



# Supplement of

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

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#### 1 Supplementary material

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

- 3 *Mineralization*: The mineralized P is added to solution P pool. The amount of active
- 4 and stable organic P are calculated as

$$5 \begin{cases} orgP_{act} = orgP_{hum} \cdot orgN_{act} / (orgN_{act} + orgN_{sta}) \\ orgP_{sta} = orgP_{hum} \cdot orgN_{sta} / (orgN_{act} + orgN_{sta}) \end{cases}$$
(S1)

- 6 where  $orgP_{act}$  and  $orgP_{sta}$  are the amounts (kg/ha) of P in active organic pool and
- stable organic pool, respectively;  $orgP_{hum}$  is the humic organic P in the layer (kg/ha);
- 8 orgNact and orgNsta are the amounts of N in active organic pool and stable organic
- 9 pool (kg/ha), respectively, which are simulated by DNDC.
- 10 The mineralized rate of humus active organic P pool (*RHP*) is calculated by

11 
$$RHP = 1.4 \cdot \beta_{\min} \cdot (\gamma_{tmp} \cdot \gamma_{SW})^{1/2}$$
 (S2)

- 12 where  $\beta_{\min}$  is the mineralization rate of humus active organic P;  $\gamma_{tmp}$  and  $\gamma_{SW}$  are 13 reduction factors of soil temperature and moisture.
- 14 The mineralized of the residue fresh organic P pool (*RRP*) is calculated as

15 
$$\begin{cases} RRP = 0.8 \cdot \delta_P \\ \delta_P = \beta_{rsd} \cdot \gamma_P \cdot (\gamma_{tmp} \cdot \gamma_{SW})^{1/2} \end{cases}$$
(S3)

- 16 where  $\delta_P$  and  $\beta_{rsd}$  are the residue decay rate and the mineralization rate of residue
- 17 fresh organic P.  $\gamma_P$  is the P cycling residue composition factor.
- 18 Decomposition: The decomposition rate of the residue fresh organic P pool (DRP) is

$$19 \quad DRP = 0.2 \cdot \delta_P \tag{S4}$$

- 20 Sorption: The P movement between soluble and active mineral pools ( $P_{sol|act}$ , kg/ha)
- and between active and stable mineral pools ( $P_{act|sta}$ , kg/ha) are

22 
$$P_{sol|act} = \begin{cases} P_{sol} - \min P_{act} \cdot pai/(1 - pai) & \text{if} \quad P_{sol} > \min P_{act} \cdot pai/(1 - pai) \\ 0.1 \cdot [P_{sol} - \min P_{act} \cdot pai/(1 - pai)] \text{if} \quad P_{sol} < \min P_{act} \cdot pai/(1 - pai) \end{cases}$$
(S5)

23 and

$$1 \qquad P_{act|sta} = \begin{cases} 0.0006 \cdot (4 \cdot \min P_{act} - \min P_{sta}) & \text{if} & \min P_{sta} < 4 \cdot \min P_{act} \\ 0.00006 \cdot \beta_{eqP} \cdot (4 \cdot \min P_{act} - \min P_{sta}) & \text{if} & \min P_{sta} > 4 \cdot \min P_{act} \end{cases}$$
(S6)

2 respectively, where  $P_{sol}$ ,  $minP_{act}$  and  $minP_{sta}$  are soluble, mineral active and stable P 3 (kg/ha), respectively; *pai* is P availability index.

4

#### 5 2. Crop growth module

#### 6 **2.1 Crop yield (Williams** *et al.*, **1989)**

7 The crop growth process depends on the accumulation of daily heat (Sharpley and

- 8 Williams, 1990). The accumulated heat  $(HU, ^{\circ}C)$  during a day and heat unit index
- 9 (*HUI*) is calculated as:

10 
$$\begin{cases} HU_{K} = (T_{mx,K} + T_{mn,K})/2 - T_{b,j} \\ HUI_{i} = \sum_{K=1}^{i} HU_{K} / PHU_{j} \end{cases}$$
(S7)

11 where  $T_{mx,K}$  and  $T_{mn,K}$  are the maximum and minimum temperatures (°C) on the k<sup>th</sup> 12 day, respectively;  $T_{b,j}$  is the base temperature of the j<sup>th</sup> crop (°C). *PHU<sub>j</sub>* is the potential 13 heat unit required for the j<sup>th</sup> crop maturity (°C). The range of *HUI* is from 0.0 at the 14 seeding time to 1.0 at the physiological maturity. *i* is the total days of crop growth. 15 The potential increased biomass for a day is estimated as follow:  $\Delta B_{p,i} = 0.001 \cdot BE_i \cdot PAR_i \cdot [1 + \Delta HRLT_i]^3$ (CO)

$$= 0.001 \cdot BE_i \cdot PAR_i \cdot [1 + \Delta HRLI_i]$$

$$= 0.0005 \cdot BE_i \cdot RA_i \cdot [1 - \exp(-0.65 \cdot LAI)] \cdot [1 + \Delta HRLT_i]^3$$
(S8)

17 where  $\Delta B_p$  is daily potential increased biomass (t/ha); *BE* is crop parameter for

18 converting energy to biomass (kg ha m<sup>2</sup>/MJ); *HRLT* and 
$$\Delta HRLT$$
 are length of a day

22 From emergence to the start of leaf decline, *LAI* is estimated with the equation:

$$LAI_{i} = LAI_{i-1} + \Delta LAI$$

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

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

2 
$$LAI_i = LAI_0 \cdot (1 - HUI_i/1 - HUI_0)^{ad_j}$$
 (S10)

3 where *HUF* is heat unit factor. *REG* is minimum crop stress factor. *Ad* is a parameter

4 controlled LAI decline rate for crop j and  $HUI_0$  is HUI value when LAI begins to

5 decline.

6 But the biomass growth is constrained by water, temperature, nutrient and aeration.

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

8 where *REG* is the crop growth regulating factor.

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

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

11 The nitrogen stress: 
$$\begin{cases} SN_{S,i} = 2[1 - \sum_{K=1}^{i} UN_{K} / (c_{NB,i} \cdot B_{i})] \\ SN_{i} = 1 - SN_{S,i} / [SN_{S,i} + \exp(3.39 - 10.93SN_{S,i})] \end{cases}$$
(S14)

12 The phosphorus stress: 
$$\begin{cases} SP_{S,i} = 2[1 - \sum_{K=1}^{i} UP_{K} / (c_{NP,i} \cdot B_{i})] \\ SP_{i} = 1 - SP_{S,i} / [SP_{S,i} + \exp(3.39 - 10.93SP_{S,i})] \end{cases}$$
(S15)

13 The aeration stress: 
$$\begin{cases} SAT = SW1/PO1 - CAF_j \\ AS_{S,i} = 1 - SAT/[SAT + \exp(-1.291 - 56.1 \cdot SAT)] & SAT > 0.0 \end{cases}$$

14 **(S16)** 

15 where  $T_g$  and  $T_0$  are average daily soil surface temperature and the optimal

- temperature (°C) for crop *j*, respectively; *SAT* is saturation factor; *SW1* and *PO1* are
- 17 water moisture and porosity of the top 1m of soil (mm), respectively; CAF is critical
- 18 aeration factor for crop j; AS is aeration stress factor.
- 19 The crop yield is estimated using the harvest index, viz.:

$$YLD_{j} = HI_{j} \cdot B_{AG}$$
(S17)

21 where *YLD* is total amount yield harvested from the field (t/ha), and *HI* is harvest

22 index; BAG is the above-ground biomass (t/ha). For non-stressed conditions, harvest

index increases nonlinearly from zero at seedling to *HI* at maturity. Affected by water
stress, the harvest index is calculated as following.

3 
$$HIA_{i} = HIA_{i-1} - HI_{j} \cdot WSYF_{j} \cdot FHU_{i} \cdot (0.9 - WS_{i})/[1 + WSYF_{j} \cdot FHU_{i} \cdot (0.9 - WS_{i})]$$
(S12)

- where  $HI_j$  is normal harvest index of crop *j*; *HIA* is adjusted harvest index; *WSYF<sub>j</sub>* is sensitivity parameter of harvest index to draught for crop *j*; *FHU* is a function of crop
- 6 growth stage. The crop growth stage function is calculated as

7 
$$FHU_{i} = \begin{cases} \sin[\pi \cdot (HUI_{i} - 0.3)/0.6] & 0.3 \le HUI_{i} \le 0.90 \\ 0. & HUI_{i} < 0.3, HUI_{i} > 0.9 \end{cases}$$
(S18)

#### 8 2.2 Water use

9 The potential water use from surface soil to any root depth is calculated as

10 
$$U_{p,i} = E_{p,i} \cdot [1 - \exp(-\Lambda \cdot Z/RZ)]/[1 - \exp(-\Lambda)]$$
 (S19)

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

13 
$$U_{p,l} = E_{p,i} \cdot \left[ \exp(-\Lambda \cdot Z_{l-1}/RZ) - \exp(-\Lambda \cdot Z_l/RZ) \right] / [1 - \exp(-\Lambda)]$$
 (S20)

- 14 where UP is the total water used to depth Z m on day i (mm); RZ is the root zone
- 15 depth (m);  $\Lambda$  is a water use distribution parameter.
- 16 Restricted by soil water content, the potential water use  $(U_l, \text{mm/day})$  in layer l is
- 17 calculated with the following equations when soil water content is less than 25% of
- 18 plant available soil water (Jones and Kiniry, 1986).

19 
$$U_{l} = \begin{cases} U_{p,l} \cdot \exp\left[20 \cdot (SW_{l,i} - WP_{l})/(FC_{l} - WP_{l}) - 1\right] & \text{if } SW_{l,i} < (FC_{l} - WP)_{l}/4 + WP_{l} \\ U_{p,l} & \text{if } SW_{l} \ge (FC_{l} - WP_{l})/4 + WP_{l} \end{cases}$$
(S21)

### 20 2.3 Nutrient uptake

- 21 The daily crop nutrient uptake (*N* and *P*) is the difference between crop nutrient
- 22 demand and ideal nutrient content for day *i*.

$$\begin{cases} UND_i = c_{NB,i} \cdot B_i - \sum_{K=1}^i UN_K \\ UPD_i = c_{PB,i} \cdot B_i - \sum_{K=1}^i UP_K \end{cases}$$
(S22)

1

where *UND* and *UNP* are *N* and *P* uptake amounts, rescpetively (kg/ha); *UN* and *UP*are the actual uptakes of *N* and *P*, rescpetively (kg/ha); *c<sub>NB</sub>* and *c<sub>NP</sub>* are the optimal *N*and *P* concentrations of the crop, rescpetively (kg/t); *B* is the accumulated biomass
for day *i* (t/ha).

- 6 The soluble N (NO<sub>3</sub>-N and NH<sub>4</sub>-N) mass flow to the roots is used to distribute
- 7 potential *N* uptake among soil layers.

$$8 \begin{cases} UN_{l,i} = u_{l,i} \cdot (WN_l / SW_l)_i \\ UNS_i = \sum_{K=1}^M UN_{l,i} \end{cases}$$
(S23)

- 9 where WN is NO<sub>3</sub>-N or NH<sub>4</sub>-N amount in the soil (kg/ha). The total N available for
- 10 uptake by mass flow *UNS* is estimated by summing *UN* of all layers.
- 11 The total *P* available for uptake is calculated using the equation.

12 
$$\begin{cases} UPS_{i} = 1.50 \cdot UPD_{i} \cdot \sum_{l=1}^{M} LF_{u,l} \cdot (RW_{l}/RWT_{i}) \\ LF_{u,l} = 0.1 + 0.9 \cdot c_{LP,l} / [c_{LP,l} + 117 \cdot \exp(-0.283 \cdot c_{LP,l})] \end{cases}$$
(S24)

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, rescpetively (kg/ha);  $LF_u$  is the labile *P* factor for uptake (g/t).

16 A portion of uptake *N* will be fixed by legumes, viz.,

17 
$$\begin{cases} WFX_i = FXR_i \cdot UND_i & WFX \le 6.0 \\ FXR = \min(1.0, FXW, FXN) \cdot FXG \end{cases}$$
(S25)

18 where FXG is the growth stage factor; FXW and FXN are the factors of soil water and

19 NO<sub>3</sub>-N, respectively. All of these factors are calculated using the follow equations.

$$20 FXG_i = \begin{cases} 0.0 HUI_i \le 0.15, HUI_i \ge 0.75 \\ 6.67HUI_i - 1.0 0.15 < HUI_i \le 0.3 \\ 1.0 0.3 < HUI_i \le 0.55 \\ 3.75 - 5.0HUI_i 0.55 < HUI_i < 0.75 \end{cases}$$
(S26)

1 
$$FXW_i = (SW_{0.3,i} - WP_{0.3})/0.85 \cdot (FC_{0.3} - WP_{0.3})$$
  $SW_{0.3} < 0.85(FC_{0.3} - WP_{0.3}) + WP_{0.3}$  (S27)  
2  $FXN_i = \begin{cases} 0.0 & WNO_3 > 300kg \cdot ha^{-1} \cdot m^{-1} \\ 1.5 - 0.005 \cdot WNO_3/RD & 100 < WNO_3 \le 300 \\ 1.0 & WNO_3 \le 100 \end{cases}$  (S28)

where SW<sub>0.3</sub>, WP<sub>0.3</sub> and FC<sub>0.3</sub> are the water contents in the top 0.3 m soil, at wilting
point and field capacity (mm), respectively.

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

7 The soil erosion by precipitation is estimated using the improved USLE equation

8 (Onstad and Foster, 1975), viz.,

9 
$$Y = \begin{cases} (0.646EI + 0.45Q \cdot q_p^{-0.333}) \cdot K \cdot CE \cdot PE \cdot LS & Q > 0. \\ 0 & Q = 0. \end{cases}$$
 (S29)

10 where *Y* is the sediment yield (t/ha); *Q* is runoff volume (mm);  $q_p$  is peak runoff rate

11 (mm/hr); *K* is soil erodibility factor determined by the soil type; *PE* is erosion control

- 12 practice factor.
- 13 *LS* is the factor of slope length and steepness:

14 
$$\begin{cases} LS = (\lambda/22.1)^{\xi} (65.41S^2 + 4.56S + 0.065) \\ \xi = 0.6 \cdot [1 - \exp(-35.835S)] \end{cases}$$
 (S30)

15 *CE* is the crop management factor:

16 
$$CE = (0.8 - CE_{mn,j})\exp(-0.00115CV) + CE_{mn,j}$$
 (S31)

17 *EI* is the rainfall energy factor:

18 
$$EI = R \cdot [12.1 + 8.9 \cdot (\log r_p - 0.434) \cdot r_{0.5}]/1000$$
 (S32)

19 where *S* and  $\lambda$  are the land surface slope (m/m) and slope length (m), both of which 20 are obtained during the procedure of preparing the spatial simulation units;  $\xi$  is a

- 21 parameter dependent upon slop;  $CE_{mn,j}$  is the minimum crop management factor of
- crop j; CV is soil cover (above ground biomass and residue) (kg/ha). R is daily rainfall
- amount (mm) and  $r_p$ ,  $r_{0.5}$  is the peak rainfall rate and maximum 0.5 h rainfall intensity
- (mm/hr). The value of  $r_p$  is obtained according to the exponential rainfall distribution.

1

## 2 **4. Overland water quality module**

#### 3 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 river network from urban wastewater discharge outlets. Thus, this amount of nutrient flux is the input to the model directly as the point source pollutant load. The nonpoint source nutrient loss in urban area takes place along the overland flow and is estimated using the export coefficient model (Johnes, 1996).

9 
$$V_{ur} = 100 \cdot c_{ur} \cdot Area_{urban}$$
(S33)

10 where  $V_{ur_N}$ ,  $c_{ur_N}$  and  $Area_{urban}$  are the amount of nutrient loss in urban area 11 (kg); the export coefficient (kg/ha/year) and urban area (km<sup>2</sup>), respectively.

12 The farm manure of rural living and livestock farming is also considered as one of

13 important nonpoint source of nutrient due to the deficiency of sewage treatment

14 facilities in the rural area. The total loss is estimated using the following equations.

15 
$$\begin{cases} V_{liv_N} = c_{liv_N} \cdot Pop_{rural} \\ V_{lst_N} = c_{lst_N} \cdot Pop_{stock} \end{cases}$$
(S34)

where  $V_{liv_N}$  and  $V_{lst_N}$  are the amount of nutrient loss from living and livestock farming in the rural area, respectively (kg/year).  $c_{liv_N}$  and  $c_{lst_N}$  are the export coefficient of living (kg/day/person) and livestock (kg/day/animal), respectively; *Pop*<sub>rural</sub> and *Pop*<sub>stock</sub> are the population and the animal stock, respectively.

#### 20 4.2 Nutrient loss of soil layer

The loss of soluble nutrient is considered to happen in both upper and lower layer of soil. The loss weight of  $NO_3$ -N,  $NH_4$ -N and soluble P are calculated using the equation (Williams *et al.*, 1989), respectively.

$$\begin{cases} V_{N_{up}} = W_{N_{up}} \cdot [1 - \exp(-\frac{R_s + R_{ss}}{UL})] \\ V_{N_{low}} = W_{N_{low}} \cdot [1 - \exp(-\frac{R_g}{UL})] \end{cases}$$
(S35)

where  $W_{N_{-}up}$  and  $W_{N_{-}low}$  are the soluble nutrient weight in the upper and lower soil layer, respectively (kg/ha); *UL* is maximum soil water content (mm);  $V_{N_{-}up}$  and  $V_{N_{-}low}$  is soluble nutrient loss in the upper and lower soil layer, respectively (kg/ha); *Rs* and *Rss* are surface runoff, and interflow (mm), respectively, which are obtained from the hydrological cycle module. The amount of insoluble nutrients migrated with the sediment is estimated using the equation (Neitsch *et al.*, 2011)

$$_{9} \quad Y_{ON} = 0.001 \cdot Y \cdot c_{ON} \cdot ER \tag{S36}$$

where  $Y_{ON}$  is loss of organic *N* or *P* (kg/ha);  $c_{ON}$  is insoluble nutrient concentration in the soil layer (g/m<sup>3</sup>); *ER* is enrich ratio.

### 12 **4.3 Overland migration (Neitsch** *et al.*, **2011)**

13 
$$N_{overl} = (N_{overl} + N_{stor,i-1}) \cdot \left[1 - \exp(-T_{retain}/T_{route})\right]$$
(S37)

14 where  $N_{overl}$  is the overland pollutant discharged into main channel including

15 sediment (tons), soluble and insoluble nutrient (kg);  $N_{overl}$  and  $N_{stor,i-1}$  are pollutant

16 load generated in the subbasin, pollutant retained from the previous day (tons for

17 sediment, kg for nutrient), respectively.  $T_{retain}$  and  $T_{route}$  are the retain time and

18 routing time of flow(days), respectively.

19

1

#### 20 **5. Water quality module of water bodies**

21 The basic equation of in-stream water quality module (Brown and Barnwell 1987) is

22 
$$dC/dt = -(R_d + R_{set}) \cdot C + \sum S_{out}$$
(S38)

- 1 where C is the pollutant concentration (mg/L);  $K_d$  and  $K_{set}$  are degradation and
- settling coefficient of pollutant (day<sup>-1</sup>), respectively; and  $\sum S_{out}$  is the external source
- 3 items (mg/L/day).
- 4 The equation of water quality module of water impounding is as follow.

5 
$$\begin{cases} dh/dt = [Q_{in} - Q_{out}]/A + P - E \\ dC_L/dt = [C_{in}Q_{in} - C_LQ_{out}]/Ah - K_{set}C_L - K_dC_L + K_{scu}C_s \cdot d/h \\ dC_s/dt = h/d \cdot K_{set}C_L - K_{scu}C_s - K_{bur}C_s \end{cases}$$
 (S39)

- 6 where h and d are water and sediment depth (m), respectively;  $Q_{in}$  and  $Q_{out}$  are inflow
- and outflow ( $m^3/s$ ), respectively;  $C_{in}$  and  $C_{out}$  are pollutant concentration into and out
- 8 of the water body (mg/L); P and E are precipitation and evapotranspiration (m/s);  $C_L$
- 9 and  $C_s$  are constituent concentration in the water body and the sediment (mg/L);  $K_{scu}$
- and  $K_{bur}$  are resuspension and decay coefficient of pollutant in the sediment (day<sup>-1</sup>),
- 11 respectively; A is water surface area  $(km^2)$ .
- 12

| ID    | Variables                           | Definition   | Unit      | Affected   |
|-------|-------------------------------------|--|-----------|------------|
| ID    | v artables                          |  | Omt       | components |
| Subba | isin paramete                       | rs   |           |            |
| 1     | $W_m$                               | Minimum water content of soil  | none      | flow       |
| 2     | Ww                                  | Wilting water content of soil  | none      | flow       |
| 3     | $W_{fc}$                            | Field capacity of soil   | none      | flow       |
| 4     | W <sub>sat,u</sub>                  | Saturated moisture capacity of upper soil layer  | none      | flow       |
| 5     | W <sub>sat,l</sub>                  | Saturated moisture capacity of lower soil layer  | none      | flow       |
| 6     | <i>g</i> <sub>1</sub>               | Basic surface runoff coefficient   | none      | flow       |
| 7     | <i>g</i> <sub>2</sub>               | Influence coefficient of soil moisture   | none      | flow       |
| 8     | K <sub>ET</sub>                     | Adjustment factor of evapotranspiration  | none      | flow       |
| 9     | K <sub>r</sub>                      | Interflow yield coefficient  | none      | flow       |
| 10    | $T_g$                               | Delay time for aquifer recharge  | day       | flow       |
| 11    | $K_g$                               | Baseflow yield coefficient   | none      | flow       |
| 12    | Ksat                                | Steady state infiltration rate of soil   | mm/hr     | flow       |
| 13    | <i>kf<sub>mx</sub></i>              | Ratio of state infiltration rate to maximum rate in soil                                   | none      | flow       |
| 14    | DtoW                                | Ratio of width to depth of channel   | none      | flow       |
| 15    | rch_k                               | Infiltration rate of channel   | mm/hr     | sediment   |
| 16    | ch_cov                              | Channel cover factor   | none      | sediment   |
| 17    | ch_erod                             | Channel erodibility factor   | cm/hr/Pa  | sediment   |
| 18    | <i>R<sub>set</sub></i> (algae)      | Algae settling rate at 20 °C   | mg/day    | algae      |
| 19    | $R_{set}(solP)$                     | Soluble P settling rate at 20 °C   | mg/m²/day | Р          |
| 20    | R <sub>set</sub> (NH <sub>4</sub> ) | Settling rate of NH <sub>4</sub> -N at 20 <sup>o</sup> C in channel                        | mg/m²/day | N          |
| 21    | <i>R<sub>set</sub></i> (orgN)       | Settling rate of organic N at 20 °C in channel   | day-1     | N          |
| 22    | <i>R<sub>set</sub></i> (orgP)       | Settling rate of organic P at 20 <sup>o</sup> C in channel                                 | day-1     | Р          |
| 23    | $R_d(\text{COD})$                   | COD deoxygenation rate at 20 °C in channel   | day-1     | COD        |
| 24    | $Rch_k_1$                           | Reaeration coefficients at 20 °C in channel  | day-1     | DO         |
| 25    | $R_{set}(\text{COD})$               | COD settling rate at 20 °C in channel  | day-1     | COD        |
| 26    | $Rch_k_2$                           | DO adsorption rate of sediment at 20 °C in channel   | day-1     | DO         |
| 27    | $R_d(\mathrm{NH}_4)$                | Bio-oxidation rate of NH <sub>4</sub> -N at 20 <sup>0</sup> C in channel                   | day-1     | N          |
| 28    | $R_d(NO_2)$                         | Oxidation rate of NO <sub>2</sub> -N to NO <sub>3</sub> -N at 20 <sup>0</sup> C in channel | day-1     | Ν          |
| 29    | $R_d(\text{orgN})$                  | Hydrolysis rate of organic N to NH <sub>4</sub> -N at 20 <sup>0</sup> C in channel         | day-1     | Ν          |
| 30    | $R_d(\text{orgP})$                  | Hydrolysis rate of organic P to soluble P at 20 <sup>o</sup> C in channel                  | day-1     | N          |
| 31    | CtoB                                | Relationship between COD and BOD   | none      | COD        |
| 32    | res_k                               | Infiltration rate in reservoir or sluice   | mm/hr     | flow       |
| 33    | K <sub>set</sub> (COD)              | Settling rate of COD at 20 °C in reservoir or sluice                                       | m/year    | COD        |
| 34    | K <sub>set</sub> (NH <sub>4</sub> ) | Settling rate of NH <sub>4</sub> -N at 20 <sup>o</sup> C in reservoir or sluice            | m/year    | N          |
| 35    | $K_{set}(NO_2)$                     | Settling rate of NO <sub>2</sub> -N at 20 <sup>o</sup> C in reservoir or sluice            | m/year    | N          |
| 36    | $K_{set}(NO_3)$                     | Settling rate of NO <sub>3</sub> -N at 20 <sup>o</sup> C in reservoir or sluice            | m/year    | N          |
| 37    | K <sub>set</sub> (orgN)             | Settling rate of organic N at 20 <sup>o</sup> C in reservoir or sluice                     | m/year    | N          |
| 38    | $K_{set}(\text{orgP})$              | Settling rate of organic P at 20 <sup>o</sup> C in reservoir or sluice                     | m/year    | Р          |

# Table S1. All the parameters in the extended model

1

| 39 | $K_{set}(solP)$                 | Settling rate of soluble P at 20 °C in reservoir or sluice   | m/year | Р        |
|----|---------------------------------|--|--------|----------|
| 40 | $K_{set}$ (DO)                  | Settling rate of DO at 20 °C in reservoir or sluice  | m/year | DO       |
| 41 | K <sub>set</sub> (algae)        | Settling rate of algae at 20 °C in reservoir or sluice   | m/year | algae    |
| 42 | $K_{set}(TN)$                   | Settling rate of TN at 20 °C in reservoir or sluice  | m/year | N        |
| 43 | $K_{set}(\mathrm{TP})$          | Settling rate of TP at 20 0C in reservoir or sluice  | m/year | Р        |
| 44 | <i>K</i> <sub>d</sub> (COD)     | COD deoxygenation rate in reservoirs at 20 °C  | day-1  | COD      |
| 45 | res_k1                          | Reaeration coefficients at 20 °C in reservoir or sluice  | day-1  | DO       |
| 46 | $K_d(NH_4)$                     | Bio-oxidation rate of NH <sub>4</sub> -N in reservoir at 20 °C   | day-1  | N        |
| 47 | $K_d(NO_2)$                     | Oxidation rate of NO <sub>2</sub> -N to NO <sub>3</sub> -N at 20 <sup>0</sup> C in reservoir or sluice | day-1  | N        |
| 48 | <i>K</i> <sub>d</sub> (orgN)    | Hydrolysis rate of organic N to NH <sub>4</sub> -N at 20 <sup>0</sup> C in reservoir or sluice         | day-1  | N        |
| 49 | <i>K</i> <sub>d</sub> (orgP)    | Hydrolysis rate of organic P to soluble P at 20 °C in reservoir or sluice                              | day-1  | Р        |
| 50 | $K_{scu}(\text{COD})$           | Resuspension rate of COD at 20 °C in reservoir or sluice   | m/year | COD      |
| 51 | $K_{scu}(NH_4)$                 | Resuspension rate of NH4-N at 20 °C in reservoir or sluice   | m/year | Ν        |
| 52 | $K_{scu}(NO_2)$                 | Resuspension rate of NO <sub>2</sub> -N at 20 <sup>0</sup> C in reservoir or sluice                    | m/year | Ν        |
| 53 | $K_{scu}(NO_3)$                 | Resuspension rate of NO <sub>3</sub> -N at 20 <sup>0</sup> C in reservoir or sluice                    | m/year | N        |
| 54 | $K_{scu}(orgN)$                 | Resuspension rate of organic N at 20 °C in reservoir or sluice   | m/year | N        |
| 55 | <i>K<sub>scu</sub></i> (orgP)   | Resuspension rate of organic P at 20 °C in reservoir or sluice   | m/year | Р        |
| 56 | $K_{scu}(solP)$                 | Resuspension rate of soluble P at 20 °C in reservoir or sluice   | m/year | Р        |
| 57 | $K_{scu}(DO)$                   | Resuspension rate of DO at 20 °C in reservoir or sluice  | m/year | DO       |
| 58 | <i>K<sub>scu</sub></i> (algae)  | Resuspension rate of algae at 20 °C in reservoir or sluice   | m/year | algae    |
| 59 | $K_{scu}(TN)$                   | Resuspension rate of TN at 20 °C in reservoir or sluice  | m/year | N        |
| 60 | $K_{scu}(\mathrm{TP})$          | Resuspension rate of TP at 20 °C in reservoir or sluice  | m/year | Р        |
| 61 | <i>K</i> <sub>bur</sub> (COD)   | Decay rate of COD at 20 °C in reservoir or sluice  | m/year | COD      |
| 62 | $K_{bur}(\mathrm{NH}_4)$        | Decay rate of NH <sub>4</sub> -N at 20 <sup>o</sup> C in reservoir or sluice                           | m/year | N        |
| 63 | $K_{bur}(NO_2)$                 | Decay rate of NO <sub>2</sub> -N at 20 °C in reservoir or sluice                                       | m/year | N        |
| 64 | $K_{bur}(NO_3)$                 | Decay rate of NO <sub>3</sub> -N at 20 <sup>0</sup> C in reservoir or sluice                           | m/year | Ν        |
| 65 | <i>K</i> <sub>bur</sub> (orgN)  | Decay rate of organic N at 20 °C in reservoir or sluice  | m/year | Ν        |
| 66 | <i>K</i> <sub>bur</sub> (orgP)  | Decay rate of organic P at 20 °C in reservoir or sluice  | m/year | Р        |
| 67 | $K_{bur}(solP)$                 | Decay rate of soluble P at 20 °C in reservoir or sluice  | m/year | Р        |
| 68 | $K_{bur}(DO)$                   | Decay rate of DO at 20 °C in reservoir or sluice   | m/year | DO       |
| 69 | <i>K</i> <sub>bur</sub> (algae) | Decay rate of algae at 20 °C in reservoir or sluice  | m/year | algae    |
| 70 | <i>K</i> <sub>bur</sub> (TN)    | Decay rate of TN at 20 °C in reservoir or sluice   | m/year | Ν        |
| 71 | $K_{bur}$ (TP)                  | Decay rate of TP at 20 °C in reservoir or sluice   | m/year | Р        |
| 72 | usle_k                          | Soil erodibility factor of USLE equation   | none   | sediment |
| 73 | usle_p                          | Erosion control practice factor of USLE equation   | none   | sediment |
| 74 | MicrIn                          | Microbe index  | none   | C, N     |
| 75 | $K_{l}$                         | Decomposition rate of labile organic C   | day-1  | С        |
| 76 | $\mu_{CLAY}$                    | Reduction factor of clay content on organic matter decomposition                                       | none   | С        |
| 77 | $\mu_t$                         | Reduction factor of soil temperature on growth of denitrifier or nitrifier                             | none   | N        |
| 78 | S                               | Labile fraction of organic C compounds   | none   | С        |
| 79 | <i>kr</i> <sub>cvl</sub>        | Decomposition rate of very labile organic C in residue pool  | day-1  | С        |
| 80 | <i>kr</i> <sub>cl</sub>         | Decomposition rate of labile organic C in residue pool   | day-1  | С        |
| 81 | <i>kr</i> <sub>cr</sub>         | Decomposition rate of stable organic C in residue pool   | day-1  | С        |

| 82                | km <sub>sc</sub>                  | Decomposition rate of stable organic C in microbial biomass pool  | day-1              | С              |
|-------------------|-----------------------------------|---|--------------------|----------------|
| 83                | <i>km</i> <sub>cl</sub>           | Decomposition rate of labile organic C in microbial biomass pool  | day-1              | С              |
| 84                | <i>km</i> <sub>h</sub>            | Decomposition rate of microbial biomass to humands  | day-1              | С              |
| 85                | K <sub>C</sub>                    | Half velocity constant of organic C on denitrifier biomass growth   | none               | N              |
| 86                | K <sub>NxOy</sub>                 | Half velocity constant of NO <sub>3</sub> -N, NO <sub>2</sub> -N, NO and N <sub>2</sub> O on denitrifier biomass growth | none               | N              |
| 87                | U <sub>NO3</sub>                  | Maximum growth rate of NO <sub>3</sub> -N denitrifier   | day <sup>-1</sup>  | N              |
| 88                | u <sub>NO2</sub>                  | Maximum growth rate of NO <sub>2</sub> -N denitrifier   | day <sup>-1</sup>  | N              |
| 89                | u <sub>NO</sub>                   | Maximum growth rate of NO denitrifier   | day-1              | N              |
| 90                | <i>u</i> <sub>N2O</sub>           | Maximum growth rate of N <sub>2</sub> O denitrifier   | day <sup>-1</sup>  | N              |
| 91                | M <sub>C</sub>                    | Maintenance coefficient of C  | hr <sup>-1</sup>   | С              |
| 92                | Y <sub>C</sub>                    | Maximum growth yield of soluble C   | kg/ha/hr           | C              |
| 93                | M <sub>NO3</sub>                  | Maintenance coefficient of NO <sub>3</sub> -N   | hr <sup>-1</sup>   | N              |
| 94                | Y <sub>NO3</sub>                  | Maximum growth yield of NO <sub>3</sub> -N  | kg/ha/hr           | N              |
| 95                | CDR <sub>D:N</sub>                | C:N ratio in bacteria   | none               | N              |
| 96                | M <sub>NO2</sub>                  | Maintenance coefficient of NO <sub>2</sub> -N   | hr <sup>-1</sup>   | N              |
| 97                | Y <sub>NO2</sub>                  | Maximum growth yield of NO <sub>2</sub> -N  | kg/ha/hr           | N              |
| 98                | $M_{NO2}$                         | Maintenance coefficient of NO   | hr <sup>-1</sup>   | N              |
| 99                | Y <sub>NO</sub>                   | Maximum growth yield of NO  | kg/ha/hr           | N              |
| 100               | $M_{N2O}$                         | Maintenance coefficient of $N_2O$   | hr <sup>-1</sup>   | N              |
| 100               | Y <sub>N20</sub>                  | Maximum growth yield of N <sub>2</sub> O  | kg/ha/hr           | N              |
| 101               | $\mu_{SW,n}$                      | Soil water content adjusted factor for denitrification  | none               | C, N           |
| 102               | $\beta_{min}$                     | Mineralization rate of humus active organic P   | day <sup>-1</sup>  | P              |
| 103               | $\beta_{rsd}$                     | Mineralization rate of residue fresh organic P  | day <sup>-1</sup>  | P              |
|                   | shed paramet                      | -   | uuy                |                |
| 105               | $C_{ur}(\text{COD})$              | Export coefficient of COD load in urban area  | kg/ha/year         | COD            |
| 105               | $C_{ur}(\text{NH}_4)$             | Export coefficient of NH <sub>4</sub> -N load in urban area   | kg/ha/year         | N              |
| 107               | $C_{ur}(TN)$                      | Export coefficient of TN load in urban area   | kg/ha/year         | N              |
| 108               | $C_{ur}(\mathrm{TP})$             | Export coefficient of TP load in urban area   | kg/ha/year         | P              |
| 109               | $C_{ur}(\text{COD})$              | Export coefficient of COD load in unused area   | kg/ha/year         | COD            |
| 110               | $C_{ur}(\mathrm{NH}_4)$           | Export coefficient of NH <sub>4</sub> -N load in unused area  | kg/ha/year         | N              |
| 111               | $C_{ur}(TN)$                      | Export coefficient of TN load in unused area  | kg/ha/year         | N              |
| 112               | $C_{ur}(\mathrm{TP})$             | Export coefficient of TP load in unused area  | kg/ha/year         | P              |
| 113               | $R_{ur}$                          | Loss rate of non-point source load from soil layer  | none               | pollutant load |
| 114               | $C_{liv}(\text{COD})$             | Export coefficient of COD load from living in rural area  | kg/year            | COD            |
| 115               | $C_{liv}(\text{NH}_4)$            | Export coefficient of NH <sub>4</sub> -N load from living in rural area   | kg/year            | N              |
| 116               | $C_{liv}(TN)$                     | Export coefficient of TN load from living in rural area   | kg/year            | N              |
| 117               | $C_{liv}(TP)$                     | Export coefficient of TP load from living in rural area   | kg/year            | P              |
| 118               | $C_{llv}(\Pi)$                    | Export coefficient of TT load from livestock in rural area  | kg/year            | COD            |
|                   | $C_{lst}(\text{NH}_4)$            | Export coefficient of NH <sub>4</sub> -N load from livestock in rural area  | kg/year            | N              |
| 119               |                                   |   |                    | - '            |
| 119<br>120        |                                   | Export coefficient of TN load from livestock in rural area  | kg/year            | N              |
| 119<br>120<br>121 | $\frac{C_{lst}(TN)}{C_{lst}(TP)}$ | Export coefficient of TN load from livestock in rural areaExport coefficient of TP load from livestock in rural area    | kg/year<br>kg/year | N<br>P         |

| 123 | <b>R</b> <sub>lst</sub>  | Loss rate of non-point source load from livestock                                  | none                                  | pollutant load |
|-----|--------------------------|--|---------------------------------------|----------------|
| 124 | $C_{pcp}(\text{COD})$    | COD concentration in precipitation   | mg/L                                  | COD            |
| 125 | $C_{pcp}(\mathrm{NH}_4)$ | NH <sub>4</sub> -N concentration in precipitation                                  | mg/L                                  | N              |
| 126 | $C_{pcp}(TN)$            | TN concentration in precipitation  | mg/L                                  | N              |
| 127 | $C_{pcp}(\text{TP})$     | TP concentration in precipitation  | mg/L                                  | Р              |
| 128 | $SF_{tmp}$               | Snowfall temperature   | <sup>0</sup> C                        | flow           |
| 129 | $SM_{tmp}$               | Snow melt base temperature   | <sup>0</sup> C                        | flow           |
| 130 | $SMF_{mx}$               | Melt factor for snow on June 21  | mm/day                                | flow           |
| 131 | $SMF_{mn}$               | Melt factor for snow on December 21  | mm/day                                | flow           |
| 132 | TIMP                     | Snow pack temperature lag factor   | none                                  | flow           |
| 133 | Coefrad                  | Factor of maximum possible radiation to net radiation                              | none                                  | flow           |
| 134 | SC <sub>max</sub>        | Minimum snow water content that corresponds to 100% snow cover                     | mm                                    | flow           |
| 135 | SC50                     | Fraction of snow volume represented by SCMX that corresponds to 50% snow cover     | none                                  | flow           |
| 136 | $SC_1$                   | Coefficients that define shape of snow curve 95% coverage at 100% snow cover       | none                                  | flow           |
| 137 | $SC_2$                   | Coefficients that define shape of snow curve 50% coverage at 100% snow cover       | none                                  | flow           |
| 138 | Surlag                   | Surface runoff lag time  | day                                   | flow           |
| 139 | n_ch                     | Roughness of Channel   | none                                  | flow           |
| 140 | msk_x                    | Weighting factor in Muskingum equation   | none                                  | flow           |
| 141 | msk_k                    | Storage time constant of channel in Muskingum equation                             | day                                   | flow           |
| 142 | $AI_1$                   | Fraction of algal biomass that is N  | none                                  | N              |
| 143 | $AI_2$                   | Fraction of algal biomass that is P  | none                                  | Р              |
| 144 | $AI_3$                   | Adjusted rate of oxygen production per unit of algal photolysis                    | none                                  | DO             |
| 145 | $AI_4$                   | Adjusted rate of oxygen uptake per unit of algal respiration                       | none                                  | DO             |
| 146 | $AI_5$                   | Adjusted rate of oxygen uptake per unit of NH4-N oxidation                         | none                                  | Ν              |
| 147 | $AI_6$                   | Adjusted rate of oxygen uptake per unit of NO <sub>2</sub> -N oxidation            | none                                  | Ν              |
| 148 | AI <sub>7</sub>          | Adjusted rate of NH <sub>4</sub> -N oxidation to NO <sub>2</sub> -N                | none                                  | Ν              |
| 149 | <i>g</i> <sub>max</sub>  | Maximum specific algal growth rate at 20 <sup>o</sup> C                            | day-1                                 | algae          |
| 150 | RHOQ                     | Algal respiration rate at 20 <sup>o</sup> C  | day-1                                 | algae          |
| 151 | TFACT                    | Fraction of solar radiation computed in temperature heat balance                   | none                                  | algae          |
| 152 | K_1                      | Half-saturation coefficient for light  | kJ/m <sup>2</sup>                     | algae          |
| 153 | K_N                      | Michaelis-Menton half-saturation constant for N                                    | mg/L                                  | algae          |
| 154 | K_P                      | Michaelis-Menton half-saturation constant for P                                    | mg/L                                  | algae          |
| 155 | Lec                      | Non-algal portion of light extinction coefficient                                  | m <sup>-1</sup>                       | algae          |
| 156 | Lec <sub>1</sub>         | Linear algal self-shading coefficient  | m <sup>-1.</sup> (µg/L) <sup>-1</sup> | algae          |
| 157 | Lec <sub>2</sub>         | Nonlinear algal self-shading coefficient   | $m^{-1}(\mu g /L)^{-2/3})$            | algae          |
| 158 | <i>P_N</i>               | Algal preference factor for ammonia  | none                                  | N              |
| 159 | PRF                      | Peak rate adjustment factor for sediment routing in channel                        | none                                  | sediment       |
| 160 | SP <sub>con</sub>        | Linear parameter for calculating maximum transport capacity of sediment in channel | none                                  | sediment       |

| 161         | SPexp                                     | Exponent parameter for calculating maximum transport capacity of sediment in channel | none | sediment       |
|-------------|---|--|------|----------------|
| 162         | f_Ph                                      | Flood PH value   | none | C, N           |
| 163         | rcn <sub>rvl</sub>                        | Ratio of C/N of very labile litter   | none | C, N           |
| 164         | <i>rcn<sub>rl</sub></i>                   | Ratio of C/N of labile litter  | none | C, N           |
| 165         | rcn <sub>rr</sub>                         | Ratio of C/N of resistant litter   | none | C, N           |
| 166         | rcn <sub>b</sub>                          | Ratio of C/N of labile biomass   | none | C, N           |
| 167         | <i>rcn</i> <sub>h</sub>                   | Ratio of C/N of labile humus   | none | C, N           |
| 168         | rcn <sub>m</sub>                          | Ratio of C/N of humads   | none | C, N           |
| 169         | pavi                                      | P availability index   | none | C, N           |
| 170         | TtoC                                      | Relationship between TOC and COD   | none | COD            |
| 171-<br>182 | <i>rpnt</i> <sub>01</sub> ~ <sub>12</sub> | Ratio of point pollutant source from Jan. to Dec.                                    | none | pollutant load |

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