Process description of NUSWALITE

A simplified model for the fate of nutrients in surface waters

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ABSTRACT

Mathematical models predicting nitrogen and phosphorus concentrations in surface waters can be useful tools to evaluate measures combating eutrophication. NUSWALITE is a water quality model to predict the nutrient concentrations in high spatial and temporal detail for catchments and 'polder areas'. The NUSWALITE model comprises the description of five main processes: i) uptake and release of nutrients by biomass, ii) mineralization of organic phosphorus and nitrogen to their mineral fractions, iii) adsorption and desorption of phosphorus and nitrogen, iv) loss of nitrogen by denitrification, sedimentation and biomass removal, and loss of phosphorus by sedimentation and biomass removal. This report includes the description of the process formulations, solution scheme, parameterization, and calculation of nutrient retention.

Keywords: water quality, simulation model, macrophytes, nutrients, nitrogen, phosphorus, mineralization, denitrification, sorption, sedimentation, retention

Contents

Preface

As the name already suggests NUSWALITE is a model derived from its predecessor NUSWA, which was never been officially published. The NUSWA model, developed in the mid 90s, has been used to simulate water quality processes in polder areas in high spatial and temporal detail. A drawback when applying this model was the amount of parameters needing proper values for which an empirical basis was often lacking. High computational running times, mainly stemming from its high resolution and detailed process descriptions, was another setback.

Another issue often encountered in regional water quality modeling projects is that at this particular scale not all information is available. Furthermore in projects like Euroharp (www.euroharp.org) the description of processes and the output does not need to be as detailed as provided by NUSWA. Therefore, some years ago, the need emerged to create a model which would be quicker and easier to use, a model which could deliver similar output but with less detailed input.

NUSWALITE is at first sight quite similar to the NUSWA model in its description of the phosphorus and nitrogen cycles. It is even somewhat 'heavier' concerning the formulation of biomass growth, which is now described as three biomass pools (two rooting and one floating) instead of one as was the case in NUSWA. However, by lumping the water and sediment compartment, lumping the dissolved and particulate organic pools, and by leaving out the oxygen cycle a more streamlined approach has been created.

NUSWALITE can be used to obtain a first and rather good impression of nutrient concentrations. The simplified and lumped process descriptions make it easy to apply NUSWALITE at large scale. As the NUSWALITE model needs few parameters it can be particular useful when limited data are available. However, smart parameterization still requires a calibration of parameters associated to aggregated processes. For more detailed problems and advanced simulations the use of a more detailed water quality model is nevertheless recommended.

The NUSWALITE model has been used in the Euroharp project and it is currently applied for Dutch catchments in the project "Monitoring Stroomgebieden" (www.monitoringstroomgebieden.nl). This report describes the state-of-the-art and forms the basis for further improvement.

For questions about the contents of this report and the modeling concepts presented, the reader is referred to the (co-)authors Mr. L. van Gerven (luuk.vangerven@wur.nl) or Mr. P. Groenendijk (piet.groenendijk@wur.nl).

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Summary

Evaluation of the effectiveness of eutrophication combating measures often requires the quantification of nutrient loads and concentrations. Mathematical models predicting nitrogen and phosphorus concentrations in surface waters can be useful tools for such quantification efforts. NUSWALITE is a water quality model to predict the nutrient concentration in catchments and 'polder areas'. It describes four main processes, namely: i) the uptake and release of nutrients by biomass; ii) the mineralization of organic phosphorus and nitrogen to mineral fractions; iii) the adsorption and desorption of mainly phosphorus; and iv) the loss of nitrogen by denitrification, sedimentation and biomass removal, and the loss of phosphorus by sedimentation and biomass removal.

NUSWALITE simulates nutrient concentrations in the surface water on basis of water quantity data and nutrient input from the soil system and point sources generated by external models. Currently it is used in combination with SWAP (water flow in the unsaturated zone) and ANIMO (soil processes and nutrient leaching) to simulate the nutrient loads from the soil system. The hydraulic model SWQN is used to simulate surface water flow. Other nutrient input sources, next to the nutrient input generated by the ANIMO model, are erosion, point sources and atmospheric deposition. The user is free to use other external models.

The main parameters for NUSWALITE are estimated by comparing NUSWALITE with processes and known parameters of the NUSWA surface water quality model from which NUSWALITE is derived. The biomass parameters are derived from literature. Indication of ranges are given were possible.

In conclusion, NUSWALITE is a simple fast running and easy to use water quality model developed to simulate the status quo of surface waters with respect to nutrient concentrations and to obtain insights in the effects of combating measures and scenario analysis. It is able to yield realistic predictions of surface water concentrations with limited parameter and data sets at hand. Some parameter calibration, however, is still needed as considerable uncertainty remains in the currently available sets while some process descriptions have been lumped which has led to new parameters. For detailed research questions a more detailed surface water quality is recommended.

The NUSWALITE model has proved its usefulness in modeling surface water quality in various European catchments (Schoumans et al., 2008). This report describes the state-of-the-art and forms the basis for further improvement.

1　Introduction

Eutrophication has been defined as "the nutrient enrichment of waters which results in the stimulation of an array of symptomatic changes, among which increased production of algae and macrophytes and deterioration of water quality, which are found to be undesirable and interfere with water uses" (OECD, 1982). Although eutrophication can have natural causes, it is generally acknowledged that human activities have triggered higher nutrient concentrations in surface and ground waters during the last thirty years.

Especially in the rural areas with intensive agriculture eutrophication is visible in many surface waters, mainly caused by the excessive inflow of nutrients into the aquatic system due to high fertilizer inputs and to discharges of effluents from waste water treatment plants. These loads cause higher production rates of biomass within the aquatic system and, as a result, the biological diversity is reduced and a bloom of algae or macrophytes occurs.

Excessive use of fertilizers leads to high emissions of nutrients from the soil system to the surface waters. The degree of leaching is dependent on soil type, type of fertilizer, way of fertilizer application, nutrient excess and climate conditions. Due to the contamination of water bottoms in the past, inorganic phosphate can also desorb and re-suspend into the water compartment. Other eutrophication sources are the inflow of waste water effluent from purification plants and the inlet of nutrient-rich water from adjacent sub-catchments. In order to reduce the eutrophication level remedial measures are unavoidable.

Implementation of the Framework Water Directive demands for the quantification of the effects of imposed measures on the surface and groundwater (European Communities, 2000). Mathematical models predicting nitrogen and phosphorus concentrations in surface water can be useful tools to evaluate measures combating eutrophication.

In this report the NUSWALITE model is presented. NUSWALITE is a water quality model to predict the nutrient concentration in catchments and 'polder areas'. In order to calculate the nutrient concentration in the surface water on a regional scale, a schematization of the area is required. NUSWALITE obtains this schematization from an external hydraulic model, e.g. SWQN (Smit et al., 2009) or SIMGRO (van Walsum et al., 2005). Such models also provide data on the discharge rates between water compartments, which form the basis of the transport of nutrients within the area. The input of nutrients from the soil system can be obtained from the ANIMO model (Renaud et al., 2004, and Groenendijk et al., 2005).

2 Overview of the NuswaLite model

2.1 NUSWALITE nutrient cycles and boundary conditions

The NUSWALITE model is derived from the NUSWA model (Kolk and Drent, 1996), a surface water quality model developed in the mid 90s. The latter model was especially developed for application in peaty areas where eutrophication manifests itself in duckweed blooms. NUSWA describes the full phosphorus, nitrogen and oxygen cycle and consists of an interconnected system of water and sediment compartments.

In contrast to its predecessor, NUSWALITE is developed for more general applications in order to obtain reasonably good estimates of the nutrient status of surface water bodies. The model lumps several processes to prevent an unacceptable performance for regional applications. The nitrogen and phosphorus cycles are simplified and only consist of a mineral and an organic pool, while the oxygen cycle is not explicitly described. The interaction between water and sediment is formulated by an equilibrium equation instead of modeling two independent compartments. Several types of coexisting floating and rooting biomass can be defined by the user.

This results in a simpler and easy to use model, having less parameters to calibrate, and which is adapted to the amount of data and scale of regional water systems.
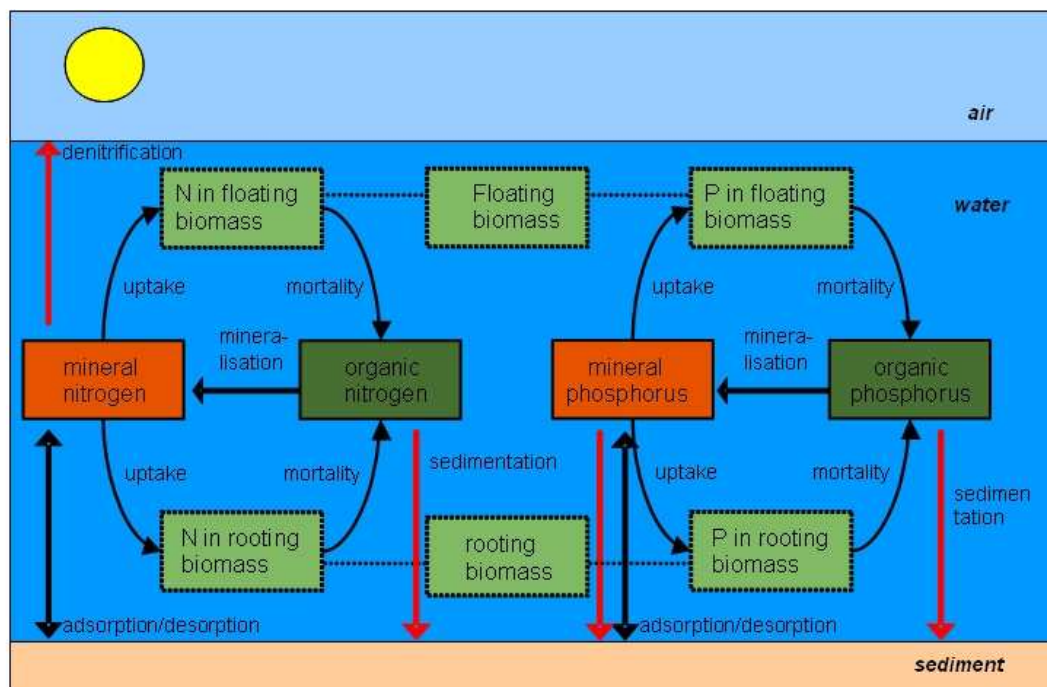
Figure 1 Processes within each section in NUSWALITE: red arrows denote removal processes

The following system state variables are considered in the NUSWALITE model:
- Living biomass - floating fraction
- Living biomass - immovable fraction
- Dissolved organic nitrogen
- Mineral nitrogen
- Dissolved organic phosphorus
- Mineral phosphorus

Figure 1 shows all internal processes that take place in the water and sediment compartment. Four main processes are modeled by the NUSWALITE model: i) first of all we have the uptake and release of nutrients by biomass; ii) the mineralization of organic phosphorus and nitrogen into mineral fractions; iii) the adsorption and desorption of mainly phosphorus and; iv) the loss of nitrogen by denitrification, sedimentation and biomass removal, and the loss of phosphorus by sedimentation and biomass removal. These processes will be explained in detail in Chapters 4 and 5.

Figure 2 shows the fluxes between two sections in NUSWALITE. Floating biomass and all dissolved nitrogen and phosphorus fractions are transported by flowing water to the adjacent downward section. Rooting biomass and sediment, with nitrogen and phosphorus adsorbed to it, are not transported. External nutrients can enter the system by nutrient leaching (e.g. agriculture), soil erosion due to surface run off, point sources, and atmospheric deposition on the water system, i.e. both dry and wet (precipitation).
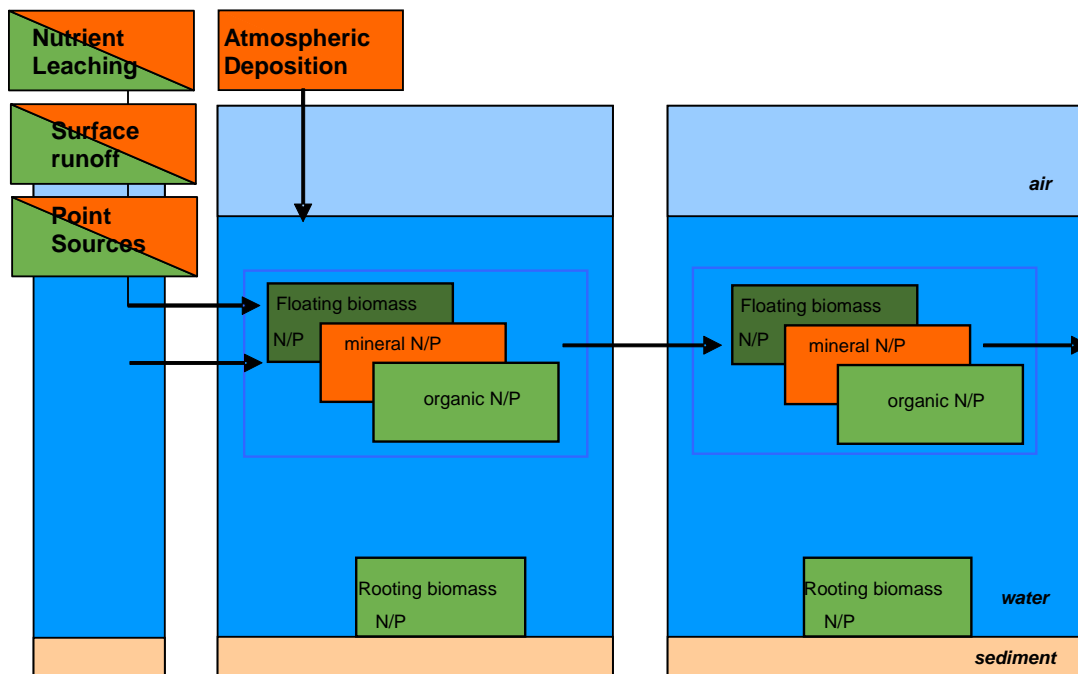
Figure 2 Fluxes between sections in NUSWALITE

The general equation governing the flow processes is described by Equation 1. Internal processes like adsorption/desorption, uptake by plants or denitrification and sedimentation, as shown in Figure 1, are not included in this equation.

$$\frac{dm_w}{dt} = \frac{d(V_w C_w)}{dt} = V_w \frac{dC_w}{dt} + C_w \frac{dV_w}{dt} =$$

$$Q_{in} C_{w,in} - Q_{out} C_w + L_{external,in} - Q_{external,out} C_w$$

(1)

where:

|		
m_w	mass of substance in water compartment	(g)
t	time	(d)
V_w	volume of water compartment	(m³)
C_w	concentration of substance in water compartment	(g m⁻³)
$C_{w,in}$	concentration of substance in upstream water compartment	(g m⁻³)
Q_{out}	flow to downstream compartment	(m³ d⁻¹)
Q_{in}	flow from upstream compartment	(m³ d⁻¹)
$L_{external,in}$	loads of external additions (e.g. nutrient leaching, surface runoff erosion, point sources and atmospheric depositions)	(g d⁻¹)
$Q_{external,out}$	external outgoing flow (e.g. drinking water inlet)	(m³ d⁻¹)

It is important to keep in mind that NUSWALITE assumes the sediment layer and the water compartment to be perfectly mixed. The thickness of this 'virtual' sediment layer can be specified for each water compartment individually and is considered to be static. Hence, sedimentation is interpreted as a sink process and therefore does not affect the volume of the sediment layer. Consequently, re-suspension and transport processes of sediment particles are not included in the model formulation either. Exchange of nutrients between the sediment and water compartment takes place via absorption and desorption which are based on a linear sorption relation (Paragraphs 4.3 and 5.3).

2.2   Relation to external models

Water quantity data and external input of nutrients to the water system form the start for NUSWALITE calculations. These data are usually obtained from external models. In its most common use NUSWALITE makes up the final step in the model chain, which starts with a soil hydrological model feeding a hydraulic model. The soil hydrological model also provides input for a nutrient leaching model. Combined together, the flows computed by the hydraulic model and the loads computed by the nutrient leaching model provide the basic input for the surface water quality model. In addition, surface water concentrations can also be influenced by external nutrient inputs from soil erosive processes caused by surface run off (Walvoort, 2008), point sources and atmospheric deposition. An example of such a model suite is NL-CAT (Schoumans et al., 2008), which is schematically presented in see Figure 3.

The water flow in the soil is described by SWAP (Van Dam, 2000, Van Dam, 2008, and Kroes et al., 2008). Precipitation, atmospheric demand, land-use, soil physical and drainage characteristics form the main input for this model. SWAP calculates the discharge to or infiltration from the surface water, which is, in short, the result of precipitation and upward seepage minus evapotranspiration and downward seepage and the difference in soil water storage.
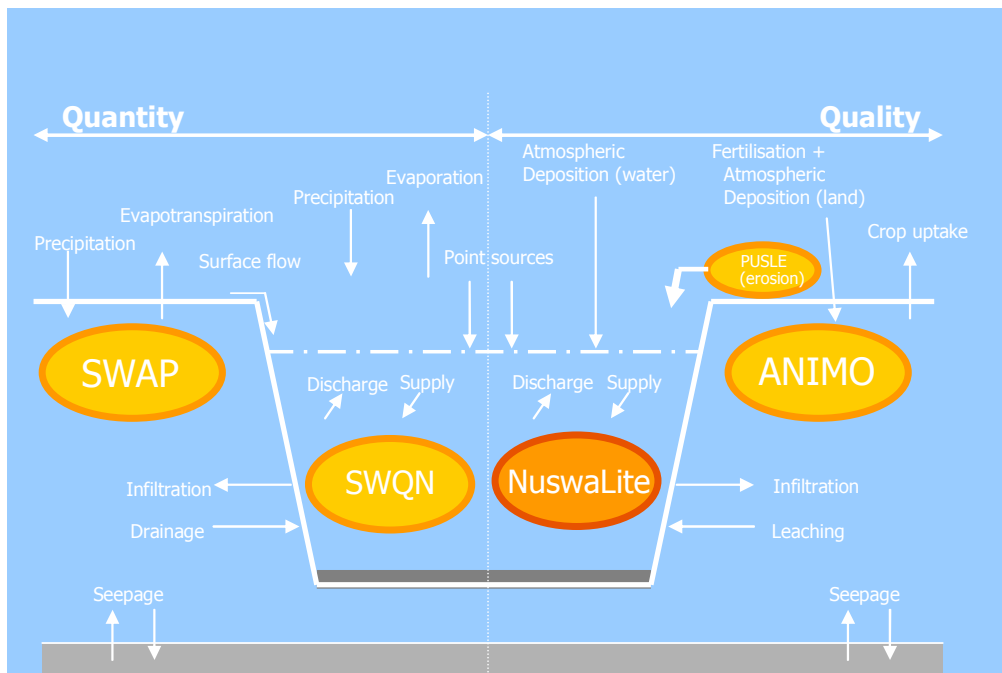
Figure 3 Relation of NUSWALITE to external models and an overview of incoming, outgoing and boundary fluxes, that influence nutrient concentrations in the surface water system.

Nutrient loads from the soil system to the surface water system are obtained from the dynamic ANIMO simulation model (Renaud et al., 2004, Groenendijk et al., 2005). ANIMO includes the carbon, nitrogen and phosphorus cycles and their interrelations using the hydrological information provided by SWAP. Depending on the local hydrological conditions, also infiltration from surface waters may occur or seepage from the deep groundwater across the lower boundary of the profile. Hence, the external concentrations should be known a priori in order to calculate the correct loads for ANIMO.

The discharges in the surface water system are simulated by SWQN, an external hydraulic model (Smit et al., 2009). In SWQN the surface water is schematized into computational nodes linked together by connectors referred to as sections. Each section is assigned a length, cross profile, bottom slope, initial depth and a Chézy friction coefficient, which essentially determine the stage-discharge (Q-h) relations. SWQN provides NUSWALITE with discharges and water volumes and depths, which are

necessary inputs for the advective transport of dissolved nutrients and floating biomass, and the water quality processes in the computational nodes.

The user is of course free to use other external models than the ones presented above as long as their output is correctly converted into the formats used by NUSWALITE (see: NUSWALITE manual by Jeuken and Van Gerven, 2009). For example, the hydraulic models SOBEK (WL│Delft Hydraulics, 2001), DUFLOW (www.duflow.nl), or one of the modules of the SIMGRO package (van Walsum, 2005) can be used as well as a pre-processor.

3   Biomass

3.1   Introduction

The growth of macrophytes has a high impact on the nutrient concentration in the surface water system, especially in summer, and is therefore an essential part of the nutrient cycle. In eutrophic aquatic systems mostly blooms of either algae or one macrophyte species occur. Macrophytes which abundantly grow in eutrophic waters are for example water thyme (Elodea), duckweed (Lemna) and reed (Phragmites Australis). Growth of algae or macrophytes depends on the light intensity (photosynthesis) and water temperature. However, living biomass can only grow in the presence of nutrients. During the period of growth, there will be an uptake of dissolved mineral nitrogen (ammonium or nitrate) and mineral phosphorus. These nutrients return to the water system when biomass dies and particulate organic-N and organic-P is formed.

Three fractions of living biomass are considered: i) a floating fraction which can be transported with the water flow, ii) an immovable fraction having its roots in the sediment, but which has most of its mass above the water surface (e.g. reed), and iii) a submerged rooting biomass fraction.

The mass balance for the floating fraction reads:

$$\frac{Storage \quad difference}{Time \quad difference} = Inflow - Outflow - Death + Growth \tag{2}$$

and the mass balance for the immovable fraction:

$$\frac{Storage \quad difference}{Time \quad difference} = - Death + Growth \tag{3}$$

In mathematical terms:

$$\frac{Storage\ difference}{Time\ difference} : \quad \frac{dV_w[L]}{dt} \tag{4.1}$$

$$Inflow: \quad \sum Q_{in}[L_f]_{in} f_{adv} \tag{4.2}$$

$$Outflow: \quad \sum Q_{out}[L_f] f_{adv} \tag{4.3}$$

$$Death: \quad k_{morT}\overline{V_w}[L] \tag{4.4}$$

$$Growth: \qquad \overline{V_w} \frac{F_T(1-a)P_{st}^* f_{light\ interception}}{\overline{H}} f_{reduction} \qquad\qquad (4.5)$$

where:

$[L]$	dry matter content of living biomass per m^3 water ($[L_f]$=floating biomass, $[L_r]$=submerged rooting biomass, $[L_{reed}]$=reed)	(g m^{-3})
V_w and $\overline{V}_w$	water volume and time averaged water volume present in the water compartment	(m^3)
Q_{in} and Q_{out}	water inflow and water outflow	(m^3 d^{-1})
k_{morT}	temperature corrected mortality rate (biomass type dependent)	(d^{-1})
P^*_{st}	unconstrained standard dry matter production	(g m^{-2} d^{-1})
$\overline{H}$	average water depth	m
a	respiration constant (biomass type dependent)	(-)
F_T	temperature response coefficient	(-)
$f_{light\ interception}$	light interception coefficient (biomass type dependent)	(-)
$f_{reduction}$	reduction factor based on nitrogen or phosphorus concentrations (biomass type dependent)	(-)
f_{adv}	reduction factor on the advective flow of floating biomass	(-)

As can be seen from Equations 4.2 and 4.3, the (in- and) outflow of floating biomass is determined by the concentration times discharge and is reduced by an advective factor between 0 and 1. This advective factor can be used to differentiate between the outflow of water and the outflow of floating biomass. If set to 0, no floating biomass will leave the compartment (or modeled water system) irrespective of the prevailing outgoing flows. If set to 1 the outgoing load will be simply a result of the floating biomass concentration times discharge. Especially for floating biomass, like duckweed, it can be expected that not all mass will leave (parts of) the system with the same flow velocity as the water itself, which is mainly due to frictional forces at the water surface or along the cross profile of the water course.

3.2 Growth

The gross growth of biomass is largely influenced by the solar radiation and the turbidity, temperature and nutrient status of the water. Growth of biomass generates a nutrient uptake demand. In NUSWALITE the nutrient content of the living biomass is considered as a constant fraction of the biomass' dry weight, irrespective of seasonal variations. This gives as nutrient uptake demand for the three types of biomass floating, rooting, and reed:

N uptake demand (g d⁻¹ N): $f_{N,f}\ Growth_f$ $f_{N,r}\ Growth_r$ $f_{N,reed}\ Growth_{reed}$ (5)

P uptake demand (g d⁻¹ P): $f_{P,f}\ Growth_f$ $f_{P,r}\ Growth_r$ $f_{P,reed}\ Growth_{reed}$ (6)

where f_N and f_P are the nitrogen and phosphorus weight fractions of the biomass dry weight (g/g) and dependent on the type of biomass. The change in the content of mineral nutrients in the surface water (in this case nitrogen) as a result of the growth of biomass is described by:

$$\left(\frac{dV_w c_{mN}}{dt}\right)_{uptake\ biomass} = -\left\{f_{N,f}\ Growth_f + f_{N,r}\ Growth_r + f_{N,reed}\ Growth_{reed}\right\}$$ (7)

where C_{mN} is the concentration of mineral nitrogen (g m⁻³) in the surface water. The uptake of mineral phosphorus is described in a similar way.

We have to keep in mind that in NUSWALITE the nutrients for growth are provided by the lumped, and perfectly mixed, water and sediment system. In reality the concentration of nutrients in the sediment pores can be different from the concentration in the water compartment, especially in upward seepage controlled areas having a thick sediment layer. For the growth of rooting biomass, driven by nutrient uptake from the sediment layer by its roots, small errors may be introduced by this assumption.

When the nutrient uptake demand exceeds the available amount of nutrients in the water the growth of biomass (and thus the nutrient uptake) will be reduced (see Paragraph 6.1).

3.2.1 Radiation

The basis for the biomass growth is provided by the standard dry matter production P_a in kg ha⁻¹ d⁻¹, which was approximated by Rijtema et al in 1999. For perfectly clear days it reads:

$$P_{st} = 435\cos(\frac{\pi\phi}{180})^{-0.72}(\cos\frac{\pi(23.45\sin(2\pi\frac{t+284}{365})-\phi)}{180})^{1+0.005|\phi|}$$ (8)

For completely overcast days it is expressed as:

$$P_{st} = 229\cos(\frac{\pi\phi}{180})^{-0.75}(\cos\frac{\pi(23.45\sin(2\pi\frac{t+284}{365})-\phi)}{180})^{1+0.008|\phi|} \qquad (9)$$

where ϕ is the latitude in degrees, positive for the northern hemisphere (see also Figure 4). The actual P^*_{st} for partly clouded days is calculated by the use of the relative duration of bright sunshine.
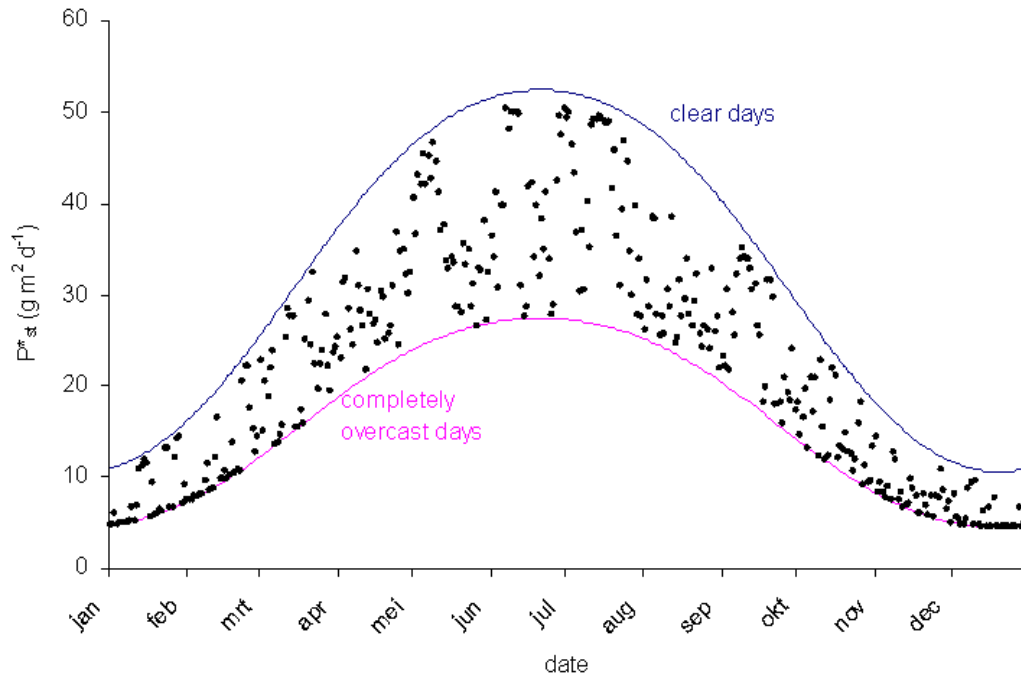
Figure 4 Example of the standard dry matter production P_{st}^* as a function of cloudiness

Light interception

The light interception by the floating and rooting fraction has been taken into account by employing the law of Lambert-Beer. The light interception of all biomass fractions (Equations 10, 11 and 12) is dependent on the amount of biomass: the more biomass per surface area the more light can be intercepted and the smaller the growth reduction will be. Furthermore, the light interception of the submerged rooting fraction is negatively effected by the floating fraction which intercepts light before it reaches the submerged rooting fraction (Equation 11). For a maximum floating biomass layer of 250 g/m2 there will be total light extinction which diminishes linearly with decreasing floating biomass densities.

$$f_{light\,int\,erception\,efficiency,\,f} = (1 - e^{-\alpha_{eff}[L_f]\overline{H}}) \tag{10}$$

$$f_{light\,int\,erception\,efficiency,r} = (1 - \min(\frac{[L_r]\overline{H}}{250},1))(1 - e^{-\alpha_{eff}[L_r]\overline{H}}) \tag{11}$$

$$f_{light\,int\,erception\,efficiency,\,reed} = (1 - e^{-\alpha_{int}[L_{reed}]\overline{H}}) \tag{12}$$

where:

α_{eff}	effective light interception coefficient	(m^2 g^{-1})
α_{int}	light interception constant for reed	(m^2 g^{-1})
$[L]$	dry matter content of living biomass per m^3 water	(g m^{-3})

The dependency of the light interception on the biomass densities makes the biomass growth a 'pseudo' first order process, whereas in Equation 4.5 the growth is presented as a zero order process. Lower values for the light interception constants yield lower light interception coefficients and thus lower growth rates, especially for low concentrations of biomass. For large biomass concentrations the light interception efficiency approaches one (except for submerged rooting biomass where light can be intercepted by floating biomass). This implies a close to zero order growth for large biomass concentrations.

The light interception for the submerged floating and submerged rooting fraction is also influenced by the turbidity and depth of the water column since these factors affect the light availability. An increasing water depth (*H*) leads also to a decreasing average light intensity in the water column at greater depths due to adsorption and extinction by other particles then biomass itself. For the submerged floating fraction the light extinction by depth is a function of the average water depth since the submerged floating fraction will be mainly present in the upper water layer.

Furthermore, increasing flow velocity (*v*) induces an increased re-suspension of suspended solids and has also a decreasing effect on the average light intensity in the water column. The effective light interception factor α_{eff} is therefore determined as a function of water depth (*f₁(H)*) and flow velocity (*f2(v)*) according to Equation 13.

Note that the water depth function and the velocity function are both equal to one for shallow floating biomass.

$$\alpha_{eff} = \alpha \, f_1(H) \, f_2(v)$$
(13)

where:

 α light interception constant $(m^2 \, g^{-1})$

 $f_1(H)$ water depth function, for submerged floating biomass: $H = \overline{H}$ (-)

 $f_2(v)$ velocity function   (-)

The function $f_1(H)$ is derived by splitting the total water depth into two zones: a top zone with full light intensity and a bottom zone with a depth averaged value of the Lambert-Beers light extinction law with depth:

$$H \leq \delta \quad f_1(H) = 1$$
$$H > \delta \quad f_1(H) = 1 - e^{-\lambda \delta} + \frac{e^{-\lambda \delta} - e^{-\lambda H}}{\lambda H - \lambda \delta}$$
(14)

where:

H	water depth	(m)
δ	depth of the top zone with full light intensity	(m)
λ	depth related light extinction constant	(m^{-1})

In the present model setup values of $\delta = 0.075$ m and $\lambda = 3$ m^{-1} were chosen (see also Figure 5), which gives a reasonable fit with values found in literature (e.g. Haag and Gorham, 1977).
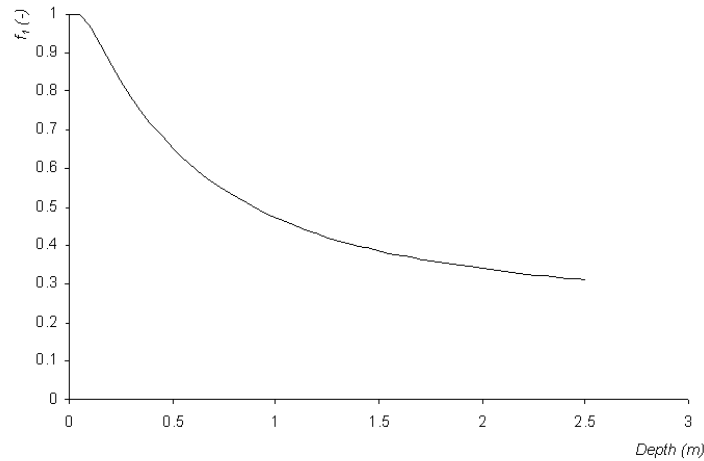
Figure 5 Light interception as function of depth (δ=0.075m and λ=3 m^{-1})

The turbidity of water is influenced by a number of factors: grain size distribution of the suspended solids, depth of the water column, wind speed, shape of the cross section, chemical composition, etc. A threshold value for the flow speed is

introduced assuming no impact of the average flow velocity below this value. According to Sundborg (1956), particles of any grain size will deposit when the flow velocity is less than 0.2 m/s. Some authors assume a proportional increase of turbidity with an increase of average flow speed. A linear relation has the disadvantage of negative results when the flow velocity exceeds a certain value. Therefore a hyperbolic relation with an asymptotic value of zero is introduced:

$$v \leq v_{thres} \qquad f_2(v) = 1$$

$$v > v_{thres} \qquad f_2(v) = 1 - \frac{\kappa\,(v - v_{thres})}{1 + \kappa\,(v - v_{thres})} = \frac{1}{1 + \kappa\,(v - v_{thres})} \qquad (15)$$

where:

v	flow velocity	(m s^{-1})
v_{thresh}	threshold flow velocity	(m s^{-1})
κ	flow related light extinction constant	(s m^{-1})

At small positive values of $\kappa(v - v_{thres})$ the function approaches to a limit according to:

$$f_2(v) \rightarrow 1 - \kappa\,(v - v_{thres})$$

The values $\kappa = 2$ s/m and $v_{thresh} = 0.2$ m/s are used in the present model setup (Figure 6).
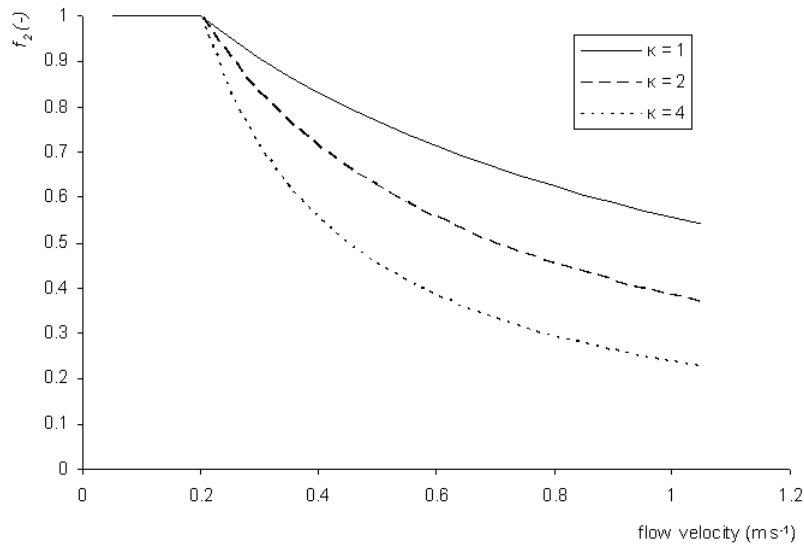
Figure 6 Velocity response as a function of the average flow velocity given for 3 values of κ

3.2.2 Temperature

The temperature response coefficient F_T for the growth of living biomass can be described as:

$$F_T = \theta^{T-20} \tag{16}$$

The Arrhenius coefficient θ is a measure for the dependence of biomass growth on temperature. This coefficient is chosen at 1.06, which corresponds to recently found values (Kadlec et al., 2001, and Bartleson et al., 2005). The response function has been approximated linearly in the reach below 17.2 °C to prevent biomass growth under freezing conditions following (and see also Figure 7):

$$
\begin{aligned}
T < 0\ ^oC & \qquad F_T = 0 \\
0 \leq T \leq 17.2\ ^oC & \qquad F_T = 0.0494\,T \\
T > 17.2\ ^oC & \qquad F_T = \theta^{T-20}
\end{aligned}
\tag{17}
$$
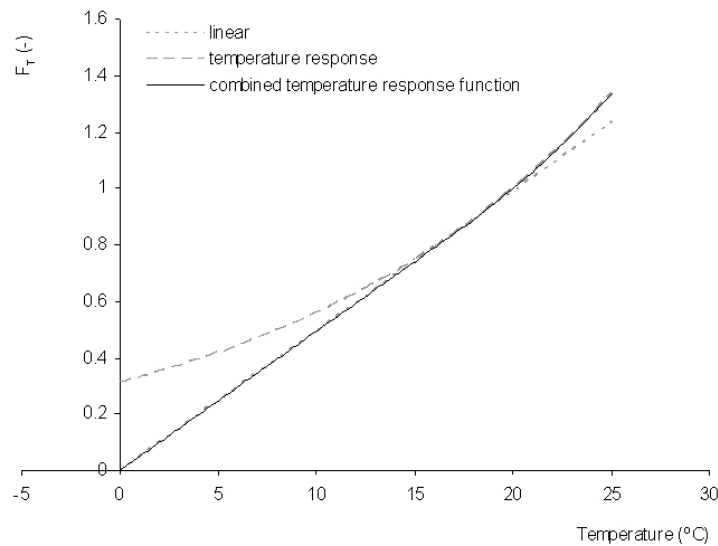
Figure 7 Temperature response curve for the growth of living biomass

3.2.3 Nutrient reduction

Finally growth is controlled by the nutrient status of the surface water in such a way that growth is reduced when nutrient concentrations are relatively low. The Michaelis-Menten (Monod type) reduction function for both nitrogen and phosphorus is applied of which the minimum value is used to reduce the growth (Equation 18). When the concentration in the surface water is equal to C_{monod}, the reduction factor will be exactly 0.5. The growth is increasingly reduced when the

concentration of mineral nitrogen or phosphorus decreases (Figure 8). The C_{monod} coefficient can hold different values for different biomasses.

$$f_{reduction} = \min\left(\left(\frac{c_{mN}}{c_{mN} + c_{N_{monod}}} \right), \left(\frac{c_{mP}}{c_{mP} + c_{P_{monod}}} \right) \right) \qquad (18)$$

where:

c_{mN}	concentration of mineral nitrogen in the water compartment	(g m^{-3})
c_{Nmonod}	Monod coefficient for mineral nitrogen	(g m^{-3})
c_{mP}	concentration of mineral phosphorus in the water compartment	(g m^{-3})
c_{Pmonod}	Monod coefficient for mineral phosphorus	(g m^{-3})
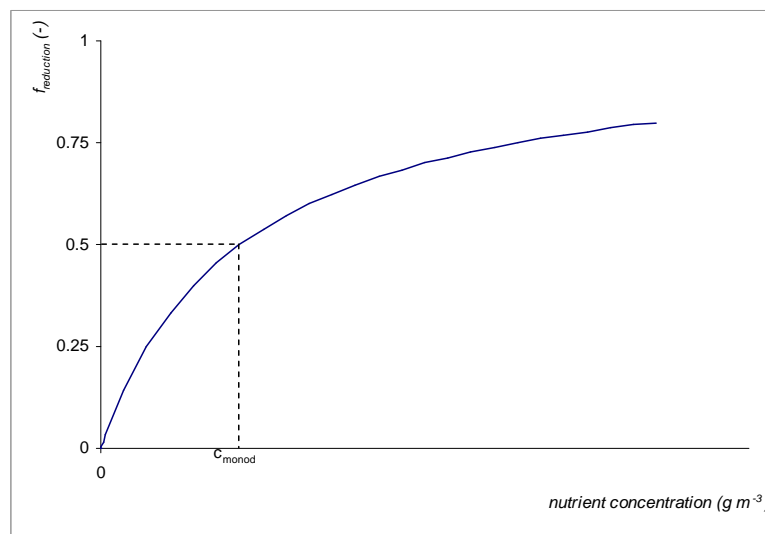
Figure 8 Reduction on growth as a result of (mineral) nutrient concentrations

3.3 Mortality

The death of biomass is considered as a first order rate process dependent on the actual density of living biomass. The decease results in a direct input to the dissolved organic nitrogen and phosphorus fractions. This is a simplification in the NUSWALITE model. In reality nitrogen and phosphorus will be stored, temporarily or definitively, in a pool of dead biomass as particulate organic material before it will be released as dissolved organic material. The absence of this definitive storage of dead biomass in NUSWALITE can partly be compensated by the nitrogen and phosphorus sedimentation rates (Paragraphs 4.2 and 5.2).

The change in content of dissolved organic nitrogen as a result of dying biomass is given by Equation 19. A similar equation holds for (dissolved) organic phosphorus.

$$\left(\frac{dV_w c_{oN}}{dt}\right)_{mortality} = k_{morT,f}\overline{V}_w f_{N,f}[L_r] + k_{morT,r}\overline{V}_w f_{N,r}[L_r] + k_{morT,reed}\overline{V}_w f_{N,reed}[L_{reed}] \qquad (19)$$

where:

c_{oN} concentration of dissolved organic nitrogen in the surface water   g m^{-3}

k_{morT} temperature corrected mortality rate (biomass type dependent)   d^{-1}

The death of biomass indirectly contributes to the amount of mineral nutrients in the surface water since dissolved organic nutrients are transformed into mineral nutrients by mineralization.

3.3.1 Temperature and seasonal response

The temperature corrected mortality rate k_{mor} for the mortality of biomass is calculated according to:

$$k_{morT} = k_{mor}\left(1+\beta_{mor}\right)^{T-20} \qquad (20)$$

where:

k_{mor} mortality rate (biomass type dependent)   d^{-1}

β_{mor} temperature response on mortality rate (biomass type dependent)   [-]

For all biomasses a seasonal difference in mortality rates can be imposed. Different values for the mortality rate can be specified for the winter season and the summer season. By default the summer starts at the 1st of April and ends at the 30th of September, but both start and end date can be specified by the user.

3.3.2 Removal of biomass by management

The NUSWALITE model accounts for the removal of biomass by management like mowing or dredging. For each water compartment individually a fraction of biomass can be removed on a specified date. This kind of management provides a good tool to directly remove nutrients (contained by the biomass) from the system. NUSWALITE, however, does not account for redistribution of nutrients over the shoot and roots for rooting biomass. During the winter nutrients are stored in the roots whereas in the growth season nutrients are translocated to the shoot. As a consequence the removal of nutrients by harvesting in the winter instead of summer can be overestimated by about 40% for reed (Meuleman et al., 2002), since only the non-submerged parts (shoot) will be mowed.

3.4 Numerical solution

The differential equations describing growth and death of living biomass are solved analytically in the NUSWALITE model. For illustrative purposes a numerical finite difference solution technique is employed here. The numerical approach yields an easier relationship between the average living biomass content during the time step and the concentration change with time. This simple relation is used in the feedback relation describing the living biomass development at nutrient constrained conditions (Chapter 6). The central difference scheme for the floating fraction is given by:

$$
\frac{V_{w,t_0+\Delta t}[L_f]_{t_0+\Delta t} - V_{w,t_0}[L_f]_{t_0}}{\Delta t} = -(\frac{[L_f]_{t_0+\Delta t} + [L_f]_{t_0}}{2})(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w) + \\
\sum Q_{in}[L_f]_{in} f_{adv} + Growth_f
\tag{21}
$$

where:

$$
Growth_f = \overline{V}_w \frac{F_T(1-a)P_{st}^*(1-e^{-\alpha_{eff}[L_f]_{t_0}\overline{H}})}{\overline{H}} f_{reduction}
\tag{22}
$$

The subscript t_0 indicates the start of the time step and the subscript $t_0 + \Delta t$ denotes the end of the time step (Δt).

Re-arranging yields:

$$
[L_f]_{t_0+\Delta t} = \frac{\left(V_{w,t_0} - \frac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w)\right)}{\left(V_{w,t_0+\Delta t} + \frac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w)\right)}[L_f]_{t_0} + \\
\frac{\Delta t \sum Q_{in}[L_f]_{in} f_{adv} + \Delta t\, Growth_f}{\left(V_{w,t_0+\Delta t} + \frac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w)\right)}
\tag{23}
$$

The central difference scheme for the immovable fraction worked out for the submerged rooting biomass fraction (these equations also hold for reed):

$$
\frac{V_{w,t_0+\Delta t}[L_r]_{t_0+\Delta t} - V_{w,t_0}[L_r]_{t_0}}{\Delta t} = -(\frac{[L_r]_{t_0+\Delta t} + [L_r]_{t_0}}{2})k_{morT,f} \overline{V}_w + Growth_r
\tag{24}
$$

where:

$$
Growth_r = \overline{V}_w \frac{F_T(1-a)P_{st}^* e^{-\alpha_{eff}[L_f]_{t_0}\overline{H}}(1-e^{-\alpha_{eff}[L_r]_{t_0}\overline{H}})}{\overline{H}} f_{reduction}
\tag{25}
$$

and re-arranging yields:

$$[L_r]_{t_0+\Delta t} = \frac{\left(V_{w,t_0} - \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w\right)}{\left(V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w\right)} [L_r]_{t_0} + \frac{\Delta t\, Growth_r}{\left(V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w\right)} \qquad (26)$$

The average values for L_f, L_r, and L_{reed} are calculated by:

$$[\overline{L}_f] = \frac{[L_f]_{t_0+\Delta t} + [L_f]_{t_0}}{2} = \frac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w)} [L_f]_{t_0} +$$

$$\frac{\dfrac{\Delta t}{2}(Growth_f + \sum Q_{in}[L_f]_{in} f_{adv})}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f} \overline{V}_w)}$$

$$[\overline{L}_r] = \frac{[L_r]_{t_0+\Delta t} + [L_r]_{t_0}}{2} = \frac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w} [L_r]_{t_0} + \frac{\dfrac{\Delta t}{2} Growth_r}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w} \qquad (27)$$

$$[\overline{L}_{reed}] = \frac{[L_{reed}]_{t_0+\Delta t} + [L_{reed}]_{t_0}}{2} = \frac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w} [L_{reed}]_{t_0} + \frac{\dfrac{\Delta t}{2} Growth_{reed}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,f} \overline{V}_w}$$

where:

$$Growth_{reed} = \overline{V}_w \frac{F_T (1-a) P_{st}^* (1 - e^{-\alpha_{int}[L_{reed}]_{t_0} \overline{H}})}{\overline{H}} f_{reduction} \qquad (28)$$

4 Nitrogen cycle

4.1 Nitrogen components in water

The nitrogen concentration in a water body depends on the inflow and outflow of nitrogen and on the internal processes. These processes are part of the nitrogen cycle as shown in Figure 9. In the nitrogen cycle four nitrogen components are described: dissolved organic nitrogen (also containing particulate organic nitrogen), mineral nitrogen (ammonium and nitrate), nitrogen in biomass and mineral nitrogen adsorbed to the sediment. The growth and death of rooting and floating biomass plays a central role in the nitrogen cycle (Chapter 3). Rooting and floating biomass require mineral nitrogen for their growth, while organic nitrogen is released to the water by decaying biomass.
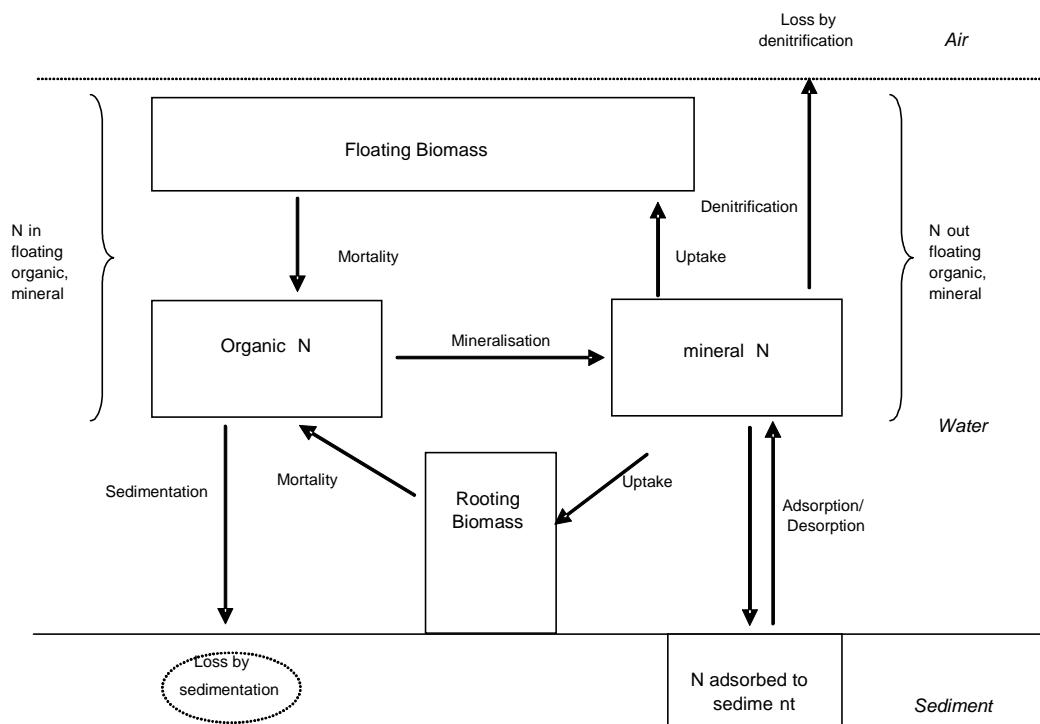
Figure 9 Schematic overview of the nitrogen cycle in NUSWALITE

In NUSWALITE it is assumed that the nitrogen concentration is not influenced by binding of N_2 from the atmosphere by micro-organisms. Also the loss of nitrogen due to NH_3 volatilization is neglected. The losses from the surface water compartment are:

- N removal by denitrification, sedimentation and biomass removal (management);
- Outflow of dissolved organic and mineral nitrogen;
- Outflow of floating biomass.

4.2 Mineralization, denitrification and sedimentation

Mineralization of dissolved organic to mineral nitrogen and denitrification, where nitrate is converted[1] into nitrogen gas, are modeled as first order processes with temperature dependent rates and coefficients given by:

$$k_{miT} = k_{mi}(1 + \beta_{mi})^{T-20} \tag{29}$$

$$k_{denT} = k_{den}(1 + \beta_{den})^{T-20} \tag{30}$$

where:

k_{mi}	constant mineralization rate for organic nitrogen	(d^{-1})
β_{mi}	mineralization temperature response factor	(-)
k_{den}	constant denitrification rate	(d^{-1})
β_{den}	denitrification temperature response factor	(-)

Mineralization, however, is a stepwise process: first particulate organic material mineralizes to the dissolved organic fraction, which then mineralizes to the mineral fraction, or ammonium to be more precise. The next step is the nitrification of ammonium to nitrate. All three steps are lumped in NUSWALITE.

Denitrification in NUSWALITE applies to the fraction of mineral nitrogen in the combined water-sediment compartment, while in the NUSWA model this has been correctly modeled, i.e. only converting nitrate in the sediment into nitrogen gas. Using the NUSWALITE approach may overestimate the actual denitrification, especially for water systems where ammonium makes up a considerable part of the amount of mineral nitrogen available and where sediments are relatively well aerated.

Deceased biomass will settle as sediment in the water courses, either until it is decomposed into particulate organic N and leached to the water compartment or until the biomass itself is re-suspended due to increased flow velocities, or when the top sediment layer is removed as a result of dredging. A certain part of the deceased biomass, however, will never be released as dissolved organic nitrogen and can be considered as a loss term. This part is modeled in NUSWALITE as a first order removal process with sedimentation rate k_{sed}. It is possible to specify for each water compartment individually if sedimentation occurs and at which rate.

---

[1] This process needs anaerobic conditions and support from denitrifying bacteria

The irreversible sedimentation rate is described as:

$$k_{sed,oN} = \frac{w_{s,oN}}{H}$$

(31)

where:

$k_{sed,oN}$ sedimentation rate for dissolved organic nitrogen   (d^{-1})

$w_{s,oN}$ sediment sink speed for dissolved organic compounds   (m d^{-1})

H water depth   (m)

Very shallow water depths would lead to very high sedimentation rates with an almost total removal of dissolved organic nitrogen as a consequence. In reality a total depletion of nitrogen will not occur. For that reason the minimum water depth in the sedimentation rate equation is limited to 10^{-4} m.

4.3 Adsorption and desorption

The ammonium component of mineral nitrogen can be ad- and desorbed to the sediment layer depending on concentration changes in the pore water. Since the sediment compartment is modeled as a 'virtual layer', no pore water exists and nitrogen concentrations will be equal to the concentrations in the water compartment. For infiltration dominated areas this hypothesis is more-or-less justified. For upward seepage controlled areas errors may be introduced.

In NUSWALITE we also use a linear Freundlich isotherm for the adsorption as it is contemplated that the generally low values for the ammonium sorption coefficients render small errors in the adsorbed fractions. Since the ammonium and nitrate pools are lumped in the model, the sorption is directly related to the complete mineral nitrogen fraction. This may give an upward distortion in the adsorption for low ammonium concentrations.

The sorption equilibrium is then represented by the following equation:

$$\left(\frac{dV_w c_{mN}}{dt} \right)_{adsorption} = k_{aN}\, \overline{V}_s \rho_s \left(\frac{dc_{mN}}{dt} \right)_{sediment}$$

(32)

where:

k_{aN} sorption coefficient for mineral nitrogen   (m$^3_{water}$ g$^{-1}_{solid}$)

$\overline{V}_s$ volume of the sediment layer   (m$^3_{solid}$)

ρ_s bulk density of the sediment layer   (g$_{solid}$ m$^{-3}_{solid}$)

The volume of the sediment layer is computed by multiplying the bottom area of the water compartment with a 'virtual sediment thickness', which can be specified for each compartment individually.

The adsorption rate of mineral nitrogen to the sediment is assumed to be constant with time. However, it is possible to introduce a seasonal variation if desired (see Equation 33).

$$k_{aN} = k_{aN\min} + (k_{aN\max} - k_{aN\min})\left(\tfrac{1}{2} + \tfrac{1}{2}\cos(2\pi\left(\frac{t - t_{k_{aN\max}}}{365.25}\right))\right)^2 \qquad (33)$$

where:

$k_{aN\min}$	minimum adsorption rate for mineral nitrogen	(m³$_{water}$ g^{-1}$_{solid}$)
$k_{aN\max}$	maximum adsorption rate for mineral nitrogen	(m³$_{water}$ g^{-1}$_{solid}$)
t	day of the year	(d)
$t_{k_{aN\max}}$	day with maximum adsorption	(d)

4.4   General nitrogen equation

Summarizing all previously discussed processes the system of equations for organic and mineral nitrogen becomes:

$$\begin{pmatrix} \dfrac{dV_w c_{oN}}{dt} \\ k_{aN}\,\bar{V}_s\rho_s\dfrac{dc_{mN}}{dt} + \dfrac{dV_w c_{mN}}{dt} \end{pmatrix} = \begin{pmatrix} -\sum Q_{out} -(k_{sed,oN} + k_{miT})\bar{V}_w & 0 \\ k_{miT}\bar{V}_w & -\sum Q_{out} - k_{denT}\bar{V}_w \end{pmatrix}\begin{pmatrix} c_{oN} \\ c_{mN} \end{pmatrix} +$$

$$\begin{pmatrix} \sum Q_{in}c_{oN,in} + \bar{V}_w\{k_{morT,f}f_{N,f}[\bar{L}_f] + k_{morT,r}f_{N,r}[\bar{L}_r] + k_{morT,reed}f_{N,reed}[\bar{L}_{reed}]\} \\ \sum Q_{in}c_{mN,in} - \{f_{N,f}\,Growth_f + f_{N,r}\,Growth_r + f_{N,reed}\,Growth_{reed}\} \end{pmatrix} \qquad (34)$$

where:

$\sum Q_{in}c_{oN,in}$	Sum of incoming loads of organic nitrogen from upstream water compartment(s) (incoming flow times concentration contained by upstream compartment)	(g d^{-1})
$\sum Q_{in}c_{mN,in}$	Sum of incoming loads of mineral nitrogen from upstream water compartment(s)	(g d^{-1})
$\sum Q_{out}$	Sum of outgoing fluxes to downstream compartment(s)	(m³ d^{-1})

The incoming loads from the upstream compartment(s) also comprise the external incoming loads on the compartment under consideration: either as direct external loads (e.g. nutrient leaching, surface runoff erosion, point sources and dry atmospheric deposition) or as indirect loads by multiplying their concentrations by the corresponding external flux (e.g. precipitation, nutrient leaching, surface runoff

erosion and point sources) (see also Chapter 2). The total outgoing flux includes external outgoing fluxes (e.g. drinking water inlet).

Substitution of Equation 27 in Equation 34 yields:

$$\begin{pmatrix} \dfrac{dV_w c_{oN}}{dt} \\[2mm] k_{aN}\,\overline{V}_s\rho_s\dfrac{dc_{mN}}{dt}+\dfrac{dV_w c_{mN}}{dt} \end{pmatrix} = \begin{pmatrix} -\sum Q_{out}-(k_{sed,oN}+k_{miT})\overline{V}_w & 0 \\[2mm] k_{miT}\overline{V}_w & -\sum Q_{out}-k_{denT}\overline{V}_w \end{pmatrix}\begin{pmatrix} c_{oN} \\ c_{mN} \end{pmatrix} + \begin{pmatrix} Constant_{oN} \\ Constant_{mN} \end{pmatrix} \quad (35)$$

where:

$$Constant_{oN} = \sum Q_{in}c_{oN,in} + \overline{V}_w\{k_{morT,f}f_{N,f}p_{f,1} + k_{morT,r}f_{N,r}p_{r,1} +$$
$$k_{morT,reed}f_{N,reed}p_{reed,1} + k_{morT,f}f_{N,f}p_{f,2}(Growth_f + \sum Q_{in}[L_f]_{in}f_{adv}) +$$
$$k_{morT,r}f_{N,r}p_{r,2}Growth_r + k_{morT,reed}f_{N,reed}p_{reed,2}Growth_{reed}\}$$

$$Constant_{mN} = \sum Q_{in}c_{mN,in} - \{f_{N,f}Growth_f + f_{N,r}Growth_r + f_{N,reed}Growth_{reed}\}$$

$$p_{f,1} = \frac{\dfrac{V_{w,t_0}+V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}(\sum Q_{out}f_{adv}+k_{morT,f}\overline{V}_w)}[L_f]_{t_0} \qquad p_{f,2} = \frac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}(\sum Q_{out}f_{adv}+k_{morT,f}\overline{V}_w)} \quad (36)$$

$$p_{r,1} = \frac{\dfrac{V_{w,t_0}+V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}k_{morT,r}\overline{V}_w}[L_r]_{t_0} \qquad p_{r,2} = \frac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}k_{morT,r}\overline{V}_w}$$

$$p_{reed,1} = \frac{\dfrac{V_{w,t_0}+V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}k_{morT,reed}\overline{V}_w}[L_{reed}]_{t_0} \qquad p_{reed,2} = \frac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t}+\dfrac{\Delta t}{2}k_{morT,reed}\overline{V}_w}$$

5 Phosphorus cycle

5.1 Phosphorus components in water

The kinetics for the phosphorus system is defined analogously to the nitrogen system. We distinguish four different phosphorus components in the water compartment, namely mineral phosphorus, (dissolved) organic phosphorus (also containing particulate organic phosphorus), phosphorus in biomass, and mineral phosphorus adsorbed to the sediment (Figure 10).

The amount of phosphorus present in biomass can be directly deduced from its dry mass P ratio in relation to the total biomass weight. Phosphorus from biomass is returned to the water phase when plants die and biomass is recycled into non-living organic matter.

Mineral phosphorus can be adsorbed to the iron and aluminum compounds in the sediment layer until an equilibrium between the adsorbed phosphorus and the concentration in the water phase is reached. This equilibrium depends on the properties and oxygen condition of the sediment layer, sorption isotherm, and the phosphorus concentration in the water compartment.
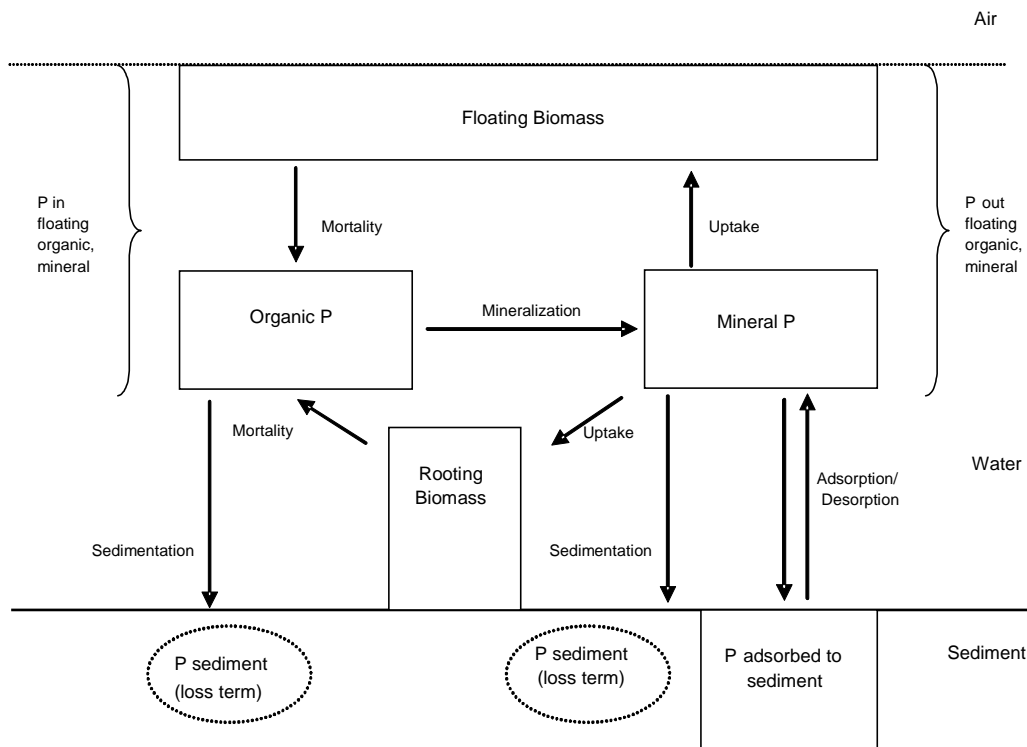
Figure 10 Schematic overview of the phosphorus cycle in NUSWALITE

Sedimentation is regarded as a loss term, representing the settled part which is not subject to re-suspension. The transport of phosphorus to other water compartments takes place via advection.

The losses from the surface water compartment thus comprise:
- P removal by irreversible sedimentation and biomass removal (management);
- Outflow of dissolved organic and mineral nitrogen;
- Outflow of floating biomass.

5.2   Mineralization and sedimentation

Mineralization of organic to mineral phosphorus is described in the same way as the mineralization of nitrogen (Paragraph 4.2). Also here the two-step mineralization process, from particulate organic to dissolved organic to mineral phosphorus, is lumped into a single step. The mineralization rate of phosphorus is hence described by an equation similar to Equation 29.

As previously explained, sedimentation is considered as an irretrievable loss term in NUSWALITE. It represents the loss of mineral phosphorus by irreversible sorption to the sediment. It also includes the loss of organic phosphorus by sedimentation of particulate organic matter, which is a product of deceased biomass, followed by burial or dredging (Brenner et al., 2006). In reality, however, not all deposited particulate matter will be retained. Some parts are re-suspended due to for example high flow velocities.

The sedimentation rate is described similar to the nitrogen sedimentation rate (Paragraph 4.2). The sediment rates for the mineral and organic fractions can hold different values.

5.3   Adsorption and desorption

The sediment layer plays an important role in the regulation of the phosphorus concentration in surface waters due to the strong adsorption of phosphate to iron- and aluminum (hydr-)oxides and clay minerals. The contaminated sediment will again release its phosphate if concentrations in the water phase fall below the equilibrium state. In analogy to the description for nitrogen sorption (Paragraph 4.3), phosphate concentrations in the water compartment are used to calculate the adsorption to and desorption from the 'virtual sediment layer'.

P-sorption is often described with a Langmuir isotherm (Enfield et al., 1977; Noordwijk et al., 1990; Schoumans and Groenendijk, 2000). The Langmuir equation approaches to a linear Freundlich isotherm for low concentration values (Equation 37).

In NUSWALITE we assume a linear Freundlich isotherm for P-sorption, which is plausible for the low concentration ranges but may be questionable for the higher ranges. However, the total adsorptive capacity of the water-sediment system is not only determined by the sorption parameters, but also by the mass of the 'virtual sediment layer' (Equation 38). This provides further options for calibration (see Paragraph 7.5).

$$\lim_{c \to 0} \frac{S_{max} k_L c}{1 + k_L c} = S_{max} \ k_L \ c \tag{37}$$

where:

c	liquid concentration	$(\text{g m}^{-3}_{\text{pore water}})$
k_L	sorption constant	$(\text{m}^3_{\text{pore water}} \text{ g}^{-1}_{\text{solid}})$
S_{max}	maximum sorption capacity	$(\text{g}_{\text{solid}} \text{ g}^{-1})$

$$\frac{dV_w c_{mP-adsorption}}{dt} = k_{aP} \ \overline{V}_s \rho_s \frac{dc_{mP}}{dt} \tag{38}$$

where:

k_{aP}	sorption coefficient for mineral phosphorus	$(\text{m}^3_{\text{water}} \text{ g}^{-1}_{\text{solid}})$
$\overline{V}_s$	volume of the sediment layer	$(\text{m}^3_{\text{solid}})$
ρ_s	bulk density of the sediment layer	$(\text{g}_{\text{solid}} \text{ m}^{-3}_{\text{solid}})$

Due to much higher sorption coefficients, the amount of mineral phosphorus adsorbed is much higher than the amount of mineral nitrogen. The phosphorus adsorption capacity can also fluctuate over time. When oxygen levels rise, Fe^{2+} oxidizes to Fe^{3+} and more phosphate can be absorbed. During the winter season, oxygen levels in the sediment are in general higher than during the summer due to lower BODs and temperatures while higher flow velocities offer better re-aeration conditions. Therefore, the maximum values of the adsorption coefficient are likely to occur in winter time (Equation 39).

$$k_{aP} = k_{aP_{min}} + (k_{aP_{max}} - k_{aP_{min}}) \left(\frac{1}{2} + \frac{1}{2} \cos(2\pi \left(\frac{t - t_{k_{aP_{max}}}}{365.25} \right)) \right)^2 \tag{39}$$

where:

$k_{aP_{min}}$	minimum adsorption rate for mineral phosphorus	$(\text{m}^3_{\text{water}} \text{ g}^{-1}_{\text{solid}})$
$k_{aP_{max}}$	maximum adsorption rate for mineral phosphorus	$(\text{m}^3_{\text{water}} \text{ g}^{-1}_{\text{solid}})$
t	day number of the year	(d)
$t_{k_{aP_{max}}}$	day number with maximum adsorption	(d)

5.4 General phosphorus equation

The final system of equations for the phosphorus component is given by:

$$\begin{pmatrix} \dfrac{dV_w c_{oP}}{dt} \\ \rho_s \overline{V}_s k_{aP} \dfrac{dc_{mP}}{dt} + \dfrac{dV_w c_{mP}}{dt} \end{pmatrix} = \begin{pmatrix} -\sum Q_{out} - (k_{miT} + k_{sed,oP})\overline{V}_w & 0 \\ k_{miT}\overline{V}_w & -\sum Q_{out} - k_{sed,mP}\overline{V} \end{pmatrix} \begin{pmatrix} c_{oP} \\ c_{mP} \end{pmatrix} + $$

$$\begin{pmatrix} \sum Q_{in} c_{oP,in} + \overline{V}_w \{ k_{morT,f} f_{P,f}[\overline{L}_f] + k_{morT,r} f_{P,r}[\overline{L}_r] + k_{morT,reed} f_{P,reed}[\overline{L}_{reed}] \\ \sum Q_{in} c_{mP,in} - \{ f_{P,f} Growth_f + f_{P,r} Growth_r + f_{P,reed} Growth_{reed} \} \end{pmatrix} \qquad (40)$$

where:

$\sum Q_{in} c_{oP,in}$	Sum of incoming loads of organic phosphorus from upstream water compartment(s) (incoming flow times concentration contained by upstream compartment)	(g d⁻¹)
$\sum Q_{in} c_{mP,in}$	Sum of incoming loads of mineral phosphorus from upstream water compartment(s)	(g d⁻¹)
$\sum Q_{out}$	Sum of outgoing fluxes to downstream compartment(s)	(m³ d⁻¹)

Similar to nitrogen, the incoming loads include external loads, whereas the total outgoing flow include external demands (see also Chapter 2).

Substitution of Equation 27 in Equation 40 yields:

$$\begin{pmatrix} \dfrac{dV_w c_{oP}}{dt} \\ \rho_s \overline{V}_s k_{aP} \dfrac{dc_{mP}}{dt} + \dfrac{dV_w c_{mP}}{dt} \end{pmatrix} = \begin{pmatrix} -\sum Q_{out} - (k_{miT} + k_{sed,oP})\overline{V}_w & 0 \\ k_{miT}\overline{V}_w & -\sum Q_{out} - k_{sed,mP}\overline{V} \end{pmatrix} \begin{pmatrix} c_{oP} \\ c_{mP} \end{pmatrix} + \begin{pmatrix} Constant_{oP} \\ Constant_{mP} \end{pmatrix} \qquad (41)$$

where:

$$Constant_{oP} = \sum Q_{in} c_{oP,in} + \overline{V}_w \{ k_{morT,f} f_{P,f} p_{f,1} + k_{morT,r} f_{P,r} p_{r,1} +$$
$$k_{morT,reed} f_{P,reed} p_{reed,1} + k_{morT,f} f_{P,f} p_{f,2} (Growth_f + \sum Q_{in}[L_f]_{in} f_{adv}) + \qquad (42)$$
$$k_{morT,r} f_{P,r} p_{r,2} Growth_r + k_{morT,reed} f_{P,reed} p_{reed,2} Growth_{reed} \}$$

$$Constant_{mP} = \sum Q_{in} c_{mP,in} - \{ f_{P,f} Growth_f + f_{P,r} Growth_r + f_{P,reed} Growth_{reed} \}$$

$$p_{f,1} = \dfrac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f}\overline{V}_w)}[L_f]_{t_0} \qquad p_{f,2} = \dfrac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2}(\sum Q_{out} f_{adv} + k_{morT,f}\overline{V}_w)}$$

$$p_{r,1} = \dfrac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,r}\overline{V}_w}[L_r]_{t_0} \qquad p_{r,2} = \dfrac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,r}\overline{V}_w}$$

$$p_{reed,1} = \frac{\dfrac{V_{w,t_0} + V_{w,t_0+\Delta t}}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,reed} \overline{V}_w} [L_{reed}]_0 \qquad p_{reed,2} = \frac{\dfrac{\Delta t}{2}}{V_{w,t_0+\Delta t} + \dfrac{\Delta t}{2} k_{morT,reed} \overline{V}_w}$$

6 Computational scheme

6.1 Mathematical solution

The final and average concentrations of organic nitrogen for a time step are found by solving the differential equation (Equation 35). The general solution to this equation reads:

$$c_{oN}(t) = \xi_1(t)c_{oN}(0) + \xi_2(t)\sum Q_{in}c_{oN,in} + \xi_2(t)\,\overline{V}_w\{k_{morT,f}f_{N,f}p_{f,1} + k_{morT,r}f_{N,r}p_{r,1} +$$
$$k_{morT,reed}f_{N,reed}p_{reed,1}\} + \xi_2(t)\,\overline{V}_w\{k_{morT,f}f_{N,f}p_{f,2}(Growth_f + \sum Q_{in}[L_f]_{in}f_{adv}) + \qquad (43)$$
$$k_{morT,r}f_{N,r}p_{r,2}Growth_r + k_{morT,reed}f_{N,reed}p_{reed,2}Growth_{reed}\}$$

and the time averaged concentration of organic nitrogen:

$$\overline{c}_{oN} = \zeta_1(t)c_{oN}(0) + \zeta_2(t)\sum Q_{in}c_{oN,in} + \zeta_2(t)\,\overline{V}_w\{k_{morT,f}f_{N,f}p_{f,1} + k_{morT,r}f_{N,r}p_{r,1} +$$
$$k_{morT,reed}f_{N,reed}p_{reed,1}\} + \zeta_2(t)\,\overline{V}_w\{k_{morT,f}f_{N,f}p_{f,2}(Growth_f + \sum Q_{in}[L_f]_{in}f_{adv}) + \qquad (44)$$
$$k_{morT,r}f_{N,r}p_{r,2}Growth_r + k_{morT,reed}f_{N,reed}p_{reed,2}Growth_{reed}\}$$

where $\xi_1(t)$, $\xi_2(t)$, $\zeta_1(t)$, and $\zeta_2(t)$ are coefficients that result from solving the differential equations (Appendix 2). The applied solution method is similar to the one used in the ANIMO model (Groenendijk et al., 2005).

It can be seen that both the resulting concentration $c_{oN}(t)$ and the average concentration $\overline{c}_{oN}$ are linear combinations of the initial concentration at the start of the time step and the zero-order inputs to the compartment. The time averaged organic nitrogen concentration is used in the mineralization term of the differential equation for the mineral compound:

$$c_{mN}(t) = \xi_3(t)c_{mN}(0) + \xi_4(t)k_{mi}\overline{V}_w\,\overline{c}_{oN} + \xi_4(t)\sum Q_{in}c_{mN,in} -$$
$$\xi_4(t)\{f_{N,f}Growth_f + f_{N,r}Growth_r + f_{N,reed}Growth_{reed}\} \qquad (45)$$

and

$$\overline{c}_{mN} = \zeta_3(t)c_{mN}(0) + \zeta_4(t)k_{mi}\overline{V}_w\,\overline{c}_{oN} + \zeta_4(t)\sum Q_{in}c_{mN,in} -$$
$$\zeta_4(t)\{f_{N,f}Growth_f + f_{N,r}Growth_r + f_{N,reed}Growth_{reed}\} \qquad (46)$$

When the uptake rate is too high, the resulting concentration at the end of the time step c_{mN} can take a value which is lower than the critical uptake concentration c_{Ncrit}. To avoid this, the resulting concentration c_{mN} at the end of the time step is checked. When $c_{mN} < c_{Ncrit}$, the nitrogen uptake is reduced by decreasing the growth rate of

living biomass. Setting the resulting mineral N concentration at c_{Ncrit}, the new average organic N concentration and the adjusted living biomass content are determined by solving the linear system of 4 equations and 4 unknowns:

$$\begin{pmatrix} \xi_4(t)k_{mi}\overline{V}_w & -\xi_4(t)f_{N,f} & -\xi_4(t)f_{N,r} & -\xi_4(t)f_{N,reed} \\ 1 & -\zeta_2(t)k_{morT,f}\overline{V}_w f_{N,f}p_{f,2} & -\zeta_2(t)k_{morT,r}\overline{V}_w f_{N,r}p_{r,2} & -\zeta_2(t)k_{morT,reed}\overline{V}_w f_{N,reed}p_{reed,2} \\ 0 & -1\!\!\big/\!Growth_f^* & 1\!\!\big/\!Growth_r^* & 0 \\ 0 & -1\!\!\big/\!Growth_f^* & 0 & -1\!\!\big/\!Growth_{reed}^* \end{pmatrix} \begin{pmatrix} \overline{c}_{oN} \\ Growth_f \\ Growth_r \\ Growth_{reed} \end{pmatrix} = \begin{pmatrix} RHS_1 \\ RHS_2 \\ RHS_3 \\ RHS_4 \end{pmatrix} \quad (47)$$

with:

$$RHS_1 = c_{N,crit} - \xi_3(t)c_{mN}(0) - \xi_4(t)\sum Q_{in}c_{mN,in}$$

$$RHS_2 = \zeta_1(t)c_{oN}(0) + \zeta_2(t)\sum Q_{in}c_{oN,in} + \zeta_2(t)\,\overline{V}_w\{k_{mor,f}f_{N,f}p_{f,1} +$$
$$\qquad k_{mor,r}f_{N,r}p_{r,1} + k_{mor,reed}f_{N,reed}p_{reed,1} + k_{mor,f}f_{N,f}p_{f,2}\sum Q_{in}[L_f]_{in}f_{adv}\}$$

$$RHS_3 = 0$$

$$RHS_4 = 0$$

and where $Growth_f^*$, $Growth_r^*$ and $Growth_{reed}^*$ are the original estimates of the growth rates. The new growth rates are a constant fraction of their original estimated values (see row 3 and 4 in Equation 47). The adjusted values of the growth rates and the average organic nitrogen concentration are substituted in the expressions for $c_{oN}(t)$ and $\overline{c}_{mN}$.

The solution of the equations describing the phosphorus concentration is derived in a similar way as the nitrogen component, taking into account an adjusted growth rate of living biomass if required:

$$c_{oP}(t) = \xi_5(t)c_{oP}(0) + \xi_6(t)\sum Q_{in}c_{oP,in} + \xi_6(t)\,\overline{V}_w\{k_{morT,f}f_{P,f}p_{f,1} + k_{morT,r}f_{P,r}p_{r,1} +$$
$$\qquad k_{morT,reed}f_{P,reed}p_{reed,1}\} + \xi_6(t)\,\overline{V}_w\{k_{morT,f}f_{P,f}p_{f,2}(Growth_f + \sum Q_{in}[L_f]_{in}f_{adv}) + \qquad (48)$$
$$\qquad k_{morT,r}f_{P,r}p_{r,2}Growth_r + k_{morT,reed}f_{P,reed}p_{reed,2}Growth_{reed}\}$$

$$\overline{c}_{oP} = \zeta_5(t)c_{oP}(0) + \zeta_6(t)\sum Q_{in}c_{oP,in} + \zeta_6(t)\,\overline{V}_w\{k_{mor,f}f_{P,f}p_{f,1} + k_{mor,r}f_{P,r}p_{r,1} +$$
$$\qquad k_{mor,reed}f_{P,reed}p_{reed,1}\} + \zeta_6(t)\,\overline{V}_w\{k_{mor,f}f_{P,f}p_{f,2}(Growth_f + \sum Q_{in}[L_f]_{in}f_{adv}) + \qquad (49)$$
$$\qquad k_{mor,r}f_{P,r}p_{r,2}Growth_r + k_{mor,reed}f_{P,reed}p_{reed,2}Growth_{reed}\}$$

The time averaged organic phosphorus concentration is used in the mineralization term of the differential equation for the mineral compound:

$$c_{mP}(t) = \xi_7(t)c_{mP}(0) + \xi_8(t)k_{mi}\overline{V}_w\,\overline{c}_{oP} + \xi_8(t)\sum Q_{in}c_{mP,in} -$$
$$\qquad \xi_8(t)\{f_{P,f}Growth_f + f_{P,r}Growth_r + f_{P,reed}Growth_{reed}\} \qquad (50)$$

and

$$\overline{c}_{mP} = \zeta_7(t)c_{mP}(0) + \zeta_8(t)k_{mi}\overline{V}_w\overline{c}_{oP} + \zeta_8(t)\sum Q_{in}c_{mP,in} -$$
$$\zeta_8(t)\{f_{P,f}Growth_f + f_{P,r}Growth_r + f_{P,reed}Growth_{reed}\} \tag{51}$$

When the uptake rate is still too high relative to the mineral phosphorus availability, the resulting concentration at the end of the time step c_{mP} can take a negative value. Then, another adjustment of the growth rate of living biomass is needed. Such an adjustment is conducted similar to the one performed for c_{mP} values below the critical uptake concentration c_{Pcrit}. After assessing the new $Growth_f$, $Growth_r$, and $Growth_{reed}$ values new concentration values for $c_{oP}(t)$ and $\overline{c}_{mP}$ can be calculated.

6.2 Numerical corrections

Before information from hydraulic preprocessors like SWQN can be inserted into NUSWALITE to solve the general concentration equations several checks are made:

- Water balance:
  NUSWALITE checks the water balance of the hydraulic input data. Substantial water balance errors can lead to disturbances and inaccuracies in the NUSWALITE calculations. Therefore large water balance errors are reported to make the user aware of possible introduced errors.

- Negative water levels:
  NUSWALITE can not handle negative water levels which can be simulated by some hydraulic models. While a negative water depth may not be a problem for a hydraulic model, NUSWALITE can not cope with it because the term with the derivative of concentration to time will have an opposite sign to the derivative itself, which is physically impossible. The hydraulic input is therefore checked for nodes with negative water volumes and, if negative values are found, a fixed volume of water is added to both begin and end volume in such a way that any volume will have a positive value. This procedure does not affect discharges.

- Circular flows:
  The present version of NUSWALITE can not handle circular flows. Circular flows can result from pump activities, wind influences, and sometimes also from model inaccuracies. NUSWALITE checks the occurrence of circular flows and disables them by subtracting the lowest flow from all the involved nodes.

7 Parameterization

7.1 Introduction

NUSWALITE is derived from the NUSWA model in which most described processes have a physical, chemical or biological basis. As a consequence most of the NUSWA process parameters can be deduced directly from experiments, measurements, or literature. In NUSWALITE several nutrient stages are lumped into pools, like for instance organic and particulate N/P, and some processes are combined, like the denitrification in the water and sediment compartments. As a result many parameters can not be derived directly from measurements or literature values.

Still it is essential to have an idea of the parameter ranges when using NUSWALITE. In deriving the NUSWALITE parameterization a three step approach is used:
* The NUSWA parameterization used in a number of polder studies (Hendriks et al., 1994, and Hendriks et al., 2002) is taken as a basis since they provide parameter estimates which are derived from literature values or field data (Appendix III);
* Then, based on similarities and differences in process description between the two models, the NUSWALITE parameters have been assembled where possible;
* Finally, in cases where parameter ranges could not be derived from the NUSWA settings, calibrated values are taken from NUSWALITE case studies in the Drentsche Aa (Roelsma et al., 2005) and the EuroHarp catchments (Schoumans et al., 2008) in combination with new insights and expert judgment.

It is essential to keep in mind that each catchment has its own characteristics and requires further evaluation and, if necessary, calibration of the NUSWALITE parameters. For the biomass parameterization this three step approach can not be applied because two additional species have been introduced which were not covered by NUSWA. The corresponding parameters are derived from literature.

7.2 Biomass

The original NUSWA model only dealt with floating biomass. In NUSWALITE two additional biomasses are defined: submerged rooting biomass and reed. In the next paragraphs parameters are derived for:
* Duckweed (Lemna), the most common floating biomass species in Dutch surface water systems;
* Elodea, the most common submerged rooting biomass species in Dutch surface water systems;

- Reed (Phragmites Australis), a fast growing water plant that can have a strong purifying effect on nutrient rich water.

There are two parameters that apply to all types of biomasses, namely indicating which minimum nutrient concentrations are needed to start biomass growth (Table 1).

Table 1 Minimum concentrations of mineral nutrients needed for biomass growth

Process	Parameter description	Symbol	Value NUSWALITE	Unit
Biomass growth	Critical uptake concentration for N	C_{Ncrit}	10^{-5}	g m^{-3}
	Critical uptake concentration for P	C_{Pcrit}	10^{-5}	g m^{-3}

7.2.1 Floating biomass

The NUSWA parameters for floating biomass are derived for duckweed (see Appendix 3), the most common floating biomass species in Dutch surface water systems. Since the growth of floating biomass is approached in a similar way, the parameters in NUSWALITE are assigned values in the same range. Some parameters, however, are modified compared to the NUSWA model. Values for the nitrogen dry mass content are derived from Zimmo (2003), who found a nitrogen dry mass ratio of 0.055 ± 0.01 for duckweed. The phosphorus ratio is an order of ten smaller.

An important parameter is the light extinction coefficient in water (α), since this parameter links the initial biomass concentration (at a time step) to the growth, making biomass growth a pseudo first order process. This parameter can be used to regulate the growth rate, which implies that its physical meaning as a light extinction coefficient is partly lost. The value is chosen in such a way that the maximum growth rate is in the range found by Peng et al. (2007), that is a value of 0.47 per day for duckweed at 20°C.

There are two additional parameters related to floating biomass that were not handled by the NUSWA model. First, not all floating biomass is subject to advective transport (by water) and therefore it is better to define a movable fraction per compartment. It is recommended to set this parameter to one for open water with high flow velocities, which means that all the floating biomass is transported by the water. For water systems with low flow velocities, for example polder areas, the advective fraction can be set to a value smaller than one, since dense beds of duckweed have a certain flow resistance which can only be removed at considerable flow velocities. As a second option, it is now possible to define a background inflow of floating biomass. This inflow applies to all model nodes. It is recommended to set this parameter to zero.

With the current parameterization (Table 2) duckweed can reach a maximum density of about 250 g/m2 in Dutch open waters under nutrient unlimited conditions (Figure 11). As the approaches for light interception differ considerably between the two models, no direct comparison can be made for their parameters.

Table 2 Growth parameters for floating biomass (derived for duckweed)

Process	Parameter description	Symbol	Value		Unit
			NUSWA	**NUSWALITE**	
Growth	Light reduction factor due to water	ε_w	0.1	-	-
	Light reduction factor due to biomass in water	ε_b	0.02	-	-
	Competition factor	α	0.05	-	$m^2\,g^{-1}$
	Light interception constant	α	-	0.23	$m^2\,g^{-1}$
	Michaelis-Menten (Monod) coefficient for N (nutrient limitation)	C_{Nmonod}	0.35	0.35	$g\,m^{-3}$
	Michaelis-Menten (Monod) coefficient for P (nutrient limitation)	C_{Pmonod}	0.07	0.07	$g\,m^{-3}$
	Respiration constant	a	0.3	0.3	-
	Nitrogen Dry Matter ratio	$f_{N,f}$	0.042	0.05	$gN\,g^{-1}$
	Phosphorus Dry Matter ratio	$f_{P,f}$	0.008	0.005	$gP\,g^{-1}$
Mortality	Mortality rate at 20°C	$k_{mor,f}$	0.05	0.15	d^{-1}
	Temperature influence on mortality	β_{mor}	0.09	0.09	-
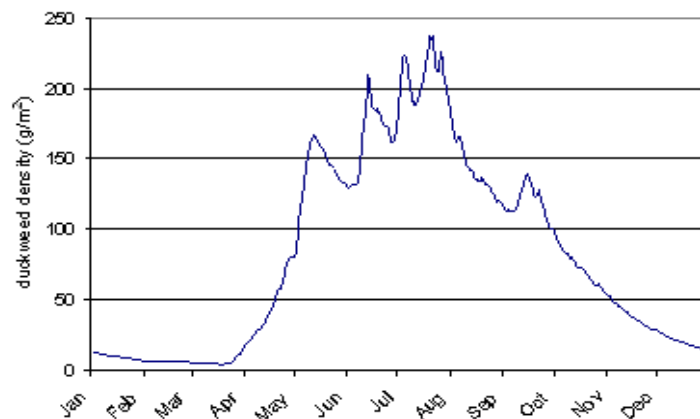
Figure 11   Example of the life cycle of duckweed using the parameters defined for a Dutch open water system with stagnant water. In this example there is no nutrient reduction on growth.

7.2.2 Submerged rooting biomass

The submerged rooting biomass parameters are derived for Elodea, the most common submerged species in Dutch open waters (e.g. water thyme or Florida Elodea). The corresponding parameters could not be derived from the NUSWA model, since NUSWA only deals with floating biomass.

Table 3 shows the parameter values for Elodea, partly found in literature. The light extinction coefficient is chosen in such a way that the maximum growth rate is similar to the growth rate found by Muhammetoglu and Soyupak, 2000. The values for the respiration rate and the mortality parameters yield realistic Elodea densities.

Table 3 Growth parameters for rooting biomass in NUSWALITE (derived for Elodea)

Process	Parameter description	Symbol	Value	Unit
Growth	Light interception constant	α	0.02	$m^2 g^{-1}$
	Michaelis-Menten (Monod) coefficient for N (nutrient limitation)	C_{Nmonod}	0.01[1]	$g\ m^{-3}$
	Michaelis-Menten (Monod) coefficient for P (nutrient limitation)	C_{Pmonod}	0.005[1]	$g\ m^{-3}$
	Respiration constant	a	0.3	-
	Nitrogen Dry Matter ratio	f_{Nr}	0.035[1]	$gN\ g^{-1}$
	Phosphorus Dry Matter ratio	f_{Pr}	0.0025[1]	$gP\ g^{-1}$
Mortality	Mortality rate at 20°C	$k_{mor,r}$	0.06	d^{-1}
	Temperature influence on mortality	β_{mor}	0.15	-

[1]*Derived from Muhammetoglu and Soyupak, 2000*

Figure 12 shows the growth of Elodea with the current parameterization under non-nutrient constrained conditions, without the presence of floating biomass. If floating biomass is present it will intercept part of the light before it reaches the submerged macrophytes with a decrease in biomass as a consequence. The growth reduction on submerged biomass can be huge under nutrient rich conditions in open waters with a small flow velocity, where large beds of duckweed can be formed.
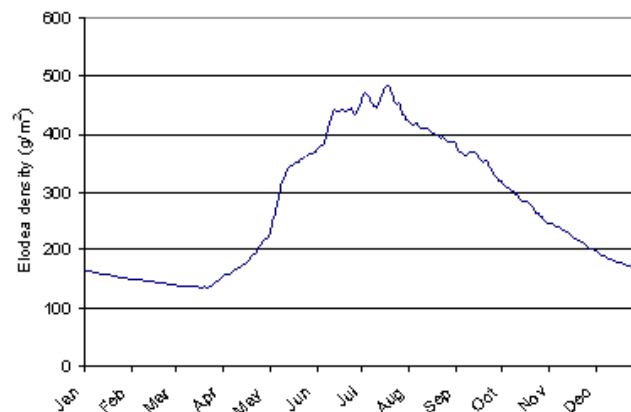
Figure 12   Example of the growth cycle of Elodea using the parameters defined in Table 3 in a Dutch open water system. In this example there is no nutrient reduction on growth.

The uptake of nutrients by Elodea is regulated by its roots. In NUSWALITE the sediment and water compartment are lumped having one nutrient concentration. This assumption is more-or-less valid for infiltration dominated systems, but errors can be introduced in upward seepage controlled areas depending on the seepage rate and its nutrient concentration.

7.2.3 Reed

Reed (Phragmites Australis) is a fast growing water plant that can have a strong purifying effect on nutrient rich water. The removal of nutrients can be increased by mowing, especially at the end of the summer when the large shoots contain high amounts of nutrients. Part of the biomass parameters for reed are derived from a Dutch site called Lankheet (Mulder and Querner, 2008), where the purifying effect of planted reed fields on the water system is investigated. The light interception constant is chosen such that realistic growth rates are guaranteed (i.e. Janse, 2005). The mortality rate of reed is derived from an average lifetime of the shoot of one year.

Figure 13 shows the growth cycle of the reed shoot as a result of the current parameterization (Table 4). There is no nutrient reduction on the growth in this example and it is assumed that the shoot represents 75% of the total biomass. The remaining 25% is contained by the roots. In practice this ratio varies over the year. Figure 13 shows a fast growth to 1,200 g/m^2 in the first year which corresponds with observations at the Lankheet site. After 5 years of non-nutrient constrained growth, an equilibrium is reached with a maximum density of almost 3,000 g/m^2 biomass in the shoot, which is in the same range as found by Janse, 2005.
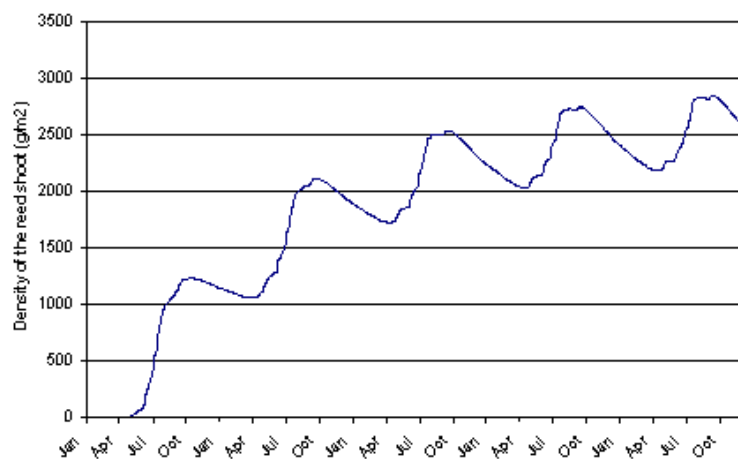

Figure 13   *Growth cycle of the shoot of reed (Phragmites Australis) using the parameters defined in Table 4 in a Dutch open water system. The reed shoot is assumed to be 75% of the total reed biomass. There is no nutrient reduction on growth.*

The NUSWALITE model does not account for (re-)translocation of nutrients. At the end of the growing season nutrients are transported from the shoot to the roots (re-translocation), whereas at the beginning of the growth season there is an opposite flux of nutrients (translocation). As a consequence, the nitrogen and phosphorus dry matter content vary throughout the year over the roots and shoot. This implies that the removal of nutrients by harvesting in the winter can be overestimated by about 40% (Meuleman et al., 2002) as only plant material above the water level is mowed.

Table 4 Growth parameters for reed in NUSWALITE (Phragmites Australis)

Process	Parameter description	Symbol	Value	Unit
Growth	Light interception coefficient	α_{int}	0.01	$m^2 g^{-1}$
	Michaelis-Menten (Monod) coefficient for N (nutrient limitation)	C_{Nmonod}	0.1	$g\ m^{-3}$
	Michaelis-Menten (Monod) coefficient for P (nutrient limitation)	C_{Pmonod}	0.01	$g\ m^{-3}$
	Respiration constant	a	0.5	-
	NitrogenDMratio	f_{Nreed}	0.015	$gN\ g^{-1}$
	PhosphorusDMratio	f_{Preed}	0.0015	$gP\ g^{-1}$
Mortality	Mortality rate at 20 °C	$k_{mor,reed}$	0.003	d^{-1}
	Temperature influence on mortality	β_{mor}	0.08	-

7.3 Mineralization

In Table 5 the parameter values for NUSWA and NUSWALITE governing the mineralization processes are presented. As described in Paragraphs 4.3, there is no separate pool of particulate nitrogen and mineralization is modeled as a single step process, from organic to mineral. Hence, the lowest NUSWA mineralization rate would be a good first estimate for NUSWALITE as this rate sets the limit in the conversion chain. However, a somewhat higher value could be considered since particulate nitrogen can also be converted directly into its mineral form.

Table 5 Mineralization parameters in the water compartment

Process	Parameter description	Symbol	Value		Unit
			NUSWA	NUSWALITE	
Minerali-zation	Mineralization rate constant – step 1 (particulate to dissolved organic)	k_{minw1}	0.15	-	d^{-1}
	Temperature coefficient	θ_m	0.04	-	-
	Mineralization rate constant – step 2 (dissolved organic to mineral)	k_{minw2}	0.25	-	d^{-1}
	Temperature coefficient	θ_m	0.04	-	-
	Mineralization rate constant – single step (dissolved organic to mineral)	k_{mi}	-	0.15	d^{-1}
	Temperature coefficient	β_{mi}	-	0.04	-

Table 6 shows that for NUSWA the limiting rate in the sediment layer lies below the limiting rate in the water compartment (Table 5). However, residence times in the sediment layer will be considerably higher than in the water compartment which will

probably offset this lower value. So, when lumping both compartments in NUSWALITE, it seems warranted to stick to a mineralization rate of about 0.15 d^{-1}. The temperature correction coefficients are assumed to be equal in both models (Table 5).

Table 6 Mineralization parameters in the sediment compartment

Process	Parameter description	Symbol	Value		Unit
			NUSWA	NUSWALITE	
Minerali-zation	Mineralization rate constant – step 1 (particulate to dissolved organic)	k_{mins1}	0.1	-	d^{-1}
	Temperature coefficient	θ_m	0.04	-	-
	Mineralization rate constant – step 2 (dissolved organic to mineral)	k_{mins2}	0.3	-	d^{-1}
	Temperature coefficient	θ_m	0.04	-	-

7.4 Nitrogen and phosphorus removal processes

7.4.1 Nitrogen

The simplifications in NUSWALITE with respect to the denitrification process make it difficult to convert the NUSWA denitrification constant into an appropriate value for NUSWALITE. Bearing in mind that NUSWA simulations were performed for polder areas, one could argue that with a nitrate-ammonium ratio of 1.5 the NUSWALITE parameter could be set at 0.06 d^{-1} for similar water systems, assuming residence times in the water compartment in the same order of magnitude as those for the sediment compartment. However, resident times in the sediments are usually much higher leading to much lower values.

In freely discharging catchment in the elevated parts of the Netherlands, ammonium concentrations are usually very low while oxygen levels in the sediment are generally higher. This would also allow for a significant reduction of the NUSWA denitrification constant if used in NUSWALITE.

For NUSWALITE a denitrification constant of 0.05 d^{-1} could be used as a starter (Table 7), but it appears from the above remarks that there is ample space for further calibration.

Sedimentation related parameters are also not directly comparable for both models. A removal mechanism is necessary to account for slow degradable fractions in deceased biomass and for fractions more-or-less definitely lost from the water system due to sedimentation of dead biomass in deep stratified lakes, dredging, or the mowing of living biomass.

In NUSWA a reaction constant is used in combination with the fraction particulate organic-N. NUSWALITE employs a sedimentation velocity which, after division by de actual water depth, is multiplied with the fraction organic dissolved nitrogen. Since NUSWALITE disregards the pool of particulate organic matter and dead biomass is directly converted into dissolved organic nitrogen, we may assume that these pools

are of more-or-less equal size. With an estimated average water depth of 0.5 m for polders, this would result in an effective sedimentation velocity of 0.05 m/d (Table 7) based on the NUSWA sedimentation constant of 0.1 d⁻¹.

For catchments in the elevated parts of the country, the average water depth will be lower but with higher flow velocities lowering the effective sedimentation velocity. Therefore, as a first estimate an effective sedimentation velocity of 0.05 m/d for dissolved organic nitrogen is proposed for NUSWALITE.

Table 7 Parameters for nitrogen removal processes

Process	Parameter description	Symbol	Value NUSWA	Value NUSWALITE	Unit
Denitrification	Denitrification constant	k_{den}	0.09	0.05	d⁻¹
	Temperature coefficient	β_{den}	0.045	0.045	-
Sedimentation	Sedimentation constant for particulate organic nitrogen	$k_{sed,oN}$	0.1	-	d⁻¹
	Sediment sink speed for dissolved organic N	$w_{s,oN}$	-	0.05	m d⁻¹

7.4.2 Phosphorus

The loss of organic phosphorus follows the loss of organic nitrogen as described in Paragraphs 4.2 and 7.4.1 with an added similar mechanism for the removal of mineral phosphorus. For the sedimentation velocity of organic-P a value of 0.05 m/d is proposed (Table 8), the same value as derived for organic-N (Table 8). As to mineral-P, an effective sedimentation velocity can be set in NUSWALITE to cover irreversible adsorption. A value of 0.15 m/d has been derived for a number of Dutch catchments (Table 8).

Table 8 Parameters for phosphorus removal processes

Process	Parameter description	Symbol	Value NUSWA	Value NUSWALITE	Unit
Sedimentation	Sedimentation constant for particulate organic phosphorus	k_{sed}	0.1	-	d⁻¹
	Sediment sink speed for dissolved organic P	$w_{s,oP}$	-	0.05	m d⁻¹
	Sediment sink speed for mineral P	$w_{s,mP}$	-	0.15	m d⁻¹

7.5 Sorption

The descriptions for sorption differ considerably between NUSWA and NUSWALITE. The latter model only uses linear sorption isotherms, aggregates nitrate and ammonium into a single mineral nitrogen pool, and uses the mineral nutrient concentrations in the water compartment for sorption instead of those in the sediment layer (Paragraphs 4.3 and 5.3). This implies that the adsorption rates need to be derived from model calibrations.

For mineral nitrogen the adsorption rates are very small, but for mineral phosphorus this is generally not the case and sorption can have a large influence on the seasonal dynamics of concentrations in the water compartment. These dynamics can also be influenced by the oxygen status of the sediments. For peaty areas a net phosphate release from the sediment has been observed during the summer period when anaerobic circumstances prevail (Oosterberg et al., 1989). During the winter a reverse situation may occur. In both NUSWA and NUSWALITE the seasonal aspect of the P-sorption is described by a cosine function (Paragraphs 4.3 and 5.3). For sandy soils, where anaerobic circumstances are less likely to occur, this seasonal variation can be eliminated by setting k_{min} equal to k_{max}.

Table 9 shows the parameterization derived for catchments with sandy sediment layers (www.monitoringstroomgebieden.nl), which can be used as a guideline. There is no seasonal variation in sorption, although this can be introduced when modeling peaty areas. For clay areas the adsorption rates can be raised as to account for the higher adsorption capacity.

Table 9 Sorption parameters in NUSWALITE

Process	Parameter	Symbol	Value	Unit
General sorption	Thickness of 'virtual sediment layer'	D	variable$_{x,y}$	m
	Bulk density of 'virtual sediment layer'	ρ_s	variable$_{x,y}$	g$_{solid}$ m^{-3}$_{solid}$
Phosphorus sorption	Minimum mineral adsorption rate	k_{aPmin}	0.0007	m^3$_{water}$ g^{-1}$_{solid}$
	Maximum mineral adsorption rate	k_{aPmax}	0.0007	m^3$_{water}$ g^{-1}$_{solid}$
	Day number with maximum adsorption rate	$t_{k_{aP\max}}$	30	d
Nitrogen sorption	Minimum mineral adsorption rate	k_{aNmin}	0.00005	m^3$_{water}$ g^{-1}$_{solid}$
	Maximum mineral adsorption rate	k_{aNmin}	0.00005	m^3$_{water}$ g^{-1}$_{solid}$
	Day number with maximum adsorption rate	$t_{k_{aN\max}}$	240	d

8 Retention

8.1 Definition

An important objective in surface water quality modeling is to derive the annual retention of nutrients in a catchment. This is done using the mass balance:

$$retention = 1 - \frac{TotalLoadOut}{TotalLoadIn} \qquad (52)$$

where:
TotalLoadOut   annual total output of mineral and organic nutrients
TotalLoadIn   annual total input of mineral and organic nutrients

The total incoming loads comprise the loads emitted from the soil, point sources, erosion and atmospheric deposition, accumulated for the whole catchment. The outgoing load is calculated by multiplying the outgoing water volume (at the outlets or via boundary extractions) with their concentration of organic and mineral nutrients. In the NUSWALITE model the retention is automatically calculated for the whole catchment on an annual basis. Optionally the user can define sub-catchments for which the retention is calculated separately.

8.2 Processes influencing retention

The annual retention of nitrogen in NUSWALITE is mainly related to four processes: denitrification, sedimentation, and removal of nitrogen containing biomass (e.g. mowing and dredging). Denitrification and to a lesser extent sedimentation are irreversible losses. Adsorption can also contribute to the annual retention in case average phosphate concentrations show a significant variability over the years, usually due to hydrological variations.

Floating biomass containing nutrients (e.g. algae or duckweed) is often (unintentionally) included in the retention calculations. The reason for this is that in field measurements water samples at the catchment's outlet are not analyzed for biomass. In NUSWALITE the retention can be calculated with or without the contribution of floating biomass.

Seasonally, there can be substantial differences in the amount of retention. During the summer half year nutrients are needed for biomass growth, whereas nutrients are returned to the surface water during the winter half year when biomass death exceeds growth. Also processes like denitrification, sorption and sedimentation are seasonally dependent. When computing the retention on an annual basis, however, these seasonal effects will level out to a large extent.

8.3   Examples of retention

In Table 10 the average retention for five European catchments calculated with the NUSWALITE model is presented (Schoumans et al., 2008). There is a large variation in incoming loads. This depends on the size of the catchment, population, erosion susceptibility and intensity of agriculture. The Vecht catchment is the largest area and is densely populated with very intensive agriculture, which is reflected in the high incoming loads. The effect of large lakes on the retention can be seen in the Zelivka and Vansjø-Hobøl, with nitrogen retentions of 36% and 49% and, especially, phosphorus retentions of 91% and 79% respectively. Lakes together with the many water level control structures result in high residence times and hence more retention.

An exception is the Ouse catchment in the north-east of England. No reservoirs or dams are present in this area, although it belongs to the catchments with the steepest slopes. Low residence times result in low retentions for both nitrogen and phosphorus.

Table 10 Average retention calculated for five European catchments

Catchment	Year	N_{in}	N_{out}	Ret. N	Ret. N	P_{in}	P_{out}	Ret. P	Ret. P
		(ton year^{-1})			(%)	(ton year^{-1})			(%)
Odense (DK)	1990-2000	1506	1109	397	29	42	26	15	40
Ouse (UK)	1989-2000	6921	6789	132	2	259	239	19	8
Vecht (NL/GE)	1990-2000	13589	8836	4753	36	730	422	308	44
Zelivka (CZ)	1995-2000	2513	1658	855	36	44	4	41	91
Vansjø-Hobøl (NK)	1990-2000	796	417	379	49	45	9	35	79

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Appendix 1 List of symbols

a	respiration constant (biomass dependent)	(-)
A^*	coefficient A^* within conservation equation	($m^3\ d^{-1}$)
A	coefficient A within conservation equation	($m^3\ d^{-1}$)
B	coefficient B within conservation equation	($g\ d^{-1}$)
BOD	Biological Oxygen Demand	($g\ m^{-3}$)
c	concentration	($g\ m^{-3}$)
$\bar{c}$	average concentration	($g\ m^{-3}$)
C_w	concentration of substance in water compartment	($g\ m^{-3}$)
$C_{w,i}$	concentration of substance in water compartment i	($g\ m^{-3}$)
$C_{w,i-1}$	concentration of substance in water compartment i-1	($g\ m^{-3}$)
c_{Nmonod}	Michaelis-Menten coefficient of mineral nitrogen	($g\ m^{-3}$)
c_{Pmonod}	Michaelis-Menten coefficient of mineral phosphorus	($g\ m^{-3}$)
c_{oN}	concentration of dissolved organic nitrogen in the water compartment	($g\ m^{-3}$)
$c_{oN,in}$	concentration of dissolved organic nitrogen of the incoming water	($g\ m^{-3}$)
c_{mN}	concentration of mineral nitrogen in the water compartment	($g\ m^{-3}$)
$c_{mN,in}$	concentration of mineral nitrogen of the incoming water	($g\ m^{-3}$)
c_{oP}	concentration of dissolved organic phosphorus in the water compartment	($g\ m^{-3}$)
$c_{oP,in}$	concentration of dissolved organic phosphorus of the incoming water	($g\ m^{-3}$)
c_{mP}	concentration of mineral phosphorus in the water compartment	($g\ m^{-3}$)
$c_{mP,in}$	concentration of mineral phosphorus of the incoming water	($g\ m^{-3}$)
$C_{N_{crit}}$	critical uptake concentration of mineral nitrogen	($g\ m^{-3}$)
$C_{P_{crit}}$	critical uptake concentration of mineral phosphorus	($g\ m^{-3}$)
f_{adv}	reduction factor on the advective flow of floating biomass	(-)
$f_{lightinterception}$	light interception coefficient	(-)
$f_{lightinterception,f}$	light interception coefficient for floating biomass	(-)
$f_{lightinterception,r}$	light interception coefficient for submerged rooting biomass	(-)
$f_{lightinterception,reed}$	light interception coefficient for reed biomass	(-)
$f_1(H)$	water depth function	(-)
$f_1(v)$	velocity function	(-)

f_N	nitrogen dry mass ratio of living biomass (biomass dependent)	(-)
f_P	phosphorus dry mass ratio of living biomass (biomass dependent)	(-)
$f_{reduction}$	reduction factor based on nitrogen and phosphorus concentration	(-)
F_T	temperature response coefficient	(-)
$Growth_f$	growth of floating biomass	(g d^{-1})
$Growth_r$	growth of submerged rooting biomass	(g d^{-1})
$Growth_f$	growth of reed biomass	(g d^{-1})
H	water depth	m
$\overline{H}$	average water depth	m
k_{mor}	mortality rate (biomass dependent)	(d^{-1})
k_{morT}	temperature corrected mortality rate (biomass dependent)	(d^{-1})
k_{mi}	mineralization rate of organic nitrogen	(d^{-1})
k_{miT}	temperature corrected mineralization rate of organic nitrogen	(d^{-1})
k_{den}	denitrification rate	(d^{-1})
k_{denT}	temperature corrected denitrification rate	(d^{-1})
k_{aN}	sorption coefficient for mineral nitrogen	(m$_{pores}^3$ g$_s^{-1}$)
$k_{aN\min}$	minimum adsorption rate for mineral nitrogen	(m$_{pores}^3$ g$_s^{-1}$)
$k_{aN\max}$	maximum adsorption rate for mineral nitrogen	(m$_{pores}^3$ g$_s^{-1}$)
k_{aP}	sorption coefficient for mineral phosphorus	(m$_{pores}^3$ g$_s^{-1}$)
$k_{aP\min}$	minimum adsorption rate for mineral phosphorus	(m$_{pores}^3$ g$_s^{-1}$)
$k_{aP\max}$	maximum adsorption rate for mineral phosphorus	(m$_{pores}^3$ g$_s^{-1}$)
$\overline{k}_a$	average value of adsorption coefficient	(m$_{pores}^3$ g$_s^{-1}$)
k_L	sorption constant	(m$_{pores}^3$ g$_s^{-1}$)
k_{sed}	sedimentation rate	(d^{-1})
$L_{external,in}$	external loads to the water compartment	(g d^{-1})
$[L]$	dry matter content of biomass per m^3 water	(g m^{-3})
$[L_f]$	dry matter content of floating biomass per m^3 water	(g m^{-3})
$[L_f]_{in}$	dry matter content of floating biomass per m^3 water in inflowing water	(g m^{-3})
$[L_f]_{t0}$	dry matter content of floating biomass per m^3 water at the start of time step	(g m^{-3})
$[L_f]_{t0+\Delta t}$	dry matter content of floating biomass per m^3 water at the end of time step	(g m^{-3})
$[L_r]$	dry matter content of submerged rooting biomass per m^3 water	(g m^{-3})
$[L_r]_{t0}$	dry matter content of submerged rooting biomass per m^3 water at the start of time step	(g m^{-3})

$[L_r]_{t0+\Delta t}$	dry matter content of submerged rooting biomass per m³ water at the end of time step	(g m⁻³)
$[L_{reed}]$	dry matter content of reed biomass per m³ water	(g m⁻³)
$[L_{reed}]_{t0}$	dry matter content of reed biomass per m³ water at the start of time step	(g m⁻³)
$[L_{reed}]_{t0+\Delta t}$	dry matter content of reed biomass per m³ water at the end of time step	(g m⁻³)
m_w	mass of substance in water compartment	(g)
P_{st}	unconstrained standard dry matter production	(kg ha⁻¹ d⁻¹)
P_{st}^*	unconstrained standard dry matter production	(g m⁻² d⁻¹)
$Q_{external,out}$	external flow leaving the water compartment	(m³ d⁻¹)
Q_i	flow from compartment i to downward water compartment	(m³ d⁻¹)
Q_{i-1}	flow from compartment i to compartment i-1	(m³ d⁻¹)
Q_{in}	water flow into water compartment	(m³ d⁻¹)
Q_{out}	water flow out of water compartment	(m³ d⁻¹)
S_{max}	Maximum sorption content	(-)
t	time	(d)
Δt	time step	(d)
$t_{k_{aN\,max}}$	day at which mineral nitrogen sorption reaches maximum value	(d)
$t_{k_{aP\,max}}$	day at which mineral phosphorus sorption reaches maximum value	(d)
v	flow velocity	(m s⁻¹)
v_{thres}	threshold flow velocity for (re)suspension	(m s⁻¹)
$\overline{V}_w$	time averaged volume of the water compartment	(m³)
V_w	volume of the water compartment	(m³)
$V_{w,t0}$	volume of the water compartment at the start of time step	(m³)
$V(t_0)$	volume of the water compartment at the start of time step	(m³)
$V_{w,t0+\Delta t}$	volume of the water compartment at the end of time step	(m³)
$\overline{V}_s$	volume of the sediment layer	(m_s³)
α	light interception coefficient	(m² g⁻¹)
α_{int}	light interception coefficient for reed biomass	(m² g⁻¹)
α_{eff}	effective light interception coefficient	(m² g⁻¹)
β	temperature response factor	(-)
β_{mor}	temperature response on mortality rate (biomass dependent)	(-)
β_{mi}	temperature response on mineralization rate	(-)
β_{den}	temperature response on nitrogen removal rate	(-)

δ	depth of the top zone with full light intensity	(m)
φ	change of water volume with time	$(m^3\ d^{-1})$
K	Flow related light extinction constant	$(m^{-1}\ s)$
λ	depth related light extinction constant	(m^{-1})
ρ_s	density of the sediment layer	$(g_s\ m_s^{-3})$

Appendix 2 Estimation of the ξ1, ξ2, ζ1 and ζ2 coefficients

The coefficients $\xi_1(t)$, $\xi_2(t)$, $\zeta_1(t)$ and $\zeta_2(t)$ can be found by solving the differential equations of Chapter 6. To derive these coefficients we use the differential equations for mineral nitrogen and phosphorus as a starting point since they are the most extended ones. They can be written as:

$$\rho_s V_s \overline{k_a} \frac{dc}{dt} + \frac{dV_w c}{dt} = -A^* c + B \qquad (A.1)$$

where:

c	concentration	(g m^3)
t	time	(d)
V_w	water volume	(m^3)
V_s	volume of the (virtual) sediment layer	(ms^3)
ρ_s	dry bulk sediment density	(g m s^{-3})
$\overline{k_a}$	average value of adsorption coefficient	(m$^3_{pores}$ g^{-1})
A^*	coefficient within conservation equation independent of time / concentration	(m^3 d^{-1})
B	coefficient within conservation equation independent of time / concentration	(g d^{-1})

The last term in the left hand side of equation A.1 can be written as:

$$\frac{dV_w c}{dt} = V_w \frac{dc}{dt} + c \frac{dV_w}{dt} \qquad (A.2)$$

where the water volume can by approximated over a time interval t by:

$$V_w \approx V(t_0) + \frac{dV_w}{dt} t = V(t_0) + \varphi t \qquad (A.3)$$

with:

$V(t_0)$	water volume at start of the time interval	(m^3)
φ	change of water volume with time	(m^3 d^{-1})

Substitution of equations A.2 and A.3 in equation A.1 results in:

$$\frac{dc}{dt} = -\frac{A}{\left(V(t_0) + \rho_s V_s \overline{k_a} + \varphi t\right)} c + \frac{B}{\left(V(t_0) + \rho_s V_s \overline{k_a} + \varphi t\right)} \qquad (A.4)$$

where: $A = A^* + \varphi$

Solving equation A.4 with initial condition $c(t_0) = c_0$ leads to:

$$c(t) = \xi_1(t)c_0 + \xi_2(t)B \tag{A.5}$$

whereas the average concentration is given by:

$$\bar{c}(t) = \frac{1}{\Delta t}\int_o^{\Delta t} c(t)dt = \zeta_1(t)c_0 + \zeta_2(t)B \tag{A.6}$$

The coefficients $\xi_1(t)$, $\xi_2(t)$, $\zeta_1(t)$, and $\zeta_2(t)$ are calculated for 4 different cases:

Case 1: $\varphi \neq 0$ and $A \neq 0$:

$$\xi_1(t) = \left(\frac{V(t_0) + \rho_s V_s \overline{k}_a + \varphi t}{V(t_0) + \rho_s V_s \overline{k}_a}\right)^{-\frac{A}{\varphi}} \quad and \quad \xi_2(t) = \frac{1 - \xi_1(t)}{A} \tag{A.7}$$

If $\varphi \neq 0$ and $A \neq 0$ and $\varphi \neq A$:

$$\zeta_1(t) = \frac{V(t_0) + \rho_s V_s \overline{k}_a}{t(\varphi - A)}\left[\left(\frac{V(t_0) + \rho_s V_s \overline{k}_a + \varphi t}{V(t_0) + \rho_s V_s \overline{k}_a}\right)^{\frac{\varphi - A}{\varphi}} - 1\right] and \quad \zeta_2(t) = \frac{1 - \zeta_1(t)}{A} \tag{A.8}$$

If $\varphi \neq 0$ and $A \neq 0$ and $\varphi = A$:

$$\zeta_1(t) = \frac{V(t_0) + \rho_s V_s \overline{k}_a}{\varphi t}\ln\left(\frac{V(t_0) + \rho_s V_s \overline{k}_a + \varphi t}{V(t_0) + \rho_s V_s \overline{k}_a}\right) and \quad \zeta_2(t) = \frac{1 - \zeta_1(t)}{A} \tag{A.9}$$

Case 2: $\varphi = 0$ and $A \neq 0$:

$$\xi_1(t) = e^{-\frac{A}{V(t_0) + \rho_s V_s \overline{k}_a}t} \quad and \quad \xi_2(t) = \frac{1 - \xi_1(t)}{A} \tag{A.10}$$

$$\zeta_1(t) = \frac{V(t_0) + \rho_s V_s \overline{k}_a}{At}\left(1 - e^{-\frac{A}{V(t_0) + \rho_s V_s \overline{k}_a}t}\right) \quad and \quad \zeta_2(t) = \frac{1 - \zeta_1(t)}{A} \tag{A.11}$$

Case 3: $\varphi \neq 0$ and $A = 0$:

$$\xi_1(t) = 1 \quad and \quad \xi_2(t) = \frac{1}{\varphi}\ln\left(\frac{V(t_0) + \rho_s V_s \overline{k}_a + \varphi t}{V(t_0) + \rho_s V_s \overline{k}_a}\right) \tag{A.12}$$

$$\zeta_1(t) = 1 \quad \text{and} \quad \zeta_2(t) = \frac{1}{\varphi}\left[\left(\frac{V(t_0) + \rho_s V_s \bar{k}_a + \varphi t}{\varphi t}\right) \ln\left(\frac{V(t_0) + \rho_s V_s \bar{k}_a + \varphi t}{V(t_0) + \rho_s V_s \bar{k}_a}\right) - 1\right] \qquad (A.13)$$

Case 4: $\varphi = 0$ and $A = 0$:

$$\xi_1(t) = 1 \quad \text{and} \quad \xi_2(t) = \frac{1}{V(t_0) + \rho_s V_s \bar{k}_a} t \qquad (A.14)$$

$$\zeta_1(t) = 1 \quad \text{and} \quad \zeta_2(t) = \frac{1}{2(V(t_0) + \rho_s V_s \bar{k}_a)} t \qquad (A.15)$$

Appendix 3 NUSWA parameter settings

A_oc	2.67	oxygen demand for degradation of carbon
f_sorp_wa	1	number of sorption fractions in water
ka_n_w	0.0160	lineair sorption coeff for NH4 in water
ka_n_s	0.0160	lineair sorption coeff for NH4 in sediment
ka_p_w	0.0160	lineair sorption coeff for PO4 in water
ka_p_max	1.12	maximum Langmuir coeff for PO4 in sediment
ka_p_min	3.00	minimum Langmuir coeff for PO4 in sediment
max_sorp_w	1.00	maximum sorption capacity in water
max_sorp_s	1.00	maximum sorption capacity in sediment
K_bod	0.100	oxygen rate constant of organic carbon
K_den	0.090	denitrification constant
K_nitr	0.250	nitrification constant
K_mn	0.025	constant for preference of ammonium uptake
K_minw1	0.150	mineralization constant in water 1st step
K_mins1	0.100	mineralization constant in sediment 1st step
K_minw2	0.250	mineralization constant in water 2nd step
K_mins2	0.300	mineralization constant in sediment 2nd step
K_om	0.000027	degradation constant of organic matter in sediment
K_l	0.050	mortality constant of duckweed
K_sed	0.100	sedimentation constant
K_resp	0.300	respiration constant
K_b	1.000	oxygen limitation constant for C decline
K_n	2.000	oxygen limitation constant for nitrification
K_d	0.500	oxygen limitation constant for denitrification
K_bd	5.000	carbon limitation constant for denitrification
K_michn	0.350	Michaelis-Menten constant for N
K_michp	0.070	Michaelis-Menten constant for P
theta_bod	1.047	temperature coefficient for degradation of C
theta_d	1.045	temperature coefficient for denitrification
theta_m	1.040	temperature coefficient for mineralisation
theta_n	1.080	temperature coefficient for nitrification
theta_r	1.028	temperature coefficient for reaeration
theta_l	1.090	temperature coefficient for mortality
frac_n	0.042	fraction N in duckweed
frac_p	0.008	fraction P in duckweed
frac_c	0.390	fraction C in duckweed
fract_on	1.000	fraction N mineralizion to dissolved orgN
fract_op	1.000	fraction P mineralizion to dissolved orgP
D_no3	0.002	diffusion coefficient for NO3
D_nh4	0.002	diffusion coefficient for NH4
D_po4	0.002	diffusion coefficient for PO4
D_orgp	0.002	diffusion coefficient for orgP
D_orgn	0.002	diffusion coefficient for orgN
D_o2	0.0002	diffusion coefficient for O2
Fd_no3	1.0	factor for effective diffusion of NO3
Fd_nh4	1.0	factor for effective diffusion of NH4
Fd_po4	1.0	factor for effective diffusion of PO4
Fd_orgp	1.0	factor for effective diffusion of orgP
Fd_orgn	1.0	factor for effective diffusion of orgN
Fd_o2	1.0	factor for effective diffusion of oxygen
f_reaera	0.010	extra flow velocity to reduce reaeration
porosity	0.90	porosity of sediment
tortuosity	0.67	tortuosity of sediment
density	140.0	bulk density of sediment
dif_layer	0.015	thickness of diffusion layer
sed_temp	4.0	maximum temperature of sediment
alpha_d	0.05	competition factor for duckweed
frac_fe	0.0047	fraction of Fe which can be reduced to Fe2+
qu	0.9	value for calculation of sorption constant of PO4
tau	2.5	value for oxydation or reduction
vred	0.8	reduction velocity
vox_red	1.0	oxydation velocity/reduction velocity
m	0.17	term to calculate sorption coefficient