig.usgs.gov).

	Model Name										
Constituent	BLTM	CE-QUAL -ICM	CE-QUAL -R1	CE-QUAL -RIV1	CE-QUAL -W2	EFDC/ HEM3D	HSPF	MIKE 11, MIKE 21, MIKE 3	QUAL2E/ QUAL2K	SWAT	WASP5/ WASP7
Algae	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Temperature	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
DO	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Total dissolved solids			Yes		Yes						
Dissolved organic matter		Yes	Yes		Yes	Yes					
Bottom sediments					Yes						
Sediment diagenesis		Yes	Yes			Yes					Yes
BOD	Yes			Yes	Yes		Yes	Yes	Yes	Yes	Yes
COD	Yes	Yes		Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
SOD									Yes		
Detritus		Yes	Yes		Yes	Yes	Yes	Yes		Yes	
N	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
P	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Silica		Yes	Yes			Yes					Yes
Total inorganic carbon							Yes			Yes	
pH			Yes		Yes		Yes		Yes	Yes	
User-defined constituent	Yes							Yes	Yes		Yes
Conservative tracer	Yes					Yes	Yes		Yes	Yes	Yes

is a series of reaches (maximum of 50) that are divided into a number of subreaches or computational elements (maximum of 20 per reach). For each computational element, a hydrologic balance in terms of flow, a heat balance in terms of temperature, and a materials balance in terms of concentration are maintained. Both advective and dispersive transport are considered in the materials balance. Mass can be gained or lost from the element by transport processes, external sources and sinks (waste discharges or abstractions), or internal sources and sinks (benthic sources or biological transformations). The model computes the major interactions between up to 15 state variables within each computational element. Those relevant to DO are:

- DO
- BOD
- Temperature
- Algae as chlorophyll a
- N (organic, ammonia, nitrite, nitrate)
- P (organic, inorganic)
- An arbitrary nonconservative constituent and three conservative constituents.

The mass transport and reaction equation is solved for the steady flow, steady-state condition in a classical implicit backward difference method (Walton and Webb, 1994). The specific equations and solution technique are described in detail in the QUAL2E documentation and user manual (Brown and Barnwell, 1987).

Ultimate BOD is the primary internal sink of DO in the model. However, detritus, an important source of BOD, is not simulated in QUAL2E. Other sinks include SOD, modeled as a zero-order reaction, respiration by algae, and nitrification, which includes the oxidation of both ammonia and nitrite. The major sources of DO are from algal photosynthesis and reaeration. QUAL2E uses chlorophyll *a* (user input) as an indicator of planktonic algae biomass and assumes a first-order reaction to describe the accumulation of algae biomass. The accumulation of biomass is calculated as a balance between growth, respiration, and settling of the algae. Maximum growth rate is light and nutrient limited. Three mathematical options are provided with which to estimate nitrogen and phosphorus limitations (Birgand, 2001). Nine methods are available for calculating the reaeration coefficient. Reaeration under ice cover and above dams is also considered. All sources and sinks except SOD are modeled as first-order reactions.

Input Data Requirements

QUAL2E requires hydraulic data, initial conditions, flow data, meteorological data, and reaction rate coefficients, some of which require considerable experience to estimate (USGS, 2005), for each reach. Input data values depend on the type of simulation and the number of state variables used. If the maximum of 15 state variables and 50 stream reaches is used, the input data requirements can be quite onerous. A detailed description of the input data requirements is presented by Brown and Barnwell (1987), Birgand (2001), and Cox (2003b).

Calibration

A major problem faced by the user when working with a complex model such as QUAL2E is model calibration and determination of the most efficient plan for collection of calibration data. This problem can be addressed through uncertainty analysis. QUAL2E-UNCAS is an enhancement to QUAL2E that allows the user to perform uncertainty analysis on the steady-state water quality simulations. Three uncertainty options are available: sensitivity analysis, first-order error analysis, and Monte Carlo simulation. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts (Brown and Barnwell, 1987). Quantification of the uncertainty in model forecasts allows assessment of the risk (probability) of a water quality variable being above or below an acceptable level. Brown and Barnwell (1987) and Melching and Yoon (1996) suggest that the uncertainty analysis be performed early in the modeling stages so that the site- and use-specific sensitive parameters be identified.

Outputs

QUAL2E produces output tables of hydraulic parameters, water quality parameters, and reaction coefficients. These tables can be easily imported into other applications such as spreadsheets for analysis. Newer versions of the model provide some graphic analysis of results. State variables can be plotted at defined distances along the reaches. In addition, the user can input observed DO data, which the model uses to plot versus predicted values. The model also produces diurnal temperature and algal biomass values on a predefined time step (Birgand, 2001).

Limitations

The QUAL models are not suited for rivers that experience temporal variations in stream flow or where the major discharges fluctuate significantly over a diurnal or shorter time period. More significant are the limitations of the model when examining the contribution of nonpoint sources of pollutants to river water quality degradation. Indeed, nonpoint source loads are often driven by rainfall events, and thus both the waste load and the stream flow vary significantly over time. Both types of variation may deviate significantly from the assumptions of QUAL2E (Shanahan et al., 1998).

QUAL2K is a modernized version of the QUAL2E model. It operates within the Microsoft Windows environment and is coded in Visual Basic for Applications (VBA). Excel is used as the graphical user interface. In addition to changes in the operating system environment, QUAL2K includes the following new elements (EPA, 2005b):

- Model segmentation: QUAL2E segments the domain into river reaches comprised of equally spaced elements. In contrast, QUAL2K uses unequally spaced reaches. It also allows for multiple loadings and abstractions within a reach.
- Carbonaceous BOD speciation: QUAL2K uses two forms of carbonaceous BOD to represent organic carbon. These forms are a slowly oxidizing form (slow CBOD) and a rapidly oxidizing form (fast CBOD). In addition, non-living particulate organic matter (detritus) is simulated. This detrital material is composed of particulate carbon, nitrogen, and phosphorus in a fixed stoichiometry.
- Anoxia: QUAL2K accommodates anoxia by reducing oxidation reactions to zero at low DO levels. In addition, denitrification is modeled as a first-order reaction that becomes pronounced at low DO concentrations.
- Sediment-water interactions: Sediment-water fluxes of DO and nutrients are simulated internally rather than being defined by the user.
- Periphyton: The model explicitly simulates periphyton (attached bottom algae).
- Light extinction: Light extinction is calculated as a function of algae, detritus, and inorganic solids.
- pH: Both alkalinity and total inorganic carbon are simulated. The river's pH is then calculated from these two parameters.

Current Support

The QUAL series of models are in the public domain and are available at no cost from the EPA. QUAL2E and QUAL2E-UNCAS are available from the EPA Office of Research and Development (www.epa.gov/ceampubl/swat - er). QUAL2K is available from the EPA Watershed and Water Quality Modeling Technical Support Center (www.e-pa.gov/ATHENS/wwqtsc).

TMDL Applications

As stated earlier, the QUAL models are frequently used for developing DO TMDLs. QUAL2E and QUAL2E-UN-CAS were applied to develop a DO TMDL for the Nanticoke River and Broad Creek in Delaware (www.epa.gov/ reg3wapd/tmdl/de_tmdl/). QUAL2E was also used to develop DO TMDLs for the Colville River in Washington (Murray and Pelletier, 2003); North Fork, Little Sugar Creek, and Sugar Creek in Ohio (www.epa.state.oh.us/dsw/tmdl); and West Creek in Kansas (KDHE, 2002). Several other similar TMDLs can be identified through the EPA's TMDL web portal (www.epa.gov/owow/tmdl). This web page provides links to all TMDLs approved by the EPA, and many of the TMDL reports are available electronically.

HSPF (Hydrological Simulation Program – FORTRAN)

HSPF is the second of the two most commonly used models for developing DO TMDLs in the U.S. In contrast to QUAL2E, whose domain is strictly rivers, lakes, and reservoirs, HSPF is a comprehensive watershed transport model and one of only a very few such models that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions. HSPF incorporates watershed-scale models into a basin-scale analysis framework that includes fate and transport in one-dimensional stream channels (Bicknell et al., 1993, 1997; Donigian et al., 1984). The model can simulate the hydrologic and associated water quality processes on pervious and impervious land surfaces and in streams and well-mixed impoundments. The model includes in-stream quality components for nutrient fate and transport, BOD, DO, pH, phytoplankton, zooplankton, and periphyton. When simulating the riverine environment, HSPF is a mechanistic, deterministic, one-dimensional, dynamic model. Steady-state conditions can also be simulated.

Model Operation

In HSPF, the various hydrologic processes are represented mathematically as flows and storages. In general, each flow is an outflow from a storage, usually expressed as a function of the current storage amount and the physical characteristic of the subsystem. Thus, the overall model is physically based, although many of the flows and storages are represented in a simplified or conceptual manner. Although this requires the use of calibrated parameters, it has the advantage of avoiding the need for giving the physical dimensions and characteristics of the flow system. This reduces input requirements and gives the model its generality (Bicknell et al., 1997).

For simulation with HSPF, the basin has to be represented in terms of land segments and reaches/reservoirs. A land segment is a subdivision of the simulated watershed. The boundaries are established according to the user's needs but, generally, a segment is defined as an area with similar hydrologic characteristics. A segment of land that has the capacity to allow enough infiltration to influence the water budget is considered pervious. Otherwise, it is considered impervious (Bicknell et al., 1997). The two groups of land segments are simulated independently. In pervious land segments, HSPF models the movement of water along three paths: overland flow, interflow, and groundwater flow.

Water, sediment, and water quality constituents leaving the watershed move laterally to a downslope segment or to a reach/reservoir (Bicknell et al., 1997). The model computes the interactions between 15 or more water quality constituents within a reach. Those relevant to DO are:

- DO
- CBOD
- Temperature
- N (organic, nitrite-nitrate, ammonia)
- P (organic, inorganic)
- Sediment detachment and transport
- pH
- Phytoplankton
- Conservative tracer(s).

The hydraulic and water quality processes that occur in the river channel network are simulated within a reach based on two assumptions: there is a fixed relationship between depth, volume, and discharge; and discharge is a function of volume. This means that flow reversals and backwater effects in an upstream reach are not simulated. The outflow from a reach or completely mixed lake may be distributed across several targets to represent normal outflow, diversions, and multiple gates on a lake or reservoir. Evaporation, precipitation, and other fluxes that take place are also represented. Routing is done using a modified version of the kinematic wave equation. Momentum is not considered in the routing computations. Snow accumulation and melt are also included, so that the complete range of physical processes affecting the generation of water and associated water quality constituents can be approximated.

HSPF uses groups of subroutines to simulate the in-stream environment. The oxygen reaction subroutine group is used to account for temporal variations in oxygen balance, and the DO and BOD state variables. The state variable DO represents the oxygen dissolved in water and immediately available to satisfy the oxygen requirements of the system. Only CBOD is considered by the model; NBOD is not included. The model considers the following principal processes in determining oxygen balance: longitudinal advection of DO and BOD, settling of BOD material, SOD, resuspension of benthic BOD, reaeration, and CBOD (Bicknell et al., 1997).

Sources and sinks, except for SOD, are simulated as first-order reactions. SOD is assigned to each reach by the user. The model accommodates anoxia by reducing oxidation reactions at low DO levels. Four methods are available for calculating the reaeration coefficient.

Additional sources and sinks of DO and BOD are simulated in other subroutines if they have been activated by the user. These include the effects of nitrification and denitrification, photosynthetic and respiratory activity by phytoplankton and/or periphyton, respiration and nonrefractory organic excretion by zooplankton, and oxygen consumption due to planktonic decomposition. The user's manual (Bicknell et al., 1997) discusses the structure of the system and presents a detailed discussion of the algorithms used to simulate various water quantity and quality processes. It also contains all of the information necessary to develop input files for applying the program, including descriptions of program options, parameter definitions, and detailed input formatting data.

Input Data Requirements

Data needs for HSPF can be extensive. HSPF is a continuous simulation program and requires continuous data to drive the simulations. At a minimum, continuous rainfall records are required to drive the runoff model, and additional records of evapotranspiration, temperature, and solar intensity are desirable (EPA, 2005c). A large number of model parameters can be specified, although default values are provided when necessary. Option flags allow bypassing entire sections of the program where data are not available. A detailed description of the input data requirements is presented by Bicknell et al. (1997).

Calibration

Because data requirements for HSPF are extensive, calibration and verification are recommended (USGS, 2005). To facilitate calibration, the USGS developed a stand-alone expert system version of the model called HSPEXP. This interface allows the user to interactively edit the input file and provides the user with advice on which parameters should be adjusted to improve calibration. The expert system uses over 35 rules involving over 80 conditions to recommend parameter adjustments. The rules are based on the experience of a worldwide network of expert HSPF users.

Outputs

HSPF produces a time history of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time history of water quantity and quality at any point in a watershed. Statistical features are incorporated into the model to allow for frequency-duration analysis of specific output parameters. Hundreds of computed time series may be selected for the output files. HSPEXP offers error statistics for simulations and provides for graphic analysis of results. Output parameters can be plotted against observed data.

Limitations

As with most models, it is up to the user to decide if HSPF is appropriate for the area being modeled. Further, the in-stream model assumes that the receiving waterbody is well-mixed with width and depth, and it is thus limited to well-mixed rivers and reservoirs. Application of this methodology generally requires a team effort because of its comprehensive nature. Finally, backwater or tailwater control situations are not explicitly modeled by HSPF.

Current Support

HSPF is in the public domain and available at no cost from the USGS. The code for the model can be downloaded from the USGS Water Resources Applications Software web page (http://water.usgs.gov/software). HSPF is included in the BASINS (Better Assessment Science Integrating Point and Nonpoint Sources) suite of models (see subsequent section).

TMDL Applications

As with the QUAL series of models, HSPF is a popular choice when developing DO TMDLs. Most frequently, it has been used to simulate the unimpaired streams in a watershed and provide loadings to the impaired stream, which is then simulated with a linked in-stream model such as EFDC (discussed below). Among others, this was done for multiple streams in the Christina River Basin in Pennsylvania-Delaware-Maryland (EPA, 2000) and the Suwannee River Basin in Georgia (Georgia EPD, 2002). The Georgia application is presented as a case study later in this article.

WASP (Water Quality Analysis Simulation Program)

The WASP modeling system interprets and predicts water quality responses to natural phenomena and man-made pollution for various pollution management decisions. It is a mechanistic, deterministic, dynamic compartment-modeling program for aquatic systems, including both the water column and the underlying benthic sediments. The time-varying processes of advection, dispersion, point and diffuse mass loading, and boundary exchange are represented in the model (DiToro et al., 1983; Connolly and Winfield, 1984; Ambrose et al., 1993; Wool et al., 2001). Based on flexible compartment modeling, WASP can be applied in one, two, or three dimensions.

Model Operation

The WASP system consists of two stand-alone computer programs, DYNHYD and WASP, which can be run in conjunction or separately. DYNHYD is a hydrodynamics program that simulates the movement of water, while the water quality program, WASP, simulates the movement and interaction of pollutants within the water. The basic principle of both the hydrodynamics and water quality program is the conservation of mass. The water volume and water quality constituent masses being studied are tracked and accounted for over time and space using a series of mass balancing equations. Transport includes advection and dispersion of water quality constituents. Most transport data, such as flows or settling velocities, must be specified by the user in a WASP input data set. For water column flow, however, the user may "link" WASP with the hydrodynamics model. If this option is specified, WASP will read the contents of a hydrodynamic file for unsteady flows, volumes, depths, and velocities (Wool et al., 2001).

DYNHYD is a simple link-node hydrodynamic program capable of simulating variable tidal cycles, wind, and unsteady flows. It uses the St. Venant equation (full dynamic wave) to calculate the flow of water through a waterbody (Lindenschmidt et al., 2005) and produces an output file that supplies flows, volumes, velocities, and depths (time averaged) for the WASP modeling system. DYNHYD solves the one-dimensional equations of continuity and momentum for a branching or channel-junction (link-node) computational network. Driven by variable upstream flows and downstream heads, simulations typically proceed at one- to five-minute intervals. The resulting unsteady hydrodynamics are averaged over larger time intervals and stored for later use by the model.

Water quality processes in WASP are represented in special kinetic subroutines that are either chosen from a library or written by the user. WASP is structured to permit easy substitution of kinetic subroutines into the overall package to form problem-specific models. WASP comes with the EUTRO submodel for simulating conventional water quality (Wool et al., 2001). Without the submodel, WASP can only be used to simulate dissolved, conservative chemicals such as chlorides or dye tracer. The EUTRO

Table 3. Interaction between level of complexity of the Streeter-Phelps equation used and state variables in the WASP model (EPA, 2005e).

State Variable	Level of Complexity[a]					
	1	2	3	4	5	6
Ammonia			Yes	Yes	Yes	Yes
Nitrate			Yes	Yes	Yes	Yes
Inorganic P				Yes	Yes	Yes
Phytoplankton C				Yes	Yes	Yes
Periphyton C						Yes
CBOD	Yes	Yes	Yes	Yes	Yes	Yes
DO	Yes	Yes	Yes	Yes	Yes	Yes
Organic N			Yes	Yes	Yes	Yes
Organic P				Yes	Yes	Yes
Sediment diagenesis					Yes	Yes

[a] 1 = Streeter-Phelps DO/BOD and descriptive SOD.
2 = Modified Streeter-Phelps with NBOD.
3 = Linear DO balance with nitrification.
4 = Simple eutrophication with descriptive SOD.
5 = Intermediate eutrophication with sediment diagenesis.
6 = Advanced eutrophication with sediment diagenesis and periphyton.

submodel combines a kinetic structure with the WASP transport structure. This model predicts DO, CBOD, phytoplankton, carbon, chlorophyll *a*, ammonia, nitrate, organic nitrogen, and orthophosphate in benthic sediments and overlying waters. EUTRO can be operated by the user at various levels of complexity to simulate some or all of these variables and interactions. To simulate only BOD and DO, for example, the user may bypass calculations for the N, P, and phytoplankton variables (the bypass option is documented in the user's manual). Six levels of complexity are available for simulations, as depicted in table 3.

The most recent version of the WASP modeling system (WASP7) simulates the transport and transformation reactions of 10 to 14 state variables (depending on how they are counted). Earlier versions of WASP (through WASP6) reported only eight state variables (Ambrose et al., 1993; Wool et al., 2001). The current state variables are:

- DO
- N (organic, ammonia, nitrite-nitrate)
- P (organic, inorganic)
- Phytoplankton and periphyton
- Particulate detritus (N, P, C)
- CBOD (fast, intermediate, slow).

The state variables can be considered as components of six interacting systems: phytoplankton kinetics, periphyton kinetics, the phosphorus cycle, the nitrogen cycle, the DO balance, and sediment diagenesis. The general WASP mass balance equation is solved for each state variable. To this general equation, the EUTRO subroutines add specific transformation processes to customize the WASP transport equation for state variables in the water column and benthic sediments. The interaction of state variables and levels of complexity in WASP is shown in table 3.

Input Data Requirements

To perform mass balance computations, the user must supply WASP with input data defining seven important characteristics:

- Simulation and output control
- Model segmentation
- Advective and dispersive transport
- Boundary concentrations
- Point and diffuse source waste loads
- Kinetic parameters, constants, and time functions
- Initial concentrations.

These input data, together with the general WASP mass balance equations and the specific chemical kinetics equations, uniquely define a special set of water quality equations. These are numerically integrated by WASP as the simulation proceeds in time. At user-specified print intervals, WASP saves the values of all display variables for subsequent retrieval and display. The WASP modeling system includes an interactive preprocessor program for entering input parameters.

Calibration

Due to the spatial and temporal variability, measurement errors, and simplifying assumptions in the model, calibration to a good set of monitoring data is definitely needed to provide credible predictions (Wool et al., 2001). Conservative tracers can used to calibrate calculated flows, dispersive coefficients, and other associated parameters (Benaman et al., 1998).

Outputs

The WASP modeling system includes a tabular post-processor program and a graphical post-processor for EUTRO and DYNHYD. The post-processor interactively produces tables of user-specified variables. Some users have reported output limitations with the WASP5 version of the modeling system.

Limitations

Dam-break situations cannot be simulated with DYNHYD nor can small mountain streams.

Current Support

Several generations of the WASP modeling system exist. All are in the public domain and are available at no cost from the EPA. The most commonly used version is WASP5, which is available from the EPA Office of Research and Development (www.epa.gov/ceampubl/swater). The most recent version is WASP7, which is available from the EPA Watershed and Water Quality Modeling Technical Support Center (www.epa.gov/ATHENS/wwqtsc).

TMDL Applications

WASP was used to develop DO TMDLs for the Appoquinimink and Murderkill Rivers in Delaware (www.epa.gov/reg3wapd/tmdl/de_tmdl/), Butcher Pen Creek in the Lower St. Johns River basin in Florida (EPA Region 4, 2005), and several other lotic systems in the U.S. WASP has also been used to develop lake or reservoir DO TMDLs. Examples include Lakes Fausse Pointe and Dauterive in Louisiana (Louisiana DEQ, 2000).

EFDC (Environmental Fluid Dynamics Code)

The EFDC and HEM3D (Hydrodynamic-Eutrophication Model) are coupled three-dimensional mechanistic, deterministic, dynamic surface water models for hydrodynamic and water quality simulations in rivers, lakes, reservoirs, wetland systems, estuaries, and the coastal ocean. EFDC is a hydrodynamic model that can be used to simulate aquatic systems in one, two, and three dimensions. It has evolved over the past two decades to become one of the most widely used and technically defensible hydrodynamic models in the world (EPA, 2006). HEM3D extends EFDC to simulate the spatial and temporal distribution of water quality parameters, including eutrophication processes and sediment beo-geochemical processes (diagenesis). The two models can execute in a fully coupled mode, simultaneously simulating hydrodynamic and water quality processes. The models can also be used in series, with EFDC transport parameters being stored and then being used by HEM3D. EFDC also provides output formatted to yield transport fields for other water quality models, including WASP, using procedures described in Hamrick (1994). EFDC will be included in EPA's TMDL Toolbox to provide necessary hydrodynamic inputs to WASP.

Model Operation

EFDC uses stretched or sigma vertical coordinates and Cartesian or curvilinear, orthogonal horizontal coordinates to represent the physical characteristics of a waterbody. The model uses a finite difference spatial representation and is capable of reduced dimension execution in one-dimensional network and two-dimensional (horizontal or vertical plane) modes. Water column transport includes three-dimensional advection and vertical and horizontal turbulent diffusion. Shear dispersion may be included for two-dimensional horizontal applications (Hamrick, 1996). EFDC solves three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable-density fluid. Dynamically coupled transport equations for turbulent kinetic energy, turbulent length scale, salinity, and temperature are also solved. The EFDC model is unique in that it allows for drying and wetting in shallow areas by a mass conservation scheme. For the simulation of flow in vegetated environments, the model incorporates both two- and three-dimensional vegetation resistance formulations (Hamrick and Moustafa, 1995). HEM3D is based on the CE-QUAL-ICM model (tables 1 and 2) and incorporates a predictive diagenesis component (DiToro and Fitzpatrick, 1993). It is capable of two- or three-dimensional spatial resolution (Park et al., 1995). The model uses 21 state variables to simulate the spatial and temporal distributions of water quality parameters including:

- DO
- Suspended algae (three groups represented in carbon equivalent units)
- N (organic, ammonia, nitrite-nitrate)
- P (organic, dissolved)
- Organic C
- COD
- Available and unavailable silica.

Model variables in the sediment bed include particulate organic C, N, and P, each in three reaction rate classes; particulate and available silica; sulfide or methane; ammonia; nitrate; inorganic phosphorus; bed-water column fluxes of ammonia, nitrate, inorganic phosphorous and silica; SOD; and release of COD. The model's formulation allows direct determination of organic C levels in the water column and sediment bed (Park et al., 1995).

Input Data Requirements

EFDC requires the user to provide volumetric inflows and inflowing concentrations of sediment and water quality state variables. Alternatively, these values can be provided by a watershed model such as HSPF, as described in a case study presented later in this article. The user must also provide wind and atmospheric thermodynamic conditions. Input file templates are included with the source code and the user's manual to aid in input data preparation. A pre-processor is supplied with the model to aid with grid generation.

Calibration

The model developers recommend making modifications to the input parameters based first on comparison of observed hydrologic data to simulated data and based second on comparisons of the water quality data (Hamrick, 1992). Extensive calibration of the model requires long-term observations for the lotic system being simulated (Hamrick, 1995). Only a few studies have calibrated the model to observed DO data. A pre-processor is supplied with the model to aid grid generation.

Outputs

The model performs harmonic and time series analysis at user-specified locations. The model outputs a variety of file formats for 3-D vector and scalar visualization and animation using several public and private visualization packages.

Limitations

The primary user-related limitations are that both models require considerable technical expertise in hydrodynamics to use EFDC effectively and in eutrophication processes to use the water quality component.

Current Support

The model code is in the public domain and is available at no cost from the EPA Watershed and Water Quality Modeling Technical Support Center (www.epa.gov/ATHENS/wwqtsc). The models are currently supported and maintained at TetraTech, which is in the process of updating the model and manuals.

Applications

EFDC linked to WASP was used to determine the level of nutrient reduction required for the Neuse Estuary during TMDL development. HSPF was used to provide loads directly to the estuary model. The linked models were applied over a three-year period and also used to determine the frequency of anoxic conditions in the lower waters of the estuary due to nutrient enrichment and the benefits gained (relative to DO) through nutrient reduction (EPA, 2006). An HSPF-EFDC modeling system was used to develop DO TMDLs in the Christina River basin in Pennsylvania-Delaware-Maryland (EPA, 2000) and to several stream segments in Georgia's Suwannee River basin. A case study of this application is presented below.

BASINS (Better Assessment Science Integrating Point and Nonpoint Sources)

To facilitate the development of TMDLs, the EPA developed the BASINS system (EPA, 2005d). BASINS integrates a geographic information system (GIS), national watershed and meteorologic data, and state-of-the-art environmental assessment and modeling tools into one software package. To simplify the development of TMDLs across the U.S., a data set has been assembled that can be easily retrieved for use with BASINS. These data are distributed by EPA through the BASINS website. Because they are readily available, these data sets are often used for developing TMDLs. BASINS contains models for estimating watershed loading including HSPF and the Soil and Water Assessment

Tool (SWAT). Like HSPF, SWAT is a river basin model developed to quantify the impact of land management practices in large watersheds (Arnold et al., 1998) but also simulates in-stream processes including DO. Extensive descriptions of the model are available (Arnold et al., 1998; Saleh et al., 2000; Spruill et al., 2000), as are several model applications (Saleh et al., 2000; Santhi et al., 2001; Srinivasan et al., 1997; Bingner, 1996; Bosch et al., 2004). SWAT has been applied alone or in conjunction with a stream model to develop DO TMDLs in at least four states. For example, SWAT was used to estimate nutrient loading to the Pineview Reservoir in Utah and the impact of the loading on DO conditions in the reservoir (Whitehead and Judd, 2002). In another application, SWAT was used in conjunction with the QUAL-TX model to develop a DO TMDL for the Long Prairie River in central Minnesota (Munir, 2004). Because SWAT is well known, widely used, and described in detail in other articles of this collection (Benham et al., 2006; Borah et al., 2006; Shirmohammadi et al., 2006), it will not be described further here.

Case Study

To this point, this article has described five different models that have been used to develop DO TMDLs in the U.S. and has presented a tabular summary of the characteristics of several other models that simulate DO (tables 1 and 2). The remainder of the article will focus on application of two of these models to develop a DO TMDL. Although it is true that dozens of DO TMDLs have been developed and approved by the EPA, it is difficult to find more than a few TMDLs developed using the same modeling techniques. It is common for TMDLs within a given river basin to be developed using the same tools but for TMDLs in the immediately adjoining watershed to be done in an entirely different way. In Georgia, for example, DO TMDLs in the Suwannee River basin (fig. 3) were contracted to a consulting firm, which chose to use a combination of HSPF and EFDC (to be described later). In the adjoining Satilla River basin, DO TMDLs were developed in-house by Georgia EPD using the Georgia DOSag model –– clearly two very different approaches.

Rather than summarizing a case study for each of the models discussed in this article, we chose instead to provide a detailed case study with which we illustrate the process of developing a DO TMDL. In general, the process is similar, regardless of the model. The case study is from Georgia and describes the development of the DO TMDL for Turkey Branch, which is located within the Suwannee River basin. The information presented here is a summary of the TMDL report submitted by Georgia EPD to the EPA (Georgia EPD, 2002). The case study is particularly interesting because it includes both point and nonpoint sources in a mixed-use watershed.

Turkey Branch DO TMDL

Turkey Branch is located in the headwaters of the Suwannee River basin near Fitzgerald, Georgia. It is within the Alapaha River 8-digit HUC (03110202), as shown in figure 3. The Turkey Branch watershed, 12-digit HUC 031102020502, is approximately 44 km^2. Turkey Branch flows into the Willacoochee River and then eventually into the Alapaha River. It was placed on the Georgia 303(d) list for violating Georgia DO standards based on data collected during 1998. The data were collected during Georgia EPD's routine rotating trend monitoring program of the state's water bodies. Trend monitoring is contracted to the USGS. The applicable DO water quality criteria for Turkey Branch were as follows: a daily average of 5.0 mg L^{-1} and no less than 4.0 mg L^{-1} at all times for waters supporting warm-water species of fish (Georgia EPD, 2000).

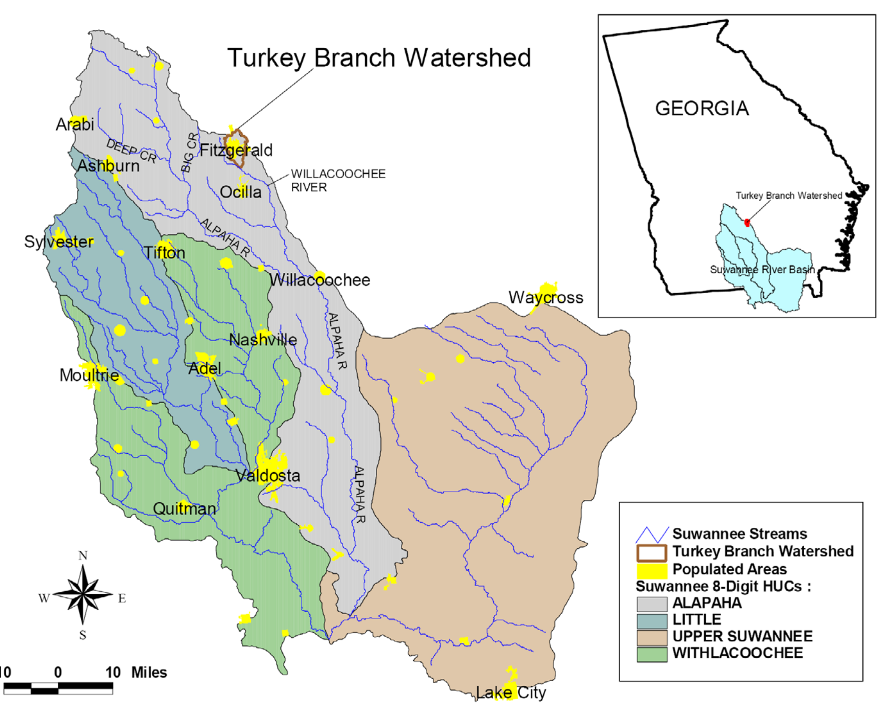

Figure 3. Location of the Turkey Branch 12-digit HUC watershed within the Suwannee River basin in southern Georgia (Georgia EPD, 2002).

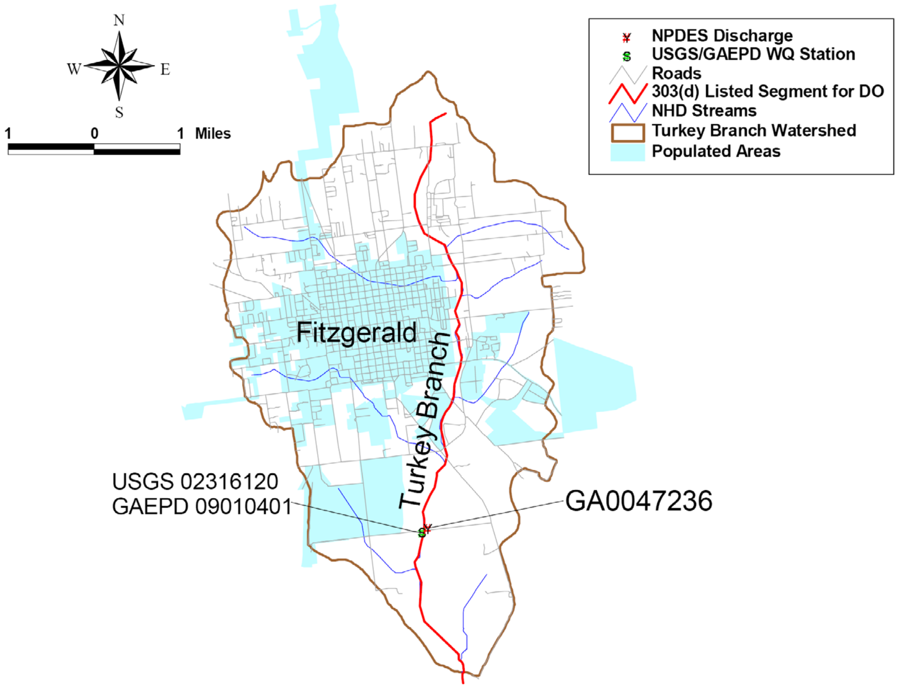

Figure 4. Turkey Branch 12-digit HUC showing (left) the location of the trend monitoring sampling site and (right) the location of the Fitzgerald waste water treatment plant, indicated by its NPDES permit number (Georgia EPD, 2002).

Turkey Branch Water Quality

There were 20 measurements during the 1998 monitoring period at the USGS 02316120 – Georgia EPD trend monitoring site (fig. 4). Figures 5 and 6 display the DO measurements versus temperature, BOD_5, and ammonia. The DO data did not meet the Georgia EPD criterion of 5.0 mg L^{-1} for the daily average and met the 4.0 mg L^{-1} minimum only 10% (2 of 20 measurements) of the time. Figures 5 and 6 show that the hypoxic conditions were prevalent from June through September. There was not a continuous flow gauge in the Turkey Branch watershed and, due to drought conditions during the 1998 monitoring year, the USGS did not report a flow measurement for each sampling event (Georgia EPD, 2002).

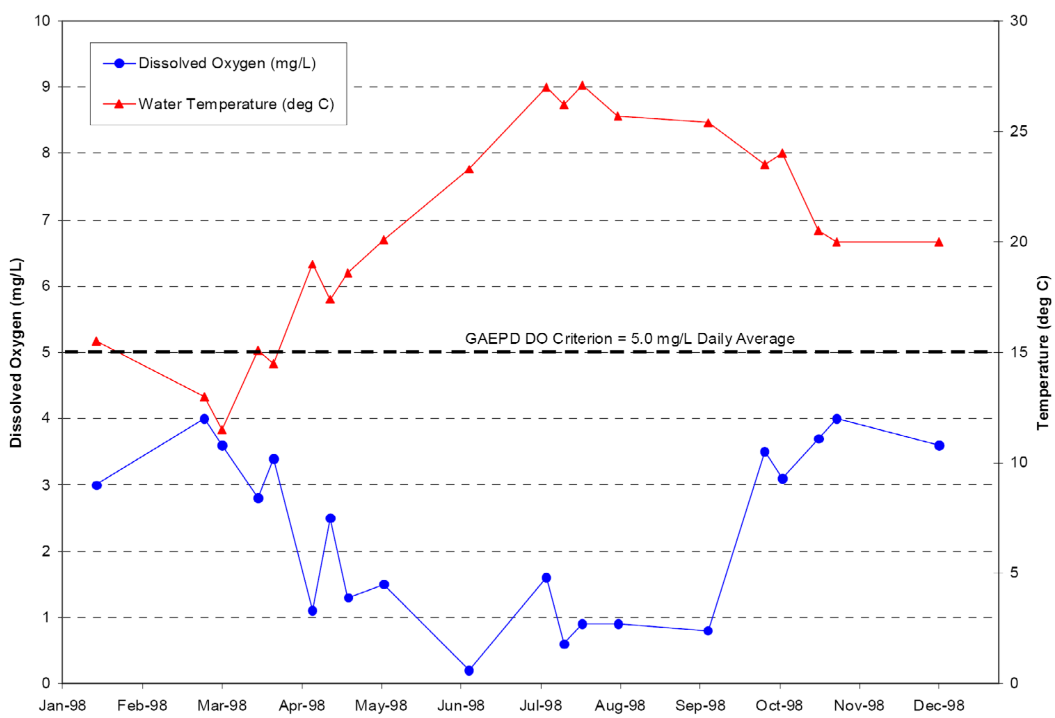

Figure 5. DO and temperature as measured during 1998 at the trend monitoring sampling site on Turkey Branch (Georgia EPD, 2002).

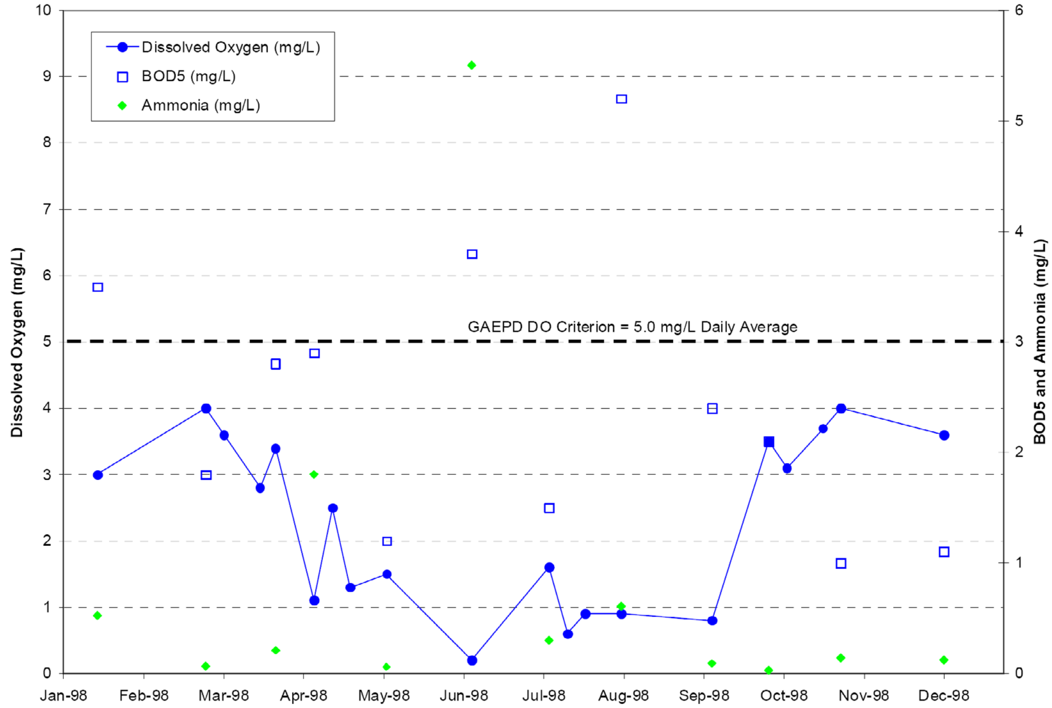

Figure 6. DO, BOD_5, and ammonia as measured during 1998 at the trend monitoring sampling site on Turkey Branch (Georgia EPD, 2002).

Source Assessment

The 303(d) listing for Turkey Branch identified municipal sources as the primary contributor to the DO impairment. An examination of permits and land use information for the watershed was used to identify all potential sources of oxygen-demanding substances in the basin. These sources (divided into point and nonpoint sources) were considered in the source loading analysis and the subsequent TMDL. The point source that contributes to this listed water is the Fitzgerald wastewater treatment plant. The facility is located approximately two miles upstream of the confluence of Turkey Branch and the Willacoochee River. Figure 4 shows its location with respect to the watershed.

Nonpoint sources of oxygen-demanding substances are typically separated into urban and rural components. In urban or suburban settings, important sources of loading are surface storm runoff, failing septic systems, and leakage and overflows from sanitary sewer systems. In rural areas, sources of oxygen-demanding substances may include diffuse runoff of agricultural fertilizer and animal wastes (from manure application or grazing animals), erosion of sediments, and runoff from concentrated animal operations. Based on a land use assessment and review of the literature, nonpoint source contributions from urban, agriculture, and forested areas were all likely in the Turkey Branch watershed. Cropland, pasture, forest, urban areas, and wetlands were all identified in the basin.

In addition to the aforementioned nonpoint sources of oxygen-demanding substances, many southern Georgia streams receive significant contributions of oxygen-demanding organic materials from local wetlands and forested stream corridors. In particular, the following sources of organic materials have been identified: adjacent wetland/swampy areas that have organically rich bottom sediments, direct leaf litterfall onto the water surface from overhanging trees and vegetation, and lateral leaf litterfall that has fallen into the floodplains.

Leaf litterfall plays a major role in the amount of carbon in the stream water column. The riparian areas of the watershed are the primary source of leaf litterfall. At higher flows, the leaf litterfall in the floodplains is picked up and transported laterally into the stream. Many streams in southern Georgia are referred to as "blackwater" streams due to the humic substances leached from surrounding watersheds that impart color to the water (Meyer, 1992). Low DO in blackwater streams is common in the summer months when the temperatures are high and the flows are low.

Technical Approach

The TMDL analysis includes an evaluation of the relationship between the sources and the impact on the receiving water. Due to the many factors that dynamically influence in-stream DO concentrations, this relationship was developed using a complex model linkage. Turkey Branch was modeled using both a dynamic receiving water model and a dynamic watershed model. The linkage of these models permitted representation of major processes associated with DO concentration variability, discussed earlier.

By developing a linked watershed-receiving water model, the impacts of various factors (including all nonpoint and point source loads) on in-stream DO were evaluated. Ultimately, the loading capacity of the waterbody for each critical pollutant affecting the DO concentration was determined. The required source-based loading reduction required to meet the in-stream standard was also calculated. This approach permitted assessment of point source and nonpoint source contributions (including both watershed and leaf litterfall, etc.).

HSPF was selected to represent nonpoint source pollutant contributions (and point source contributions as necessary) to Turkey Branch. The impaired stream was modeled using the

Environmental Fluid Dynamics Code (EFDC), a 3-D hydrodynamic and water quality model capable of simulating DO and a full suite of DO interactions (table 1). Output from HSPF was applied directly to EFDC in order to provide the linkage between source and waterbody response (Georgia EPD, 2002).

The year 1998 was selected as the calibration period because it contained a wide range of hydrologic conditions, including heavy rainfall and drought conditions. More importantly, this period contained the most extensive monitoring data, which were necessary for model calibration. HSPF was run for ten years to examine the watershed water quality loading over an extended period of time. The 1998 watershed loading rates were compared directly to 1997 rates to see if there were any anomalies in the loading rates. Hourly precipitation, air temperature, dew point, wind speed, solar radiation, and percent cloud cover data were obtained from a nearby weather station.

Land Use Representation

HSPF uses land use data as the basis for representing hydrology and nonpoint source loading. Land use categories for modeling were selected based on the USGS Multi-Resolution Land Classification (MRLC) data set, and included urban, forest, cropland, pasture, and wetlands. The USGS data represented conditions in the early to middle 1990s. The modeling categories and their corresponding USGS classifications are reported by Georgia EPD (2002).

Per the earlier description of the model, HSPF requires division of land uses in each subwatershed into separate pervious and impervious land units. In this application, this division was based on typical imperviousness percentages from individual land use categories, such as those used in the NRCS TR-55 method. For modeling purposes, the percent imperviousness of a given land category was calculated as an area-weighted average of land use classes encompassing the modeling land category (Georgia EPD, 2002).

Hydrologic Representation

Watershed hydrology plays an important role in the determination of nonpoint source flow and, ultimately, nonpoint source loadings to a waterbody. The watershed model must appropriately represent the spatial and temporal variability of hydrologic characteristics within a watershed. Key hydrologic characteristics include interception storage capacities, infiltration properties, evaporation and transpiration rates, and watershed slope and roughness. The HSPF modules used to represent watershed hydrology for TMDL development include PWATER (water budget simulation for pervious land units) and IWATER (water budget simulation for impervious land units).

EFDC was used to simulate all in-stream DO processes for the impaired stream. Unimpaired streams contributing to the impaired stream were represented using HSPF's in-stream algorithms. Key components of the in-stream representation included: hydrodynamic representation, water quality configuration, unimpaired waterbody representation, and hydrodynamic representation.

An independent grid system was developed to represent the impaired stream within EFDC. The longitudinal extent of the impairment, as defined in the Georgia 303(d) list, was used to determine the grid coverage. The extent of impairment in Turkey Branch was 12 km. Each cell was rectangular and represented a single vertical water layer (one dimension). Cells were typically on the order of 1 to 3.22 km in length. The lateral dimension (width) was derived from USGS cross-sectional data obtained from the USGS monitoring station located on Turkey Branch. Tributary inflows, point sources, and nonpoint source contributions were applied directly to applicable cells in the grid. Upstream inflows (represented in the watershed model) were applied directly to the most upstream cell in the EFDC grid. Flow from the 12-digit subwatershed in the immediate vicinity of Turkey Branch (also represented in the watershed model) was distributed evenly among the cells. Flow from incoming tributaries (represented as stream networks in the watershed model) and point sources were applied directly to the most appropriate cell in the configuration.

Source Representation

In this case study, nonpoint sources were simulated with HSPF. A total of four water quality parameters were simulated using the watershed model: BOD, total nitrogen (TN), total phosphorus (TP), and total suspended solids (TSS). These parameters (either directly or indirectly) constitute the primary nonpoint sources contributing to DO depletion and/or replenishment. The buildup and washoff of these pollutants were represented using the PQUAL (simulation of quality constituents for pervious land segments) and IQUAL (simulation of quality constituents for impervious land segments) modules in HSPF. Different buildup and washoff rates were used to represent the different land categories (e.g., fertilizer and manure application generally result in a higher nutrient buildup and washoff from cropland than nutrient washoff from urban lands). Upon application to the receiving water model, many parameters simulated in the watershed model were converted into more applicable constituents for in-stream modeling with EFDC (Georgia EPD, 2002).

Loadings of leaf litterfall were assumed to be consistent with a study performed on the Ogeechee River in southern Georgia (Meyer et al., 1997). The direct leaf litterfall was reported as 843 g m^{-2} $year^{-1}$, and lateral leaf litterfall was reported as 3,520 g m^{-2} $year^{-1}$. The surface area of the stream channel was used to derive loading rates in the model. The lateral leaf litterfall was flow dependent to simulate the loading increase when the flows are large enough to inundate the floodplains and pick up the organic material deposited in the floodplain. The leaf litterfall loading was only applied to the receiving water model grid segments. Loadings from the HSPF model (particularly BOD, which was ultimately converted to TOC, discussed below) were assumed to account for residual leaf litterfall from upstream segments (transported to the impaired segment). The majority of leaf litter was assumed to be deposited on the stream bottom within each segment, thus forming an organic-enriched bed, resulting in higher simulated SOD. SOD values were estimated from the literature (Bowie et al., 1985; Chapra, 1997; Fuss and Smock, 1996).

Because the point source in the Turkey Branch watershed was on the impaired stream, it was represented in EFDC. If it were on a non-impaired tributary, it would have been represented with HSPF (only the impaired stream was simulated with EFDC). The point source was represented using a constant flow and pollutant loading. Permitted flows and loads were used to represent initial conditions for TMDL development. The monthly average permitted conditions were loaded into EFDC for the allocation runs. For example, where BOD_5 is permitted at a maximum of 45 mg L^{-1} and an average of 30 mg L^{-1}, the average of 30 mg L^{-1} would be multiplied by the average daily permitted flow to produce a daily mass loading (kg day^{-1}). The monthly average permitted values, versus the monthly maximum, are more representative in determining assimilative capacity in the system. Water quality constituents represented include BOD, TN, TSS, and TP. BOD and TSS values were represented using Discharge Monitoring Report (DMR) and permitted values. TN values were based on monitored NH_3 values for the facility. TP values were assumed to be 5 mg L^{-1} (due to the absence of DMR data and permitted values).

Calibration and Validation

After parameterizing, the watershed and receiving water models were calibrated. HSPF was calibrated first and simulation outputs were applied to EFDC for that model's calibration. Calibration of EFDC required further calibration of HSPF, resulting in an iterative approach to calibration. The HSPF subwatershed model runs were calibrated primarily to BOD_5 and TSS. EFDC is a C-based water quality model that simulates organic matter as C rather than BOD. Because of this, BOD_5 watershed loads from HSPF were converted to TOC prior to use by EFDC. This was achieved by using the relationship: TOC = 10.8 BOD_5. The relationship was derived by first developing a BOD_u/BOD_5 ratio for the Turkey Branch watershed, which was calculated to be 4.0. This ratio was then multiplied by a literature value for converting BOD_u to TOC of 2.7 (Thomann and Mueller, 1987).

Hydrologic calibration involved an adjustment of parameters related to all components of the hydrologic cycle including overland flow, infiltration, groundwater flow, and evapotranspiration. Adjustments were made during a comparison of in-stream flow monitoring data to modeled in-stream flow at a representative location for the region. Because the TMDL for Turkey Branch was a component of the overall TMDL development effort in the Suwannee River basin, additional data outside the Turkey Branch watershed were available for calibration and validation. Flow data from gauged USGS stream monitoring sites were used for this effort. For calibration purposes, in-situ temperature data measured concurrently with DO were input into the model. For the TMDL load allocation model runs, a representative seasonal distribution of temperature was created.

Once hydrology was calibrated and validated for HSPF, calibration focused on water quality parameters. Water quality calibration consisted of adjusting TSS, BOD, TN, and TP buildup and washoff parameters within a reasonable range to achieve a good match between model output and in-stream water quality observations. Key considerations in the water quality calibration for the watershed model were baseflow concentrations, background concentrations, seasonal variations, and stormflow concentrations. Initial buildup and washoff parameters were based on past studies.

Kinetic parameters that required adjustment included selection of an appropriate reaeration equation, ratios for nutrient splits, leaf litterfall nutrient split, and density of periphyton. For the EFDC model runs, the primary water quality parameters for evaluating a calibrated model were DO and TOC. Secondary parameters include ammonia, nitrate-nitrite, TN, and TP. SOD was also examined to see how much oxygen demand is derived from benthic sediment. The oxygen balance was calibrated by making adjustments to reaeration, algal growth and death, in-stream kinetic rates, partitioning coefficients for sediment fluxes, and water temperatures. In addition to the water quality calibration, flow, velocity, and depth were examined to ensure proper calibration of the hydrodynamics. DO calibration curves for Turkey Branch are shown in figure 7. The model overpredicted DO concentrations during the early spring, a time when DO typically decreases rapidly in coastal plain streams. The mechanisms causing this rapid decline are not well understood and consequently not well simulated.

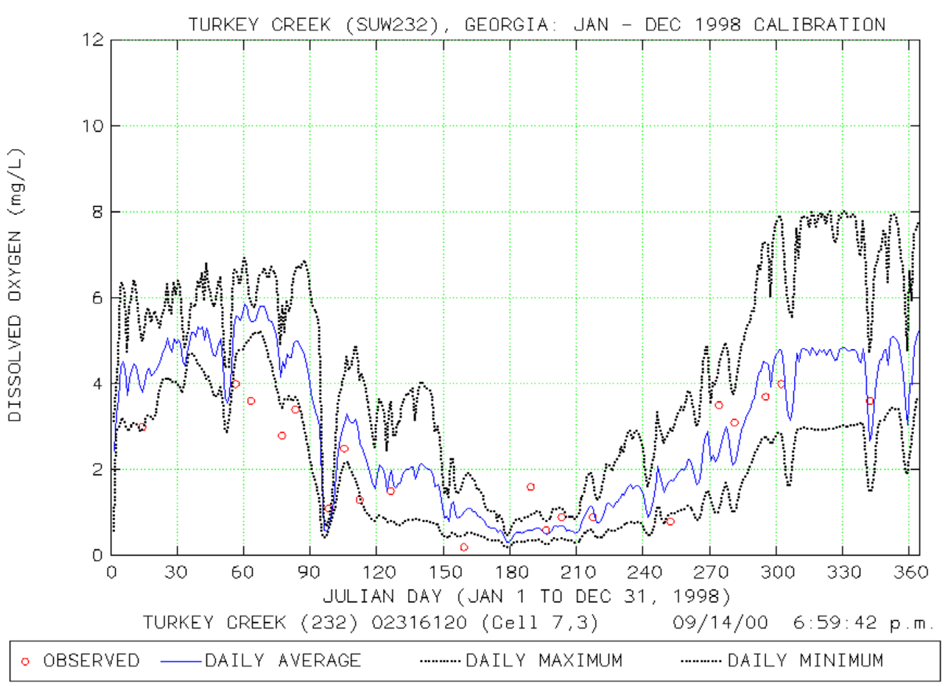

Figure 7. Turkey Branch final DO calibration curves compared to observed data (Georgia EPD, 2002).

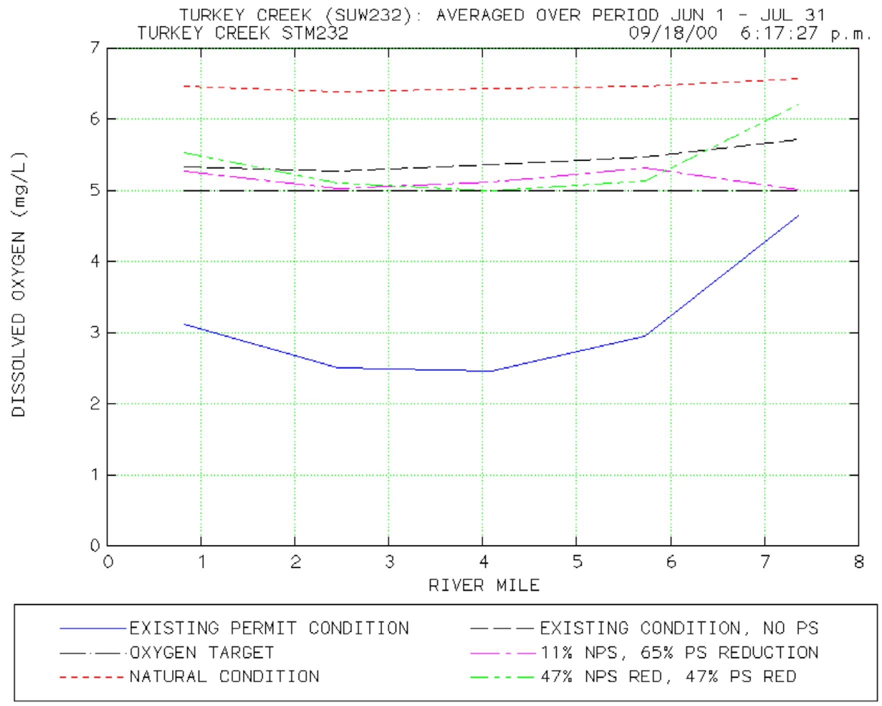

Figure 8. Longitudinal DO concentrations in Turkey Branch for various load allocation alternatives. These data are the monthly average for July, during which DO and flow are typically at their lowest data (Georgia EPD, 2002).

TMDL Development

The tested model was ultimately used to identify the allowable loading capacity for the listed segment. This was done through a series of simulations aimed at meeting the DO target limit by varying source contributions. The first step in the process was to determine naturally occurring DO concentrations for the impaired waterbody. To determine the naturally occurring DO concentrations, the in-stream model was run using watershed model input representing pristine conditions (entirely forest and wetland contributions) and leaf litterfall. The resulting in-stream DO concentrations represented natural conditions (fig. 8). However, these concentrations do not reflect low DO measurements reported by Ice and Sugden (2003) and Carey et al. (2005, 2006) in forested watersheds in Louisiana and Georgia, respectively. The models were then run to determine the loading capacity of Turkey Branch (fig. 8). The final acceptable scenario represented the TMDL (and acceptable loading of the waterbody).

Several partitioning scenarios met the in-stream DO criteria of 5.0 mg L^{-1} for a daily average, as shown in figure 8. The scenario selected for the TMDL calls for a 25% point source reduction in TOC, TN, and TP and a 57% nonpoint source reduction of the same constituents. Load estimates for this scenario are presented in table 4. Achieving a 57% nonpoint source load reduction appears difficult, if not impossible. In contrast, it is possible to achieve higher point source load reduction than the allocated 25% by significantly upgrading the Fitzgerald wastewater treatment plant. The partitioning of allocations between point and nonpoint sources to meet the TMDL was based on modeling results and professional judgment. These types of allocation decisions are affected by total available resources, the most efficient allocation of these resources, actions that will result in the quickest water quality improvements, and social and political factors.

Margin of Safety

According to EPA, there are two accepted methods for incorporating a margin of safety (MOS) during TMDL development (EPA, 1991). These are to implicitly incorporate a MOS using conservative model assumptions to develop allocations, or to explicitly specify a portion of the total TMDL as the MOS and use the remainder for allocations (EPA, 1991). In the Turkey Branch TMDL, a MOS was incorporated using the first method. Specifically, this was achieved by running a dynamic model, using average month–ly permit values to load permitted point sources into the mod–

Table 4. Existing loads and TMDL allocation loads for the Turkey Branch watershed (Georgia EPD, 2002).

	Water Quality Parameters								
	Existing Loads			TMDL Allocation Loads			Percent Reduction		
	TOC (kg $year^{-1}$)	TN (kg $year^{-1}$)	TP (kg $year^{-1}$)	TOC (kg $year^{-1}$)	TN (kg $year^{-1}$)	TP (kg $year^{-1}$)	TOC (%)	TN (%)	TP (%)
Nonpoint Source[a]	1,273,048	38,231	3,828	547,410	16,440	1,645	57	57	57
Point Source[b]	728,163	27,704	41,510	546,122	20,778	31,133	25	25	25
Total	2,001,211	65,935	45,338	1,093,532	37,218	32,778			

[a] Turkey Branch 12-digit HUC.
[b] Fitzgerald Wastewater Treatment Plant.

el for allocation runs, taking into account the daily maximum loads, running the model with actual flow and temperature during one or more annual cycles including a critical summer period, and using a 41% saturation for upstream DO (Meyer, 1992).

Conclusions

At least 13 constituent transport or flow and constituent transport models are widely used in the U.S. for simulating DO concentrations in rivers, lakes, reservoirs, estuaries, and other coastal areas. The majority of these models are in the public domain and supported by federal agencies, usually the EPA or the USGS. The two most commonly used models for DO TMDL development are QUAL2E and HSPF. Intended users of these models are engineers, scientists, and regulatory agencies with some degree of modeling experience.

Although some DO models are no longer being updated, most models continue to be enhanced. For example, most now have graphical user interfaces (GUIs), which allow easier parameterization, calibration, and visualization of results. More importantly, however, the models continue to become more sophisticated and thus better able to simulate the natural environment. These advancements do not guarantee better application and better predictions from the models. This is dependent on proper parameterization, calibration, and validation of the models. In a companion article, Shirmohammadi et al. (2006) address issues of inappropriate use and uncertainty of model predictions.

Despite advancements, many DO models are still not capable of simulating some of the most complex drivers of DO dynamics, partly because the scientific community does not yet fully understand these processes, and continue to require user-estimated inputs for these processes. The most obvious example is SOD. Because these processes are complex and difficult to quantify, users are forced to rely on the few published data, which may or may not be applicable to their conditions. To overcome these limitations, future research must focus on understanding these processes and creating comprehensive and easily accessible databases of DO parameters.

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