

DEVELOPMENT AND APPLICATION OF A THREE DIMENSIONAL WATER QUALITY MODEL FOR A SHALLOW OXBOW LAKE

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ABSTRACT

A three-dimensional numerical model was developed for simulating the concentration of water quality constituents. Four interacting systems were simulated, including phytoplankton dynamics, nitrogen cycle, phosphorus cycles, and dissolved oxygen balance. The effects of suspended and bed sediment on the water quality were also considered. The model was tested using analytical solutions for the transport of non-conservative substances in open channel flow, then calibrated and applied to a shallow oxbow lake to simulate the concentration of phytoplankton (as chlorophyll) and nutrients. The simulated trends and magnitudes of water quality constituents were generally in good agreement with field observations.

1. INTRODUCTION

Agricultural activities are a major source of nonpoint-source pollution in the United States, contributing sediment, nutrients, and pesticides to aquatic ecosystems. The Mississippi Delta Management System Evaluation Area (MDMSEA) project is part of a national program designed to evaluate the impact of agricultural production on water quality and to develop best management practices (BMPs) to minimize adverse effects. Deep Hollow Lake, an oxbow lake located in Leflore County, Mississippi, was selected as a test location for MDMSEA. Deep Hollow receives runoff from a ~200 ha watershed which is heavily cultivated. Others have reported results of studies of inflow and in-lake water quality and fish (Rebich and Knight, 2001). Previous studies (Rebich and Knight, 2001) have shown that the concentration of suspended sediment is relatively high and exceeds the level for fish growth and health. In addition, the lake water quality is sensitive to suspended sediment concentrations because photosynthetic activity is limited by elevated turbidity levels following runoff events. Work by others in systems similar to Deep Hollow have shown that

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the nutrients may be released from suspended and bed sediments.

In the past few decades, many researchers have studied water quality characteristics of water bodies using numerical models (Cerco and Cole 1993, Gin et al 2001, Jin et al 1998). Some well-established models, such as WASP, CE-QUAL-ICM, RMA10, MIKE3, ECOM/RCA, CE-QUAL-W2, SMS are used currently to simulate variables in river, lake, estuary and ocean water quality. These models generally simulate the basic physical, chemical and biological processes of the aquatic ecosystems, but few consider the effects of sediment on the water quality constituents.

Two- and three-dimensional numerical models have already been developed and used to simulate flow fields and mass transport in Deep Hollow Lake (Zhu et al 2003, Chao et al 2004). The objective of this study is to develop a 3D water quality model for Deep Hollow Lake that reproduces the effects of sediment on the growth of phytoplankton, and the processes of adsorption-desorption and bed release of nutrients from sediment.

2. MODEL DESCRIPTION

The proposed 3D water quality model was developed to simulate the temporal and spatial variations of water quality with respect to phytoplankton, nutrients and DO. The model scheme generally followed WASP6 (Wool et al. 2001), including algorithms representing phytoplankton dynamics, N cycle, P cycles, and DO balance. Eight state variables were simulated in the proposed water quality model, including: ammonia nitrogen, nitrate nitrogen, inorganic phosphorus, phytoplankton, carbonaceous biochemical oxygen demand, DO, organic nitrogen, and organic phosphorus.

Sediment has been identified as one of the leading nonpoint-source pollutants in the United States. Excessive sediment reduces light penetration needed for the growth of phytoplankton. In addition, nutrients may be released from stream or lake beds. Furthermore, nutrients can interact with suspended sediments through the processes of adsorption and desorption in the water. To study those complex processes, the effects of sediment on the phytoplankton, nutrients and DO were considered in the water quality model.

2.1 Governing Equations

Each one of the water quality variables can be described by the following mass transport equation:

$$\frac{\partial C_i}{\partial t} + \frac{\partial(UC_i)}{\partial x} + \frac{\partial(VC_i)}{\partial y} + \frac{\partial(WC_i)}{\partial z} = \frac{\partial}{\partial x}(D_x \frac{\partial C_i}{\partial x}) + \frac{\partial}{\partial y}(D_y \frac{\partial C_i}{\partial y}) + \frac{\partial}{\partial z}(D_z \frac{\partial C_i}{\partial z}) + \sum S_i \quad (1)$$

in which U , V , W are the water velocity components in longitudinal(x), lateral(y) and vertical(z) directions, respectively; C_i is the concentration of the i th water quality constituent; D_x , D_y and D_z are the diffusion coefficients in x , y and z directions respectively; $\sum S_i$ is the effective source term, which includes the kinetic transformation rate, external loads and sinks for i th water quality constituent. Herein the velocity field was obtained from the 3-D hydrodynamic model CCHE3D (Jia et al. 1999)

2.2 Interaction Systems of the Water Quality Model

2.2.1 Phytoplankton kinetics

Phytoplankton, the group of planktonic plants that float in waters, plays a central role in the carbon and nutrient cycles that comprise the model ecosystem. The conceptual framework for

phytoplankton kinetics is mainly based on the models WASP6 (Wool et al 2001) and CE-QUAL-ICM (Cerco and Cole 1993). Total chlorophyll is used as an aggregated variable providing a simple measure of total phytoplankton biomass. The governing equation for phytoplankton concentration (as total chlorophyll) is shown in Eq. (1). The effective source terms can be obtained based upon growth and death rates.

$$\sum S_{chl} = [P_x - D_p] C_{chl} \quad (2)$$

in which P_x is the growth rate of phytoplankton (day^{-1}); D_p is the death rate of phytoplankton (day^{-1}); and C_{chl} is the concentration of chlorophyll ($\mu g/L$).

The growth rate of phytoplankton is determined by the availability of nutrients, the intensity of light, and by the ambient temperature. The effects of each factor are considered to be multiplicative:

$$P_x = P_{mx} f(N) f(I) f(T) \quad (3)$$

in which P_{mx} is the production under optimal conditions (day^{-1}); and $f(N)$, $f(I)$ and $f(T)$ are the limitations due to nutrient concentration, light intensity and temperature respectively. The limits $f(N)$, $f(I)$ and $f(T)$ may be calculated as follows:

$$f(N) = \min\left(\frac{CIN}{CIN + MIN}, \frac{CPH}{CPH + MPH}\right) \quad (4)$$

$$f(I) = \frac{2.72}{Kess\Delta z} \left[\exp\left(-\frac{I_0}{I_m} e^{-Kess(zd+\Delta z)}\right) - \exp\left(-\frac{I_0}{I_m} e^{Kess\cdot zd}\right) \right] \quad (5)$$

$$f(T) = \exp\left[-KTg_1(T - Tm)^2\right] \quad \text{when } T \leq Tm \quad (6a)$$

$$f(T) = \exp\left[-KTg_2(Tm - T)^2\right] \quad \text{when } T > Tm \quad (6b)$$

in which CIN and CPH are the concentration of inorganic nitrogen and phosphate, respectively; MIN and MPH are the half-saturation constants for N and P uptake respectively; Δz is the model segment thickness; zd is the distance from the water surface to the top level of a computational element in the water; I_0 is the daily illumination at the water surface; I_m is the light intensity required for maximum productivity; T is the temperature; Tm is the optimal temperature for phytoplankton growth; KTg_1 is the effect of temperature below Tm on growth and KTg_2 is the effect of temperature above Tm on growth; $Kess$ is the total light attenuation coefficient, and it is determined by the effects of water, chlorophyll and suspended sediment, and can be expressed by

$$Kess = K_0 + f(C_{chl}) + f(s) \quad (7)$$

where K_0 is the background light attenuation; $f(C_{chl})$ is the attenuation by chlorophyll; $f(s)$ is the attenuation by suspended sediment.

Phytoplankton losses mainly include endogenous respiration, mortality, grazing by herbivorous zooplankton and exudation. The death rate of phytoplankton is given as follows:

$$D_p = BM + PR \quad (8)$$

where BM and PR are the rates of basal metabolism and predation respectively. They can be given as:

$$BM = BMr \exp[KTb(T - Tr)] \quad (9)$$

$$PR = PRr \exp[KTb(T - Tr)] \quad (10)$$

where Tr is the reference temperature for metabolism; BMr is the metabolic rate at Tr ; KTb is the effect of temperature on metabolism; PRr is the predation rate at Tr .

2.2.2 Nutrient cycle

Ammonia and nitrate are taken up by phytoplankton for growth. For physiological reasons, NH_4 is the preferred form of inorganic nitrogen for phytoplankton. Nitrogen is returned from the phytoplankton biomass pool to particulate and dissolved organic nitrogen pools as a result of phytoplankton death and endogenous respiration and zooplankton grazing and mortality. Organic nitrogen is converted to NH_4 at a temperature-dependent mineralization rate, and NH_4 is then converted to NO_3 at a temperature- and oxygen-dependent nitrification rate. In the absence of oxygen, NO_3 can be converted to nitrogen gas (denitrification) at a temperature-dependent rate. Ammonia nitrogen may interact with sediment through the processes of adsorption and desorption. Dissolved inorganic and organic nitrogen at the bed sediment layer may also be released to the water column under certain conditions.

Phosphorus kinetics are basically similar to the nitrogen kinetics except there is no process analogous to denitrification. Inorganic phosphorus is utilized by phytoplankton for growth and is incorporated into phytoplankton biomass. Phosphorus is returned to the water column from dead or decaying phytoplankton biomass in the bed. The various forms of organic phosphorus undergo settling, hydrolysis and mineralization, and are converted to inorganic phosphorus at temperature-dependent rates. In addition, phosphorus may interact with sediment through the processes of adsorption, desorption and bed release.

2.2.3 BOD-DO balance

The sources of oxygen included in the model are atmospheric reaeration and phytoplankton photosynthesis. The sinks of oxygen include phytoplankton respiration, CBOD (carbonaceous biochemical oxygen demand), nitrification and sediment oxygen demand.

2.2.4 The processes of adsorption, desorption and bed release of nutrient by sediment

There is an adsorption-desorption interaction between dissolved nutrients and suspended sediment in the water column. Because the reaction rates for adsorption-desorption are much faster than that for the biological kinetics, an equilibrium assumption can be made (Wool et al. 2001). This assumption implies that the dissolved and particulate phases respond instantaneously to nutrient inputs (e.g., runoff or shoreline erosion) so as to redistribute the nutrients between the dissolved and solid-phase compartments. Thus, the processes of adsorption-desorption are assumed to reach equilibrium at each time step.

In some models, the adsorption-desorption of nutrients by sediment is described by a linear isotherm (Ishikawa and Nishimura 1989; Wool et al. 2001). Most experimental results show the Langmuir equilibrium isotherm is a better representation of the relations between the dissolved and particulate nutrient concentrations (Fox et al. 1989; Appan and Wang 2000; Bubba et al 2003). In

this study, the Langmuir equation was adopted to calculate the adsorption and desorption rate. The equilibrium adsorption content (Q) can be expressed as

$$Q = \frac{Q_m K C_d}{1 + K C_d} \quad (11)$$

where C_d is the dissolved nutrient concentration after the adsorption reaches equilibrium; Q_m is the maximum adsorption capacity; and K is the ratio of adsorption and desorption rate coefficients. It is assumed that the volume of the nutrient/water/sediment mixture solution is V_0 , which is a constant before and after adsorption. C_0 is the initial nutrient concentration at each time step in the solution, and s is the sediment concentration. Since the initial amount of nutrient in the solution is same as when the adsorption reaches equilibrium, it can be expressed as:

$$C_0 V_0 = C_d V_0 + s V_0 Q \quad \text{or} \quad C_d = C_0 - s Q \quad (12)$$

so

$$C_d = C_0 - C_p \quad (13)$$

where the particulate concentration C_p can be written as

$$C_p = s Q \quad (14)$$

By substituting Eqs.(13) and (14) into Eq.(11) and simplifying, it can be shown that:

$$C_p = \frac{1}{2} \left[\left(C_0 + \frac{1}{K} + s Q_m \right) - \sqrt{\left(C_0 + \frac{1}{K} - s Q_m \right)^2 + \frac{4 s Q_m}{K}} \right] \quad (15)$$

$$C_d = \frac{1}{2} \left[\left(C_0 - \frac{1}{K} - s Q_m \right) + \sqrt{\left(\frac{1}{K} + C_0 - s Q_m \right)^2 + \frac{4 s Q_m}{K}} \right] \quad (16)$$

Eqs. (15) and (16) are used to calculate the concentration of particulate and dissolved nutrients due to adsorption-desorption.

Bed release is an important source of inorganic and organic nutrient diffuses from bed sediment to the water column. The release rate of nutrients from the bed sediment layer is affected by the concentration gradient across the water-sediment interface, pH, temperature, DO concentration, as well as flow conditions. Based on Romero's study (2003), the bed release rate can be expressed as

$$S_{diff} = f(T_{sed}) S_c \left(\frac{K_{dos}}{K_{dos} + DO} + \frac{|pH - 7|}{K_{pHS} + |pH - 7|} \right) / \Delta z_b \quad (17)$$

where S_c is the diffusive flux of nutrient; K_{dos} and K_{pHS} are the values that regulate the release of nutrient according to the DO (DO) and pH in the bottom layer of the water column of depth Δz_b ; and $f(T_{sed})$ is the temperature coefficient.

2.3 Numerical Simulation

The proposed water quality model is decoupled with CCHE3D hydraulic model (Jia et al 2001). This model uses the Efficient Element Method, a special Finite Element technique. The grid system in the horizontal plane is a structured conformal mesh generated on the boundary of the computational domain. The mesh lines are generally placed with finer resolution near the wall, bed and free surface.

The unsteady equations are solved by using the time marching scheme. The velocity correction method has been applied to solve the dynamic pressure and enforce mass conservation. Provisional velocities have been solved first without the pressure term, and the final solution of the velocity is obtained by correcting the provisional velocities with the pressure solution (Jia et al 2001). The system of the algebraic equations is solved using the Strongly Implicit Procedure (SIP). Based on the flow fields computed by CCHE3D, the concentration distribution of water quality constituents in water column can be obtained by solving mass transport equations (1) numerically.

3. MODEL VERIFICATION

To verify the water quality model, simulation results were compared with test case results and analytical solutions.

3.1 Nonconservative Substance Transport – Steady Case

The numerical model was tested against an analytical solution for predicting concentrations of a non-conservative substance in a one-dimensional river flow with constant depth and velocity. At the middle of the river, there is a point source with constant concentration (Fig 1).

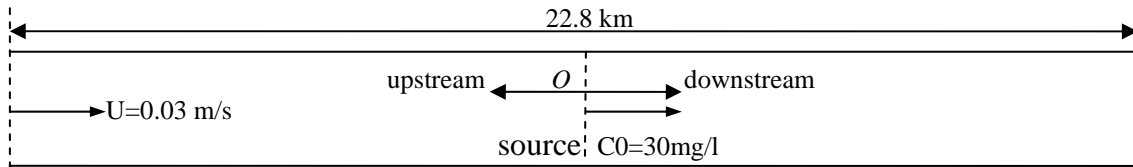


Fig. 1. Test river for case 3.1

Under the steady-state condition, the concentration of the substance throughout the river can be expressed as:

$$U \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} - KC \quad (18)$$

where U is the velocity; C is the substance concentration; C_0 is the concentration at O point; D_x is the dispersion coefficient; x is the displacement from O point; and K is the decay rate. An analytical solution given by Thomann and Mueller (1988) is:

$$C(x) = C_0 \exp \left[\left(\frac{u + \sqrt{u^2 + 4KD_x}}{2D_x} \right) x \right] \quad (\text{upstream, } x \leq 0) \quad (19)$$

$$C(x) = C_0 \exp\left[\left(\frac{u - \sqrt{u^2 + 4KD_x}}{2D_x}\right)x\right] \quad (\text{downstream, } x > 0) \quad (20)$$

For the hypothetical conditions shown in Fig. 1 and with depth = 10 m and $D_x=30 \text{ m}^2/\text{s}$, the values of $K = 0, 1.0/\text{day}$ and $2.0/\text{day}$, respectively, Fig. 2 shows the concentration distributions obtained by the numerical model and analytical solution. The maximum error is less than 3%.

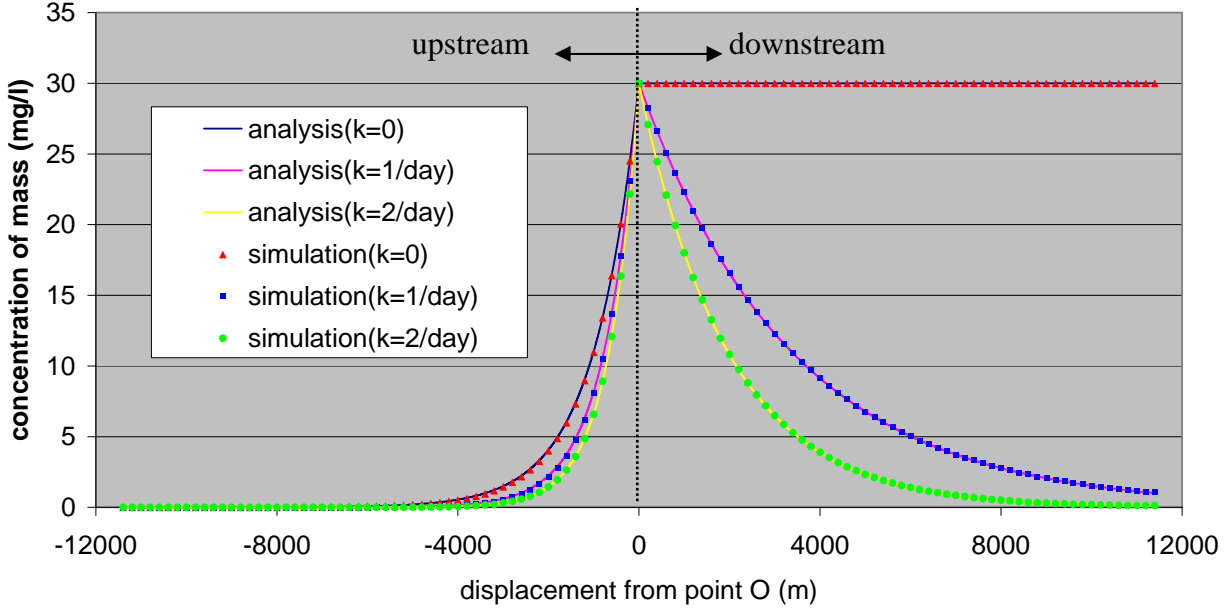


Fig. 2 The concentration distribution along the river

3.2 Nonconservative Substance Transport – Unsteady Case

The capability of the model to simulate unsteady, non-conservative mass transport in a one-dimensional river flow was tested. The hypothetical case involved a river as in the first case, but with a continuous source of a nonconservative substance for a finite period of time, τ . The mass transport equation for this case is:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} - KC \quad (21)$$

Chapra (1997) gave an analytical solution for this case:

$$C(x, t) = \frac{C_0}{2} \left[\exp\left(\frac{Ux}{2D_x}(1-\Gamma)\right) \operatorname{erfc}\left(\frac{x-Ut\Gamma}{2\sqrt{D_x t}}\right) + \exp\left(\frac{Ux}{2D_x}(1+\Gamma)\right) \operatorname{erfc}\left(\frac{x+Ut\Gamma}{2\sqrt{D_x t}}\right) \right] \quad (t < \tau) \quad (22)$$

$$C(x, t) = \frac{C_0}{2} \left\{ \exp\left(\frac{Ux}{2D_x}(1-\Gamma)\right) \left[\operatorname{erfc}\left(\frac{x-Ut\Gamma}{2\sqrt{D_x t}}\right) - \operatorname{erfc}\left(\frac{x-U(t-\tau)\Gamma}{2\sqrt{D_x(t-\tau)}}\right) \right] \right\}$$

$$+ \exp\left(\frac{Ux}{2D_x}(1+\Gamma)\right) \left[\operatorname{erfc}\left(\frac{x+U\Gamma}{2\sqrt{D_x t}}\right) - \operatorname{erfc}\left(\frac{x+U(t-\tau)\Gamma}{2\sqrt{D_x(t-\tau)}}\right) \right] \quad (t > \tau) \quad (23)$$

where $\Gamma = \sqrt{1+4\eta}$, and $\eta = \frac{KD_x}{U^2}$. For the river conditions shown in Fig. 3, with a depth of 10 m and $D_x=30 \text{ m}^2/\text{s}$, $\tau = 6 \text{ hr}$, and the values of $K = 0, 1.0/\text{day}$ and $2.0/\text{day}$, respectively. Fig. 4 shows the concentration at $x = 2000 \text{ m}$ obtained by the numerical model and by the analytical solution. Again, the maximum error is less than 3%.

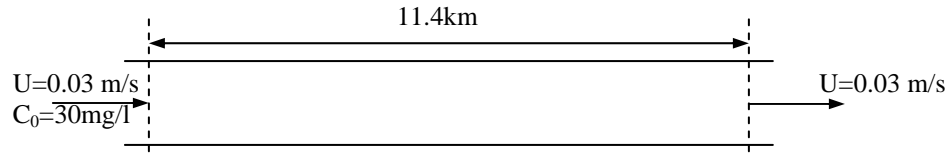


Fig. 3. Test river for case 3.2

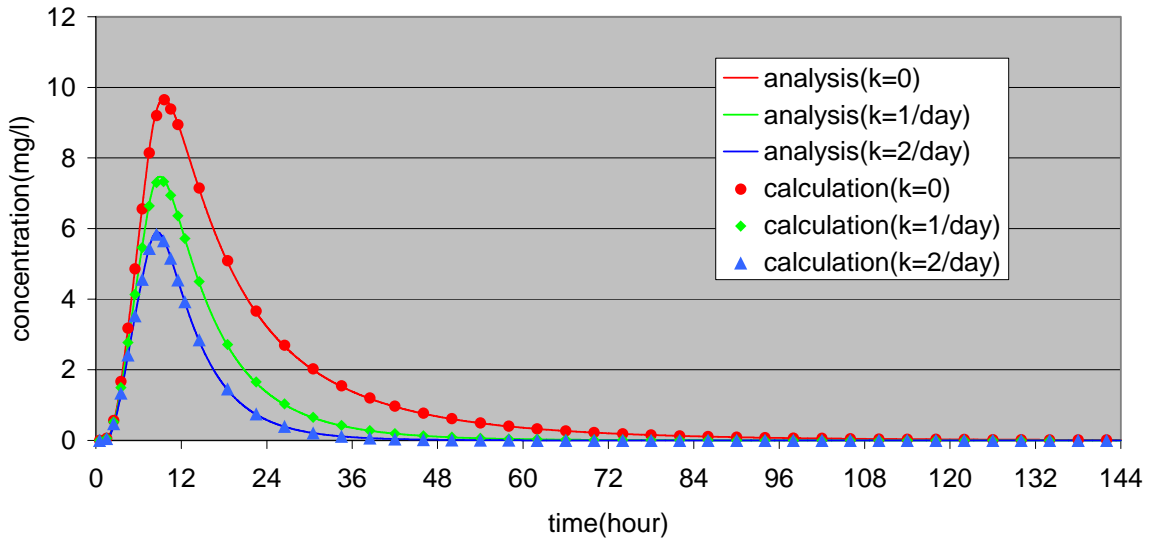


Fig. 4 The time serial concentration distribution at the section $x = 2000\text{m}$

4. MODEL APPLICATION TO THE DEEP HOLLOW LAKE

4.1 Study Area

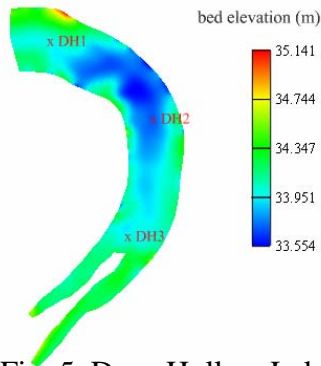


Fig. 5. Deep Hollow Lake

Fig. 5 shows the study area of Deep Hollow Lake. It has a morphology typical of an old oxbow lake, with a length of $\sim 1 \text{ km}$ and a width of $\sim 100 \text{ m}$. Lake water depth ranged from 0.5 m to 2.6 m , with greatest depth in the middle. Stations DH1, DH2 and DH3 were sampled weekly or biweekly for suspended sediment, nutrients, chlorophyll, bacteria, and other selected water quality variables (Rebich and Knight, 2001). The lake was bordered by a wooded buffer, likely mediating the wind-driven currents. Two of the major inflows (ephemeral channels draining

agricultural fields) were monitored for water quality and quantity by the U.S. Geological Survey (Rebich and Knight, 2001), and the inlet boundaries of water quality constituents were calculated based on those field measurements.

The nutrient levels in Deep Hollow Lake are mainly dependent on the fertilizer loadings in the surrounding farmland and the quantity of runoff. Suspended sediment concentrations are relatively high, exceeding published levels for fish growth and health (Rebich and Knight 2001). Field measurements also show that the concentrations of nitrate and ammonia in the lake are very low, while the concentration of phosphorus is relatively high in comparison with other areas of USA. The available field measurements at these three stations were used for model calibration and validation. In general, the data show that water quality conditions at the three stations are similar. Only data from Station DH1 are presented here.

Based on bathymetric data, the computational domain was discretized into a conformal grid using the CCHE Mesh Generator. In the horizontal plane, the computational domain was represented by a 95×20 irregular structure mesh. In the vertical direction, it was divided into 8 levels with finer spacing near the bed.

4.2 Model Calibration

The proposed water quality model was calibrated using biweekly field data and analysis of lake water samples obtained between April to June, 1999. For calibration runs, water currents induced by wind and runoff were obtained from runs of CCHE3D (Jia et al. 2001 and Chao et al. 2004). Much adjustment of model parameters was required to obtain reasonable agreement between the numerical results and field data. In addition, supplemental data were collected in order to develop a predictive relationship for the light attenuation coefficient K_{ess} in Eq. (5). Wool et al.(2001) proposed a formula for K_{ess} based on the sum of the background light attenuation, K_0 and the phytoplankton self-shading attenuation, but ignoring the effect of suspended sediment:

$$K_{ess} = K_0 + 0.0088C_{chl} + 0.054C_{chl}^{0.67} \quad (24)$$

In fact, the suspended sediment increases both the surface reflectivity and light attenuation in the water. To obtain a more reasonable formula for application to Deep Hollow Lake, the National Sedimentation Laboratory concurrently measured the distribution of light intensity along the water column and the concentrations of suspended sediment and chlorophyll. Measured light attenuation coefficients ranged from 9 to 20 m^{-1} . Given the form of the relationships in Eq. (7) above, and work by Stefan (1983) that showed attenuation by suspended sediment can be given by:

$$f(s) = \alpha s \quad (25)$$

where s is the concentration of suspended sediment and α is a coefficient, Eq (7) can be written as

$$K_{ess} = 1.2 + 0.0088C_{chl} + 0.054C_{chl}^{0.67} + 0.0458s \quad (26)$$

The adsorption and desorption of ammonium nitrogen and phosphate by sediment was simulated by the Langmuir equation. For Deep Hollow Lake, the concentration of ammonium is very low, so the ammonium adsorption and desorption from sediment was expected to be insignificant and was not incorporated. At equilibrium, the concentration of dissolved and particulate phosphate due to adsorption-desorption was calculated using Eqs. (15) and (16). Dissolved inorganic and organic nutrients at the bed sediment layer may also be released to the

water column. In the proposed model, ammonium, nitrite, organic nitrogen, phosphate, and organic phosphorus were calculated using Eq (17).

Since there was not enough measured data in Deep Hollow Lake, the authors had to borrow some other measured results obtained from laboratory experiments and field observations to simulate the processes of adsorption-desorption and bed release (Portielje and Lijklema 1993; DiToro 2001; Wool et al. 2001; Hipsey et al. 2003; Bubba et al. 2003).

The calibration results of the proposed water quality model at DH1 Station were shown in Figs. 6, 7 and 8. It can be observed that good agreements for chlorophyll and nutrients between the numerical results and field measurements are obtained.

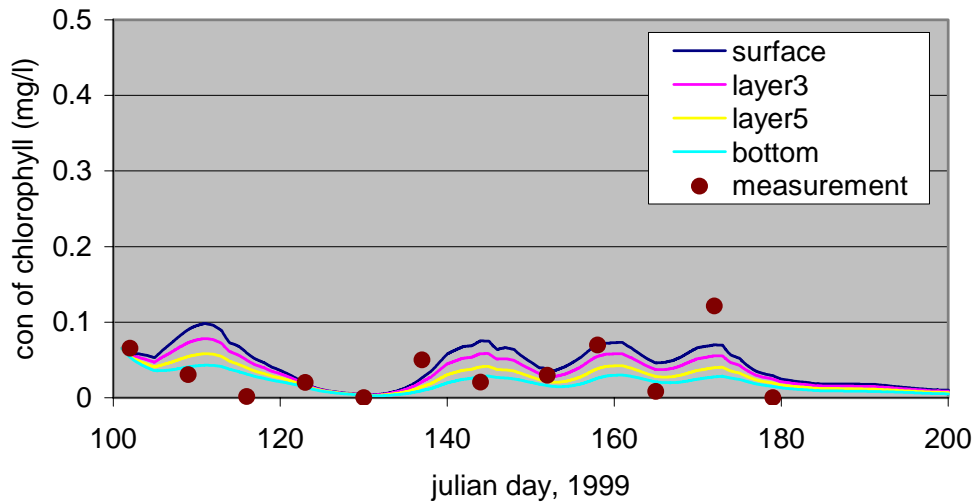


Fig. 6 The concentration of chlorophyll at Station DH1(calibration)

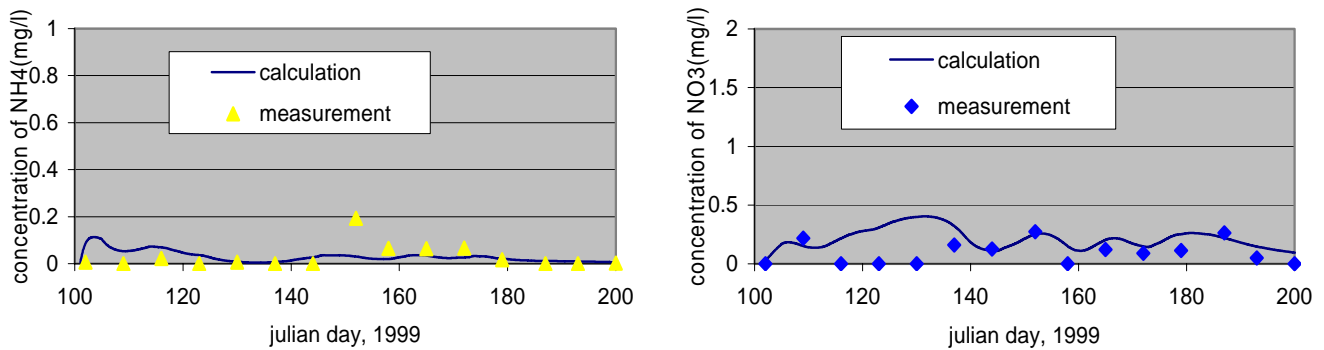


Fig. 7 The concentration of nitrogen at Station DH1 (calibration)

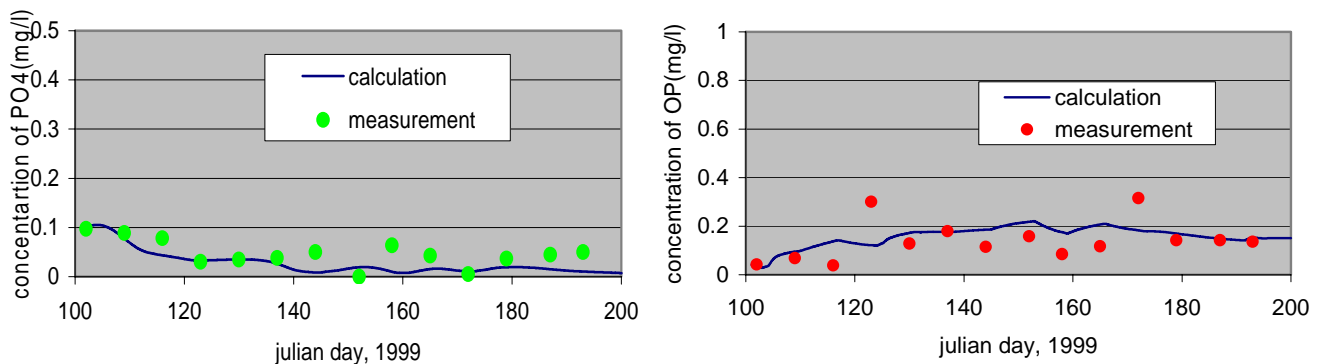


Fig. 8 The concentration of phosphorus at Station DH1 (calibration)

4.3 Model validation

The period from September to December 1999 was chosen for model validation. Flow currents, boundary conditions, weather data and suspended sediment concentrations were provided to the model as inputs and concentrations of other water quality constituents were predicted. Parameter values in the water quality model were held equal to the April – June 1999 calibrated values. Figs. 9 and 10 show the simulated and observed concentrations of chlorophyll and nitrogen. Some differences between measurement and prediction may arise from the fact that measurements occurred weekly while the time step for the simulation was 3600 seconds. However, trends and quantities of concentration of chlorophyll and nutrients obtained from the numerical model were generally in agreement with the observations.

Fig. 11 shows the simulated and observed concentrations of ortho-phosphorus and total organic phosphorus, respectively. Without considering the processes of adsorption, desorption and bed release, the model overestimated ortho-phosphorus concentration and underestimated organic phosphorus. After considering those processes, the root mean square error (RMSE) of ortho-phosphorus was reduced from 0.029 to 0.019, and for organic phosphorus was reduced from 0.051 to 0.037.

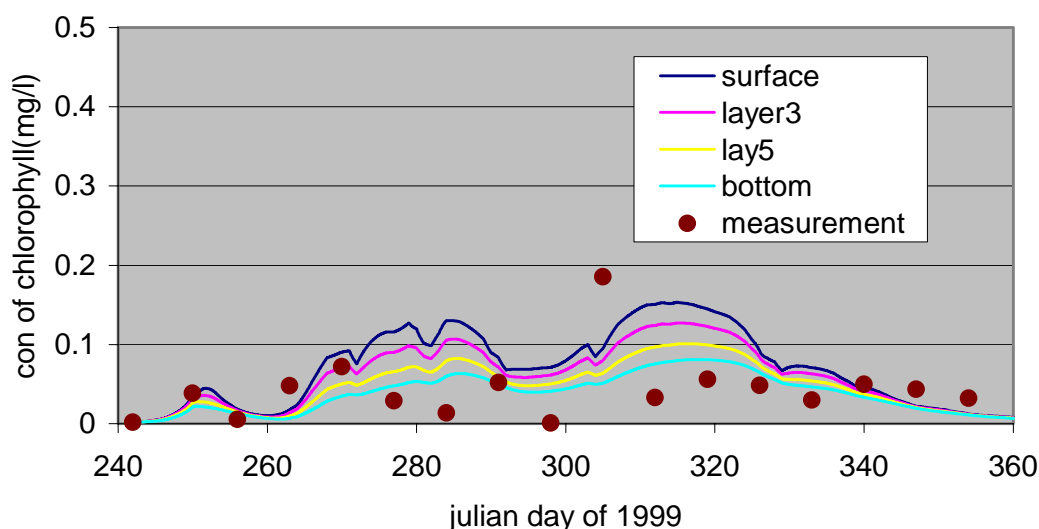


Fig. 9 The concentration of chlorophyll at Station DH1(validation)

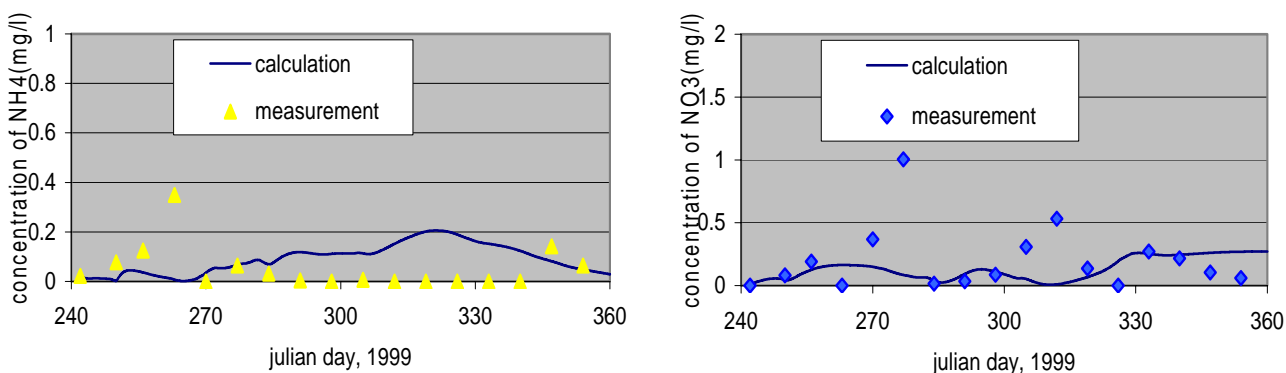


Fig. 10 The concentration of nitrogen at Station DH1 (validation)

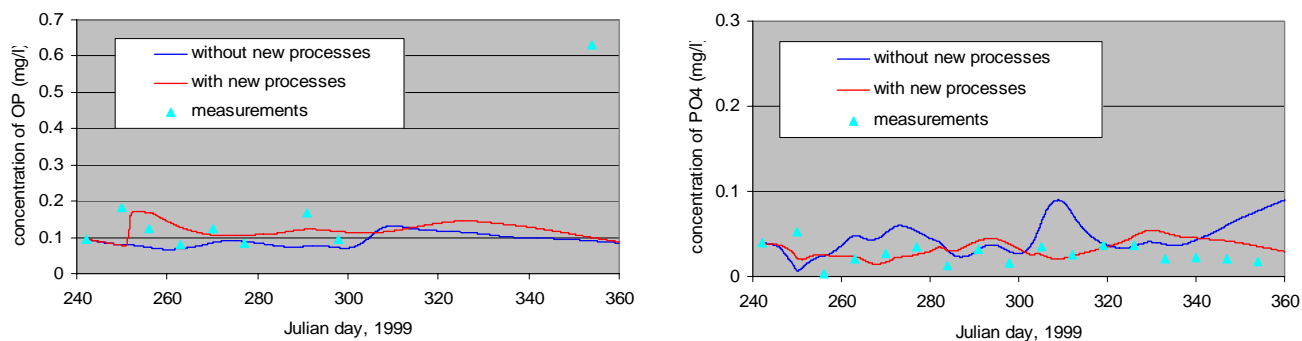


Fig. 11 The concentration of phosphorus at Station DH1(validation)

SUMMARY AND CONCLUSIONS

A three-dimensional numerical model was developed to simulate the concentration of water quality constituents in shallow oxbow lakes where sediment-related processes are important. In this model the effects of sediment on the growth of phytoplankton, and the processes of adsorption-desorption and bed release of nutrients from sediment were simulated. The model was verified using analytical solutions of pollutant transport in open channel flow, and the agreement between computed and theoretical solutions was excellent. The model was successfully applied to simulate the concentration of water quality constituents in Deep Hollow Lake. Trends and magnitudes of nutrient and phytoplankton concentrations obtained from the numerical model generally agreed with field observations. Since these concentrations are governed by agricultural practices, the model described here may be used to assess effects of agricultural conservation measures on adjacent shallow lake ecosystems.

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