Supplementary Materials:

Explore the nonlinear water quality response to an in-situ phosphorus control method through numerical simulation

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Supplementary Material I: Basic description of EFDC

This document won't present all the equations and numerical schemes here for the sake of simplicity, but only sketch the framework of EFDC, more detailed information cloud be found in Hamrick (1992) and Park et al. (1995). The hydrodynamic model, water quality model, and endogenous dynamics model are tightly coupled in EFDC. The water quality and endogenous dynamics simulation provide data to each other, and both them require the output of hydrodynamic simulation. The general governing equation of the water quality module of EFDC can be mathematically represented as:

$$\frac{\partial(m_x m_y HC)}{\partial t}+\frac{\partial(m_y HuC)}{\partial x}+\frac{\partial(m_x HvC)}{\partial y}+\frac{\partial(m_x m_y wC)}{\partial z}=$$

$$\frac{\partial}{\partial x}\left(\frac{m_y HA_x}{m_x}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{m_x HA_y}{m_y}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(m_x m_y\frac{A_z}{H}\frac{\partial C}{\partial z}\right)+m_x m_y HS_c \tag{1}$$

where C is a state variable represents the concentration of water quality; u, v, w represents velocity components in the curvilinear, sigma x-, y-, and z-directions, respectively; A_x, A_y, A_z represents turbulent diffusivities in the x-, y-, and z-directions, respectively; S_c represents internal and external sources and sinks per unit volume; H means water column depth; mx, my denote horizontal curvilinear coordinate scale factors.

The last three terms on the left-hand side of Eq. (1) account for transport and the first three terms on the righthand side account for diffusive transport. These six terms for physical transport are solved using the same numerical method for temperature and salinity in the hydrodynamic model (Hamrick 1992). The last term in Eq. (1) represents the kinetic processes and external loads for each of the state variables. In EFDC, Eq. (1) is solved using a fractional step procedure that decouples the kinetic terms from the physical transport terms:

$$\frac{\partial(m_x m_y HC)}{\partial t_p}+\frac{\partial(m_y HuC)}{\partial x}+\frac{\partial(m_x HvC)}{\partial y}+\frac{\partial(m_x m_y wC)}{\partial z}=$$

$$\frac{\partial}{\partial x}\left(\frac{m_y HA_x}{m_x}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{m_x HA_y}{m_y}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(m_x m_y\frac{A_z}{H}\frac{\partial C}{\partial z}\right)+m_x m_y HS_{cp} \tag{2}$$

$$\frac{\partial C}{\partial t_K}=\mathrm{S}_{CK} \tag{3}$$

Leading to:

$$\frac{\partial(m_x m_y HC)}{\partial t}=\frac{\partial(m_x m_y HC)}{\partial t_p}+(m_x m_y H)\frac{\partial C}{\partial t_K} \tag{4}$$

In Eqs. (2) and (3), the source–sink term in Eq. (1) has been split into physical sources and sinks (S_{CP}), which are associated in volumetric inflows and outflows, and kinetic sources and sinks (S_{CK}).

The main steps for conducting EFDC include grid generation and preprocessing, input file preparation, code compiling and executing, diagnostic options and output, time series output and analysis, results output and visualization (Hamrick 1992). EFDC simulates 21 water column state variables as listed in Table 1. Water temperatures are needed for computation of the water quality state variables and they are provided by the internally coupled hydrodynamic model.

In addition to representing the water column dynamics, a predictive water quality model must quantitatively represent the interactions between the water column and sediment in evaluating the response of water quality to external loadings for water bodies when internal nutrient loadings from sediments are significant. With highly enriched sediment of Xingyun Lake, the internal nutrient loading from the benthic flux can be a significant contributor to the long-term eutrophication problem in the lake. Therefore, a critical component of the water quality model for Xingyun Lake is to have the capability of simulating the interactions between the sediment bed and water column water quality. The modeling framework for the sediment-water interaction simulation is the sediment diagenesis module in EFDC, which has 27 state variables representing the kinetic processes occurring in the sediment bed. The sediment module, upon receiving the particulate organic matter deposited from the overlying water column, simulates the diagenesis and the resulting fluxes of inorganic substances (phosphate, ammonium, nitrate, and silica) and sediment oxygen demand (SOD) back to the water column. The coupling of the sediment process model with the water column eutrophication model allows the water quality model to have a predictive capability that enables long-term simulations of water quality following various load reduction conditions (Park et al. 1995).

Table 1 EFDC model water quality state variables (Wang et al., 2014)

(1) Algae group 1 (Bc)	(12) Labile particulate organic nitrogen (LPON)
(2) Algae group 2 (Bd)	(13) Dissolved organic nitrogen (DON)
(3) Algae group 2 (Bg)	(14) Ammonia nitrogen (NH_4)
(4) Refractory particulate organic carbon (RPOC)	(15) Nitrate nitrogen (NO_3)
(5) Labile particulate organic carbon (LPOC)	(16) Particulate biogenic silica (SU)
(6) Dissolved organic carbon (DOC)	(17) Dissolved available silica (SA)
(7) Refractory particulate organic phosphorus (RPOP)	(18) Chemical oxygen demand (COD)
(8) Labile particulate organic phosphorus (LPOP)	(19) Dissolved oxygen (DO)
(9) Dissolved organic phosphorus (DOP)	(20) Total active metal (TAM)
(10) Total phosphate (PO_4t)	(21) Fecal coliform bacteria (FCB)
(11) Refractory particulate organic nitrogen (RPON)	(22) Macrophyte/periphyton (Bm)

References:

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Hamrick JM (1992) A three-dimensional environmental fluid dynamics computer code: theorectical and computational aspects.Special paper 317, the College of William and Mary, Virginia Institute of Marine Science, Williamsburg.

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Supplementary Material II: Phoslock module

1. Phoslock transport in water

The development of Phoslock module is based on the knowledge of the phoslock's behavior in water. Generally speaking, after spraying the phoslock into lake, the physical and chemical processes of dissolution, diffusion, PO_4^{3-} adsorption, and settlement are happened in sequence. In particularly, the fine simulation of PO_4^{3-} adsorption and settlement is realized by parameterizing the solubility of phoslock under different dissolved oxygen level, the sedimentation rate after phoslock combined with PO_4^{3-}, the potential phosphorus locking capacity of phoslock, the semi-saturated PO_4^{3-} conc of phosphorus locking coefficient and other relevant factors. The hydrodynamic and water quality model provide the essential data for quantifying the processes, such as the flow, dissolved oxygen, PO_4^{3-} conc, water temperature and so on. Design parameters such as the positions, the dose, the starting and ending time of the phoslock release are also set in the phoslock module.

For considering the influence of the topography of the lake bottom on the flow, the model uses the sigma coordinate in the vertical direction. In other words, the free surface and the lakebed are respectively mapped to Z = 1 and z = 0 in Cartesian coordinates. This approach not only reflects the smooth terrain and has the same order of accuracy for shallow water and deep water, but also saves computing resources. The σ coordinate system is defined as follows:

$$\boldsymbol{z} = \frac{\boldsymbol{z^{*}+h}}{\boldsymbol{\xi+h}} \tag{1}$$

where z^* represents the original vertical physical coordinate; z represents the ordinate under the σ coordinate; ξ denotes the water surface elevation and h is the lakebed elevation. The value range of z is [0, 1].

Based on Boussinesq approximation and quasi-static assumption, momentum equation, continuity equation, state equation, phoslock transport equation are as follows.

(a) Momentum equation

$$\frac{\partial(mHu)}{\partial t} + \frac{\partial(m_yHuu)}{\partial x} + \frac{\partial(m_xHvu)}{\partial y} + \frac{\partial(mwu)}{\partial z} - \left(mf + v\frac{\partial m_y}{\partial x} - u\frac{\partial m_x}{\partial y}\right)\mathrm{Hv} =$$
$$-m_yH\frac{\partial(g\zeta+P)}{\partial x} - m_y\left(\frac{\partial \hbar}{\partial x} - z\frac{\partial H}{\partial x}\right)\frac{\partial p}{\partial z} + \frac{\partial}{\partial z}\left(m\frac{1}{H}A_v\frac{\partial u}{\partial z}\right) + Q_u \tag{2}$$

$$\frac{\partial(mHv)}{\partial t} + \frac{\partial(m_yHuv)}{\partial x} + \frac{\partial(m_xHvv)}{\partial y} + \frac{\partial(mwv)}{\partial z} + \left(mf + v\frac{\partial m_y}{\partial x} - u\frac{\partial m_x}{\partial y}\right)\mathrm{Hu} =$$
$$-m_xH\frac{\partial(g\zeta+P)}{\partial y} - m_x\left(\frac{\partial \hbar}{\partial y} - z\frac{\partial H}{\partial y}\right)\frac{\partial p}{\partial z} + \frac{\partial}{\partial z}\left(m\frac{1}{H}A_v\frac{\partial v}{\partial z}\right) + Q_v \tag{3}$$

$$\frac{\partial(m\zeta)}{\partial t} = -\frac{\mathrm{gH}(\rho-\rho_0)}{\rho_0} = -gHb \tag{4}$$

(b) Continuity equation

$$\frac{\partial m\xi}{\partial t} + \frac{\partial m_yHu}{\partial x} + \frac{\partial m_xHv}{\partial y} + \frac{\partial mw}{\partial z} = Q_H \tag{5}$$

$$\frac{\partial(m\zeta)}{\partial t} = -\frac{\mathrm{gH}(\rho-\rho_0)}{\rho_0} = -gHb \tag{6}$$

(c) State equation

$$\rho = \rho(S,\ T) \tag{7}$$

(d) Phoslock transport equation

$$\frac{\partial(m\Theta)}{\partial t}+\frac{\partial(m_yHu\Theta)}{\partial x}+\frac{\partial(m_xHv\Theta)}{\partial y}+\frac{\partial(mw\Theta)}{\partial z}=\frac{\partial}{\partial z}\left(m\frac{1}{H}A_b\frac{\partial\Theta}{\partial z}\right)+Q_\Theta \quad (8)$$

In the horizontal direction, X and Y orthogonal curvilinear coordinates are used, u and V represent the velocity components in X and Y directions of orthogonal curvilinear coordinates; W denotes the velocity in Z direction after vertical transformation; mx and my represent the square root of diagonal elements of metric tensor respectively; m equals the square root of determinant of metric tensor; A_v represents the vertical turbulent vortex viscosity coefficient; A_b denotes the vertical turbulent diffusion coefficient; f represents the Coriolis coefficient; P is the pressure; ρ and ρ_0 represent the mixing density and reference density respectively; S and T represent the salinity and temperature; Θ denotes S or T; Q_u and Q_v represent the source and sink term of momentum in X and Y directions; Q_Θ is the source and sink term of phoslock. The Q_H in equation 13 could be used as rainfall, evaporation, groundwater exchange, water intake, other point sources and non-point sources.

2. Forms and transformation of phosphorus in water

There are four phosphorus variables in the model which represent the sum of dissolved and particulate phosphorus in the aqueous phase, but excluding phosphorus in algae cells, these variables are inert organic phosphorus, unstable organic phosphorus, dissolved organic phosphorus and inorganic phosphorus, which expressed as the equations below.

(a) Particulate phosphorus

The sources and sinks of particulate phosphorus in the model are: algae metabolism and excretion, particulate organic phosphorus decomposition, precipitation and exogenous load. The kinetic equation of inert and unstable particulate organic phosphorus is as follows:

$$\frac{\partial RPOP}{\partial t}=\sum_{x=c,d,g,m}(FPR_x\cdot BM_x+FPRP_x\cdot PR_x)\cdot APC_x\cdot B_x$$
$$-K_{RPOP}\cdot RPOP+\frac{\partial}{\partial Z}(WS_{RP}\cdot RPOP)+\frac{WRPOP}{V} \quad (9)$$
$$\frac{\partial LPOP}{\partial t}=\sum_{x=c,d,g,m}(FPL_x\cdot BM_x+FPLP_x\cdot PR_x)\cdot APC_x\cdot B_x$$
$$-K_{LPOP}\cdot LPOP+\frac{\partial}{\partial Z}(WS_{LP}\cdot LPOP)+\frac{WLPOP}{V} \quad (10)$$

where RPOP represents the concentration of inert particulate organic phosphorus; LPOP represents the concentration of unstable particulate organic phosphorus; FPR_x represents the fraction of inert particulate organic phosphorus produced by the metabolism of algae; FPL_x represents the fraction of unstable particulate organic phosphorus produced by the metabolism of algae; FPRP represents the fraction of inert particulate organic phosphorus produced by predation; FPLP represents the fraction of unstable particulate organic phosphorus produced by predation; APC represents the average ratio of phosphorus to carbon of all algae; K_{RPOP} represents the hydrolysis rate of inert particulate organic phosphorus; K_{LPOP} represents the hydrolysis rate of unstable particulate organic phosphorus; WRPOP represents the external load of inert particulate organic phosphorus; WLPOP represents the exogenous load of unstable particulate organic phosphorus.

(b) Dissolved organic phosphorus

The sources and sinks of soluble organic phosphorus in the model consist of algae metabolism and excretion, decomposition of inert and unstable organic phosphorus, mineralization to phosphate, and external load. The dynamic equation describing this process is:

$$\frac{\partial DOP}{\partial t}=\sum_{x=c,d,g,m}(FPD_x\cdot BM_x+FPDP_x\cdot PR_x)\cdot APC_x\cdot B_x \quad (11)$$
$$+K_{RPOP}\cdot RPOP+K_{LPOP}\cdot LPOP-K_{DOP}\cdot DOP+\frac{WDOP}{V}$$

where DOP represents the concentration of dissolved organic phosphorus; FPD_x represents the fraction of dissolved organic phosphorus produced by algae metabolism; $FPDP_x$ represents the fraction of dissolved organic phosphorus produced by predation; K_{DOP} represents the mineralization rate of dissolved organic phosphorus; WDOP denotes the external load of dissolved organic phosphorus.

(c) Total phosphate

Total phosphate includes dissolved and adsorbed phosphorus in aqueous phase. The sources and sinks included in the model are: basic metabolism, predation and ingestion of algae; mineralization of dissolved organic phosphorus; deposition of adsorbed phosphorus; exchange between bottom sediment and soluble phosphate; and exogenous load. These processes are expressed by kinetic equations as:

$$\frac{\partial}{\partial t}(PO_4p + PO_4d) = \sum_{x=c,d,g,m}(FPI_x \cdot BM_x + FPIP_x \cdot PR_x - P_x) \cdot APC_x \cdot B_x$$

$$+K_{DOP} \cdot DOP + \frac{\partial}{\partial Z}(WS_{TSS} \cdot PO_4p) + \frac{BFPO_4d}{\Delta Z} + \frac{WPO_4p}{V} + \frac{WPO_4d}{V} \tag{12}$$

where PO_4d and PO_4p represents dissolved phosphate and particulate (adsorbed) phosphate respectively; FPI represents the fraction of inorganic phosphorus produced by algae metabolism; FPIP represents the fraction of inorganic phosphorus produced by predation; WSTSS represents suspended solid sedimentation rate, provided by hydrodynamics model; $BFPO_4d$ represents the coefficient of phosphate sediment exchanging with water; WPO_4p and WPO_4d represents the dissolved phosphate and particulate phosphate external load.

(d) Mineralization and hydrolysis

$$K_{RPOP} = \left(K_{RP} + \left(\frac{KHP}{KHP + PO_4d}\right)K_{RPalg}\sum_{x=c,d,g,m}B_x\right)exp\left(KT_{HDR}(T - TR_{HDR})\right) \tag{13}$$

$$K_{LPOP} = \left(K_{LP} + \left(\frac{KHP}{KHP + PO_4d}\right)K_{LPalg}\sum_{x=c,d,g,m}B_x\right)exp\left(KT_{HDR}(T - TR_{HDR})\right) \tag{14}$$

$$K_{DOP} = \left(K_{DP} + \left(\frac{KHP}{KHP + PO_4d}\right)K_{DPalg}\sum_{x=c,d,g,m}B_x\right)exp\left(KT_{HDR}(T - TR_{HDR})\right) \tag{15}$$

where K_{RP} represents the minimum hydrolysis rate of inert particulate organic phosphorus; K_{LP} represents the minimum hydrolysis rate of unstable particulate organic phosphorus; K_{DP} represents the minimum mineralization rate of dissolved organic phosphorus; K_{RPalg} and K_{LPalg} represent the correlation constants between the hydrolysis process of inert and unstable organic phosphorus and algae biomass respectively; KHP represents the average half saturation constant of phosphorus fed by algae.