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Integrated water system simulation by considering hydrological and biogeochemical processes: model development, with parameter sensitivity and autocalibration

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Supplementary material

1. Soil P cycle simulation (Neitsch *et al.*, 2011)

Mineralization: The mineralized P is added to the solution P pool, and the amounts of active and stable organic P pools ($orgP_{act}$ and $orgP_{sta}$, kg/ha) are calculated by

$$\begin{cases} orgP_{act} = orgP_{hum} \cdot orgN_{act} / (orgN_{act} + orgN_{sta}) \\ orgP_{sta} = orgP_{hum} \cdot orgN_{sta} / (orgN_{act} + orgN_{sta}) \end{cases} \quad \text{(S1)}$$

where $orgP_{hum}$ is the humic organic P amount (kg/ha); $orgN_{act}$ and $orgN_{sta}$ are the amounts of N in the active organic pool and stable organic pool (kg/ha), respectively, which are simulated by DNDC.

The mineralization rate of the humus active organic P pool (*RHP*) is calculated by

$$\begin{cases} RHP = 1.4 \cdot \beta_{\min} \cdot (\gamma_{tmp} \cdot \gamma_{SW})^{1/2} \\ \gamma_{tmp} = 0.9 \cdot T_{soil} / [T_{soil} + \exp(9.93 - 0.312 \cdot T_{soil})] \\ \gamma_{SW} = SW / W_{sat} \end{cases} \quad \text{(S2)}$$

where β_{min} is the mineralization rate of the humus active organic P; γ_{tmp} and γ_{SW} are the reduction factors of soil temperature and moisture, respectively.

The mineralization rate of the residue fresh organic P pool (*RRP*) is calculated by

$$RRP = 0.8 \cdot \delta_P = 0.8 \cdot \beta_{rsd} \cdot (\gamma_{tmp} \cdot \gamma_{SW})^{1/2} \quad \text{(S3)}$$

where δ_P and β_{rsd} are the decay rate and the mineralization rate of the residue fresh organic P, respectively.

Decomposition: The decomposition rate of the residue fresh organic P pool (*DRP*) is given as

$$DRP = 0.2 \cdot \delta_P \quad \text{(S4)}$$

Sorption: The P movement between the dissolved and active mineral pools ($P_{dis|act}$, kg/ha) and between active and stable mineral pools ($P_{act|sta}$, kg/ha) are

$$P_{dis|act} = \begin{cases} P_{dis} - \min P_{act} \cdot pai / (1 - pai) & if \quad P_{dis} > \min P_{act} \cdot pai / (1 - pai) \\ 0.1 \cdot [P_{dis} - \min P_{act} \cdot pai / (1 - pai)] & if \quad P_{dis} < \min P_{act} \cdot pai / (1 - pai) \end{cases} \quad \text{(S5)}$$

and

$$P_{act|sta} = \begin{cases} 0.0006 \cdot (4 \cdot \min P_{act} - \min P_{sta}) & if \quad \min P_{sta} < 4 \cdot \min P_{act} \\ 0.00006 \cdot \beta_{eqP} \cdot (4 \cdot \min P_{act} - \min P_{sta}) & if \quad \min P_{sta} > 4 \cdot \min P_{act} \end{cases} \quad \text{(S6)}$$

respectively. Here P_{sol}, $minP_{act}$ and $minP_{sta}$ are the amounts of dissolved, mineral active and stable P (kg/ha), respectively; and *pai* is the P availability index.

2. Crop growth module

2.1 Crop yield (Williams *et al.*, 1989)

The crop growth depends on the accumulation of thermal time (Sharpley and Williams, 1990). The daily thermal time (HU, °C) and the thermal time index for j^{th} crop (HUI) are calculated as:

$$\begin{cases} HU_K = (T_{mx,K} + T_{mn,K})/2 - T_{b,j} \\ HUI_i = \sum_{K=1}^{i} HU_K \Big/ PHU_j \end{cases} \quad \text{(S7)}$$

where $T_{mx,K}$ and $T_{mn,K}$ are the maximum and minimum temperatures (°C) on the K^{th} day, respectively; $T_{b,j}$ is the base temperature of the j^{th} crop (°C). Crop growth will stop when HU_K is below 0.0. PHU_j is the required cumulative thermal time for the j^{th} crop from sowing to physical maturity (°C). The range of HUI is from 0.0 at sowing to 1.0 at maturity. i is the total days of crop growth.

The daily potential biomass accumulation (ΔB_p, t/ha/d) is estimated as:

$$\begin{aligned} \Delta B_{p,i} &= 0.001 \cdot BE_i \cdot PAR_i \cdot [1 + \Delta HRLT_i]^3 \\ &= 0.0005 \cdot BE_i \cdot RA_i \cdot [1 - \exp(-0.65 \cdot LAI)] \cdot [1 + \Delta HRLT_i]^3 \end{aligned} \quad \text{(S8)}$$

where BE is the crop parameter for converting energy to biomass (kg·ha·m^2/MJ); $HRLT$ and $\Delta HRLT$ are the length of a day (hr) and its variation (hr/d), respectively; PAR is the intercepted photosynthetic active radiation (MJ/m^2). RA is the solar radiation (MJ/m^2). LAI is the leaf area index (m^2/m^2), which is a function of heat units, crop stress and crop development stages.

From emergence to the start of leaf decline, LAI is estimated by the following equation:

$$LAI_i = LAI_{i-1} + \Delta LAI \\ = LAI_{i-1} + (\Delta HUF)(LAI_{mx})(1-\exp(5\cdot(LAI_{i-1} - LAI_{mx})))\cdot\sqrt{REG_i} \tag{S9}$$

From the start of leaf decline to the end of the growing season,

$$LAI_i = LAI_0 \cdot \left(1 - HUI_i / 1 - HUI_0\right)^{ad_j} \tag{S10}$$

where HUF is a thermal time factor; REG is the minimum crop stress factor; ad is a parameter controlling LAI decline rate for crop j; HUI_0 is the HUI value when LAI begins to decline.

The biomass accumulation is constrained by the stresses of soil water, temperature, and nutrients (N and P).

$$\Delta B = \Delta B_p \cdot REG = \Delta B_p \cdot \min(WS, TS, SN, SP) \tag{S11}$$

where REG is the crop growth regulating factor.

The water stress: $WS_i = \sum_{l=1}^{M} U_{l,i} \Big/ E_{P,i}$ (S12)

The temperature stress: $TS_i = \sin[\pi\cdot(T_{soil,i} - T_{b,j})/2(T_{o,j} - T_{b,j})] \quad 0 \le TS_i \le 1$ (S13)

The N stress: $\begin{cases} SN_{S,i} = 2[1 - \sum_{K=1}^{i} UN_K \Big/ (c_{NB,i}\cdot B_i)] \\ SN_i = 1 - SN_{S,i}/[SN_{S,i} + \exp(3.39 - 10.93 SN_{S,i})] \end{cases}$ (S14)

The P stress: $\begin{cases} SP_{S,i} = 2[1 - \sum_{K=1}^{i} UP_K \Big/ (c_{NP,i}\cdot B_i)] \\ SP_i = 1 - SP_{S,i}/[SP_{S,i} + \exp(3.39 - 10.93 SP_{S,i})] \end{cases}$ (S15)

where T_{soil} and T_0 are the average daily soil surface temperature and the optimal temperature (°C) for crop j, respectively.

The crop yield (YLD, t/ha) is estimated by using the harvest index, viz.:

$$YLD_j = HI_j \cdot B_{AG} \tag{S16}$$

where HI is the harvest index for cop j; B_{AG} is the above-ground biomass (t/ha)..

2.2 Water use

The daily potential water use from surface soil to any root depth is calculated by

$$U_{p,i} = E_{p,i} \cdot [1-\exp(-\Lambda \cdot Z/RZ)]/[1-\exp(-\Lambda)] \quad \text{(S17)}$$

The potential water use ($U_{p,l}$, mm/day) in layer l is calculated by taking the difference between $U_{p,i}$ values at the layer boundaries, viz.,

$$U_{p,l} = E_{p,i} \cdot [\exp(-\Lambda \cdot Z_{l-1}/RZ) - \exp(-\Lambda \cdot Z_l/RZ))]/[1-\exp(-\Lambda)] \quad \text{(S18)}$$

where $U_{p,i}$ is the total water used to depth Z m on day i (mm); RZ is the root zone depth (m); Λ is a water use distribution parameter.

Restricted by soil moisture, the water use ($U_{l,i}$, mm/day) in layer l on day i is calculated with the following equations (Jones and Kiniry, 1986).

$$U_{l,i} = \begin{cases} U_{p,l} \cdot \exp\left[20 \cdot (SW_{l,i} - W_{p,l})/(W_{fc,l} - W_{p,l}) - 1\right] & \text{if } SW_{l,i} < (W_{fc,l} - W_{p,l})/4 + W_{p} \\ U_{p,l} & \text{if } SW_{l,i} \geq (W_{fc,l} - W_{p,l})/4 + W_{p} \end{cases} \quad \text{(S19)}$$

2.3 Nutrient uptake

The daily crop nutrient (N and P) demands are the differences between crop nutrient demands and potential nutrient contents.

$$\begin{cases} UND_i = c_{NB,i} \cdot B_i - \sum_{K=1}^{i} UN_K \\ UPD_i = c_{PB,i} \cdot B_i - \sum_{K=1}^{i} UP_K \end{cases} \quad \text{(S20)}$$

where UND and UNP are the potential daily N and P demands, respectively (kg/ha); UN and UP are the actual uptakes of N and P, respectively (kg/ha); c_{NB} and c_{NP} are the optimal N and P concentrations of the crop, rescpetively (kg/t); B is the daily biomass accumulation (t/ha).

The actual dissolved N (NO_3-N and NH_4-N) mass uptaken by crops is calculated as.

$$\begin{cases} UN_{l,i} = U_{l,i} \cdot (WN_l/SW_l)_i \\ UNS_i = \sum_{K=1}^{M} UN_{l,i} \end{cases} \quad \text{(S21)}$$

where $UN_{l,i}$ is the actual uptakes of N in the layer l on day i. WN is the NO_3^-N or NH_4-N amount in the soil (kg/ha). The amount of N supplied by soil (UNS) is estimated by summing UN in all layers (kg/ha).

The soil P availability is calculated as

$$\begin{cases} UPS_i = 1.50 \cdot UPD_i \cdot \sum_{l=1}^{M} LF_{u,l} \cdot (RW_l / RWT_i) \\ LF_{u,l} = 0.1 + 0.9 \cdot c_{LP,l} / [c_{LP,l} + 117 \cdot \exp(-0.283 \cdot c_{LP,l})] \end{cases} \quad \text{(S22)}$$

where UPS is the amount of P supplied by soil (kg/ha); RW and RWT are the root weights in layer l and in total, respectively (kg/ha); LF_u is the labile P factor for uptake (g/t).

A portion of N uptake is fixed by legumes, viz.,

$$\begin{cases} WFX_i = FXR_i \cdot UND_i & WFX \le 6.0 \\ FXR = \min(1.0, FXW, FXN) \cdot FXG \end{cases} \quad \text{(S23)}$$

where FXG is the growth stage factor; FXW and FXN are the factors of soil water and NO_3-N, respectively. All of these factors are calculated by the follow equations.

$$FXG_i = \begin{cases} 0.0 & HUI_i \le 0.15, HUI_i \ge 0.75 \\ 6.67 HUI_i - 1.0 & 0.15 < HUI_i \le 0.3 \\ 1.0 & 0.3 < HUI_i \le 0.55 \\ 3.75 - 5.0 HUI_i & 0.55 < HUI_i < 0.75 \end{cases} \quad \text{(S24)}$$

$$FXW_i = (SW_{0.3,i} - W_{p,0.3}) / 0.85 \cdot (W_{fc,0.3} - W_{p,0.3}) \quad SW_{0.3} < 0.85(W_{fc,0.3} - W_{p,0.3}) + W_{p,0.3}$$

(S26)

$$FXN_i = \begin{cases} 0.0 & WNO_3 > 300 kg \cdot ha^{-1} \cdot m^{-1} \\ 1.5 - 0.005 \cdot WNO_3 / RD & 100 < WNO_3 \le 300 \\ 1.0 & WNO_3 \le 100 \end{cases} \quad \text{(S25)}$$

where $SW_{0.3}$, $W_{p,0.3}$ and $W_{fc,0.3}$ are the moistures in the top 0.3 m soil, at wilting point and field capacity (mm), respectively.

3. Soil erosion module (Onstad and Foster, 1975)

The soil erosion by precipitation is estimated by the improved USLE equation (Onstad and Foster, 1975), viz.,

$$V_{sed} = \begin{cases} (0.646EI + 0.45Q_{overl} \cdot q_p^{\ 0.333}) \cdot K \cdot CE \cdot PE \cdot LS & Q_{overl} > 0. \\ 0 & Q_{overl} = 0. \end{cases} \quad \text{(S26)}$$

where V_{sed} is the sediment yield (t/ha); q_p is the peak runoff rate (mm/hour); K is the soil erodibility factor; PE is the erosion control practice factor.

LS is the factor of slope length and steepness:

$$\begin{cases} LS = (\lambda/22.1)^{\xi}(65.41S^2 + 4.56S + 0.065) \\ \xi = 0.6 \cdot [1 - \exp(-35.835S)] \end{cases} \quad \text{(S27)}$$

CE is the crop management factor:

$$CE = (0.8 - CE_{mn,j})\exp(-0.00115CV) + CE_{mn,j} \quad \text{(S28)}$$

EI is the precipitation energy factor:

$$EI = P \cdot [12.1 + 8.9 \cdot (\log r_p - 0.434) \cdot r_{0.5}]/1000 \quad \text{(S29)}$$

where S and λ are the land surface slope (m/m) and slope length (m), both of which are obtained during the procedure of preparing the spatial simulation units; ζ is a parameter depending on the slope; $CE_{mn,j}$ is the minimum crop management factor of crop j; CV is the soil cover (above ground biomass and residue) (kg/ha); P is the daily precipitation (mm); r_p and $r_{0.5}$ are the peak precipitation rate and maximum 0.5 h precipitation intensity (mm/hr). The value of r_p is obtained according to the exponential precipitation distribution.

4. Overland water quality module

4.1 Nutrient loss in urban and rural area

Generally, the inhabitant and industrial sewage in the urban area are collected, treated and discharged into the river system from the wastewater discharge outlets. This amount of nutrient flux is the model input as the point source pollutant load. The diffuse nutrient loss in urban area takes place along the flow pathways and is estimated by the export coefficient model (Johnes, 1996) as

$$V_{ur\_N} = 100 \cdot R_{ur} \cdot c_{ur\_N} \cdot Area_{urban} \quad \text{(S30)}$$

where V_{ur_N}, c_{ur_N} and $Area_{urban}$ are the amount of nutrient loss in the urban area (kg); the export coefficient (kg/ha/year) and urban area (km^2), respectively. R_{ur} is the loss rate from urban area.

The farm manure of rural living and livestock farming is also considered as one of important diffuse source of nutrient due to the deficiency of sewage treatment facilities in the rural area. The total loss is estimated as

$$\begin{cases} V_{liv\_N} = R_{liv} \cdot c_{liv\_N} \cdot Pop_{rural} \\ V_{lst\_N} = R_{lst} \cdot c_{lst\_N} \cdot Pop_{stock} \end{cases} \quad \text{(S31)}$$

where V_{liv_N} and V_{lst_N} are the amounts of nutrient loss from living and livestock farming in the rural area, respectively (kg/year); R_{liv} and R_{lst} are the loss rates from living and livestock farming. C_{liv_N} and C_{lst_N} are the export coefficients of living (kg/day/person) and livestock (kg/day/animal), respectively; Pop_{rural} and Pop_{stock} are the human and livestock populations, respectively.

4.2 Nutrient loss of soil layer

The loss of dissolved nutrient is considered to happen in both upper and lower soil layers. The loss amounts of NO_3-N, NH_4-N and dissolved P are calculated respectively by

$$\begin{cases} V_{sol\_N} = V_{sol\_N\_up} + V_{sol\_N\_low} \\ V_{sol\_N\_up} = W_{N\_up} \cdot [1 - \exp(-\frac{R_s + R_{ss}}{SW})] \\ V_{sol\_N\_low} = W_{N\_low} \cdot [1 - \exp(-\frac{R_{bs}}{SW})] \end{cases} \quad \text{(S32)}$$

(Williams *et al.*, 1989), where W_{N_up} and W_{N_low} are the dissolved nutrient amounts in the upper and lower soil layers, respectively (kg/ha); V_{soil_N}, $V_{soil\_N\_up}$ and $V_{soil\_N\_low}$ is the total dissolved nutrient loss, the loss in the upper and lower soil layers, respectively (kg/ha); *Rs*, *Rss* and *Rbs* are the surface runoff, interflow and baseflow (mm), respectively, and are obtained from the hydrological cycle module.

The amount of insoluble nutrients migrated with the sediment is estimated by

$$V_{sed\_ON} = 0.001 \cdot V_{sed} \cdot c_{ON} \cdot ER \qquad (S33)$$

(Neitsch *et al.*, 2011), where V_{sed_ON} is loss of organic N or P (kg/ha); c_{ON} is the insoluble nutrient concentration in the soil layer (g/m^3); ER is the enrich ratio.

4.3 Overland migration (Neitsch *et al.*, 2011)

$$\begin{cases} V_{dif,i} = (V'_{dif,i} + V_{stor,i-1}) \cdot [1 - \exp(-T_{retain}/T_{route})] & \\ V_{stor,i} = V'_{dif,i} + V_{stor,i-1} - V_{dif,i} & \\ V'_{dif,i} = V_{ur\_N,i} + V_{liv\_N,i} + V_{lst\_N,i} + V_{soil\_N,i} & for \quad soluble \quad nutrient \\ V'_{dif,i} = V_{sed\_ON,i} & for \quad insoluble \quad nutrient \\ V'_{dif,i} = V_{sed,i} & for \quad sediment \end{cases} \qquad (S34)$$

where $V_{dif,i}$ is the amount of overland pollutant discharged into river system on day i including sediment (tons/day), dissolved and insoluble nutrient (kg/day); $V'_{dif,i}$ and $V_{stor,i}$ are the pollutant loads generated in the sub-basin on day i, retained from the previous day (tons for sediment, kg for nutrient), respectively. T_{retain} and T_{route} are the retain time and routing time of flow (days), respectively.

5. Water quality module of water bodies

5.1 In-stream water quality module (Brown and Barnwell 1987; Neitsch *et al.*, 2011)

The water temperature (T_{water}, ^{o}C) has a strongly positive relationship with the air temperature and is calculated as

$$T_{water} = 5.0 + 0.375 \cdot (T_{\min} + T_{\max}) \qquad (S35)$$

where T_{min} and T_{max} are the daily minimum and maximum air temperatures, respectively (^{o}C), which are obtained as the model inputs.

The basic equation of in-stream water quality module is

$$dC/dt = V_{dif} + rpnt \cdot V_{point} - V_d - V_{set} \qquad (S36)$$

where C is the water quality concentration (mg/L); V_d and V_{set} are the degradation and settling load of pollutant (mg/L/day), respectively; *rpnt* is the monthly ratio of point source pollutant; and V_{point} is the annual point source pollution loads (mg/L/day), which are all the model inputs.

$$V_{set} = C \cdot R_{set,20} \cdot 1.024^{(T_{water}-20)} \tag{S37}$$

where $R_{set,20}$ is the settling coefficient of pollutant at 20 °C.

For algae growth, the growth rate (G_{alg}, day^{-1}) is constrained by the stresses of light, nutrients, and water temperature, viz.,

$$G_{alg} = g_{max} \cdot R_{light} \cdot R_N \cdot R_P \cdot 1.047^{(T_{water}-20)} \tag{S38}$$

where g_{max} is the maximum growth rate of algae (day^{-1}); R_{light}, R_N and R_P are the stress of light, N and P.

The light stress: $$\begin{cases} R_{light} = I_{hr} \cdot fr_{pho} \cdot \exp(-k_l \cdot h) / [I_{hr} \cdot fr_{pho} \cdot \exp(-k_l \cdot h) + K_L] \\ k_l = 1.0 + 0.0088 \cdot C_{alg} + 0.054 \cdot C_{alg}^{2/3} \end{cases} \tag{S39}$$

The N stress: $$R_N = (C_{NO_3} + C_{NH_4}) / (C_{NO_3} + C_{NH_4} + K_N) \tag{S40}$$

The P stress: $$R_P = C_{solP} / (C_{solP} + K_P) \tag{S41}$$

where k_l is the light extinction coefficient (m^{-1}); h is the water depth (m); I_{hr} is the solar radiation reaching to the water surface per hour (MJ/m^2/hr); fr_{pho} is the fraction of solar radiation for photosynthesis. K_L, K_N and K_P are the half-saturation coefficients for light (MJ/m^2/hr), N (mg/L) and P (mg/L).

The algae death rate (D_{alg}, day^{-1}) is calculated as

$$D_{alg} = d_{20} \cdot 1.047^{(T_{water}-20)} \tag{S42}$$

where d_{20} is the death rate of algae at 20°C (day^{-1}).

For N cycle, the transformation sequence in degradation is organic N→NH_4-N→NO_2^--N→NO_3^--N. The degradation load of every form is calculated as follows.

$$\begin{cases} V_{d,orgN} = [R_{d,20,orgN} \cdot C_{orgN} - AI_N \cdot R_{d,20,a\lg} \cdot C_{a\lg}] \cdot 1.047^{(T_{water}-20)} \\ V_{d,NH_4} = [R_{d,20,NH_4} \cdot C_{NH_4} - R_{d,20,orgN} \cdot C_{orgN} \\ \qquad + AI_N \cdot G_{a\lg} \cdot A\_N \cdot C_{a\lg}] \cdot 1.047^{(T_{water}-20)} \\ V_{d,NO_2} = [R_{d,20,NO_2} \cdot C_{NO_2} - R_{d,20,NH_4} \cdot C_{NH_4}] \cdot 1.047^{(T_{water}-20)} \\ V_{d,NO_3} = [AI_N \cdot G_{a\lg} \cdot (1 - A\_N) \cdot C_{a\lg} - R_{d,20,NO_2} \cdot C_{NO_2}] \cdot 1.047^{(T_{water}-20)} \end{cases} \quad \text{(S43)}$$

where $R_{d,20}$ is the degradation coefficient at 20 °C (day^{-1}); AI_N is the N fraction of algal biomass; A_N is the algal preference factor for NH_4-N.

For P cycle, the transformation sequence in degradation is organic P → dissolved P. The degradation load of every form is calculated as follows.

$$\begin{cases} V_{d,orgP} = [AI_P \cdot R_{d,20,a\lg} \cdot C_{a\lg} - R_{d,20,orgP} \cdot C_{orgP}] \cdot 1.047^{(T_{water}-20)} \\ V_{d,disP} = [R_{d,20,orgP} \cdot C_{orgP} - AI_P \cdot G_{a\lg} \cdot C_{a\lg}] \cdot 1.047^{(T_{water}-20)} \end{cases} \quad \text{(S44)}$$

where AI_P is the P fraction of algal biomass.

For BOD and COD variables,

$$\begin{cases} V_{d,BOD} = R_{d,20,BOD} \cdot C_{BOD} \cdot 1.047^{(T_{water}-20)} \\ C_{COD} = CtoB \cdot C_{BOD} \end{cases} \quad \text{(S45)}$$

where $CtoB$ is the ratio of COD to BOD concentrations.

The DO concentration are the functions of atmospheric reaeration, photosynthesis, algae respiration, sediment demand, biochemical oxygen demand, nitrification and water temperature, and are given as

$$\begin{cases} V_{d,DO} = \left(AI_{a\lg,r} \cdot D_{a\lg} - AI_{a\lg,p} \cdot G_{a\lg}\right) \cdot C_{a\lg} + V_{d,BOD} + \\ \qquad [AI_{NH4} \cdot R_{d,20,NH_4} \cdot C_{NH_4} + AI_{NO2} \cdot R_{d,20,NO_2} \cdot C_{NO_2}] \cdot 1.047^{(T_{water}-20)} \\ V_{rea,DO} = Rch\_k_{1,20} \cdot (C_{DO,sat} - C_{DO}) \cdot 1.024^{(T_{water}-20)} \end{cases} \quad \text{(S46)}$$

where $AI_{alg,r}$ is the rate of oxygen production per unit of algal photosynthesis, $AI_{alg,p}$ is the rate of oxygen uptake per unit of algal respiration; AI_{NH4} is the rate of oxygen uptake per unit of NH_4-N oxidation, AI_{NO2} is the rate of oxygen uptake per unit of NO_2-N oxidation; $Rch\_k_{1,20}$ is the reaeration coefficient at 20 ^{0}C in channel. $C_{DO,sat}$ is the equilibrium saturation DO in channel and is estimated using the equation developed by APHA (1985) as

$$C_{DO,sat} = \exp[-139.34410 + \frac{1.575701\times10^{5}}{T_{water}+273.15} - \frac{6.642308\times10^{7}}{(T_{water}+273.15)^{2}} + \frac{1.243800\times10^{10}}{(T_{water}+273.15)^{3}} - \frac{8.621949\times10^{11}}{(T_{water}+273.15)^{4}}] \quad \text{(S47)}$$

5.2 Water quality module of water impounding

In the water impounding, the degradation and settling processes of pollutants are basically the same as those in channels and are estimated using the equations (S37-S47). Additionally, given that the sedimentation of water impounding is a global issue, the resuspension and decay processes of sediment are further developed.

The equations of water quality module of water impounding are

$$\begin{cases} dh/dt = [Q_{in} - Q_{out}]/A + P - E \\ dC_L/dt = [C_{in}Q_{in} - C_L Q_{out}]/A\cdot h - K_{set}C_L - K_d C_L + K_{scu}C_s \cdot d/h \\ dC_s/dt = h/d \cdot K_{set}C_L - K_{scu}C_s - K_{bur}C_s \end{cases} \quad \text{(S48)}$$

where h and d are the depths of water and sediment (m), respectively; Q_{in} and Q_{out} are inflow and outflow (m^3/day), respectively; C_{in} and C_{out} are water quality concentrations into and out of the water body (mg/L), respectively; C_L and C_s are the water quality concentrations in the water body and the sediment (mg/L), respectively; P and E are the precipitation and evapotranspiration (m/day); K_{scu} and K_{bur} are the resuspension and decay coefficients of pollutant in the sediment (day^{-1}), respectively; A is the water surface area (km^2).

Table S1. All the parameters in the extended model

ID	Parameters	Definition	Unit	Affected components
Sub-basin parameters				
1	W_m	Minimum soil moisture	none	flow
2	W_p	Soil moisture at permanent wilting point	none	flow
3	W_{fc}	Field capacity of soil	none	flow
4	$W_{sat,u}$	Saturated moisture capacity of upper soil layer	none	flow
5	$W_{sat,l}$	Saturated moisture capacity of lower soil layer	none	flow
6	g_1	Basic surface runoff coefficient	none	flow
7	g_2	Influence coefficient of soil moisture	none	flow
8	K_{ET}	Adjustment factor of evapotranspiration	none	flow
9	K_{ss}	Interflow yield coefficient	none	flow
10	T_g	Delay time for aquifer recharge	day	flow
11	K_{bs}	Baseflow yield coefficient	none	flow
12	K_{sat}	Steady-state infiltration rate of soil	mm/hr	flow
13	kf_{mx}	Ratio of state infiltration rate to maximum rate in soil	none	flow
14	*rch_k*	Infiltration rate of channel	mm/hr	sediment
15	*ch_cov*	Channel cover factor	none	sediment
16	*ch_erod*	Channel erodibility factor	cm/hr/Pa	sediment
17	$R_{set,20}$(alg)	Settling rate of Algae at 20 ^{0}C	mg/day	algae
18	$R_{set,20}$(disP)	Settling rate of dissolved P at 20 ^{0}C	mg/m^2/day	P
19	$R_{set,20}$(NH_4)	Settling rate of NH_4-N at 20 ^{0}C in channel	mg/m^2/day	N
20	$R_{set,20}$(orgN)	Settling rate of organic N at 20 ^{0}C in channel	day^{-1}	N
21	$R_{set,20}$(orgP)	Settling rate of organic P at 20 ^{0}C in channel	day^{-1}	P
22	$R_{set,20}$(BOD)	Settling rate of BOD at 20 ^{0}C in channel	day^{-1}	COD
23	$Rch\_k_{1,20}$	Reaeration coefficients at 20 ^{0}C in channel	day^{-1}	DO
24	$Rch\_k_{2,20}$	Sediment oxygen demand rate at 20 ^{0}C in channel	day^{-1}	DO
25	$R_{d,20}$(BOD)	BOD deoxygenation rate at 20 ^{0}C in channel	day^{-1}	COD
26	$R_{d,20}$(NH_4)	Bio-oxidation rate of NH_4-N at 20 ^{0}C in channel	day^{-1}	N
27	$R_{d,20}$(NO_2)	Oxidation rate of NO_2-N to NO_3-N at 20 ^{0}C in channel	day^{-1}	N
28	$R_{d,20}$(orgN)	Hydrolysis rate of organic N to NH_4-N at 20 ^{0}C in channel	day^{-1}	N
29	$R_{d,20}$(orgP)	Hydrolysis rate of organic P to dissolved P at 20 ^{0}C in channel	day^{-1}	N
30	*CtoB*	Ratio between COD and BOD	none	COD
31	*res_k*	Infiltration rate in reservoir or sluice	mm/hr	flow
32	$K_{set,20}$(BOD)	Settling rate of BOD at 20 ^{0}C in reservoir or sluice	m/year	COD
33	$K_{set,20}$(NH_4)	Settling rate of NH_4-N at 20 ^{0}C in reservoir or sluice	m/year	N
34	$K_{set,20}$(NO_2)	Settling rate of NO_2-N at 20 ^{0}C in reservoir or sluice	m/year	N
35	$K_{set,20}$(NO_3)	Settling rate of NO_3-N at 20 ^{0}C in reservoir or sluice	m/year	N
36	$K_{set,20}$(orgN)	Settling rate of organic N at 20 ^{0}C in reservoir or sluice	m/year	N
37	$K_{set,20}$(orgP)	Settling rate of organic P at 20 ^{0}C in reservoir or sluice	m/year	P
38	$K_{set,20}$(disP)	Settling rate of dissolved P at 20 ^{0}C in reservoir or sluice	m/year	P

39	$K_{set,20}$ (DO)	Settling rate of DO at 20 ^{0}C in reservoir or sluice	m/year	DO
40	$K_{set,20}$(alg)	Settling rate of algae at 20 ^{0}C in reservoir or sluice	m/year	algae
41	$K_{set,20}$(TN)	Settling rate of TN at 20 ^{0}C in reservoir or sluice	m/year	N
42	$K_{set,20}$(TP)	Settling rate of TP at 20 0C in reservoir or sluice	m/year	P
43	$K_{d,20}$(BOD)	BOD deoxygenation rate in reservoirs at 20 ^{0}C	day^{-1}	COD
44	$res\_k_{1,20}$	Reaeration coefficients at 20 ^{0}C in reservoir or sluice	day^{-1}	DO
45	$K_{d,20}$(NH_4)	Bio-oxidation rate of NH_4-N in reservoir at 20 ^{0}C	day^{-1}	N
46	$K_{d,20}$(NO_2)	Oxidation rate of NO_2-N to NO_3-N at 20 ^{0}C in reservoir or sluice	day^{-1}	N
47	$K_{d,20}$(orgN)	Hydrolysis rate of organic N to NH_4-N at 20 ^{0}C in reservoir or sluice	day^{-1}	N
48	$K_{d,20}$(orgP)	Hydrolysis rate of organic P to dissolved P at 20 ^{0}C in reservoir or sluice	day^{-1}	P
49	$K_{scu,20}$(BOD)	Resuspension rate of BOD at 20 ^{0}C in reservoir or sluice	m/year	COD
50	$K_{scu,20}$(NH_4)	Resuspension rate of NH_4-N at 20 ^{0}C in reservoir or sluice	m/year	N
51	$K_{scu,20}$(NO_2)	Resuspension rate of NO_2-N at 20 ^{0}C in reservoir or sluice	m/year	N
52	$K_{scu,20}$(NO_3)	Resuspension rate of NO_3-N at 20 ^{0}C in reservoir or sluice	m/year	N
53	$K_{scu,20}$(orgN)	Resuspension rate of organic N at 20 ^{0}C in reservoir or sluice	m/year	N
54	$K_{scu,20}$(orgP)	Resuspension rate of organic P at 20 ^{0}C in reservoir or sluice	m/year	P
55	$K_{scu,20}$(disP)	Resuspension rate of dissolved P at 20 ^{0}C in reservoir or sluice	m/year	P
56	$K_{scu,20}$(DO)	Resuspension rate of DO at 20 ^{0}C in reservoir or sluice	m/year	DO
57	$K_{scu,20}$(alg)	Resuspension rate of algae at 20 ^{0}C in reservoir or sluice	m/year	algae
58	$K_{scu,20}$(TN)	Resuspension rate of TN at 20 ^{0}C in reservoir or sluice	m/year	N
59	$K_{scu,20}$(TP)	Resuspension rate of TP at 20 ^{0}C in reservoir or sluice	m/year	P
60	$K_{bur,20}$(BOD)	Decay rate of BOD at 20 ^{0}C in reservoir or sluice	m/year	COD
61	$K_{bur,20}$(NH_4)	Decay rate of NH_4-N at 20 ^{0}C in reservoir or sluice	m/year	N
62	$K_{bur,20}$(NO_2)	Decay rate of NO_2-N at 20 ^{0}C in reservoir or sluice	m/year	N
63	$K_{bur,20}$(NO_3)	Decay rate of NO_3-N at 20 ^{0}C in reservoir or sluice	m/year	N
64	$K_{bur,20}$(orgN)	Decay rate of organic N at 20 ^{0}C in reservoir or sluice	m/year	N
65	$K_{bur,20}$(orgP)	Decay rate of organic P at 20 ^{0}C in reservoir or sluice	m/year	P
66	$K_{bur,20}$(disP)	Decay rate of dissolved P at 20 ^{0}C in reservoir or sluice	m/year	P
67	$K_{bur,20}$(DO)	Decay rate of DO at 20 ^{0}C in reservoir or sluice	m/year	DO
68	$K_{bur,20}$(alg)	Decay rate of algae at 20 ^{0}C in reservoir or sluice	m/year	algae
69	$K_{bur,20}$(TN)	Decay rate of TN at 20 ^{0}C in reservoir or sluice	m/year	N
70	$K_{bur,20}$ (TP)	Decay rate of TP at 20 ^{0}C in reservoir or sluice	m/year	P
71	*usle_k*	Soil erodibility factor of USLE equation	none	sediment
72	*usle_p*	Erosion control practice factor of USLE equation	none	sediment
73	*MicrIn*	Microbe index	none	C, N
74	K_{cl}	Decomposition rate of labile organic C	day^{-1}	C
75	μ_{CLAY}	Reduction factor of clay content on organic matter decomposition	none	C
76	μ_t	Reduction factor of soil temperature on growth of denitrifier or nitrifier	none	N
77	S	Labile fraction of organic C compounds	none	C
78	kr_{cvl}	Decomposition rate of very labile organic C in residue pool	day^{-1}	C
79	kr_{cl}	Decomposition rate of labile organic C in residue pool	day^{-1}	C
80	kr_{cr}	Decomposition rate of stable organic C in residue pool	day^{-1}	C

81	km_{sc}	Decomposition rate of stable organic C in microbial biomass pool	day^{-1}	C
82	km_{cl}	Decomposition rate of labile organic C in microbial biomass pool	day^{-1}	C
83	km_{h}	Decomposition rate of microbial biomass to humands	day^{-1}	C
84	K_{C}	Half velocity constant of organic C on denitrifier biomass growth	none	N
85	K_{NxOy}	Half velocity constant of NO_3-N, NO_2-N, NO and N_2O on denitrifier biomass growth	none	N
86	u_{NxOy}	Maximum growth rate of NO_3-N, NO_2-N, NO and N_2O denitrifier	day^{-1}	N
87	M_{C}	Maintenance coefficient of C	hr^{-1}	C
88	Y_{C}	Maximum growth yield of dissolved C	kg/ha/hr	C
89	M_{NxOy}	Maintenance coefficient of NO_3-N, NO_2-N, NO and N_2O	hr^{-1}	N
90	Y_{NxOy}	Maximum growth yield of NO_3-N, NO_2-N, NO and N_2O	kg/ha/hr	N
91	$CDR_{D:N}$	C:N ratio in bacteria	none	N
92	$\mu_{SW,n}$	Soil water content adjusted factor for denitrification	none	C, N
93	β_{min}	Mineralization rate of humus active organic P	day^{-1}	P
94	β_{rsd}	Mineralization rate of residue fresh organic P	day^{-1}	P
Watershed parameters				
95	C_{ur}(COD)	Export coefficient of COD load in urban area	kg/ha/year	COD
96	C_{ur}(NH_4)	Export coefficient of NH_4-N load in urban area	kg/ha/year	N
97	C_{ur}(TN)	Export coefficient of TN load in urban area	kg/ha/year	N
98	C_{ur}(TP)	Export coefficient of TP load in urban area	kg/ha/year	P
99	R_{ur}	Loss rate of diffuse source load from urban area	none	pollutant load
100	C_{liv}(COD)	Export coefficient of COD load from living in rural area	kg/year	COD
101	C_{liv}(NH_4)	Export coefficient of NH_4-N load from living in rural area	kg/year	N
102	C_{liv}(TN)	Export coefficient of TN load from living in rural area	kg/year	N
103	C_{liv}(TP)	Export coefficient of TP load from living in rural area	kg/year	P
104	R_{liv}	Loss rate of diffuse source load from living	none	pollutant load
105	C_{lst}(COD)	Export coefficient of COD load from livestock in rural area	kg/year	COD
106	C_{lst}(NH_4)	Export coefficient of NH_4-N load from livestock in rural area	kg/year	N
107	C_{lst}(TN)	Export coefficient of TN load from livestock in rural area	kg/year	N
108	C_{lst}(TP)	Export coefficient of TP load from livestock in rural area	kg/year	P
109	R_{lst}	Loss rate of diffuse source load from livestock	none	pollutant load
110	SF_{tmp}	Snowfall temperature	^{0}C	flow
111	SM_{tmp}	Snow melt base temperature	^{0}C	flow
112	SMF_{mx}	Melt factor for snow on June 21	mm/day	flow
113	SMF_{mn}	Melt factor for snow on December 21	mm/day	flow
114	*TIMP*	Snow pack temperature lag factor	none	flow
115	*Coefrad*	Factor of maximum possible radiation to net radiation	none	flow
116	SC_{max}	Minimum snow water content that corresponds to 100% snow cover	mm	flow
117	SC_{50}	Fraction of snow volume represented by SC_{max} that corresponds to 50% snow cover	none	flow
118	SC_{1}	Coefficients that define shape of snow curve 95% coverage at 100% snow cover	none	flow

119	SC_2	Coefficients that define shape of snow curve 50% coverage at 100% snow cover	none	flow
120	*Surlag*	Surface runoff lag time	day	flow
121	*n_ch*	Channel roughness	none	flow
122	*msk_x*	Weighting factor in Muskingum equation	none	flow
123	*msk_k*	Storage time constant of channel in Muskingum equation	day	flow
124	AI_N	N fraction of algal biomass	none	N
125	AI_P	P fraction of algal biomass	none	P
126	$AI_{alg,p}$	Rate of oxygen production per unit of algal photosynthesis	none	DO
127	$AI_{alg,r}$	Rate of oxygen uptake per unit of algal respiration	none	DO
128	AI_{NH4}	Rate of oxygen uptake per unit of NH_4-N oxidation	none	N
129	AI_{NO2}	Rate of oxygen uptake per unit of NO_2-N oxidation	none	N
130	g_{max}	Maximum specific algal growth rate at 20^0C	day^{-1}	algae
131	d_{max}	Algal respiration rate at 20^0C	day^{-1}	algae
132	fr_{pho}	Fraction of solar radiation for photosynthesis	none	algae
133	K_L	Half-saturation coefficient for light	kJ/m^2	algae
134	K_N	Half-saturation coefficient for N	mg/L	algae
135	K_P	Half-saturation coefficient for P	mg/L	algae
136	*A_N*	Algal preference factor for NH_4-N	none	N
137	*PRF*	Peak rate adjustment factor for sediment routing in channel	none	sediment
138	SP_{con}	Linear parameter for calculating maximum transport capacity of sediment in channel	none	sediment
139	*SPexp*	Exponent parameter for calculating maximum transport capacity of sediment in channel	none	sediment
140	pH_{flood}	Flood PH value	none	C, N
141	rcn_{rvl}	C:N ratio of very labile litter	none	C, N
142	rcn_{rl}	C:N ratio of labile litter	none	C, N
143	rcn_{rr}	C:N ratio of resistant litter	none	C, N
144	rcn_b	C:N ratio of labile biomass	none	C, N
145	rcn_h	C:N ratio of labile humus	none	C, N
146	rcn_m	C:N ratio of humads	none	C, N
147	*pai*	P availability index	none	C, N
148	*TtoC*	Ratio between TOC and COD	none	COD
149-160	$rpnt_{01\sim12}$	Ratio of point source pollutant from Jan. to Dec.	none	pollutant load

Table S2. The detailed information of data sets for the case study

Category	Data	Spatial scale	Temporal scale	Source
GIS	DEM	Grid: 90m*90 m	none	Institute of Geographic Science and Natural Resources Research, Chinese Academy of Sciences
	Land use	1:1,000,000	none	
	Soil	1:4,000,000	none	
Weather	Precipitation	65 stations	daily (from 2003 to 2008)	Hydrological Yearbooks of Henan Province, China
	Maximum and minimum temperature	6 stations	daily (from 2003 to 2008)	National Meteorological Information Center of China
Hydrology	Total runoff, high and low flows	6 stations	daily (from 2003 to 2008)	Hydrological Yearbooks of Henan Province, China
Water quality	Wastewater discharge outlets and the discharge load (wastewater, NH_4-N, etc.)	over 200 outlets	annual (from 2003 to 2008)	Water Resources Protection Bureau of Huai River Basin, China
	Water quality variable concentrations (NH_4-N)	6 stations	daily (from 2003 to 2008)	Water Resources Protection Bureau of Huai River Basin, China
	Nonpoint source load (NH_4-N)	9 administrative regions	average annual (from 2003 to 2005)	Huai River Commission, China
Ecology	Corn yield	9 administrative regions	average annual (from 2003 to 2005)	Henan Statistical Yearbook, China
Economy	Populations in rural area, breeding stock of large animals and livestock, water withdrawal	9 administrative regions	annual (from 2003 to 2008)	Henan Statistical Yearbook, China
Water projects	Water storage capacities of dead, usable, flood control and maximum flood levels and the corresponding water surface areas; the relationship among water level, storage volume and outflow	5 reservoirs and 12 sluices	none	Water Resources Protection Bureau of Huai River Basin, China
Agricultural management	Fertilization and irrigation types, timing and amount, the time of seeding and harvest, crop types	9 administrative regions	average annual (from 2003 to 2008)	Henan Statistical Yearbooks, China, Wang *et al.* (2008) and Zhai *et al.* (2014)

Table S3. The agricultural management scheme in the Shaying River Catchment

Crop	Management	Time		Ratio distribution of annual TN fertilizer	Ratio distribution of annual TP fertilizer	Fertilizer intensity (kg/ha)	
		Start (month-day)	Duration (day)			TN	TP
Early rice	Base fertilization	4-1	1	0.60	0.86	40.60-86.17	25.46-59.47
	Plant	4-15	1	-	-		
	Additional Fertilization	5-1	1	0.40	0.14	27.06-57.45	4.14-9.68
	Harvest & Kill	7-31	1	-	-		
Late rice	Base fertilization	8-1	1	0.50	0.86	33.83-71.81	25.46-59.47
	Plant	8-15	1	-	-		
	Additional Fertilization	9-1	1	0.50	0.14	33.83-71.81	4.14-9.68
	Harvest & Kill	10-31	1	-	-		
Winter wheat	Base fertilization	10-1	1	0.64	0.02	43.30-271.04	0.59-4.10
	Plant	10-15	1	-	-		
	Additional Fertilization	1-1	1	0.36	0.98	24.36-152.46	29.00-201.11
	Harvest & Kill	6-1	1	-	-		
Cron	Base fertilization	6-1	1	0.41	0.88	27.74-173.63	26.05-180.59
	Plant	6-15	1	-	-		
	Additional Fertilization	7-15	1	0.59	0.12	39.92-249.86	3.55-24.62
	Harvest & Kill	9-30	1	-	-		