

S1. The benthic biogeochemistry module

S1.1. The nitrogen cycle in the sediment layer

The processes involving N in the sediment layer in the model are described by the following state variables, as described in [86] and [87-96]:

- SON for organic N in sediment
- SNH representing total NH_4-N in sediment pore water
- SNO_3 indicating total NO_3 in sediment,
- $SNIM$ for immobilized N in sediments.

Within the sediment, N can undergo mineralization into NH_4 , while NO_3 may be denitrified or exchanged with inorganic N in the water column. NH_4 and NO_3 are considered as inorganic N (IN), with the assumption that the ratio of NH_4 to NO_3 in the water column just above the sediment surface mirrors that of the sediment. Additionally, NH_4 in sediment may undergo exchange with inorganic N or be nitrified into NO_3 in the uppermost sediment layer with the presence of O_2 . It is assumed that a fraction is available for nitrification and for flux across the sediment surface. Given that nitrification is an aerobic process, it is confined to the sediment layer with O_2 .

The processes involving the N -cycle in the sediments are depicted in Figure 3 and represent by the following differential equations:

$$\frac{d SON}{dt} = RSON - RSONNH - RSNIM \quad (S1)$$

$$\frac{dSNIM}{dt} = RSNIM + RDENIT \quad (S2)$$

$$\frac{d SNH}{dt} = \frac{RSONNH - RSNIT - FNH}{(1 - DM) * VF * HDO_2} \quad (S3)$$

$$\frac{d SNO_3}{dt} = \frac{RSNIT - RDENIT - FNO_3}{(1 - DM) * VF * HDS} \quad (S4)$$

The variables DM , VF , HDS , and HDO_2 denote, respectively, the fraction of dry sediment matter in water (g/g), the specific gravity (g/m³), the depths of the active sediment layer (m), and the depth of O_2 penetration into the sediment. The latter depends on the thickness of the water layer above the sediment (m) and is calculated accordingly:

$$HDO_2 = HKA + KKB * DO - KKC * ODSC * WADE \quad (S5)$$

where HKA represents the minimum depth required for O_2 penetration (m), while KKB and KKC are specific parameters governing the penetration of O_2 into sediment (m⁴/g O_2). DO denotes the dissolved oxygen concentration. Additionally, $ODSC$ and $WADE$ stand for the total sediment oxygen consumption (g O_2 /m³/day) and the thickness of the water layer above the sediment layer (m), respectively.

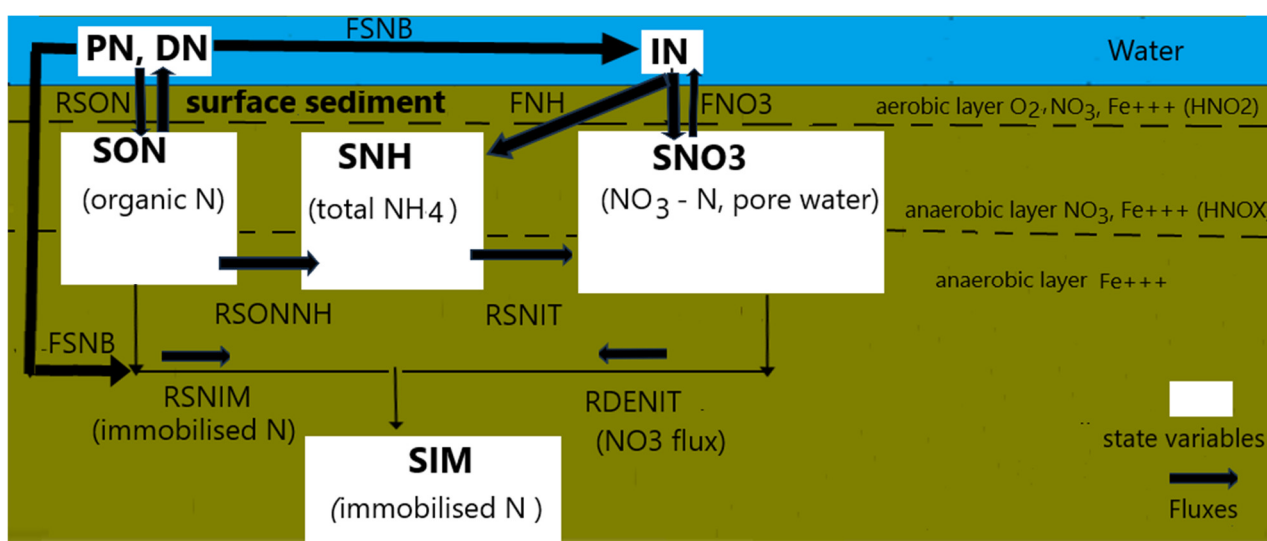


Figure S1_1. The N-cycle in the sediments.

Each equation within the (S1-S4) system, as depicted in Figure S1_1, incorporates specific processes calculated as linear functions of the following biogeochemical state variables described below.

RSO_N accounts for the remaining organic N in the sediment that contributes to the **S_{O_N}** pool. It is considered as a linear function of:

- the sedimentation of the phytoplankton N (**P_N**), **SEP_N**, ($\text{g N m}^{-3} \text{ day}^{-1}$), the sedimentation of the detritus N (**D_N**), **SED_N**, ($\text{g N m}^{-3} \text{ day}^{-1}$)
- the input to sediment of N from dead eelgrass, **SEEN**, ($\text{g N m}^{-3} \text{ day}^{-1}$), and of the fraction of the newly settled organic N which is fast mineralized, **FSNB** ($\text{g N m}^{-2} \text{ day}^{-1}$), which linearly depend on **SEP_N**, **SED_N** and **SEEN**, as well as on a function **TETN** (T^{-20}), where **T** is the water temperature and **TETN** is a number of the order of 1.0.

RSO_{NNH} accounts for the fraction of **S_{O_N}**, which is mineralized into NH_4 . It is supposed proportional to:

- S_{O_N}** (with a constant mineralized rate) and temperature dependent (**TETN** (T^{-20})).

RSNIM accounts for the fraction of the settled nitrogen which is assumed to be buried into the sediment layer. It is calculated as a linear function of the of the following variables described below:

- the sedimentation of the plankton C, **SEPC** ($\text{g C m}^{-3} \text{ day}^{-1}$)
- the sedimentation of the detritus C, **SEDC** ($\text{g C m}^{-3} \text{ day}^{-1}$)
- the input to sediment of C from the dead eelgrass, **SEEC** ($\text{g C m}^{-3} \text{ day}^{-1}$)
- the ratio N:C, of immobile N below which no mineralization occurs
- KNIM** and **WADE**.

RDENIT ($\text{g N m}^{-2} \text{ day}^{-1}$) accounts for the flux of NO_3 into sediment, corresponding to a denitrification process. It is calculated with the help of a Fick law on the concentration of NO_3 in sediment ($\text{g NO}_3\text{-N/m}^3$) for the water sediment interface. A more complex formulation is adopted for the deeper layers of the sediment layer based on, the square root function of **DIFN**, the maximum denitrification rate **DNM3** and of **TETN** (T^{-20});

RSNIT ($\text{g N m}^{-2} \text{ day}^{-1}$) accounts for the nitrification of NH_4 in the sediment. It is supposed linear dependent on the water temperature **TETN** (T^{-20}) and on two Monod-kinetics function for NH_4 in the sediment, and for the squared of O_2 concentration in the pore water, respectively. The potential nitrification rate in sediment at 20 °C is defined as **KNIT**.

FNH ($\text{g N m}^{-2} \text{ day}^{-1}$) accounts for the flux of **S_{NH}** between the sediment and the pore water. It is set proportional to **FNHNO₃** ($\text{g N m}^{-2} \text{ day}^{-1}$) and to the ration rate $\text{NH}_4/(\text{NH}_4 + \text{NO}_3)$:

-**FNO₃** ($\text{g N m}^{-2} \text{ day}^{-1}$) corresponds to the flux of NO_3 between the bottom sediment layer and the water. It is calculated as: **FNO₃** = **FNHNO₃** – **FNH**:

$FNHNO_3$ corresponds to the flux of NH_4+NO_3 between the sediment and the pore water, which is calculated with the help of a Fick law on the gradient of concentration of NH_4+NO_3 relatively to IN :

$$FNHNO_3 = DIFN * \frac{SNH+SNNO_3-IN}{KDOX} \quad (S6)$$

where $HDOX$ is the depth of the anoxic NO_3 sediment layer and $DIFN$ (m^2/day) is the diffusion coefficient of NO_3 into the sediment layer.

S1.2. The phosphorus cycle in the sediment layer

Phosphorus interacts with solids interface in various ways, including exchanges occurring at the solid-liquid interface and precipitation/dissolution reactions involving solid-phase elements such as iron, calcium, and aluminum as described in [86] and [87,88, 90, 93, 97-99]

The processes involving P in the sediment layer are described in the model by the following state variables:

- SOP which accounts for the organic P in sediment, which is mineralized into PO_4 . The exchanges of SOP through the sediment surface occur through sedimentation of algae and detritus P . A fraction of the settled SOP can be as well mineralized into PO_4 on the sediment surface;

- SIP which accounts for the total PO_4-P in sediment pore water;

- $SPFE$, which accounts for the sediment PO_4-P adsorbed to Fe^{+++} ; and $SPIM$ which accounts for the immobile P in the sediment.

The processes involving the P cycle as depicted in Figure 3 are represented by the following differential equations:

$$\frac{d SOP}{dt} = RSOP + ROPSIP - SPIM \quad (S7)$$

$$\frac{d SIP}{dt} = \frac{ROPSIP - RFSEIP - FSIP}{(1 - DM) * VF * HDS} \quad (S8)$$

$$\frac{d SPFE}{dt} = RFESIP \quad (S9)$$

$$\frac{d SPIM}{dt} = RSPIM \quad (S10)$$

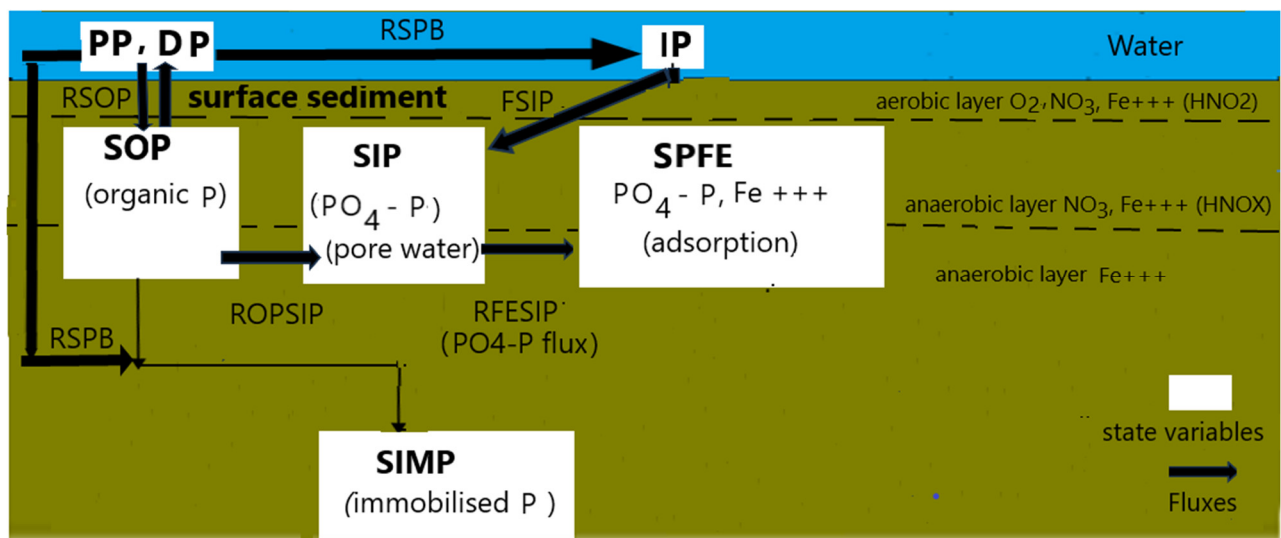


Figure S1_2. The P -cycle in the sediments.

Each equation within the (S7-S10) system, as depicted in Figure S1_2, incorporates specific processes calculated as linear functions of the following biogeochemical state variables described below.

RSOP accounts for the remaining organic in the sediment P which flows into the organic P pool. It is considered as a linear function of the following variable:

- the sum of the sedimentation of the plankton P , $SEPP$ ($\text{g P m}^{-3} \text{ day}^{-1}$), of the sedimentation of the detritus P , $SEDP$ ($\text{g P m}^{-3} \text{ day}^{-1}$);
- the input to sediment of P from the dead eelgrass, $SEEP$ ($\text{g P m}^{-3} \text{ day}^{-1}$), discounted from $FSPB$; The last one corresponds to fraction of the settled organic P which is mineralized on the sediment surface;
- the dept of the water layer above the sediment layer, $DEWA$;

ROPSIP accounts for the fraction of the organic P in the sediment, SOP , which is mineralized into PO_4 , and is released into the pore water pool of PO_4 (SIP). It is supposed to be temperature dependent ($TETN^{(T-20)}$) and a linear function of SOP , with a constant rate $RSP1$.

FSIP accounts for the flux of PO_4 between sediment and water. It is calculated with the help of a Fick law on the concentration of $SIP-IP$ in the sediment layer, with a constant diffusion coefficient, $KFIP$ (m^2/day), and inversely proportional to corresponding to the depth of PO_4 penetration in sediment, $HDOX$ (m).

RFSEIP accounts for the sorption and desorption of PO_4 to Fe^{+++} . It is supposed to obey to a Monod-kinetics for SIP and a linear function of:

- the Fe^{+++} concentration in the surface sediment, KFE (gP/gFe);
- the chemisorption of P to Fe^{+++} , $KFEPO$ (g P/g Fe);
- the depth penetration depth, the same as $HDOX$ (m), and of DM (gDM/gW) and VM (g W/g cm^3), which are respectively the dry matter of sediment relative to the water mass (W), and the specific gravity.

It should be pointed out that in the model:

- the Fe content in the O_2 or NO_3 layer will only be considered in the oxidized form.
- the time rate of $SPIM$, which accounts for the immobile fraction of P in the sediment is supposed to be equivalent to the rate of burial of organic P in sediment, $RSPIM$. The last one is considered proportional to the organic P fraction, $RSOP$, with a constant rate, $KPIM$.

Table S2_1: Main parameters for the N and P cycle in the sediment 107=58

Parameters for the N and P cycle in the sediment	range	Value	References
Fraction of settled N mineralised on sediment	0-1	0.1	-
Mineralisation of SON, 1/day	0-0.1	0.0024	[62]
N:C ratio of immob. Org. N in sediment, g N/g C	0.064	0.064	[62]
Teta. mineralisation of SON in sediment	1.04	1.04	-
Nitrification rate sediment, g N/m ³ /day	0-150	84	[62-65]
Denitrification rate sediment, g N/m ³ /day	0-500	84	[62-65]
Nitrification sediment half saturation conc., g N/m ³	0.5	0.5	-
Halfsaturation conc. For eelgrass uptake of SNH, g N/m ³	0.9	0.9	[66-68]
Teta for temperature. mineralisation of SOP	1.04	1.04	-
Immobile P fraction of settled P	0.15	0.15	[62]
Fraction of settled P mineralised at surface	0-1	0.1	-
Mineralisation of SOP, 1/h	0-0.1	0.0024	[62]
Depth of active sediment layer, m	0-1	1	-
Chemosorption of P to Fe ⁺⁺⁺ , g P/g Fe	0-1	0.005	[69, 71, 72]
Const1. DO penetration in sediment. m	0-0.1	0.00124	[73]
Const2. DO penetration in sediment, m ³ day/DO	0-0.01	0.00132	[73]
Const3. DO penetration in sediment, m/DO	0-0.1	0.000403	[73]
Diffusion for SIP, m ² /day	0-0.001	0.000024	[73]
Halfsaturation Fe ⁺⁺⁺ sorption of SIP, g P/m ³	0.25	0.25	[71, 72]
Rate for Sorption and desorption of PO ₄ to Fe ⁺⁺⁺ , 1/day	0.0004-0.001	0.001	[68]
Diffusion of NO ₃ and NH ₄ in sediment, m ² /h	0-0.001	0.000024	[64, 74]
Teta temp dependency of denitrification	1.087	1.087	[75]

SON-Sediment organic N; SOP-Sediment organic P; SIP-Sediment inorganic P, DO-Dissolved oxygen; SNH-Sediment NH₄.

The sensitivity analysis presented here focuses on parameters related to the nitrogen (N) and phosphorus (P) cycles in sediments, as they encompass both inorganic and organic phases. These parameters play a crucial role in influencing the dynamics of *TN* and *TP*, making them key factors to consider in model validation. The following experiments were considered for a typical spring situation.

- Sens1:** Sediment mineralization rate for organic N and P, *Sed_minerali_rt_NP* (1/day).
- Sens2:** Nitrification and Denitrification rates, maximum values per m³ of sediment, *Nit_Dnit_rt* (g N/(m³ day)).
- Sens3:** NO₃ penetration rate into sediment, *NO3_penet_rt* (1/day).
- Sens4:** Diffusion coefficient of the NO₃ and NH₄ into sediment, *Diffu_coef* (m²/day).
- Sens5:** Fe-P sorption and desorption of PO₄ to Fe⁺⁺ into sediment, maximum value, *Fe_Psor_dsor* (g P/ g Fe).
- Sens6:** Fraction of the settle N and P to mineralization and immobilization, *Fra_N_mineral./immob.* and *Fra_P_mineral./immob* (number).
- Sens7:** Oxygen penetration into sediment constant, *Oxygen_pene1* (m).
- Sens8:** Oxygen penetration into sediment constant, *Oxygen_pene2* m²/(g DO).

The parameters and their reference values are listed in Table 6 (see Annex for the remaining parameters).

Table S2_2. The sensitivity parameter for the experiments. (a)Baseline (calibrated values); (b) Experiment.

Parameter	Sens1	Sens2	Sens3	Sens4	Sens5	Sens6	Sens7	Sens8
Sed_minerali_rt_NP (1/day)	2.4E-3 (a); 1.0E-1 (b)	-	-	-	-	-	-	-
Nit_Dnit_rt g N/(m ³ day)	-	84 (a); 0.84 (b)	-	-	-	-	-	-
NO3_penet_rt (1/day)	-	-	5.0E-1 (a); 1.0E+0 (b)		-	-	-	-
Diffu_coef (m ² /day)	-	-	-	2.4E-5 (a); 5.0E-4 (b)	-	-	-	-
Fe_Psor_dsor (g P/ gFe)	-	-	-	-	5.0E-3 (a); 1.0E-1 (b)	-	-	-
Fra_N_mineral./im- mob. (number)	-	-	-	-	-	1.0E-1 (a); 3.0E-1 (b)	-	-
Fra_P_mineral./im- mob. (number)	-	-	-	-	-	1.0E-2 (a); 1.0E-1 (b)	-	-
Oxygen_pene1 (m)	-	-	-	-	-	-	1.0E-3 (a); 1.0E-2 (b)	-
Oxygen_pene2 (m ² /(g DO))	-	-	-	-	-	-	-	1.0E-2 (a); 1.0E-1 (b)

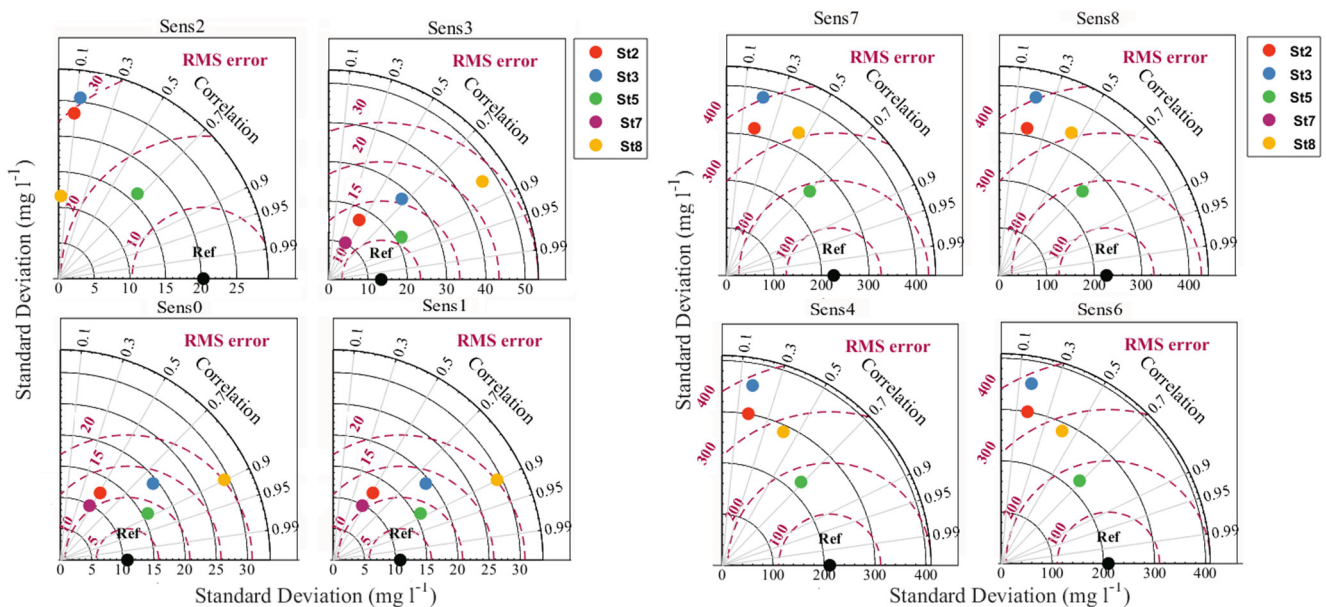


Figure S2_1 Taylor diagrams for TN parameter's sensitivity analysis
The concentrations are multiplied by 1000; *St* means station (Figure 1)
Sens means sensitivity; *Ref* means St1; *Sens0* refers to the baseline simulation.

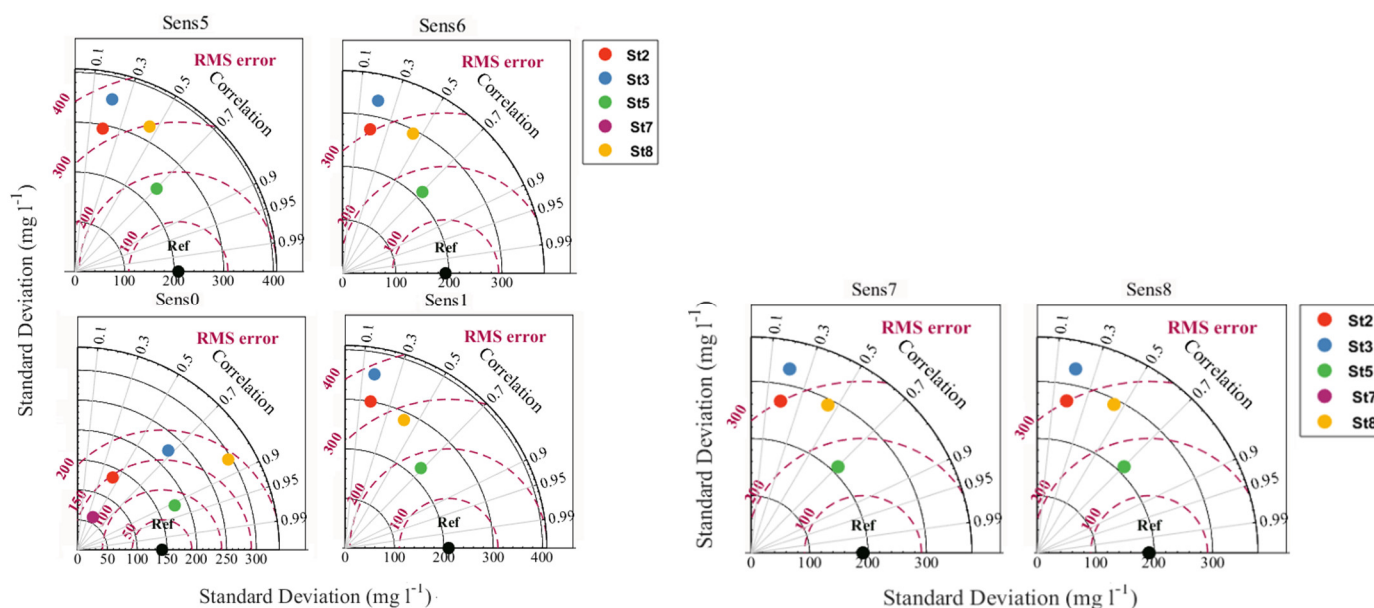


Figure S2_2 Taylor diagrams for TP parameter's sensitivity analysis
 The concentrations are multiplied by 10000; *St* means station (Figure 1)
Sens means sensitivity; *Ref* means *St1*. *Sens0* refers to the baseline simulation.

Remarks:

Figures S2_1 and S2_2 plot the Taylor diagrams for the parameter's sensitivity analysis of Table S2_2 and for five stations. Each plot is related to *St1*. The simulations are compared to the baseline *Sens0*, corresponding to a typical spring situation (average river flows). In the diagram, *Ref* refers to a reference station (*St1*).

Sens4, 6, 7 and 8 present the highest RMSE values for *TN*, varying within the range of (0.1-0.3) mg l^{-1} , while *Sens0*, 1, 2 and 3 the lowest, varying within (0.01-0.03) mg l^{-1} . Considering that *TN* typical mean values for *Sens0* are of the order of 0.3 mg l^{-1} , it can be concluded that *Sens4*, 6, 7 and 8 seem to be the most sensitive parameters for *TN*. When considering the stations influence, it seems like *St2*, 3 and 7 show the highest RMSE values, but, since *St8* is situated outside the diagrams, the last one corresponds, indeed, to the highest values. *TP* present low RMSE values for *Sens0* and 1 (<0.02) mg l^{-1} , while high for *Sens5*, 6 7 and 8 present relatively higher values ((0.02-0.03) mg l^{-1}). Likewise, *St2*, 3, 7 and 8 show the highest RMSE values. Considering that *TP* typical mean values for *Sens0* are of the order of 0.02 mg l^{-1} , it can be concluded that *Sens4*, 6, 7 and 8 seem to be the most sensitive parameters for *TN*.