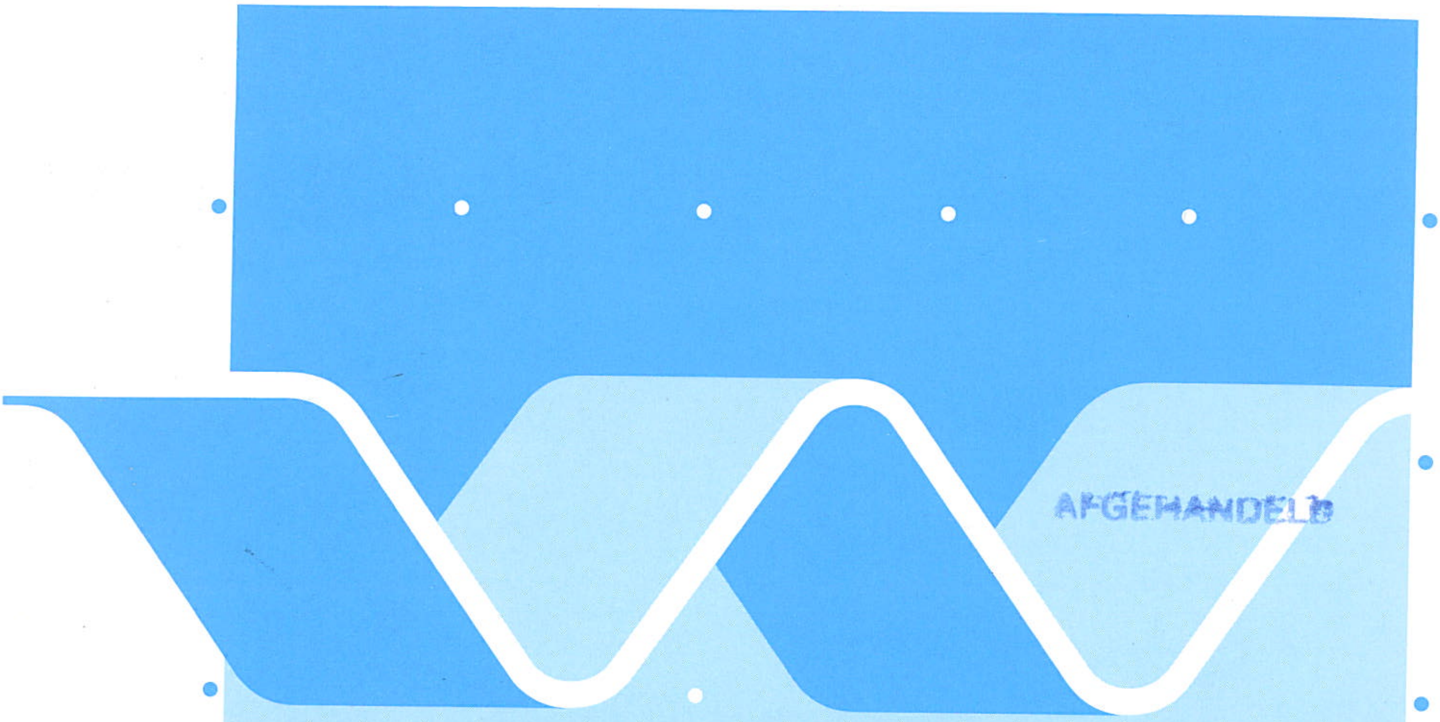

Switch, a Model for Sediment-Water Exchange of Nutrients

Part 3: Reformulation and recalibration for Lake Veluwe

Research report

March 1994

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Contents

Preface

The development of the first version of SWITCH was commissioned by the Institute for Inland Water Management and Waste Water Treatment (RIZA) and DELFT HYDRAULICS as a part of the development of the userfriendly eutrophication model DBS. The development started in 1989 and resulted in an operational first version in the summer of 1990. The first application of stand-alone SWITCH, which was carried out in 1991, aimed at calibration of the model. SWITCH and its application were documented (DELFT HYDRAULICS, 1991a) and published (Smits and Van der Molen, 1993).

Several shortcomings of SWITCH were detected during the application of the model for Lake Veluwe, overprediction of the return flux of phosphorus from the sediment to the overlying water in particular. It was decided in 1993 to reformulate SWITCH to take away the most important shortcomings. The new formulations were put to the test by means of recalibration of SWITCH for Lake Veluwe. The activities have been carried out within the framework of the DELFT HYDRAULICS research programme.

The present report is to be considered an extension of and in some respects a replacement of the previous report (DELFT HYDRAULICS, 1991a).

SWITCH was developed and calibrated by J.G.C. Smits. N.M. de Rooij and J.J.G. Zwolsman contributed to the process of reformulation by means of literature research, field data analysis, chemical modelling and discussions. The model was encoded in FORTRAN 77 by A. Hendriks.

Summary

The reformulation and recalibration of SWITCH, a model for the prediction of the nutrient fluxes across the sediment-water interface, are described and discussed. The model distinguishes four sediment layers and calculates the thicknesses of the aerobic and denitrifying layers on the basis of a steady state approach. The concentrations of detritus, ammonium, nitrate, phosphate and silicate in the sediments and the pore water are simulated dynamically using mass balance equations.

The reformulation concerned:

- the phosphorus chemistry in the sediment in order to achieve quantitatively correct prediction of the phosphate return flux in stead of overprediction;
- the extension of SWITCH with refractory organic carbon, nitrogen and phosphorus in order to link up with the existing formulations in the water quality part of DBS; and
- the replacement of the formulation for the sediment oxygen demand by a formulation which is also valid at anaerobic conditions in the water column.

The phosphorus chemistry was reformulated as follows:

- The dissolution of vivianite in the oxidized layer was changed from an instantaneous process into a slow process.
- The precipitation of phosphate as a stable mineral was added to the model next to the precipitation as vivianite.
- The adsorption capacity of the sediment has been made a function of the thickness of the oxidized layer.

The calibration of the new SWITCH-model for Lake Veluwe (1978-83) as an integral part of DELWAQ-BLOOM-SWITCH (DBS) was successful. The results show that SWITCH simulates realistically and consistently layer thicknesses, concentrations and mass fluxes connected with the transport and conversion processes. SWITCH reproduces the phenomenon of the "explosive" phosphate return flux to the overlying water at total reduction of the top sediments to a large extent. Overprediction of the phosphate return flux has disappeared. DBS predicts the net retention of phosphate in Lake Veluwe for each year in the period 1978-83.

The improvement of SWITCH also resulted in improvement of the performance of DBS, which appears from the good matching of the simulated and observed water quality in Lake Veluwe. This implies that DBS with SWITCH is capable of reliable prediction of the response of a surface water system to a large reduction of the external phosphorus load in terms of water quality and phytoplankton biomass.

1 Introduction

1.1 Background

SWITCH is a model for the prediction of the nutrient fluxes across the sediment-water interface in surface water systems. Its main objective is to contribute to the long-term modelling of eutrophication processes in aquatic systems with changing (improving) water quality. It should reproduce the important phenomenon of the 'explosive' phosphate return fluxes occurring in hypertrophic systems. The 'explosive' phosphate return flux is defined as the sudden release of large amounts of phosphate by the sediment into the overlying water as a consequence of complete chemical reduction of the top sediments (Boers and Van Hese, 1988).

The model distinguishes four sediment layers and calculates the thicknesses of the aerobic and denitrifying layers on the basis of a steady state approach. The concentrations of detritus, ammonium, nitrate, phosphate and silicate in the sediments and the pore water are simulated dynamically using mass balance equations. The details with respect to the background, the objectives and the starting-points of SWITCH have been described in DELFT HYDRAULICS (1991a). This report also describes the formulations and the calibration of the model for Lake Veluwe. SWITCH and the application for Lake Veluwe have also been published in Hydrobiologia (Smits and Van der Molen, 1993).

SWITCH has be become an integrated part of the userfriendly eutrophication model DELWAQ-BLOOM-SWITCH (DBS; DELFT HYDRAULICS, 1992). DELWAQ is a general water quality model, the overall framework taking care of mass transport and water quality processes (DELFT HYDRAULICS, 1990). BLOOM II is the phytoplankton module in DBS (DELFT HYDRAULICS, 1991b).

The development of SWITCH was and will be fed with the results (mechanisms, simplified formulations, parameter values) of research on the sediment chemistry and the water-sediment exchange processes. This research is carried out using the complicated modelling tool HADES (DELFT HYDRAULICS, 1991d) which allows a spatially detailed simulation of the sediment chemistry. HADES is based on the chemical model CHARON (DELFT HYDRAULICS, 1991c).

1.2 Objective for the reformulation

As a result of the first calibration of SWITCH for Lake Veluwe, it was established that the original model:

- predicts both the concentrations in pore water and sediment and the mass fluxes connected with the processes realistically and consistently;
- reproduces the 'explosive' phosphate return fluxes and the main long-term trends in fluxes and concentrations;
- overpredicts the phosphate return flux to the overlying water; and
- does not take into account the formation of refractory organic matter.

The overprediction of the phosphate return flux appeared from mass balance calculations that showed that net retention of phosphorus occurred in the sediments during the simulated period. The predicted net release of phosphorus from the sediment was connected with the 'observed' and therefore reproduced decrease of the phosphorus content of the sediment (period 1981-1990).

Several additional explanations were given for the decrease of the sediment phosphorus content. The redistribution of sediments from shallow parts to the deeper parts, leading to dilution of phosphorus in the sediments, was among them. The loss of phosphorus from the sediments may partionally be related to seepage. Misinterpretation of the measurements may have been the case too. The decrease of the sediment phosphorus content may have been overestimated on the basis of mean values, as the data have a large standard deviation. However, these explanations were not satisfactory and the hypothesis was formulated that the phosphorus precipitated in minerals cannot remobilize as easy as was being assumed in SWITCH.

The application of DBS for Lake Veluwe, that followed later on, showed that the overprediction of the return flux created a severe problem (unreported calibration). The overprediction could only be prevented by imposing an unrealistically high burial rate (1 cm/year net sedimentation!) in combination with a distorted initial sediment composition.

Another conclusion arose from the calibration of SWITCH that it was hampered by:

- the stand-alone application of SWITCH, which did not allow a direct coupling of the return fluxes and the overall mass balances for Lake Veluwe; and
- the averaging over two types of sediment, sandy sediment in the shallow parts and silty sediment in the deeper parts.

Considering the above, the objectives for the next step in the development of SWITCH were formulated as follows:

- reformulation of the phosphorus chemistry in order to obtain quantitatively correct prediction of the phosphate return flux;
- extension of SWITCH with refractory organic carbon, nitrogen and phosphorus in order to link up the existing formulations in the water quality part of DBS; and
- recalibration of SWITCH as an integrated part of DBS for Lake Veluwe, making the return flux fit into the overall mass balance.

2 The new formulations of SWITCH

Figure 2.1 depicts the vertical schematization of the sediment layer in SWITCH. An overview of the processes included in SWITCH is given in Figure 2.2. The formulations pertaining to these processes are described in DELFT HYDRAULICS (1991a) and below as far as the revised parts are concerned.

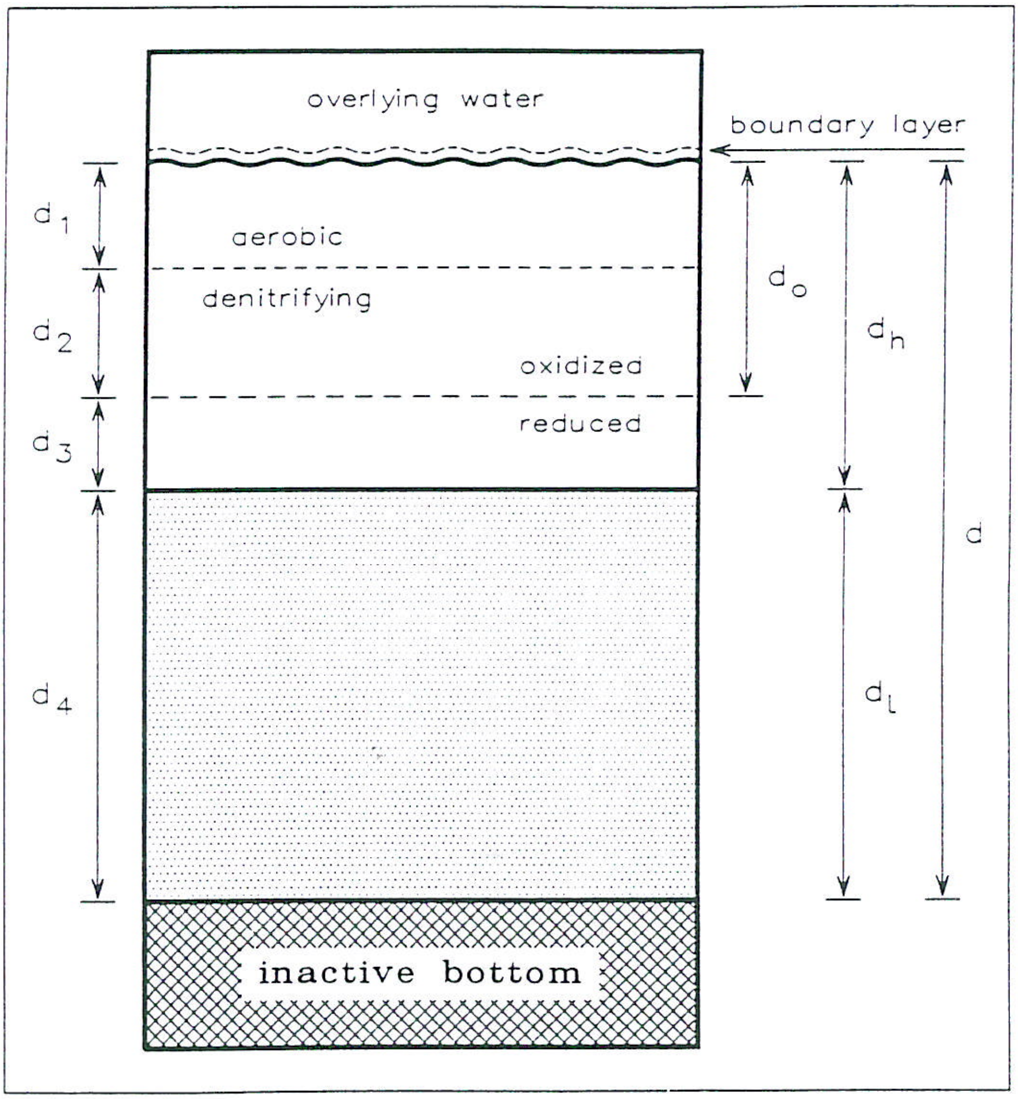


Figure 2.1 The schematization of the sediment layer in SWITCH.

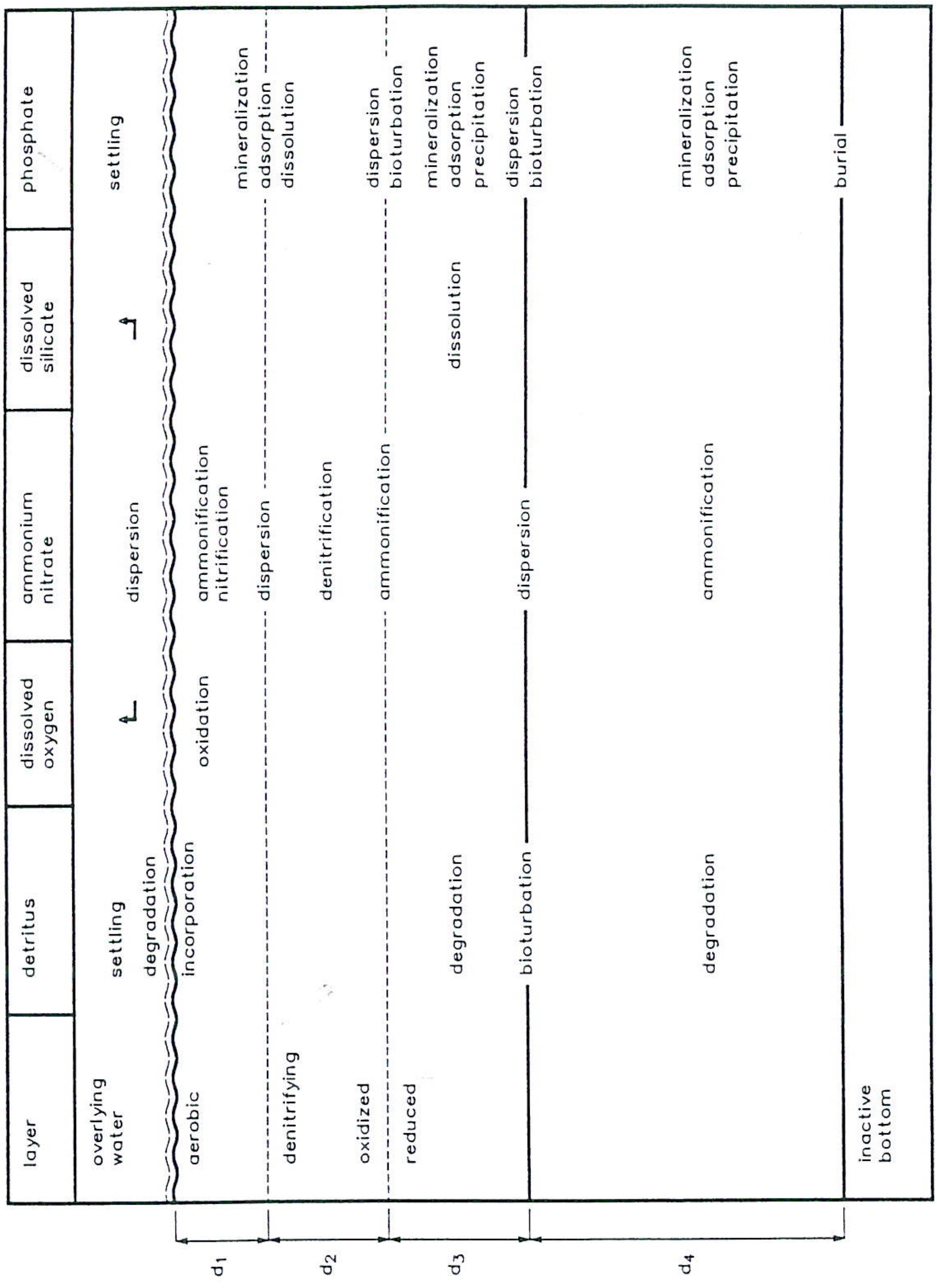


Figure 2.2 Overview of the processes included in SWITCH.

2.1 The aerobic layer and the sediment oxygen demand

The formulations for the thickness of the aerobic layer have remained the same, but are given here as the context for the reformulated sediment oxygen demand. The thickness of the aerobic layer is dependent on the oxygen consumption rate according to:

$$d_1 = \sqrt{(2\ p_1.D.fo.Co_0/Ro)} \qquad (2.1)$$

$$d_1 = do_m \text{ if } d_1 < do_m$$

in which:
Co_0 = oxygen concentration in the overlying water (g m^{-3})
do_m = minimal thickness of the oxidized layer (m)
D = dispersion coefficient (m^2 d^{-1})
fo = ratio of the oxygen concentrations at the upper and lower sides of the water boundary layer (-)
p = porosity (-)
Ro = oxygen consumption rate (g m^3 bottom d^{-1})
A subscript figure indicates a layer number or an interface number !

The introduction of ratio fo relates to the existence of a relatively stagnant boundary layer in the overlying water, which contains a part of the oxygen gradient at the sediment-water interface. The oxygen concentration at the interface is a certain fraction of the average oxygen concentration in the water column.

Oxygen is consumed in the degradation of detritus in the boundary layer (complex-detritus in the terminology of DBS) and of detritus in the aerobic layer, in the nitrification and in the chemical oxidation. The oxygen consumption rate Ro is formulated as follows:

$$Ro = Fo_b/d_1 + ac.kc_1.Cd_1 + p_1.an.kn.Ca_1 + Fo_c/d_1 \qquad (2.2)$$

in which:
ac = stoichiometric constant (gO_2 gC^{-1})
an = stoichiometric constant (gO_2 gN^{-1})
Cd_1 = detritus concentration in the upper layer (gC m^{-3}B)
Ca_1 = ammonium concentration in the aerobic layer (gN m^{-3}PW)
Fo_b = oxygen consumption in the boundary layer (gO_2 m^{-2} d^{-1})
Fo_c = chemical oxygen demand (gO_2 m^{-2} d^{-1})
kc_1 = degradation rate of detritus in the upper layer (d^{-1})
kn = nitrification rate (d^{-1}), equal to zero if $Co_0 = 0.0$

The oxygen consumption in the boundary layer is connected with the degradation of detritus on top of the sediments and is equal to:

$$Fo_b \quad = ac.kc_b.Cd_b \tag{2.3}$$

in which:

Cd_b = amount of complex-detritus in the boundary layer (gC m^2)

kc_b = degradation rate of complex-detritus in the boundary layer (d^{-1})

The chemical oxygen demand concerns the oxidation of reduced substances, such as iron(II), manganese(II), sulphide and methane originating from the degradation of detritus in the anaerobic part of the 'active' bottom. However, the reduced substances will not be oxidized completely. A part of the sulphide resulting from sulphate reduction precipitates with iron and may accumulate in the reduced part of the sediments. Methane may escape from the sediments in gasbubbles. Consequently, the actual chemical oxygen demand is formulated as a fraction of the potential chemical oxygen demand:

$$Fo_c \quad = (1\text{-}fro).ac.(kc_1.Cd_1.(d_2+d_3) + kc_4.Cd_4.d_4) \tag{2.4}$$

in which:

fro = fraction reduced substances permanently removed or fixed (-)

kc_4 = degradation rate of detritus in the lower layer (d^{-1})

Note that the degradation of detritus in the denitrifying layer has been included entirely in the chemical oxygen demand. This is not correct as such, since the elementary nitrogen produced by denitrification is chemically inert. It is not oxidized, but escapes from the bottom. A correction for the amount of nitrate consumed by denitrification can be made with fro. No correction was made in the second version of SWITCH.

The sediment oxygen demand is quantified with (modified formulation!):

$$Fo \quad = Fo_b + (ac.kc_1.Cd_1 + p_1.an.kn.Ca_1).d_1 + Fo_c \tag{2.5}$$

Maintaining a bottom oxygen demand under anaerobic conditions in the water column (kn = 0.0 !) leads to a negative oxygen concentration in the water quality model representing the surplus of reduced substances.

2.2 Detritus

Organic carbon

All organic matter, which settles on the sediments is considered as detritus, regardless of its origin. DBS distinguishes:

- live phytoplankton (DET), which enters the complex-detritus pool in the boundary layer due to settling;
- fast decomposing dead phytoplankton (DET), which enters the complex-detritus pool in the boundary layer as the net result of settling and resuspension;
- slow decomposing dead phytoplankton (OOC), which enters the slowly decomposing sediment-detritus due to settling; and
- other organic matter (BODC), which also enters the slowly decomposing sediment-detritus pool due to settling.

SWITCH transfers the complex-detritus to the relatively fast decomposing sediment-detritus pool. Resuspension (if occurring) leads to reincorporation of the sediment-detitus into the water column as fast decomposing detritus. The model converts a fraction of the sediment-detritus into refractory humic matter, which is stored in the sediment.

Summarizing, detritus is subjected to settling, resuspension, incorporation from the boundary layer into the sediment, degradation, humification and burial (Berner, 1974). The degradation rate decreases while the organic matter is transported downwards in the sediment. The concentrations of detritus in the boundary layer and the bottom layers are described with the following differential equations:

$$\frac{dCd_b}{dt} = Fd_s - Fd_b - kc_b.Cd_b \tag{2.6}$$

$$\frac{dCd_1}{dt} = (Fd_b - Fb_3.Cd_1 + Fd_3)/dh - kc_1.Cd_1 \tag{2.7}$$

$$\frac{dCd_4}{dt} = (Fxd_s + Fb_3.Cd_1 - Fd_3)/d_4 - (1+frf).kc_4.Cd_4 \tag{2.8}$$

with:

$Fd_s = sc.Cd_0$

$Fd_b = rc.Cd_b$

$Fb_3 = Fs - Fr \geq 0.0$

$Fb_4 = Fb_3.(1-p_1)/(1-p_4)$

$Fd_3 = 2\ Db.(Cd_4/(1-p_4) - Cd_1/(1-p_1))\ /\ (dh+d_4)$

$Fxd_s = sc.Cxd_0$

in which:

Cd_0 = detritus concentration in the overlying water (gC m^{-3})
Cd_b = amount of detritus in the boundary layer (gC m^{-2})
Cd_1 = detritus concentration in the upper layer (gC m^{-3}B)
Cd_4 = detritus concentration in the lower layer (gC m^{-3}B)
Cxd_0 = slow decomposing detritus (OOC) concentration in the overlying water (g m^{-3})
Db = bioturbation dispersion coefficient (m^2 d^{-1})
frf = factor for the conversion of detritus into refractory organic matter (-)
Fb = burial flux based on displaced bottom volume (m^{3}B m^{-2} d^{-1})
Fd = bioturbation flux (gC m^{-2} d^{-1})
Fd_b = flux of detritus incorporated in the upper layer (gC m^{-2} d^{-1})
Fd_s = flux of detritus settled from the overlying water (gC m^{-2} d^{-1})
Fr = resuspension flux based on displaced bottom volume (m^{3}B m^{-2} d^{-1})
Fs = sedimentation flux based on displaced bottom volume (m^{3}B m^{-2} d^{-1})
kc_b = degradation rate of detritus in the boundary layer (d^{-1})
rc = rate of incorporation in the upper layer (d^{-1})
sc = sedimentation rate for detritus (m d^{-1})
Fxd_s = flux of slow decomposing detritus (OOC) incorporated in the sediment (gC m^{-2} d^{-1})

The amount of detritus in the boundary layer (Cd_b) is not calculated in SWITCH but in the complex-module of DBS.

Notice that the conversion of detritus into refractory organic matter has been formulated as a process that is proportional and additive to decomposition at the same time. frf can be seen as an amplification factor. frf/(1-frf) delivers the fraction of the degradable organic matter that is converted into refractory organic matter.

The slow decomposing detritus (OOC) in the water column has been linked up with the detritus in the lower sediment layer because the degradation rates have comparable magnitudes.

The present version of SWITCH has only one input parameter with respect to sedimentation and resuspension. This parameter is equal to Fs-Fr and is in fact the net sedimentation/erosion rate or the burial rate in case of a positive value. Notice that the formulations in SWITCH are only valid for burial. Moreover, it is assumed that all detritus has been degraded or converted before it arrives at the lower boundary of the 'active' bottom layer, so that burial does not remove degradable detritus from the lower layer.

Only the 'average' concentration of the refractory organic matter is calculated for the 'active' bottom. The concentration is derived from:

$$\frac{dCrd_1}{dt} = (-Fb_4.Crd_1 + frf.kc_4.Cd_4.d_4) \;/\; (dh+d_4) \qquad (2.9)$$

Organic nitrogen

Similar equations have been formulated for organic nitrogen. The decomposable organic nitrogen in detritus is converted into ammonium and into refractory organic nitrogen in the following way:

$$\frac{dCnd_b}{dt} = Fnd_s - Fnd_b - knd_b.Cnd_b \qquad (2.10)$$

$$\frac{dCnd_1}{dt} = (Fnd_b - Fb_3.Cnd_1 + Fnd_3)/dh - (1+fa_1).kc_1.Cnd_1 \qquad (2.11)$$

$$\frac{dCnd_4}{dt} = (Fxn_s + Fb_3.Cnd_1 - Fnd_3)/d_4 - (1+fa_4+frf).kc_4.Cnd_4 \qquad (2.12)$$

with:

$fa_1 = (Cnd_1/Cd_1 - aa) \;/\; aa$

$fa_4 = (Cnd_4/Cd_4 - aa) \;/\; aa$

$Fnd_s = sc.Cnd_0$

$Fnd_b = rc.Cnd_b$

$Fnd_3 = 2\ Db.(Cnd_4/(1\text{-}p_4) - Cnd_1/(1\text{-}p_1))\ /\ (dh+d_4)$

$Fxn_s = sc.Cxn_0$

in which:

aa = stoichiometric constant for nitrogen in refractory detritus ($gN\ gC^{-1}$)
Cnd_0 = detritus nitrogen concentration in the overlying water ($gN\ m^{-3}$)
Cnd_b = amount of detritus nitrogen in the boundary layer ($gN\ m^{-2}$)
Cnd_1 = detritus nitrogen concentration in the upper layer ($gN\ m^{-3}B$)
Cnd_4 = detritus nitrogen concentration in the lower layer ($gN\ m^{-3}B$)
Cxn_0 = slow decomposing detritus nitrogen (OON) concentration in overlying water ($gN\ m^{-3}$)
fa = correction factor for organic nitrogen degradation rate (-)
Fnd = bioturbation flux ($gN\ m^{-2}\ d^{-1}$)
Fnd_b = flux of detritus nitrogen incorporated in the upper layer ($gN\ m^{-2}\ d^{-1}$)
Fnd_s = flux of detritus nitrogen settled from the overlying water ($gN\ m^{-2}\ d^{-1}$)
Fxn_s = flux of slow decomposing detritus nitrogen (OON) incorp. in sediment ($gN\ m^{-2}\ d^{-1}$)
knd_b = degradation rate of detritus nitrogen in the boundary layer (d^{-1})

The amount of detritus nitrogen in the boundary layer (Cnd_b) is not calculated in SWITCH but in the complex-module of DBS.

The degradation rates of organic nitrogen are adjusted in such a way that the organic matter is gradually stripped from nitrogen in excess of the nitrogen in refractory organic matter.

The 'sediment-average' concentration of the refractory organic nitrogen follows from:

$$\frac{dCrn_1}{dt} = (-Fb_4.Crn_1 + frf.kc_4.Cnd_4.d_4)\ /\ (dh+d_4) \qquad (2.13)$$

Organic phosphorus

The following equations describe the organic phosphorus in accordance with the above:

$$\frac{dCpd_b}{dt} = Fpd_s - Fpd_b - kpd_b.Cpd_b \qquad (2.14)$$

$$\frac{dCpd_1}{dt} = (Fpd_b - Fb_3.Cpd_1 + Fnd_3)/dh - (1+fp_1).kc_1.Cpd_1 \qquad (2.15)$$

$$\frac{dCpd_4}{dt} = (Fxp_s + Fb_3.Cpd_1 - Fnd_3)/d_4 - (1+fp_4+frf).kc_4.Cpd_4 \tag{2.16}$$

with:

$fp_1 = (Cpd_1/Cd_1 - ap) / ap$

$fp_4 = (Cpd_4/Cd_4 - ap) / ap$

$Fpd_s = sc.Cpd_0$

$Fpd_b = rc.Cpd_b$

$Fpd_3 = 2\ Db.(Cpd_4/(1-p_4) - Cpd_1/(1-p_1)) / (dh+d_4)$

$Fxp_s = sc.Cxp_0$

in which:
ap = stoichiometric constant for phosphorus in refractory detritus (gP gC^{-1})
Cpd_0 = detritus phosphorus concentration in the overlying water (gP m^{-3})
Cpd_b = amount of detritus phoshorus in the boundary layer (gP m^{-2})
Cpd_1 = detritus phosphorus concentration in the upper layer (gP m^{-3}B)
Cpd_4 = detritus phosphorus concentration in the lower layer (gP m^{-3}B)
Cxp_0 = slow decomposing detritus phosphorus (OOP) concentration overlying water (gP m^{-3})
fp = correction factor for organic phosphorus degradation rate (-)
Fpd = bioturbation flux (gP m^{-2} d^{-1})
Fpd_b = flux of detritus phosphorus incorporated in the upper layer (gP m^{-2} d^{-1})
Fpd_s = flux of detritus phosphorus settled from the overlying water (gP m^{-2} d^{-1})
Fxp_s = flux of slow decomp. detritus phosphorus (OOP) incorp. in sediment (gP m^{-2} d^{-1})
kpd_b = degradation rate of detritus phosphorus in the boundary layer (d^{-1})

The amount of detritus phosphorus in the boundary layer (Cpd_b) is not calculated in SWITCH but in the complex-module of DBS.

The 'sediment-average' concentration of the refractory organic phosphorus follows from:

$$\frac{dCrp_1}{dt} = (-Fb_4.Crp_1 + frf.kc_4.Cpd_4.d_4) / (dh+d_4) \tag{2.17}$$

2.3 Ammonium

Ammonium is released the degradation of detritus and is nitrified by bacteria under aerobic conditions (Berner, 1974; Vanderborght et al., 1977b). Ammonium adsorbs to a certain extent to clays in the sediments. The adsorption equilibrium is pH dependent. It is estimated that about 25 to 50 % of the ammonium present in silty sediments may be adsorbed (partition coefficient ≈ 1, pers. comm. P.C.M. Boers, RIZA) . This is a relatively small quantity compared to the high turn-over rates of ammonium in sediments. Thus, the adsorption offers only a small buffering capacity, which implies that no large mass fluxes are involved in the adsorption of ammonium. A change of ammonification is quickly followed by a proportional change of the ammonium concentration in the pore water. It is therefore justified to ignore the adsorption of ammonium in SWITCH.

The ammonium concentrations in the aerobic toplayer, the remaining part of the upper layer (d_2+d_3) and the lower reduced layer (dl) are described with:

$$\frac{dCa_1}{dt} = (Fa_b - Fa_0 + Fa_1 + Fas_0 - Fas_1)/(p_1.d_1) + (1+fa_1).kc_1.Cnd_1/p_1 - kn.Ca_1 \qquad (2.18)$$

$$\frac{dCa_2}{dt} = (- Fa_1 + Fa_3 + Fas_1 - Fas_3)/(p_1.(d_2+d_3)) + (1+fa_1).kc_1.Cnd_1/p_1 \qquad (2.19)$$

$$\frac{dCa_4}{dt} = (-Fa_3 + Fas_3 - Fas_4)/(p_4.d_4) + (1+fa_4).kc_4.Cnd_4/p_4 \qquad (2.20)$$

with:

$Fa_b = knd_b.Cd_b$

$Fa_0 = 2\ p_1.D.(Ca_1-Ca_0)\ /\ (1+d_1)$

$Fa_1 = 2\ p_1.D.(Ca_2-Ca_1)\ /\ do$

$Fa_3 = (p_1+p_4).D.(Ca_4-Ca_2)\ /\ (d-d_1)$

$Fas_0 = -\ vs.Ca_0$ if $vs < 0.0$
$Fas_1 = -\ vs.Ca_1$
$Fas_3 = -\ vs.Ca_2$

$Fas_0 = - vs.Ca_1$ if $vs > 0.0$
$Fas_1 = - vs.Ca_2$
$Fas_3 = - vs.Ca_4$

$Fas_4 = - vs.Ca_4$

in which:
Fa_b = flux from degradation detritus in boundary layer (gN m^{-2} d^{-1})
Fa_0 = dispersive return flux to the overlying water (gN m^{-2} d^{-1})
Fa_{1-3} = dispersive flux between two adjacent layers (gN m^{-2} d^{-1})
Fas_0 = seepage flux at the sediment-water interface (gN m^{-2} d^{-1})
Fas_{1-3} = seepage flux between two adjacent layers (gN m^{-2} d^{-1})
Fas_4 = seepage flux at the lower boundary (gN m^{-2} d^{-1})
knd_b = degradation rate of detritus nitrogen in the boundary layer (d^{-1})
vs = seepage velocity (m d^{-1})

It is assumed that no dispersive transport occurs across the interface of the 'active' and 'inactive' parts of the bottom. The assumption implies that the concentration of a dissolved substance is the same at both sides of the lower boundary of the bottom in the model. It is a reasonable assumption when seasonal variations in the concentration of a dissolved substance is small at the lower boundary. Moreover, a long-term shift in the ammonium concentration in the 'inactive' bottom does hardly affect the sediment-water exchange fluxes.

SWITCH stops nitrification (kn=0.0) when the dissolved oxygen concentration in the water column is equal to or less than 0.0.

2.4 Phosphate

Bacterial activity liberates phosphate from organic matter just like ammonium. In contrast with ammonium, phosphate adsorbs strongly to several components of the sediments, the hydroxides of iron(III) and aluminum in particular. Iron(III) hydroxide is present in a relatively high concentration in the oxidized layer, where it is stable. The concentration declines at the interface of the oxidized and reduced layers and goes down further in the reduced layer under the influence of reduction processes. Consequently, the adsorption is much stronger in the oxidized layer than in the reduced layer (Van Raaphorst et al., 1988; Brinkman and Van Raaphorst, 1986; Lyklema, 1980; Berner, 1974).

Phosphate also precipitates in minerals, the identity of which has not been determined unequivocally (DELFT HYDRAULICS, 1994). Vivianite (iron(II)phosphate) is being mentioned as the main mineral, but vivianite is not stable under oxidized conditions. However, coprecipitation with several carbonates and sulphides is also possible. The presence of apatite (calcium phosphate) in fresh water sediments in a stable form is not very likely.

SWITCH assumes equilibrium for the adsorption process, whereas precipitation and dissolution are formulated as slow processes. The assumption of equilibrium has the advantage, that only inorganic phosphate and precipitated phosphate need to be calculated explicitly on the basis of mass balances. The dissolved and adsorbed phosphate concentrations follow from the equilibrium condition for adsorption. The following four fractions are distinguished:

$$\begin{aligned} Cpp &= fpp.Cp \\ Cmp &= fmp.Cp \\ Cdp &= fdp.Cp/p \\ Cap &= fap.Cp \end{aligned} \tag{2.21}$$

$$fap + fdp + fpp + fmp = 1$$

in which:

Cp = total inorganic phosphate concentration (gP m^{-3}B)
Cap = adsorbed phosphate concentration (gP m^{-3}B)
Cdp = dissolved phosphate concentration (gP m^{-3}PW)
Cmp = concentration of phosphate in a stable mineral (gP m^{-3}B)
Cpp = concentration of phosphate in vivianite (gP m^{-3}B)
fap = adsorbed fraction (-)
fdp = dissolved fraction (-)
fmp = stable mineral fraction (-)
fpp = vivianite fraction (-)

These fractions are relevant for the mass balance equation for total inorganic phosphate, because the processes affect only one or two of the fractions.

The mineral phosphate fractions can be determined after solution of the mass balance equations for these components. The precipitation process is formulated with first order kinetics. The driving force is the difference between the actual concentration and the saturation concentration of ortho-phosphate dissolved in the pore water. In principle, the latter may be determined from the solubility product of the phosphate mineral, when its identity has been established. No distinction was made between the precipitation rates and the saturation concentrations of vivianite and the stable mineral, as the in-situ properties of these minerals are unknown.

The precipitation rate is a function of the driving force, the nature of which depends on the rate limiting mechanism. The function is linear when diffusion to the surface of the mineral is the rate limiting process. In case that the surface reaction is rate limiting, the function may be non-linear. However, the assumption of simple first order reaction kinetics ignoring the role of coprecipitants seems reasonable in this stage, considering that the precipitation rate has not yet been determined accurately and that the dissolved iron concentration is not simulated.

The development of the concentrations of the stable mineral phosphate is described with:

$$\begin{aligned}\frac{dCmp_1}{dt} = {} & + p_1.fm.kp.\ (fdp_1.Cp_1/p_1 - Cdp_s) + \\ & (-Fr.fmp_1.Cp_1 - Fb_2.fmp_1.Cp_1) / do + \\ & 2\ Db.\ (fmp_3.Cp_3 - fmp_1.Cp_1) / (1-p_1) / (do+d_3) / do\end{aligned} \tag{2.22}$$

$$\begin{aligned}\frac{dCmp_3}{dt} = {} & + p_1.fm.kp.\ (fdp_3.Cp_3/p_1 - Cdp_s) + \\ & (Fb_2.fmp_1.Cp_1 - Fb_3.fmp_3.Cp_3) / d_3 - \\ & 2\ Db.\ (fmp_3.Cp_3 - fmp_1.Cp_1) / (1-p_1) / (do+d_3) / d_3 + \\ & 2\ Db.\ (fmp_4.Cp_4/(1-p_4) - fmp_3.Cp_3/(1-p_1)) / (d_3+d_4) / d_3\end{aligned} \tag{2.23}$$

$$\begin{aligned}\frac{dCmp_4}{dt} = {} & + p_4.fm.kp.\ (fdp_4.Cp_4/p_4 - Cdp_s) + \\ & (Fb_3.fmp_3.Cp_3 - Fb_4.fmp_4.Cp_4) / d_4 - \\ & 2\ Db.\ (fmp_4.Cp_4/(1-p_4) - fmp_3.Cp_3/(1-p_1)) / (d_3+d_4) / d_4\end{aligned} \tag{2.24}$$

in which:
Cdp_s = saturation concentration for dissolved ortho-phosphate (gP m^{-3}PW)
fm = fraction of precipitated phosphorus stored in the stable mineral (-)
Fr = resuspension flux based on bottom volume (m^3 m^{-2} d^{-1})
kp = precipitation rate (d^{-1})

Vivianite forms in the reduced parts of the sediments. It dissolves gradually when transported into the oxidized layer by means of bioturbation of the sediments. This hypothesis can be justified as follows:

- Vivianite (iron(II) phosphate) is unstable under oxidized conditions (Lijklema, 1980).
- The concentration of dissolved Fe(II), and in some parts also the concentration of dissolved ortho-phosphate, is much higher in the reduced layer than in the oxidized layer. The solubility product is probably only exceeded in the reduced layer.

The formulation of the dissolution process is not straight forward. The dissolution is probably characterized by two steps: a) the oxidation of dissolved Fe^{2+}, b) the dissolution of vivianite at a very low dissolved Fe^{2+}-concentration. The driving force may therefore be the difference between the Fe^{2+}-concentration near the vivianite crystals and the average dissolved Fe^{2+}-concentration. The latter may approximately be equal to zero, due to oxidation.

The dissolution rate may then be formulated as follows:

$$Rdis = kdis.Cpp.Cfe \tag{2.25}$$

in which:

Cfe = the dissolved Fe2+-concentration near the surface of vivianite crystals (gFe m^{-3})

kdis = the (second order) dissolution rate constant (m^3 gFe^{-1} d^{-1})

Rdis = the dissolution rate (gP m^{-3} d^{-1})

The dissolved Fe^{2+}-concentration near the surface of the crystals is calculated from the solubility product (equilibrium constant) and the dissolved phosphate concentration with:

$$Cfe = (L_s / Cdp)^{0.33} \tag{2.26}$$

in which:

L_s = solubility product of vivianite

Equations 2.22 and 2.23 have been combined to make the dissolution rate dependent on the dissolved phosphate concentration (power -0.67). The solubility product becomes an implicit part of the dissolution rate constant. The resulting formulation meets the demand that the dissolution process slows down when the dissolved phosphate concentration increases.

The mass balances for phosphate in vivianite in three layers are:

$$\frac{dCpp_1}{dt} = - kdp.fpp_1.Cp_1.\ (fdp_1.Cp_1/p_1)^{-0.67} + \tag{2.27}$$

$$(-Fr.fpp_1.Cp_1 - Fb_2.fpp_1.Cp_1) / do +$$

$$2\ Db.\ (fpp_3.Cp_3 - fpp_1.Cp_1) / (1-p_1) / (do+d_3) / do$$

$$\frac{dCpp_3}{dt} = + p_1.kp.\ (fdp_3.Cp_3/p_1 - Cdp_s) + \tag{2.28}$$

$$(Fb_2.fpp_1.Cp_1 - Fb_3.fpp_3.Cp_3) / d_3 -$$

$$2\ Db.\ (fpp_3.Cp_3 - fpp_1.Cp_1) / (1-p_1) / (do+d_3) / d_3 +$$

$$2\ Db.\ (fpp_4.Cp_4/(1-p_4) - fpp_3.Cp_3/(1-p_1)) / (d_3+d_4) / d_3$$

$$\frac{dCpp_4}{dt} = + p_4.kp.\ (fdp_4.Cp_4/p_4 - Cdp_s) + \qquad (2.29)$$

$$(Fb_3.fpp_3.Cp_3 - Fb_4.fpp_4.Cp_4) / d_4 -$$

$$2\ Db.\ (fpp_4.Cp_4/(1-p_4) - fpp_3.Cp_3/(1-p_1)) / (d_3+d_4) / d_4$$

in which:

kdp = dissolution rate ($m^{-2.01}$ $gP^{0.67}$ d^{-1})

The dissolved fraction can be derived from the following Langmuir adsorption isoterm:

$$Cap = Cam.Cdp / (Ks+Cdp) \qquad (2.30)$$

$$Cam = Cac.(1-p).Ws$$

in which:

Cac = adsorption capacity (gP kg^{-1}DM)
Cam = maximal concentration of adsorbed phosphate (gP m^{-3}B)
Ks = half saturation concentration (gP m^{-3}PW)
Ws = specific weight of the sediments (kg m^{-3})

The adsorption capacity depends on the oxidized iron (III) and aluminum contents of the sediments. This sediment property is different for the oxidized layer and the reduced layer. The oxidized iron content and (therefore) the adsorption capacity decrease in a downward direction. Iron(III) is reduced to iron(II) in connection with the degradation of organic matter. The oxidized iron gradient is smoothed by bioturbation of the sediment, which results in upward transport of iron(II) formed in the reduced layer and in downward transport of iron(III) formed in the oxidized layer. Moreover, the adsorption capacities change in time due to changes of the temperature dependent rates of degradation of organic matter and bioturbation. Both processes affect the position of the interface between the layers and the amounts of oxidized iron present in the layers. This is taken into account in SWITCH, whereas the dependency on pH and salinity of the adsorption parameters is not considered explicitly.

Tentative simulations with HADES showed that the iron(III) contents of the oxidized layer and the reduced layer are related to the thickness of the oxidized layer (DELFT HYDRAULICS, 1991d). The adsorption capacity increases with increasing thickness of the oxidized layer. However, it has not been possible yet to formulate this relation deterministically. Empirical relations, determined by means of model calibration for Lake Veluwe, have been introduced in SWITCH in stead.

The relations used in SWITCH are:

$$\begin{aligned}
Cam_1 &= fac_1.Cac.(1-p_1).Ws \\
Cam_3 &= fac_1.fac_3.Cac.(1-p_1).Ws \\
Cam_4 &= 0.5\ fac_4.Cac.(1-p_4).Ws
\end{aligned} \tag{2.31}$$

$$\begin{aligned}
fac_1 &= ((d_1+d_2)\ /\ 0.005)^{0.25} \\
fac_3 &= ((d_1+d_2)\ /\ dh)^{0.25} \\
fac_4 &= dh\ /\ (dh+d_4)
\end{aligned}$$

in which:

Cam_1 = maximal concentration of adsorbed phosphate in the oxidized layer (gP m^{-3}B)

Cam_3 = maximal concentration of adsorbed phosphate in the upper reduced layer (gP m^{-3}B)

Cam_4 = maximal concentration of adsorbed phosphate in the lower reduced layer (gP m^{-3}B)

Cac = time average adsorption capacity of the oxidized layer (gP kg^{-1}DM)

fac = empirical factor linking up the ads. capacity with layer thickness (-)

The adsorption capacity of the oxidized layer becomes bigger than the 'average' capacity (Cac) when the thickness of the oxidized layer becomes bigger than 0.005 m, which is about half the maximal thickness of the oxidized layer. The adsorption capacities of the reduced layers depend also on the values of dh and d_4 (input parameters for SWITCH). The thicker the reduced layers are, the smaller their depth average adsorption capacities are. This is logical considering the fact that the capacity decreases with depth.

The original approach, which defined the adsorption capacities of reduced layers as constant fractions of the adsorption capacity of the oxidized layer, has been maintained in SWITCH as an alternative option.

SWITCH generates 'explosive' fluxes by means the following mechanism. When the thickness of the oxidized layer falls below a certain critical value (< 1 mm), the adsorption capacity of this layer obtains the value of the capacity of the upper reduced layer (d_3). At the same time the adsorption capacities obtain minimal values according to the above formulations. As a result, a large part of the previously adsorbed phosphate is released into the pore water. The concentration gradient at the sediment-water interface becomes much steeper and, consequently, the dispersive flux increases suddenly. The transition between the adsorption capacities for oxidized and reduced sediments occurs instantly in SWITCH, whereas the reduction of the sediments will take some time in reality.

A quadratic equation in fdp is obtained when equation 2.30 is substituted in equations 2.21. The positive root is:

$$\begin{aligned} fdp = [\ &(1\text{-}fmp\text{-}fpp).Cp - p.Ks - Cam + \\ &\sqrt{\ }\{((1\text{-}fmp\text{-}fpp).Cp - p.Ks - Cam)^2 + \\ &4\ (1\text{-}fmp\text{-}fpp).Cp.p.Ks\}\ ]\ /\ (2\ Cp) \end{aligned} \tag{2.32}$$

Having defined al four phosphate fractions, the mass balances for total inorganic phosphate in the oxidized layer, the upper reduced layer and the lower reduced layer have been formulated as follows:

$$\begin{aligned} \frac{dCp_1}{dt} = &(Fp_b + Fp_s - Fp_0 + Fp_2 + Fps_0 - Fps_2 - \\ &Fr.Cp_1 + Fpd_2 - Fb_2.Cp_1)\ /\ do + \\ &(1+fp_1).kc_1.Cpd_1 \end{aligned} \tag{2.33}$$

$$\begin{aligned} \frac{dCp_3}{dt} = &(-\ Fp_2 + Fp_3 + Fps_2 - Fps_3 - \\ &Fpd_2 + Fpd_3 + Fb_2.Cp_1 - Fb_3.Cp_3)\ /\ d_3 + \\ &(1+fp_1).kc_1.Cpd_1 \end{aligned} \tag{2.34}$$

$$\begin{aligned} \frac{dCp_4}{dt} = &(-\ Fp_3 + Fps_3 - Fps_4 - \\ &Fpd_3 + Fb_3.Cp_3 - Fb_4.Cp_4)\ /\ d_4 + \\ &(1+fp_4).kc_4.Cpd_4 \end{aligned} \tag{2.35}$$

with:

$Fp_b \quad = kpd_b.Cpd_b$

$Fp_0 \quad = 2\ p_1.D.\ (fdp_1.Cp_1/p_1\text{-}fdp_0.Cp_0)\ /\ (1+do)$

$Fp_2 \quad = 2\ D.\ (fdp_3.Cp_3\text{-}fdp_1.Cp_1)\ /\ (do+d_3)$

$Fp_3 = (p_1+p_4).D.\ (fdp_4.Cp_4/p_4\text{-}fdp_3.Cp_3/p_1)\ /\ (d_3+d_4)$

$Fpd_2 = 2\ Db.\ ((fpp_3+fap_3).Cp_3\text{-}fap_1.Cp_1)\ /\ (1\text{-}p_1)\ /\ (do+d_3)$

$Fpd_3 = 2\ Db.\ ((fpp_4+fap_4).Cp_4/(1\text{-}p_4)\text{-}(fpp_3+fap_3).Cp_3/(1\text{-}p_1))\ /\ (d_3+d_4)$

$Fps_0 = -\ vs.fdp_0.Cp_0/p_1 \quad \text{if} \quad vs < 0.0$
$Fps_2 = -\ vs.fdp_1.Cp_1/p_1$
$Fps_3 = -\ vs.fdp_3.Cp_3/p_1$

$Fps_0 = -\ vs.fdp_1.Cp_1/p_1 \quad \text{if} \quad vs > 0.0$
$Fps_2 = -\ vs.fdp_3.Cp_3/p_1$
$Fps_3 = -\ vs.fdp_4.Cp_4/p_4$

$Fps_4 = -\ vs.fdp_4.Cp_4/p_4$

in which:
Fb = burial flux based on bottom volume ($m^3\ m^{-2}\ d^{-1}$)
Fr = resuspension flux based on bottom volume ($m^3\ m^{-2}\ d^{-1}$)
Fp_b = flux from degradation detritus in boundary layer ($gP\ m^{-2}\ d^{-1}$)
Fp_s = sedimentation flux of adsorbed phosphate ($gP\ m^{-2}\ d^{-1}$)
Fp_0 = dispersive return flux to the overlying water ($gP\ m^{-2}\ d^{-1}$)
$Fp_{2\text{-}3}$ = dispersive flux between two adjacent layers ($gP\ m^{-2}\ d^{-1}$)
$Fpd_{2\text{-}3}$ = bioturbation flux between two adjacent layers ($gP\ m^{-2}\ d^{-1}$)
Fps_0 = seepage flux at the sediment-water interface ($gP\ m^{-2}\ d^{-1}$)
$Fps_{2\text{-}3}$ = seepage flux between two adjacent layers ($gP\ m^{-2}\ d^{-1}$)
Fps_4 = seepage flux at the lower boundary ($gP\ m^{-2}\ d^{-1}$)

The resuspension of phosphate is taken into account explicitly, because of the importance for the phosphate budget in the overlying water. Phosphate adsorbed to resuspended sediments may desorb in the water column.

2.5 Numerical aspects

An optimized integration algorithm has been implemented in the second version of SWITCH (N.M. de Rooij, pers. com.). This resulted in a large reduction of the computer time required for the computations with the model.

The new algorithm uses a maximal allowable timestep for SWITCH (MT), which is evaluated each timestep of DBS. A criterion for the maximal timestep (MT) was found in the maximal change of mass in a layer during a timestep, at which stability is maintained. The number of SWITCH-loops (N) taken every DBS-timestep (DELT) is equal to DELT/MT. Generally, N is small when the layers are relatively thick and the concentration gradients are relatively weak. This happens in the winter half year. Computation on the basis of a varying optimal value of N in stead of a fixed value turned out to be very efficient in saving computer time.

3 The recalibration of SWITCH for Lake Veluwe

3.1 Introduction

Lake Veluwe is a rather well mixed and shallow lake with an average depth of 1.45 m (Fig. 3.1). The depth varies from a few decimeters to 3.5 meters. The average residence time is 2.5 months. Two rather distinct types of sediments are found in Lake Veluwe. The sediments of the shallow eastern and northern zones, which make up roughly 50% of the total area, consist basically of sand. The sediments of the deeper western zone and the shipping gully contain a high percentage of silt. The silty sediments contain significantly more water, fine material, organic matter, phosphate, iron and calcium. Detailed data on the lake are provided by Van Ballegooien et al. (1991), PER (1986) and DELFT HYDRAULICS (1991a).

Before 1980 Lake Veluwe was extremely eutrophicated, giving rise to high blooms of bluegreen algae up to 400 μg chlorophyll per liter. Oscillatoria Aghardii was dominant continuously. The phosphate load from waste water was substantially reduced in 1979 in order to improve the water quality. Additionally, Lake Veluwe was flushed with phosphate-poor water from the Flevopolder located on the west side each winter from 1979/80 on. As of 1985 additional flushing was carried out during the summer. The flushing water was also relatively rich in calcium and iron. Due to the flushing the water quality in Lake Veluwe underwent at least two major changes in the period 1978-1990 (Jagtman et al., 1992).

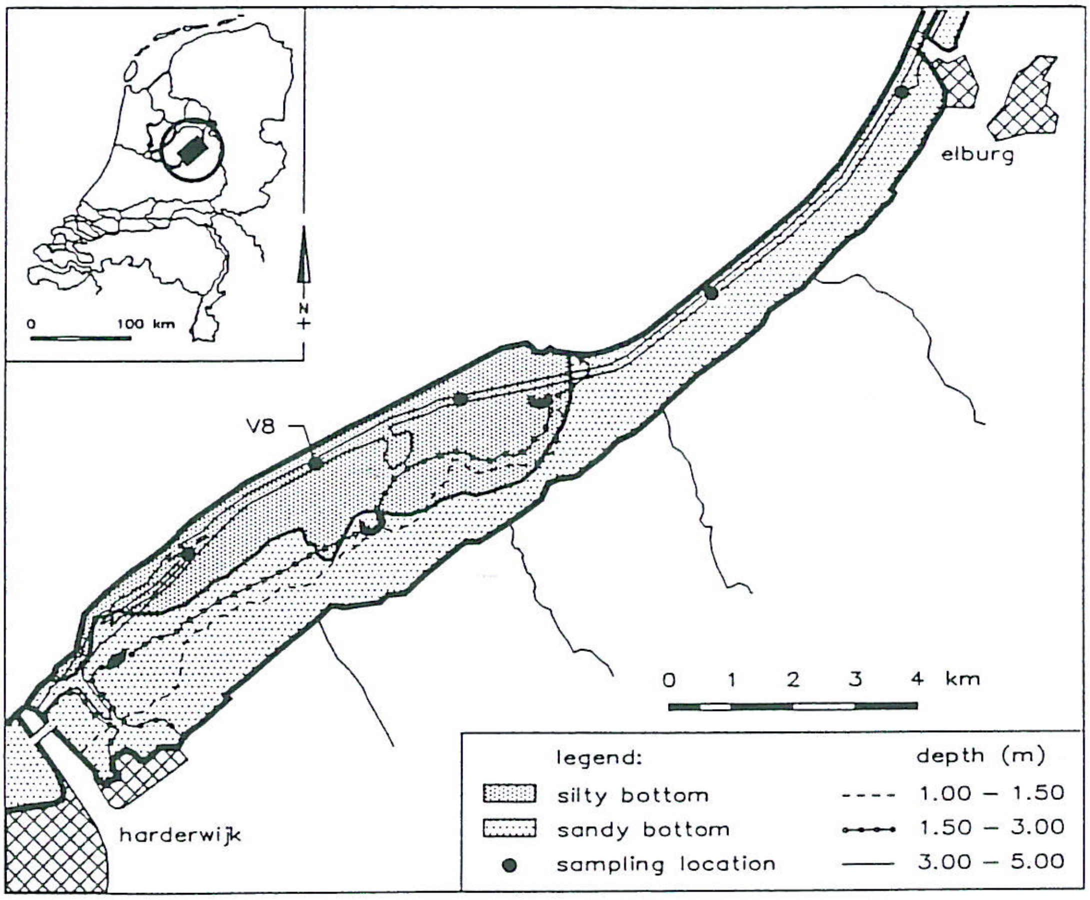


Figure 3.1 The sampling locations, the depth and the types of sediments of Lake Veluwe

The first change occurred immediately after the beginning of the flushing in the winter of 1979-80. The total phosphate concentration dropped to one third of the value in the previous years, which resulted in phosphorus limitation of the bluegreen algae. Consequently, the chlorophyll-a concentrations were reduced with 40%. The algae species composition showed a gradual shift towards diatoms and green algae. A more detailed picture of the development of the water quality in the period 1978-1983 is given by DELFT HYDRAULICS (1988) and Van der Molen et al. (1992).
The second major change took place in the beginning of 1985, when Oscillatoria disappeared rather suddenly from the lake and was replaced by diatoms and green algae. The chlorophyll-a and total phosphate concentrations dropped further with 50%.

3.2 The approach

The first time SWITCH was calibrated for Lake Veluwe for the period 1978-1990 as a stand-alone model in a DELWAQ-framework (DELFT HYDRAULICS, 1991a). SWITCH has now been recalibrated as an integrated part of DBS for the period 1978-1983. So, in stead of imposing the observed water quality as a boundary condition, the water quality was simulated with DBS imposing the 'observed' loads (water and substances). The simulated period was restricted to 1983 because a DBS-input file (loads) is not available for 1984. It has not been possible within the framework of this research to extend the modelling to the period 1985-1987, for which input files are available (Van der Molen et al., 1993).

The calibration was based on comparison of the simulated concentrations with the observed average water quality data for 1978-1983, derived from the WAQWAL and WORSRO databases which contains the data produced by the routine water quality monitoring programme of Rijkswaterstaat (RIZA). The average water quality was calculated on the basis of the data of four sampling points (DELFT HYDRAULICS, 1988). Data on concentrations in sediment and pore water, and on the return phosphate flux, which were used for the first calibration of SWITCH, have been used mainly as check-up information.

As discussed in DELFT HYDRAULICS (1991a), the horizontal inhomogeneity of the sediments of Lake Veluwe is a distinct source of inaccuracy in the calibration. The problem of inhomogeneity was solved in a practical way by assuming that all sediments are silty sediments. This approach has remained unchanged, as the constraints of the present research did not allow for a two-compartment approach with DBS.

The recalibration has been combined with reformulation in a stepwise way. The following steps were taken:

1 Evaluation of the simulation results of DBS with the existing input file.
2 Recalibration of the DBS input parameters after implementation of slow dissolution kinetics for vivianite in the oxidized layer.
3 Recalibration of the SWITCH input parameters after implementation of the formulations for refractory organic matter (C,N,P).
4 Recalibration of the phosphorus related input parameters of SWITCH after implementation of the formulations for the formation of a stable phosphate mineral.
5 Recalibration of the phosphorus related input parameters of SWITCH after implementation of the oxidized layer thickness related adsorption capacity.

Below the adjustment of existing and new input parameters is described for each step. Some parameters mentioned in DELFT HYDRAULICS (1991a) became obsolete and have therefore been omitted from this report. These parameters were mostly related to the imposed water quality boundary condition. The function of the following parameters has been taken over by DBS:

- adsorbed fraction of inorganic phosphate in water the column (fra);
- sedimentation rate (sc);
- degradation rate of detritus in boundary layer at 20 °C (kc_b^{20}); and
- sedimentation rate of adsorbed phosphate (sp).

Step 1: Evaluation

DBS had been calibrated tentatively for Lake Veluwe in an earlier stage (unreported application without bottom algae). The results were not very realistic as far as the sediment composition was concerned. The main reason for this was to be found in the shortcomings of SWITCH with respect to the phosphate chemistry, e.g. the overprediction of the phosphate return flux. The calibration delivered a distorted set of process parameters and of initial concentrations that compensated the shortcomings. In order to obtain more or less correct return fluxes it had been necessary to impose an unrealistic burial rate of 1 cm/year.

Moreover, it seemed that some of the process parameters had been quantified rather arbitrarily. This concerned the parameter for the degradation and settling of the slowly degradable detritus (OOX) in particular. The parameter setting was related to the way OOX was simulated. It was removed to a sink without any feedback to the detritus and nutrient pools in the sediment. The selected parameter values resulted in a large uncontrolled removal of nutrients from the system, nitrogen in particular.

Step 2: Recalibration of DBS with slow dissolution of vivianite

The recalibration of DBS as a whole resulted in the adjustment of:

- the burial rate (new-old value: 0.1-1.0 cm/year);
- the thickness of the sediment layers (new-old values: dh = 2-3 cm and dl = 8-7 cm);
- the initial concentrations of detritus, phosphate, ammonium and dissolved silicate in the sediment; and
- quite a few rates of processes, simulated in the DELWAQ and SWITCH modules of DBS.

The adjustments took place in the following order, as was argued in DELFT HYDRAULICS (1991a):

1) parameters referring to detritus and dissolved oxygen;
2) parameters referring to ammonium and nitrate;
3) parameters referring to phosphate; and
4) parameters referring to dissolved silicon.

The adjustment of process parameters involved:

- increase of the detritus incorporation rate (rc) in balance with decrease of the resuspension rate of complex detritus (new-old value 0.005-0.025 day^{-1}) and increase of the degradation rates (kc) in the sediment;
- increase of the temperature coefficient (kt) of the detritus degradation rates (new-old value 1.07-1.047) in order to slow down the degradation rates in winter time;
- decrease of the sedimentation rate (new-old value 0.02-0.035 m day^{-1}) and increase of the mineralisation rate (new-old value 0.008-0.001 day^{-1}) of slowly degradable detritus in the water column (OOX) in order to keep more nitrogen (Kj-N) in the water column;
- tuning of the nitrification rate in the water column (new-old value 0.2-0.0 day^{-1}) and the critical temperatures for nitrification and denitrification in the water column (new-old value 4-5 °C);
- decrease of the critical nitrate concentration (Cn_c) for determination of the oxidized layer thickness in the sediment (new-old value 0.05-0.1 gN/m^3) in order to increase the oxidized layer thickness;
- tuning of the vivianite dissolution rate (kdp); and
- increase of the dissolution rate (ks, new-old value 0.09-0.01 day^{-1}) and the saturation concentration (Cs_s, new-old value 10.0-0.5 gSi/m^3) of silicate in order to compensate for decreasing of the detritus silicate dissolution rates in the water column and the boundary layer (new-old value 0.005-0.01 day^{-1}).

These changes brought about a very much improved simulation with a realistic development of the detritus and nutrient pools in the sediment. However, SWITCH failed to reproduce the decline of the phosphate and phytoplankton concentrations in the overlying water. The concentrations were overpredicted two times for 1982-1983. In other words, the phosphate return flux was still too high.

Step 3: Recalibration of SWITCH with refractory organic matter

The input parameter 'concentration of refractory organic matter (Cd_r)' became obsolete due to reformulation and was therefore removed from the input module of DBS.

Some further tuning of the initial concentrations of the detritus and phosphorus components in the sediment appeared necessary. In addition to this the following adjustments took place:

- tuning of the factor for the conversion of detritus into refractory organic matter (frf);
- further increase of the degradation rates in the sediment layer (kc_1 and kc_4, new-old value respectively 0.055-0.03 and 0.0065-0.0022 day^{-1});
- decrease of the stoichiometric constants for nitrogen (aa) and phosphorus (ap) in refractory detritus (new-old values respectively 0.05-0.09 gN gC^{-1} and 0.005-0.0065 gP gC^{-1}); and
- further tuning of the vivianite dissolution rate (kdp).

The carbon and nitrogen compounds were simulated satisfactory after these manipulations. Once again it turned out to be impossible to prevent overprediction of the phosphate return flux. The storage of phosphorus in refractory organic matter only had a minor effect.

Step 4: Recalibration of SWITCH with a stable phosphate mineral

The initial concentrations of the phosphorus components in the sediment were adjusted to the concurrent presence of the stable phosphate mineral and vivianite. The other adjustments concerned:

- tuning of the fraction of precipitated phosphorus stored in the stable mineral (fm); and
- decrease of the precipitation rate in the sediment layer (kp, new-old value 0.86-1.2 day^{-1}).

The overprediction of the phosphate concentration in the water column and the return phosphate flux disappeared. However, a new problem arose. Both the seasonal variation and the magnitude of the 'explosive' phosphate flux had been severely reduced, resulting in an unrealistic smooth curve of the total phosphate concentration in the water column. This experience lead to the conclusion that the adsorption capacity of the sediment had to fluctuate much stronger.

Step 5: Recalibration of SWITCH with new formulations for the adsorption capacity

The reformulation was in fact done in two steps. The first attempt to link up the adsorption capacities of the reduced layers with the thickness of the oxidized layer did not give much improvement with respect to both the seasonal variation and the overprediction of the phosphate return flux. The second attempt (equations 2.31) was successful, because also the adsorption capacity of the oxidized layer was formulated as a function of the thickness of the oxidized layer.

The final adjustments were restricted to tuning of the 'average' adsorption capacity of the oxidized layer (Cac).

The original formulations for the adsorption capacities (DELFT HYDRAULICS, 1991a) have been maintained in SWITCH as the alternative option. This approach involves the following input parameters:

- the adsorption capacity of the oxidized layer (Cac_o); and
- the adsorption capacity of the upper reduced layer (Cac_r).

The adsorption capacity of the lower reduced layer is calculated in SWITCH as 0.2 times the capacity of the upper reduced layer.

3.3 The input parameters

A number of constant input parameters have not been determined during the calibration, because they could be estimated rather accurately. These constants most of which have lake specific values have been gathered in Table 3.1. Some of the parameters have been set to zero, mostly because it was assumed that they are unimportant for the sediments of Lake Veluwe.

Nevertheless, the ratio between the dissolved oxygen concentrations at the sediment-water interface and at the upper side of the water boundary layer has changed slightly since the first calibration in order to improve the performance of SWITCH, mainly with respect to the 'explosive' phosphate return flux. A similar remark can be made for the critical nitrate concentration.

Table 3.1 Basic and lake specific input parameters for SWITCH.

Parameter	Symbol	Value	Units
Substances			
Ratio oxygen in water boundary layer*	(fo)	0.675	-
Frac. red. subst. esc. sediments;	(fro)	0.0	-
average		0.0	-
amplitude		365	day
period		0.2	-
phase			
Sediments			
Thickness of the upper layer	(dh)	0.02	m
Thickness of the lower layer	(dl)	0.08	m
Thickness of the water boundary layer	(l)	0.001	m
Porosity of the upper layer	(p_1)	0.71	m^3W/m^3B
Porosity of the lower layer	(p^4)	0.68	m^3W/m^3B
Specific weight of sediment	(Ws)	2500	kb/m^3
Mass transport			
Nett seepage velocity	(vs)	-0.0035	m/day
Sedimentation flux (= burial rate)	(Fs)	$2.5\ 10^{-6}$	$m^3b/m^2/day$
Resuspension flux on basis of bottom volume	(Fr)	0.0	$m^3B/m^2/day$
Molecular diffusion coefficient oxygen	(Dm_o)	$5.5\ 10^{-5}$	m^2/day
Molecular diffusion coefficient ammonium	(DM_a)	9.0 ,,	m^2/day
Molecular diffusion coefficient nitrate	(DM_n)	9.3	m^2/day
Molecular diffusion coefficient phosphate	(DM_p)	4.2 ,,	m^2/day
Molecular diffusion coefficient silicon	(DM_s)	4.7 ,,	m^2/day
bio-irrigation multiplier;	(bt)		
average		3.0	-
amplitude		2.0	-
period		365	day
phase		0.2	-
Bioturbation disp. coeff.;	(Db)		
average		$1.0\ 10^{-6}$	m^2/day
amplitude		$1.0\ 10^{-6}$	m^2/day
period		365	day
phase		0.2	-
Numerics			
Minimal thickness of the aerobic layer	($d1_m$)	0.0005	m
Critical thickness for oxidized layer	(do_m)	0.0009	m
Critical nitrate concentration*	(Cn_c)	0.05	gN/m^3
* Adjusted during the recalibration			

The other input parameters are given in Table 3.2. Except the stochiometric constants all values have been determined by means of calibration. However, back-up data are available, except for the parameters rc, frf, fm and kdp. A minority of the parameters did not need to be recalibrated.

Table 3.2 The input parameters for processes in SWITCH.

Parameter	Symbol	Value	Units
Detritus			
Rate of incorporation in upper layer at 20°C*	(rc^{20})	0.04	1/day
Degradation rate in upper layer at 20°C*	(kc$_1^{20}$)	0.055	1/day
Degradation rate in lower layer at 20°C*	(kc$_4^{20}$)	0.0065	1/day
Temperature coefficient for degr. and incorp.*	(ktc)	1.07	-
conversion factor refractory organic matter**	(frf)	1.1	-
Ammonium and Nitrate			
Nitrification rate at 20°C	(kn^{20})	50.0	1/day
Denitrification rate at 20°C	(kd^{20})	50.0	1/day
Temperature coefficient for nitrification	(ktn)	1.07	-
Temperature coefficient for denitrification	(ktd)	1.07	-
Stoch. constant nitrogen in refractory detritus**	(aa)	0.05	gN/gC
Phosphate			
Average adsorption capacity oxidized sediment*	(Cac)	0.93	gP/kgDM
Half saturation concentration for adsorption	(Ks)	0.1	gP/m^3
Precipitation rate*	(kp)	0.857	1/day
Fraction prec. phosph. stored in stable mineral**	(fm)	0.4	-
Saturation concentration for precipitation	(Cdp$_s$)	0.05	gP/m^3
Temperature coefficient for precipitation	(ktp)	1.0	-
Dissolution rate vivianite**	(kdp)	0.01	(m$^{-2.01}$ gP$^{0.67}$ d^{-1})
Temperature coefficient for dissolution**	(ktd)	1.0	-
Stoch. constant phosphorus refractory detritus**	(ap)	0.005	gP/gC
Silicon			
Dissolution rate of opaline silicate*	(ks)	0.09	1/day
Saturation concentration for dissolution*	(Cs$_s$)	10.0	gSi/m^3
Temperature coefficient for dissolution	(kts)	1.0	-
Oxygen			
Stoch. constant for consump. in degr. detritus	(ac)	3.1	gO$_2$/gC
Stoch. constant for consump. in nitrification	(an)	4.57	g0$_2$/gN
* Adjusted during the recalibration ** New parameter			

3.4 The results

The final results of the calibration are presented in Figures 3.2-3.17. Not all simulated parameters are shown. A representative selection of concentrations and fluxes was made for this purpose.

3.4.1 Concentrations

Phytoplankton, detritus and dissolved oxygen (Fig. 3.2-5)

The phytoplankton concentration (chlorophyll-a) shows a dramatic decline between 1979 and 1980, which is reproduced by DBS. Some underprediction may occur in the summer, whereas some overprediction (1978 and 1983!) occurs during most winters. The extent of phosphate-limitation of the primary production increases from 1978 upto 1980, followed by permanent phosphate-limitation afterwards. Nitrogen-limitation occurs in summer. Its importance decreases gradually during the simulation period. The species composition shifts gradually from bluegreen algae to green algae and diatoms.

The detritus concentrations in the water column, the boundary layer and the sediment layers decrease in accordance with the behaviour of the phytoplankton. The detritus content of the lower sediment layer decreases much less than the other detritus pools, which has a relation with its slow degradation. The sediment content of refractory organic matter increases steadily. The production is by far not compensated by burial. The production of about 18 $gC/m^2/year$ seems realistic. It can be estimated on the basis of an observed 1% organic carbon in the silty sediments, that the accumulation of refractory organic matter has been about 18 $gC/m^2/year$ during 30 years (the life-time of Lake Veluwe).

The dissolved oxygen concentration seems to be overpredicted during the summer. However, the measurements are not fully representative for the daily average concentration because of diurnal variation connected with the production and respiration of phytoplankton.

The thickness of the oxidized layer (Fig. 3.6)

The aerobic layer (d_1) gets gradually thicker from 1978 to 1983. The minimal thickness does no longer occur as of 1980. The maximal thickness of the denitrifying layer (d_2) remains more or less the same. The width of the peak, however, increases substantially. The collapsing of the oxidized layer may be too severe during the winters of 1978-80. It gets restricted to a short period in 1983.

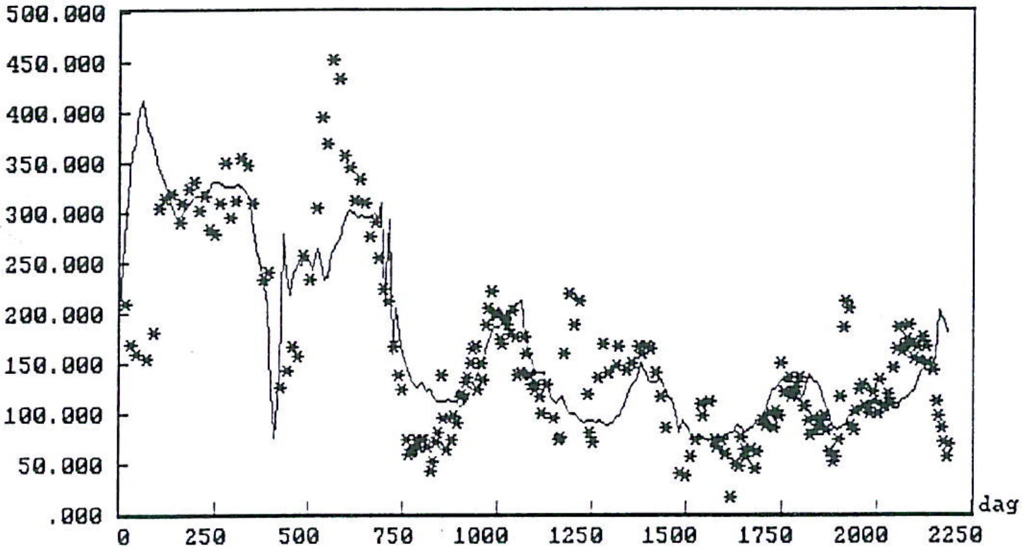


Figure 3.2 The predicted and observed phytoplankton concentration (μg chlorophyll/l) in Lake Veluwe for 1978-83.

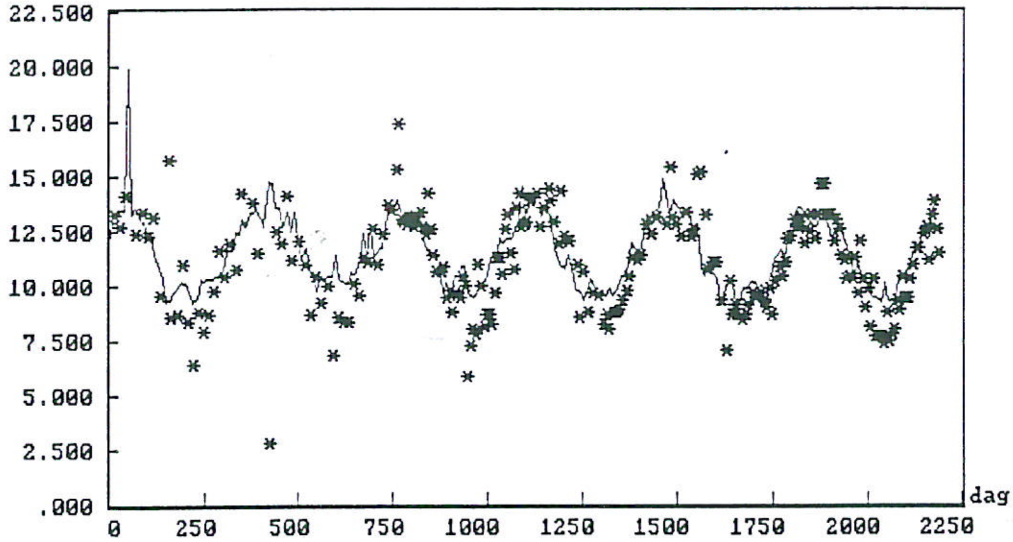


Figure 3.3 The predicted and observed dissolved oxygen concentration (g/m^3) in Lake Veluwe for 1978-83.

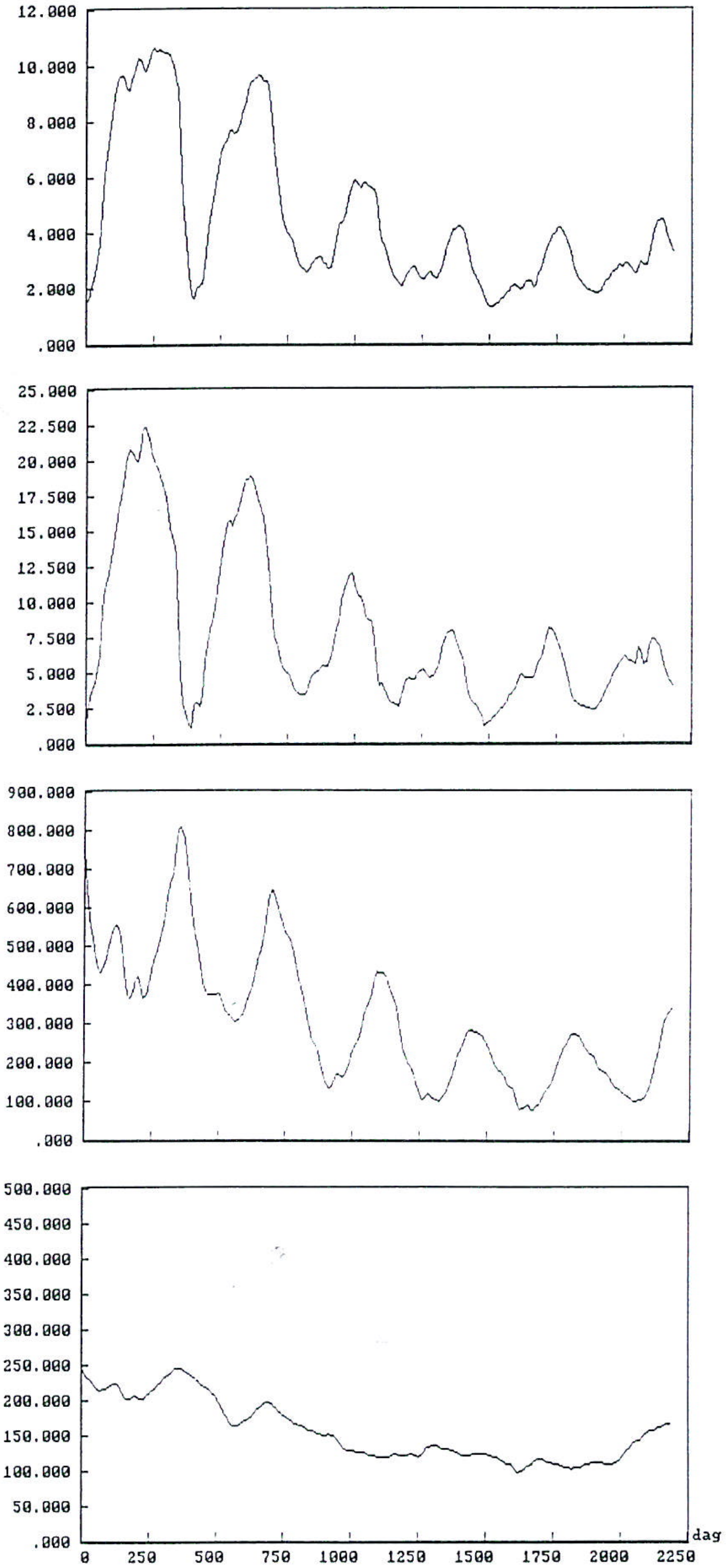


Figure 3.4 The predicted detritus concentrations (gC/m^3) in Lake Veluwe for 1978-83: a) the water column, b) the boundary layer, c) the upper sediment layer, d) the lower sediment layer.

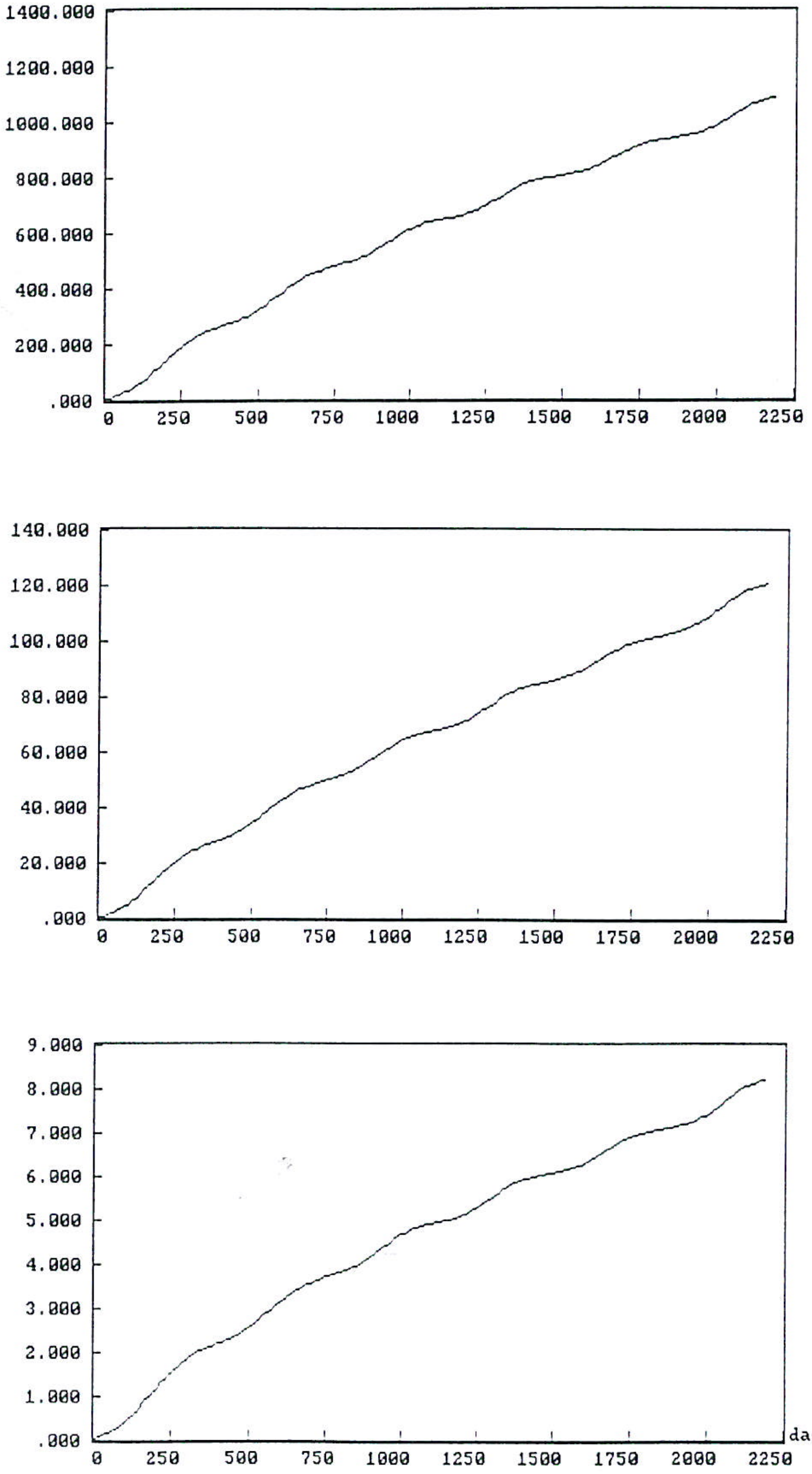


Figure 3.5 The predicted refractory organic matter concentration (g/m^3) in the sediment of Lake Veluwe for 1978-83: a) carbon, b) nitrogen, c) phosphorus.

The nitrogen compounds (Fig. 3.5, 3.7-9)

Some overprediction of Kj-N occurs in the winter, which is connected with the overprediction of phytoplankton. The ammonium concentration remains low in the water column due to nitrification and primary production. Nevertheless, the concentration seems to be somewhat underpredicted. The ammonium concentration in the pore water decrease gradually. The decrease of the concentration in the aerobic layer is relatively small, due to the increase of the thickness of this layer.

The refractory organic nitrogen content of the sediment increases. The nitrogen/carbon ratio in refractory organic matter is rather high (0.11). This is due to the influx of slowly degradable organic matter (OOX) in the detritus pool of the lower sediment layer, which has a N/C-ratio of 0.15.

The situation with respect to nitrate does not change very much, although the width of the concentration peaks increases. The nitrate concentration is buffered rather efficiently by denitrification. The underprediction in the winter season is connected with the overprediction of primary production.

The phosphorus compounds (Fig. 3.5, 3.10-13)

The total phosphate concentration in the water column goes down dramatically due to reduction of both the external and internal loads. Nevertheless, DBS predicts net retention of phosphate in Lake Veluwe for each year, from 10% in 1978 down to 50% in 1983. The overpredictions of the total phosphate concentration are connected with the concurrent overpredictions of the primary production.

'Explosive' phosphate return fluxes occur frequently in 1978-79. The magnitude of the predicted fluxes is more or less correct. The first and the second flux are simulated at the right time. The third flux may not have occurred in reality. The fourth flux comes too late and persists too long. Both the frequence and the duration of the explosive fluxes decrease enormously after 1979.

The underprediction of the inorganic phosphate concentration in the water column in the summer of 1978 may have to do with the fact that the adsorption parameter in DBS is a constant in stead of a function of the pH. Consequently, the adsorption and therefore the sedimentation of phosphate adsorbed to suspended solids remains at a constant level. The high pH during the summer season brings about a lower adsorption parameter in reality, resulting in the reduced removal of phosphate from the water column.

The phosphate content of the sediment increases until 1979 and starts to decrease thereafter. The decrease is about 5% in four years. This implies that the net retention of phosphate in the lake is exceeded by burial and seepage after 1979. A decrease of about 15% between 1980 and 1990 is to be expected. The data on the phosphate content of the sediment suggest a substantial decrease. The earlier suggestion (DELFT HYDRAULICS, 1991a) that this decrease might be as large as 40% must be based on misinterpretation of the data, the mean values of which have large standard deviations.

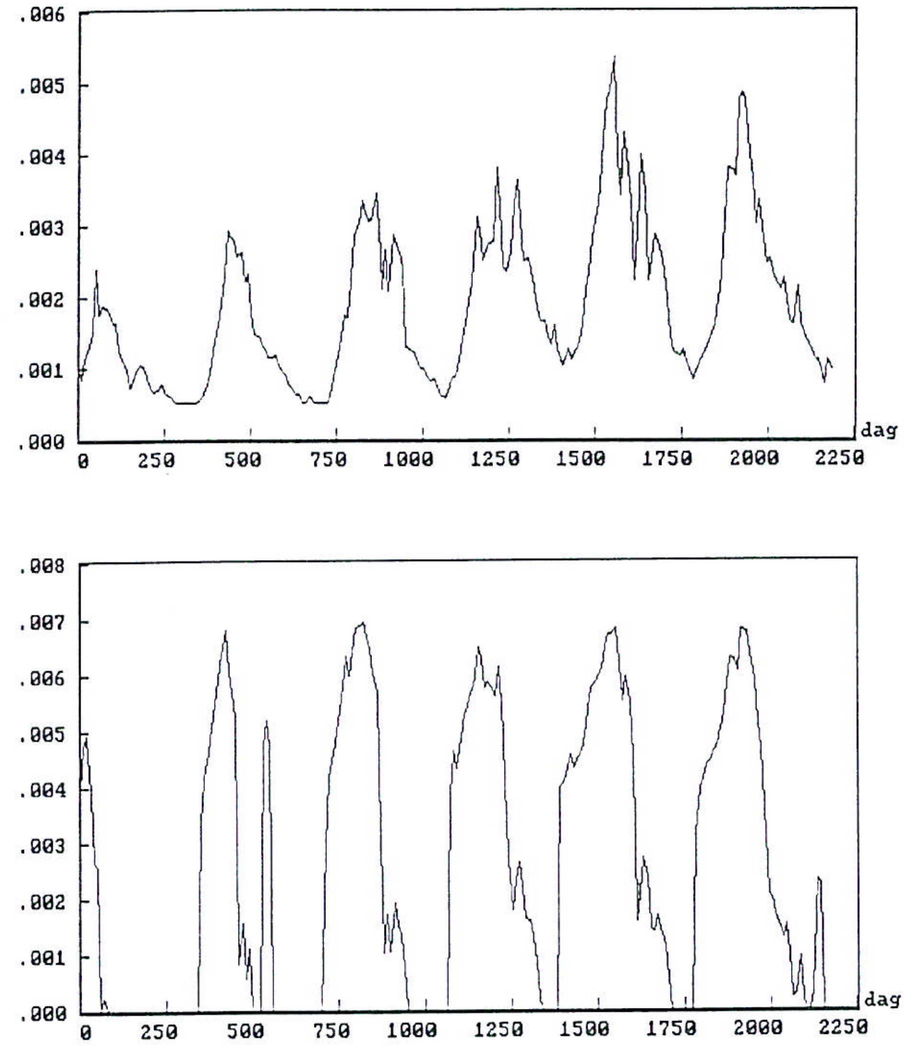


Figure 3.6 The predicted thickness of several layers (m) in the sediment of Lake Veluwe for 1978-83: a) the aerobic layer, b) the denitrifying layer.

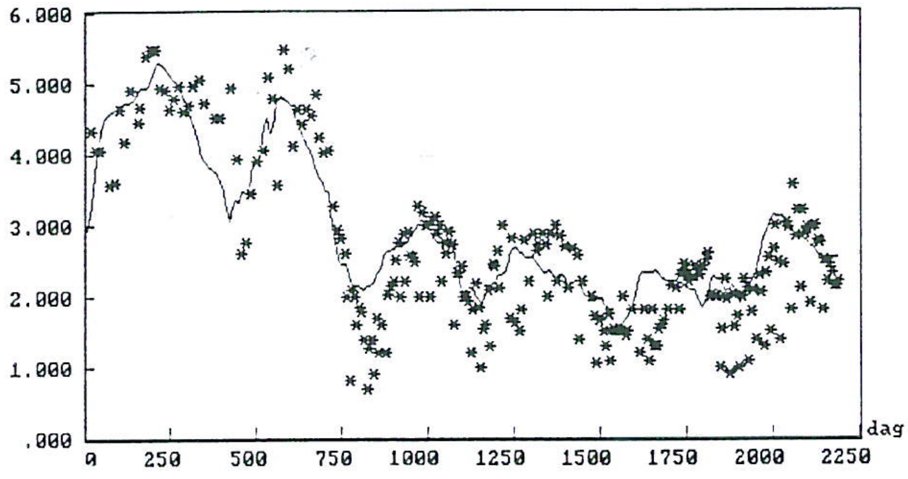


Figure 3.7 The predicted and observed Kjeldahl-N concentration (gN/m^3) in Lake Veluwe for 1978-83.

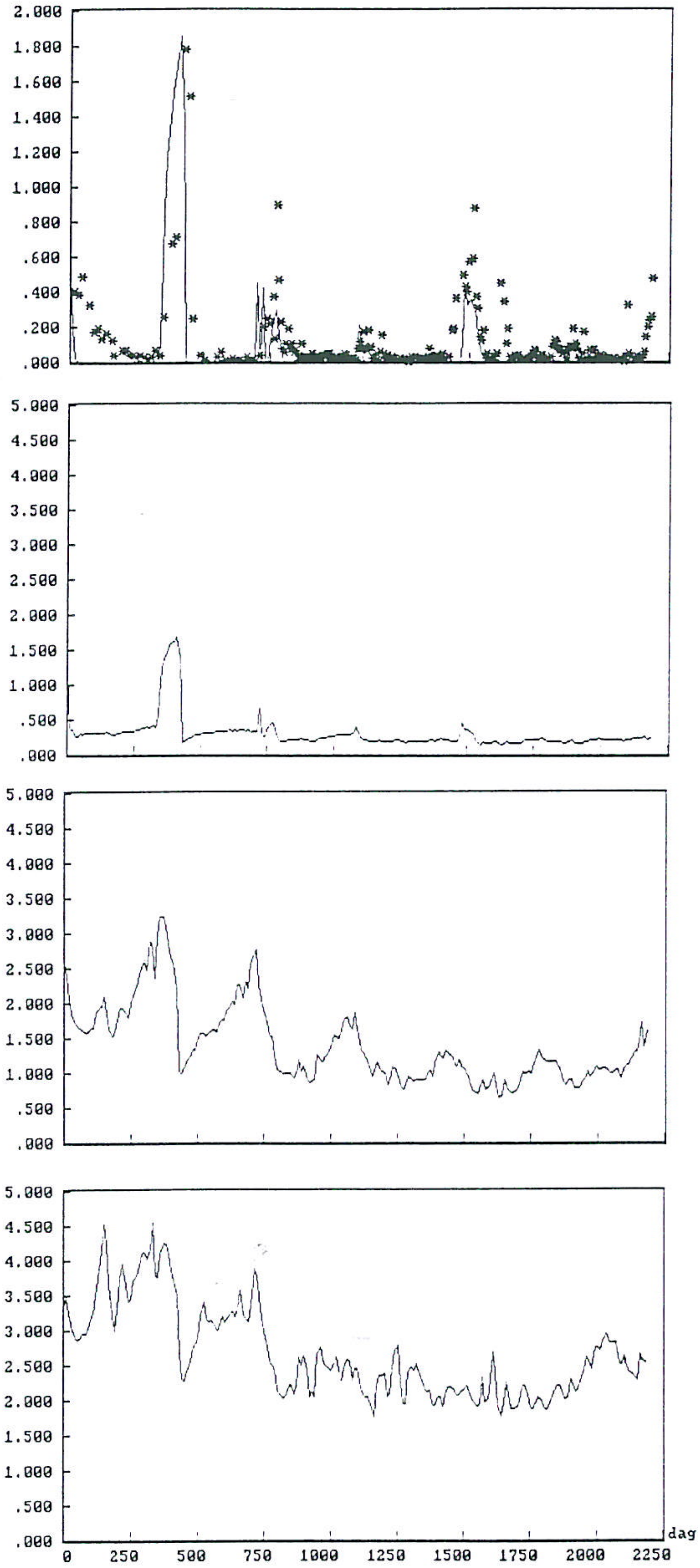


Figure 3.8 The predicted and observed ammonium concentrations (gN/m^3) in Lake Veluwe for 1978-83: a) the water column, b) the aerobic sediment layer, c) the remaining part of the upper sediment layer, d) the lower sediment layer.

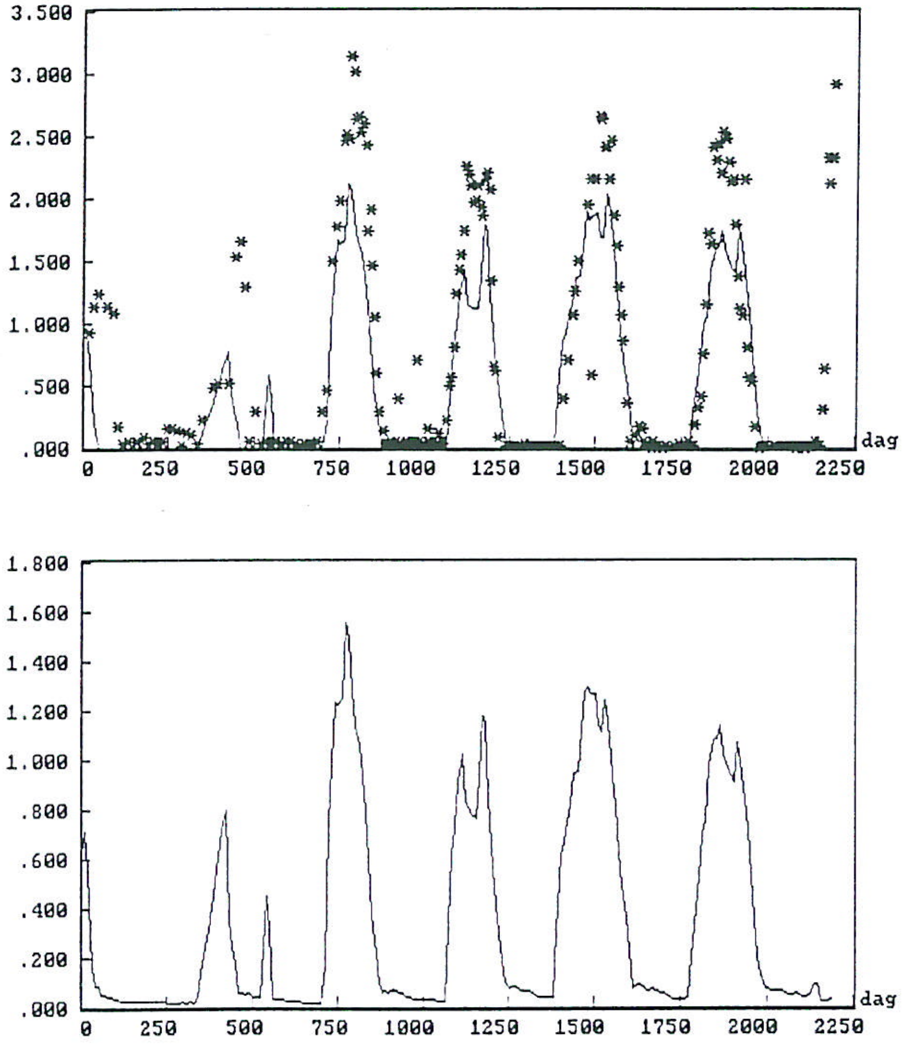


Figure 3.9 The predicted and observed nitrate concentrations (gN/m^3) in Lake Veluwe for 1978-83: a) the water column, b) the aerobic sediment layer.

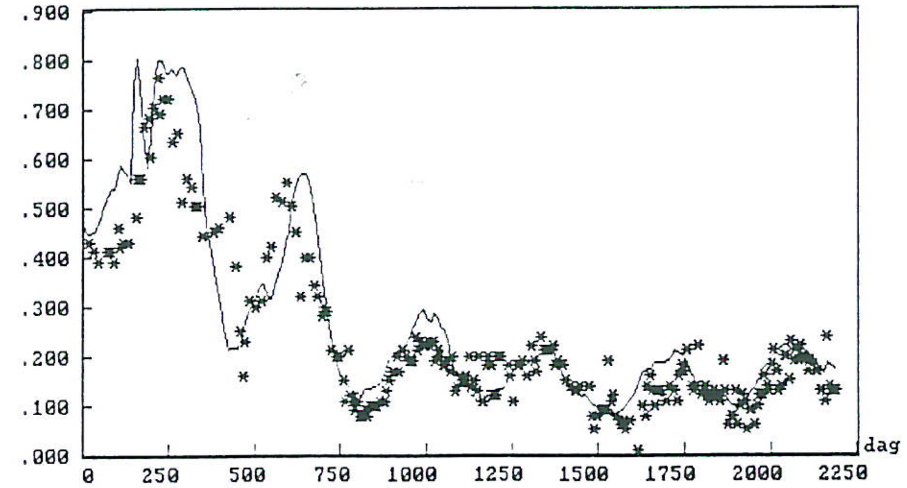


Figure 3.10 The predicted and observed total phosphate concentration (gP/m^3) in Lake Veluwe for 1978-83.

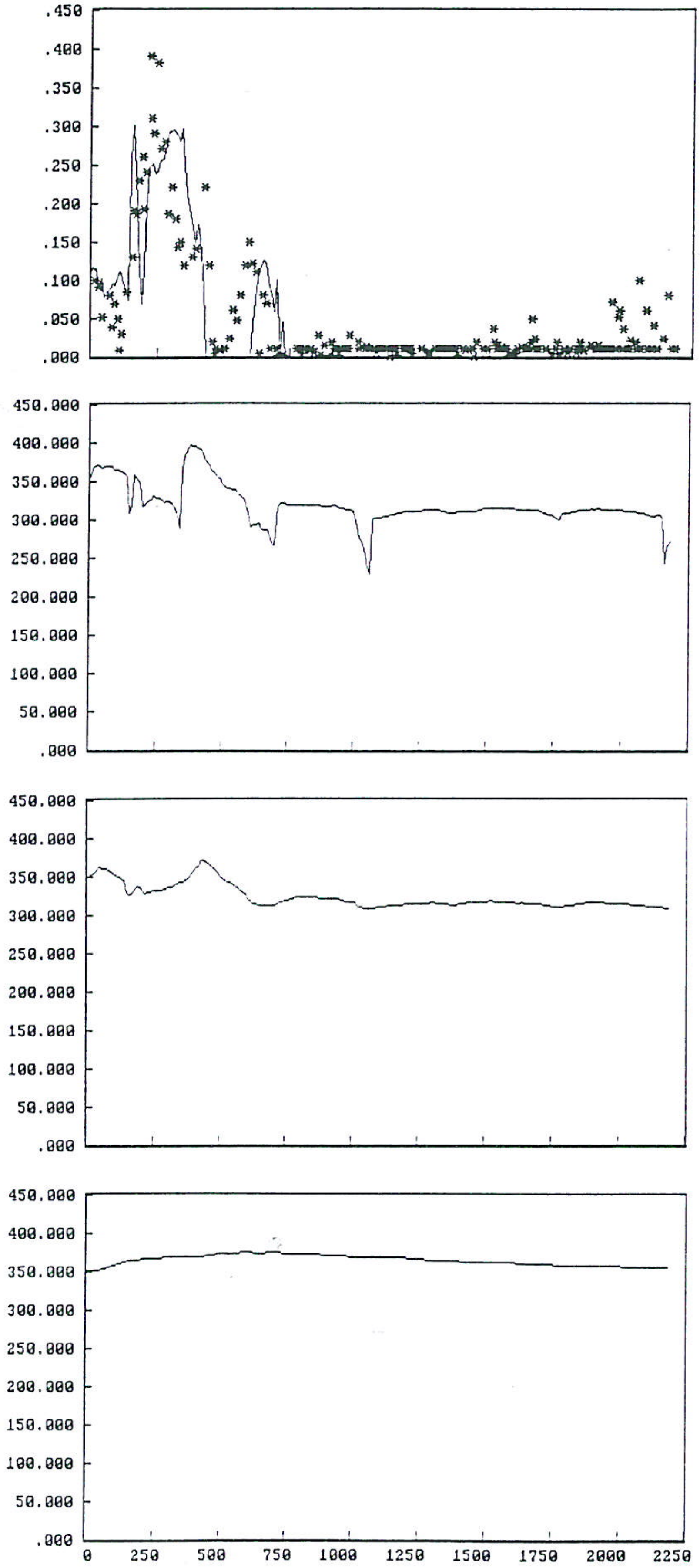


Figure 3.11 The predicted and observed inorganic phosphate concentrations (gP/m^3) in Lake Veluwe for 1978-83: a) the water column, b) the oxidized sediment layer, c) the upper reduced sediment layer, d) the lower reduced sediment layer.

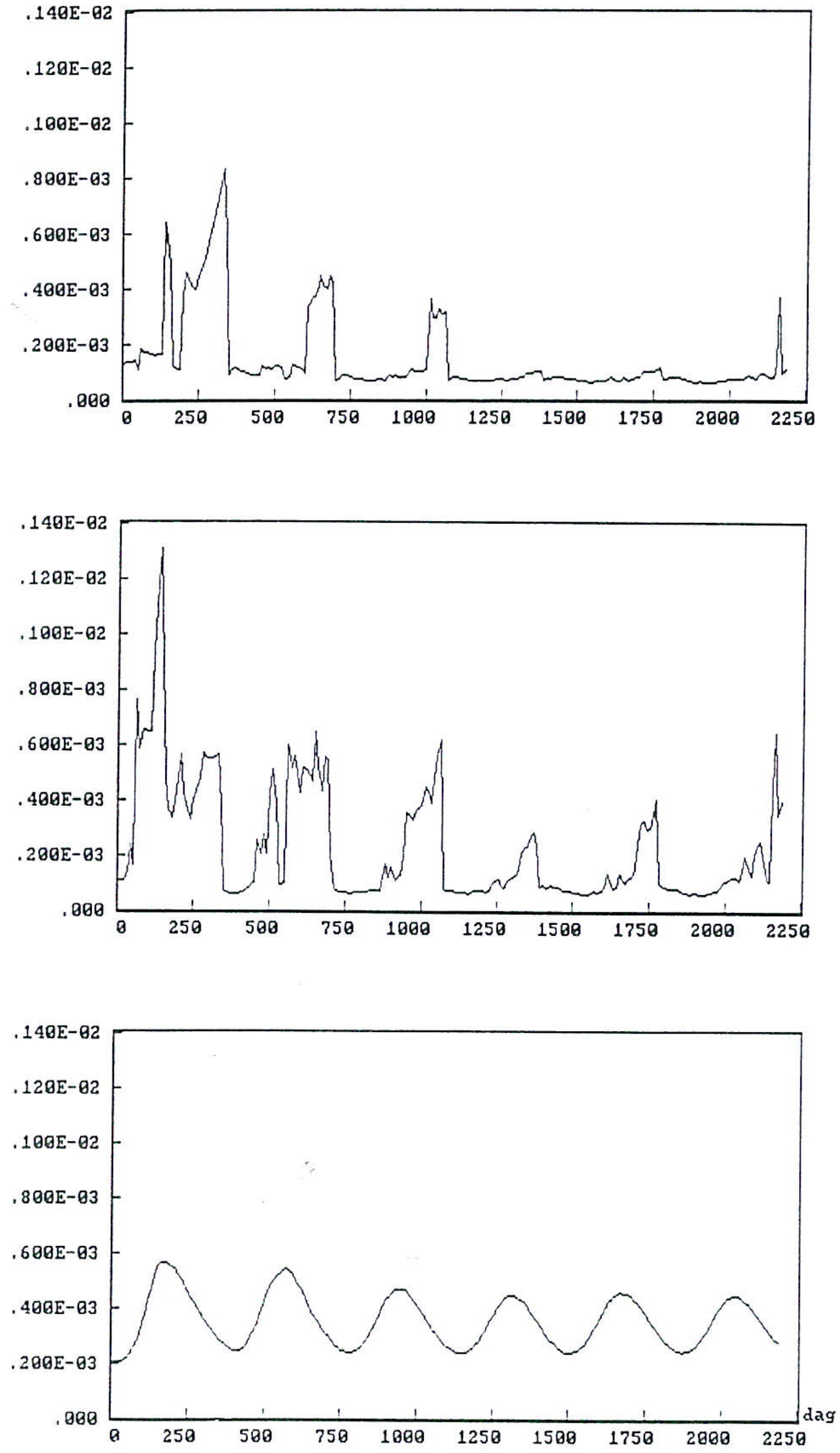


Figure 3.12 The predicted dissolved phosphate fraction (-) in the sediment of Lake Veluwe for 1978-83: a) the oxidized sediment layer, b) the upper reduced sediment layer, c) the lower reduced sediment layer.

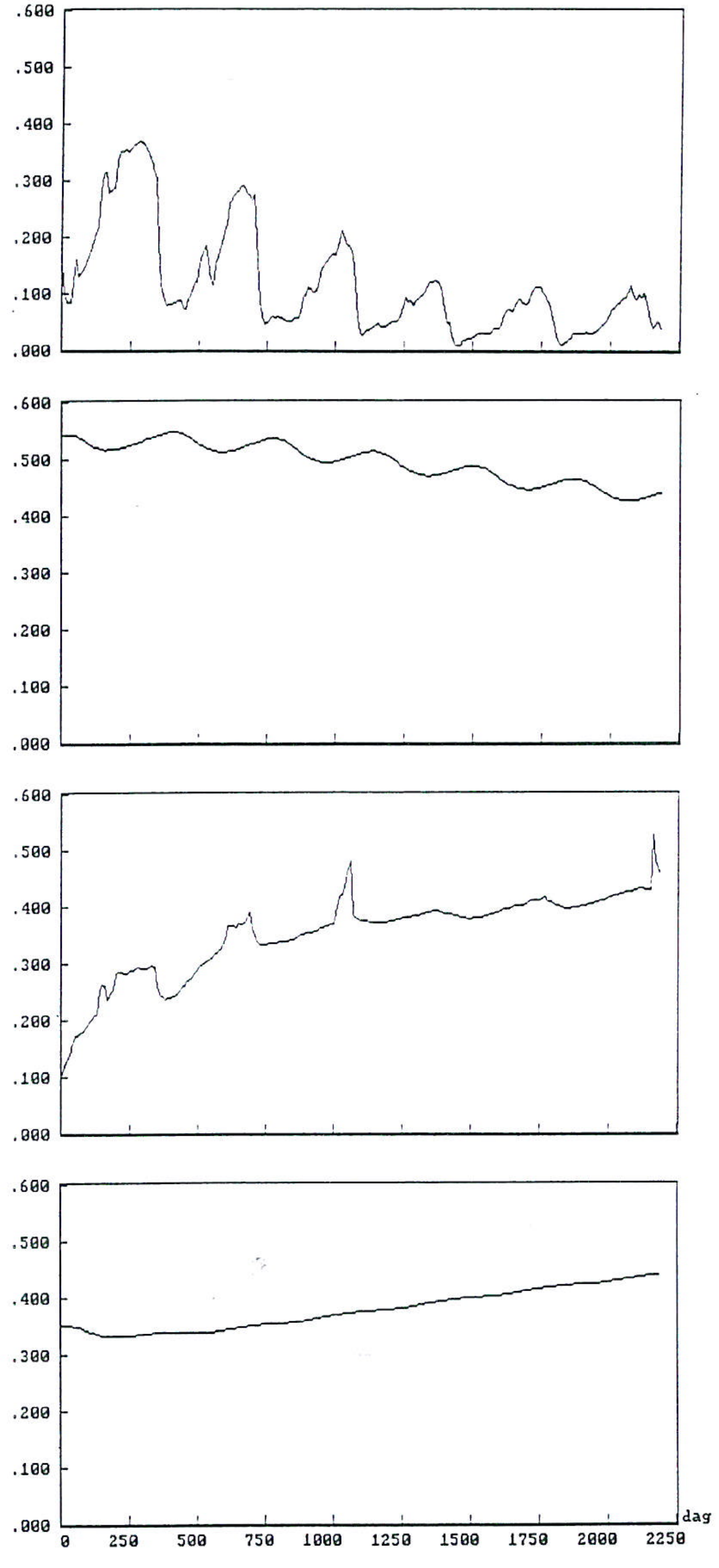


Figure 3.13 The predicted mineral phosphate fractions (-) in the sediment of Lake Veluwe for 1978-83: a) vivianite in the oxidized sediment layer, b) vivianite in the lower reduced sediment layer, c) stable mineral in the oxidized sediment layer, d) stable mineral in the lower reduced sediment layer.

The dissolved phosphate fraction in the pore water of the top sediment layer shows large peaks during 'explosive' fluxes. The dissolved phosphate concentrations vary from 0.25 to 0.05 gP/m^3 in the top layer and from 0.21 to 0.1 gP/m^3 in the lower layer.

The two mineral phosphate fractions develop mutually consistent. The stable mineral fraction get more important, whereas the vivianite fraction becomes smaller due to the increasing thickness of the oxidized layer (dissolution) and the decline of the input of phosphate into the sediment. Together they continue to make up about 90% of the total inorganic phosphate content of the sediment.

The refractory organic phosphorus content of the sediment increases. The phosphorus/carbon ratio in refractory organic matter (0.007) gets close to the expected value (0.005).

The silicon compounds (Fig. 3.14)

The dissolved silicon concentration in the water column get depleted over longer periods as the diatoms are succeeding to make up a larger part of the primary production. The observed and simulated concentrations run out of phase to some extent.

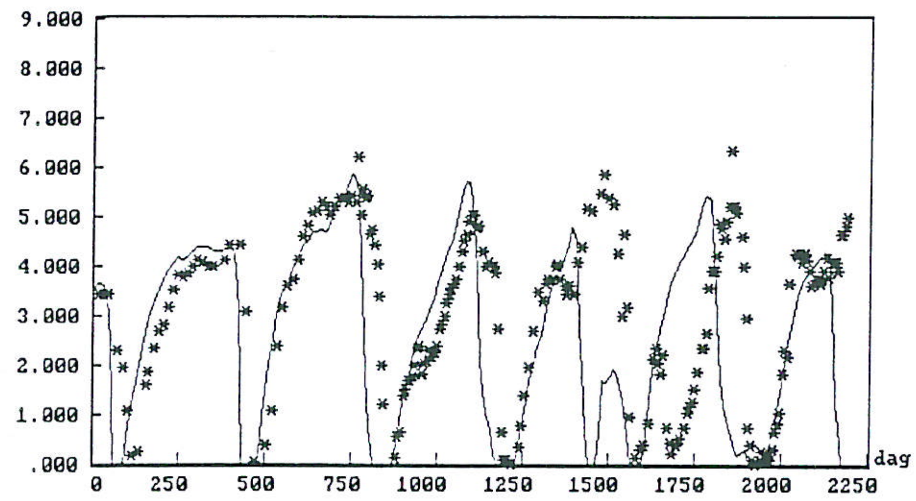
3.4.1 Fluxes

An extensive overview of all process fluxes in SWITCH was given in DELFT HYDRAULICS (1991a). Most of the data were meant to provide a quantitative view on the relative importance of the processes. The picture has remained the same in broad outlines after the recalibration. Therefore, only the return fluxes from the sediment to the water column are presented here in detail, although all fluxes have changed and some new fluxes have been added to SWITCH. Figures 3.15-3.17 provide an overall picture of the calculated nutrient fluxes in Lake Veluwe.

Table 3.3 shows the nutrient return fluxes. The yearly average return phosphate flux in DBS decreases from 0.0063 gP/m^2/day in 1978 to 0.002 gP/m^2/day in 1983. The decline occurs mainly between 1979 and 1980. The phosphate return flux calculated with the improved SWITCH-model as part of DBS is only 33% of the flux calculated with the stand-alone first version of SWITCH.

The mean observed phosphate return flux in March 1983 is 0.003 gP/m^2/day (Brinkman and Van Raaphorst, 1986; σ=0.0022, n=3). The calculated flux averaged over decades 10-18 is equal to 0.0017 gP/m^2/day, and lies well within the range of the observed values.

The return flux of ammonium decreases to a similar extent as the phosphorus flux. The nitrate-N return flux, however, shows a break between 1979 and 1980. Denitrification causes net removal of nitrate from the water column from 1980 on. As a consequence the total nutrient-N return flux becomes much smaller.



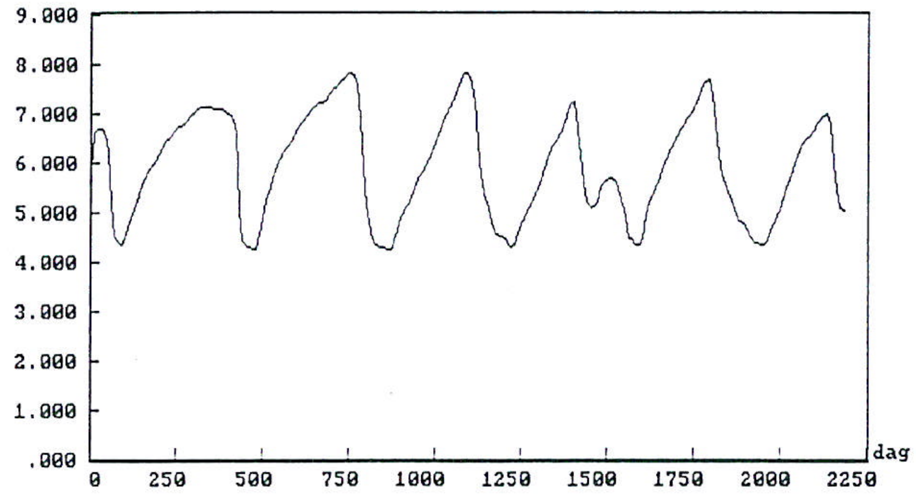


Figure 3.14 The predicted and observed dissolved silicon concentrations (gSi/m^3) in Lake Veluwe for 1978-83: a) the water column, b) the sediment layer.

Table 3.3 Calculated return fluxes from the sediment of Lake Veluwe (dispersive exchange with the pore water, seepage ignored).

Year	Phosphate gP/m^2/day	Ammonium gN/m^2/day	Nitrate gN/m^2/day	Nutrient-N gN/m^2/day	Silicon gSi/m^2/day
1978	0.0063	0.042	0.0026	0.045	0.0058
1979	0.0051	0.031	0.0012	0.032	0.0053
1980	0.0031	0.021	-0.0083	0.013	0.0063
1981	0.0022	0.015	-0.0086	0.006	0.0066
1982	0.0019	0.011	-0.0080	0.003	0.0060
1983	0.0020	0.015	-0.0080	0.007	0.0065

The net removal of organic nitrogen from the water column into the sediment (including the boundary layer) is -0.073 gN/m^2 in 1978 and -0.040 gN/m^2 in 1983. It appears that the sediment has become more important as a sink of nitrogen, when the organic-N fluxes are added to the total nutrient-N return fluxes. The addition results in -0.028 gN/m^2 in 1978 versus -0.033 gN/m^2 in 1983.

The dissolved silicon return flux increases slightly due to the increased productivity of diatoms.

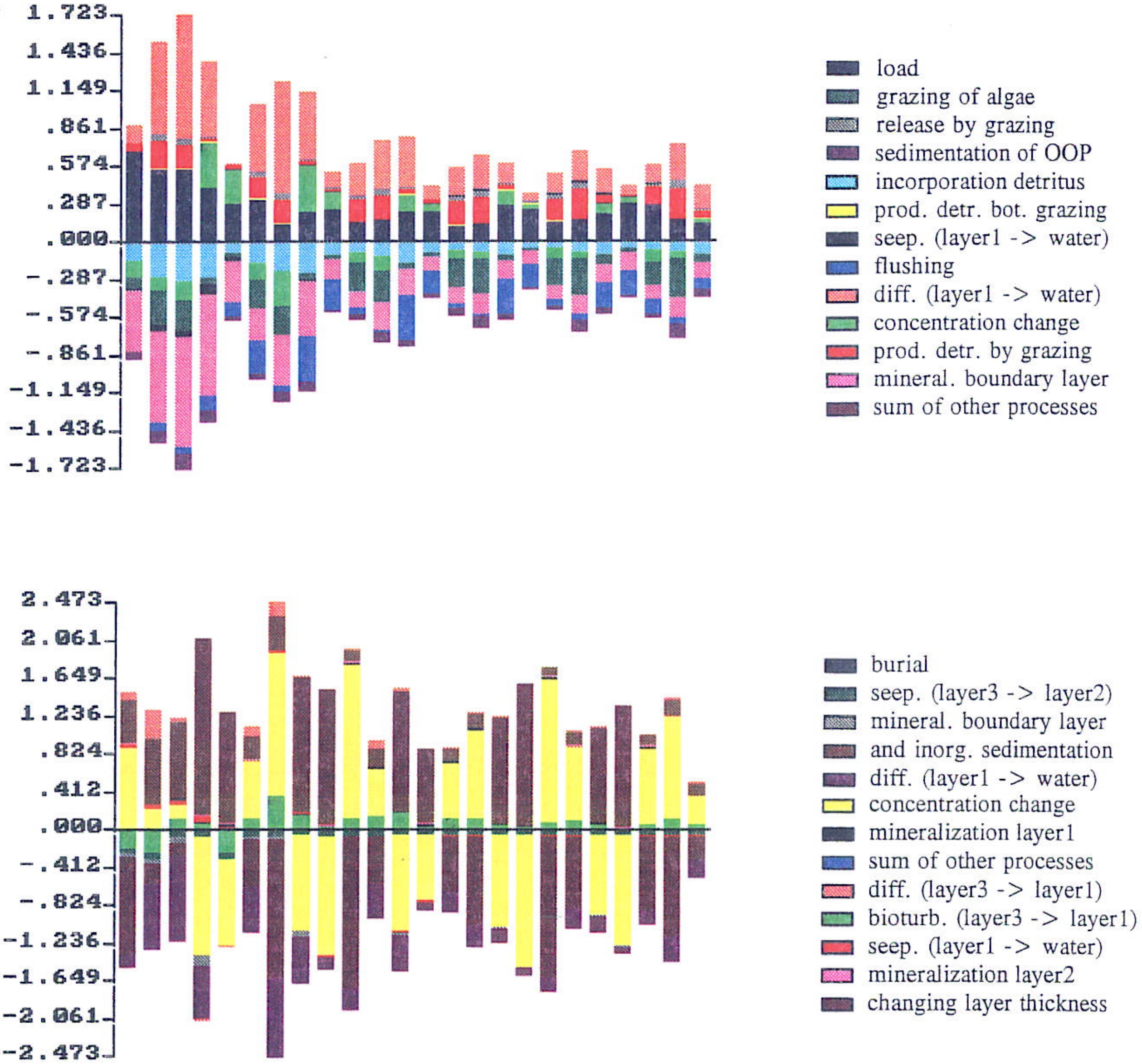


Figure 3.15 Predicted mass balances for phosphorus in Lake Veluwe for 1978-83: a) total phosphorus in the water column and the boundary layer, b) inorganic phosphorus in the oxidized sediment layer and the boundary layer; all fluxes in gP/m^2/year.

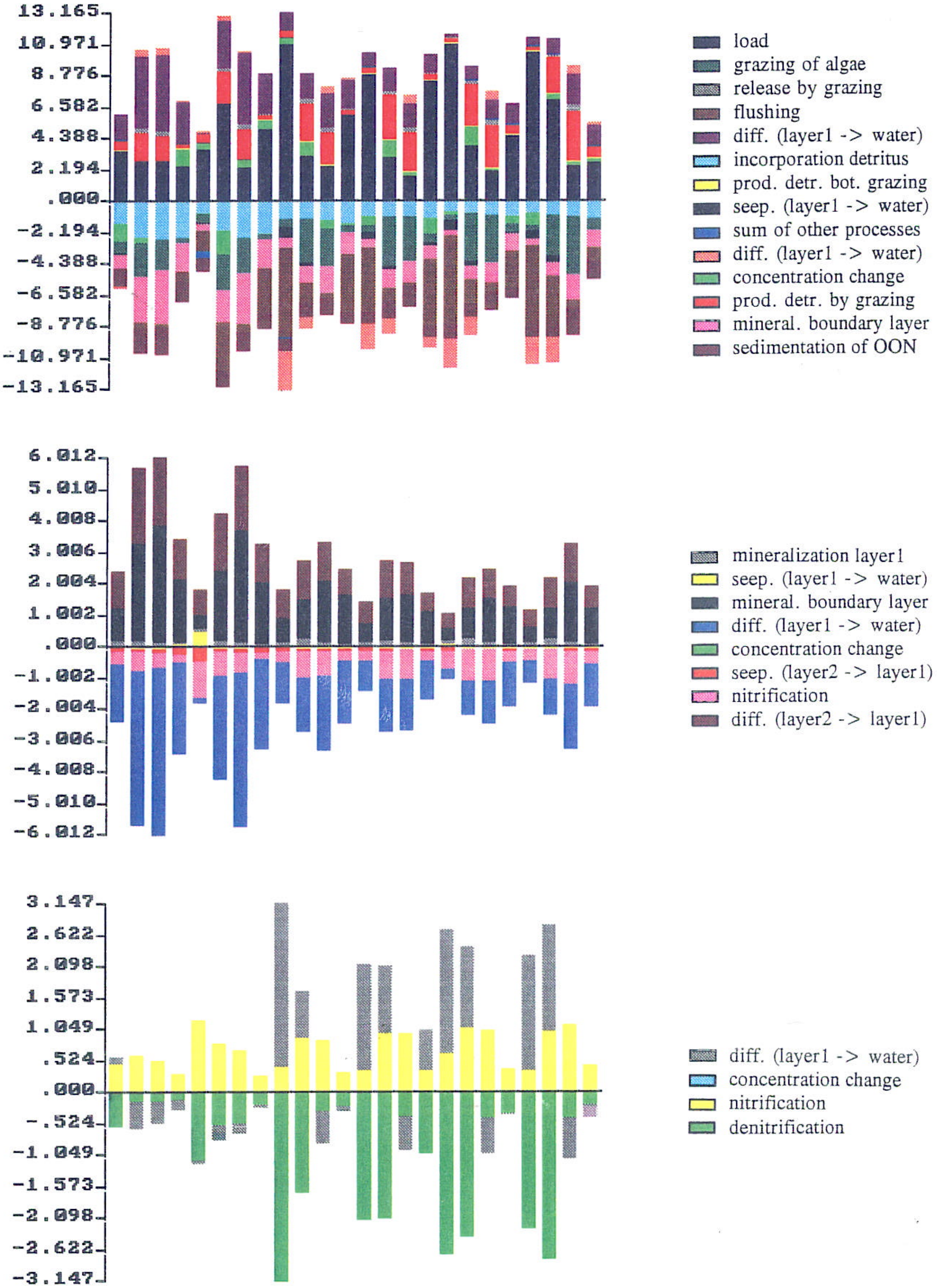


Figure 3.16 Predicted mass balances for nitrogen in Lake Veluwe for 1978-83: a) total nitrogen in the water column and the boundary layer, b) ammonium in the aerobic sediment layer and the boundary layer, c) nitrate in the aerobic sediment layer and the boundary layer; all fluxes in gN/m^2/year.

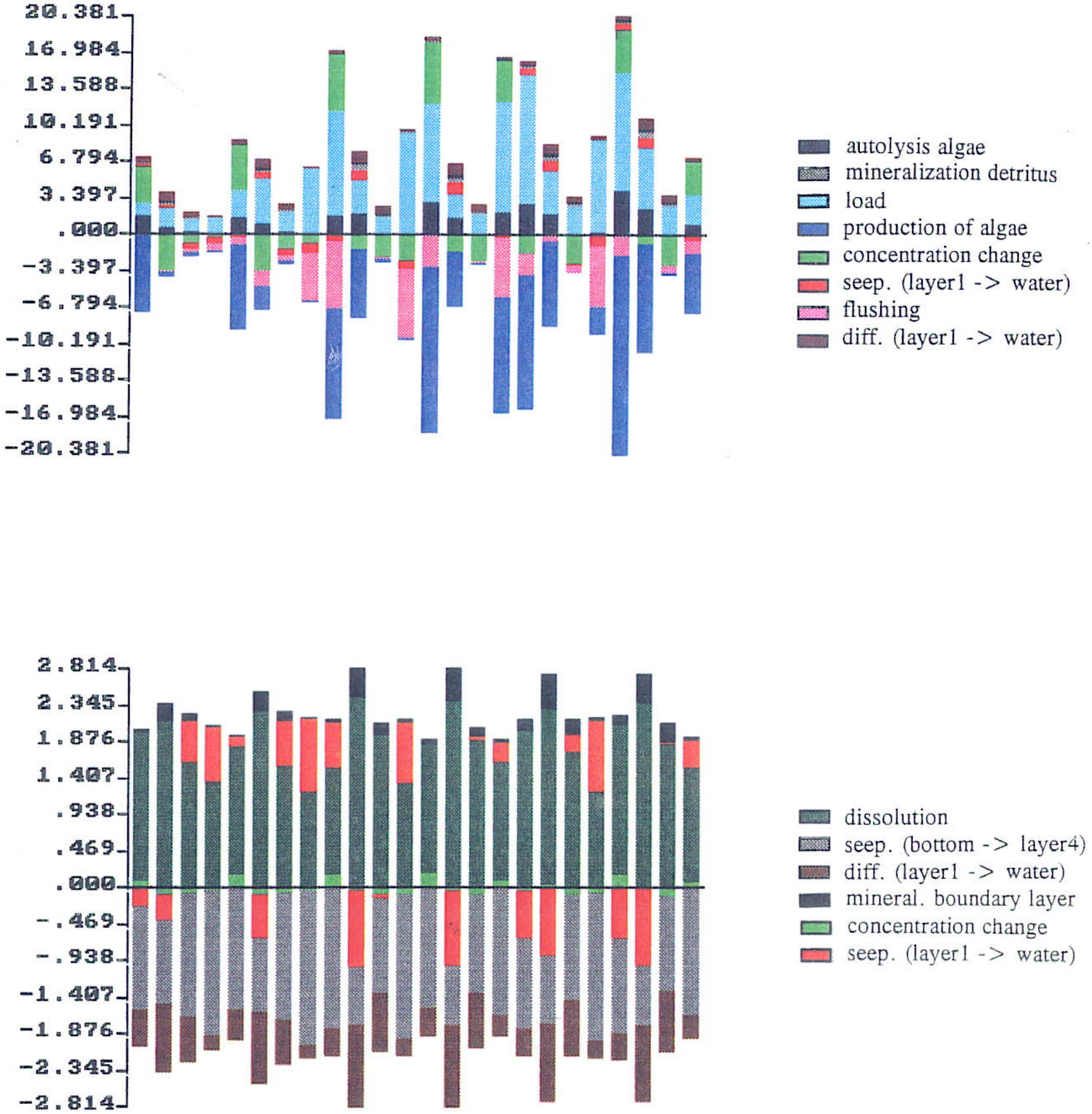


Figure 3.17 Predicted mass balances for silicon in Lake Veluwe for 1978-83: a) the water column and the boundary layer, b) dissolved in the sediment layer and the boundary layer; all fluxes in gSi/m^2/year.

4 Conclusions and discussion

The reformulation of SWITCH concerned:

- the replacement of instantaneous dissolution of vivianite in the oxidized sediment layer by slow dissolution;
- the introduction of a second mineral phosphate fraction, a stable mineral of unknown composition, next to the existing vivianite fraction;
- the relating of the phosphate adsorption capacity to the thickness of the oxidized layer;
- the addition of refractory organic matter (C,N,P); and
- the replacement of the formulation for the sediment oxygen demand by a formulation which is also valid at anaerobic conditions in the water column.

A few remarks must be made with respect to the new formulations. The formation of a stable phosphate mineral in the sediment of Lake Veluwe next to vivianite has not been proved. It has to be considered as a usable working hypothesis. Moreover, the empirical functions relating the phosphate adsorption capacity of the sediment to the thickness of the oxidized layer are tentative. The phosphate chemistry in sediment, in particular the above aspects, should be the subject of further research with HADES.

The recalibration of the new SWITCH-model for Lake Veluwe as an integral part of DELWAQ-BLOOM-SWITCH (DBS) showed that the reformulation improved the performance of both SWITCH and DBS. The recalibration was successful, which appears from the good matching of the simulated and observed water quality in Lake Veluwe for the period 1978-83. SWITCH simulates realistically and consistently layer thicknesses, concentrations and mass fluxes connected with the transport and conversion processes. The model reproduces the phenomenon of the "explosive" phosphate return flux to the overlying water too a large extent. The overprediction of the phosphate return flux has disappeared. DBS predicts net retention of phosphorus in Lake Veluwe for each year in the period 1978-83.

The improvement of SWITCH implies that DBS with SWITCH is capable of reliable prediction of the response of a surface water system to a large reduction of the external phosphorus load in terms of water quality and phytoplankton biomass.

The assessment of the performance of SWITCH must take into account that the simulation of the water and sediment quality with DBS is driven by the primary production simulated with BLOOM II. Therefore, the deviation of the calculated water quality from the observed water quality is strongly related to the predictions of BLOOM II. This goes in particular for the 'explosive' fluxes. Further improvement of SWITCH can not be disconnected of further improvement of the other modules in DBS: DELWAQ and BLOOM II.

The first calibration of SWITCH was troubled by:

1. the stand-alone application of the model, which did not allow feedback from the overall mass balances for Lake Veluwe to the calculated return fluxes;
2. the one-compartment approach, whereas the differences in sediment composition demanded for a two-compartment approach; and
3. the 'observed' decrease of the phosphate content in the sediment between 1980 and 1990, which seemed to be contradictory with the net retention of phosphate in Lake Veluwe.

Problem 1 was taken away by the calibration of SWITCH as an integrated part of DBS. Problem 2 continued to exist. The problem of horizontal inhomogeneity of the sediment, sandy in the shallow eastern part of Lake Veluwe and silty in the deeper western part, was solved in a practical way by assuming that all sediments are silty sediments. This allowed calibration on the basis of one compartment, resulting in the determination of lake-average parameter values. This implies that a part of the process parameters would have to undergo further calibration for a correct simulation with two compartments. The parameter values established in a two-compartment approach will be closer to the actual parameter values.

The third problem seems to be solved in the following way. The assumed 40%-decrease of the phosphorus content in the sediment was due to misinterpretation of the available data. Considering the large standard deviations of the mean concentrations, the decrease may well have been about 15% as was predicted with DBS. The decrease of the phosphate content in the upper sediment layer (10 cm) is then explained by the net input of phosphate from the water column being smaller than the removal through seepage and burial. The removal by burial may mainly take place in the deeper part of Lake Veluwe and may be the consequence of the transport to the deeper part of sediment eroded in the shallow part.

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6 List of symbols used

The list contains all parameter names used in this report and in DELFT HYDRAULICS (1991a).

A subscript figure indicates either a layer number (0 = overlying water) or an interface number (4 = the lower boundary of the 'active' bottom).

aa = stoichiometric constant for nitrogen in refractory detritus ($gN\ gC^{-1}$)
ac = stoichiometric constant for oxidation of detritus ($gO_2\ gC^{-1}$)
an = stoichiometric constant for nitrification ($gO_2\ gN^{-1}$)
ap = stoichiometric constant for phosphorus in refractory detritus ($gP\ gC^{-1}$)
bt = amplification factor for bio-irrigation (-)
Ca = ammonium concentration ($g\ N\ m^{-3}$ water)
Cam = maximal concentration of adsorbed phosphate ($g\ P\ m^{-3}$ bottom)
Cac = time average adsorption capacity of the oxidized layer ($gP\ kg^{-1}DM$)
Cap = adsorbed phosphate concentration ($g\ P\ m^{-3}$ bottom)
C = concentration ($g\ m^{-3}$)
Cd = detritus concentration ($g\ C\ m^{-3}$ water or bottom)
Cd_b = amount of detritus in the boundary layer ($g\ C\ m^{-2}$)
Cdp = dissolved phosphate concentration ($g\ P\ m^{-3}$ pore water)
Cdp_s = saturation concentration for ortho-phosphate ($g\ P\ m^{-3}$ pore water)
Cfe = the dissolved Fe2+-concentration near the surface of vivianite crystals ($gFe\ m^{-3}$)
Cmp = concentration of phosphate in a stable mineral ($gP\ m^{-3}B$)
Cn = nitrate concentration ($g\ N\ m^{-3}$ water)
Cn_c = critical nitrate concentration ($g\ N\ m^{-3}$ water)
Cnd_0 = detritus nitrogen concentration in the overlying water ($gN\ m^{-3}$)
Cnd_b = amount of detritus nitrogen in the boundary layer ($gN\ m^{-2}$)
Cnd = detritus nitrogen concentration ($gN\ m^{-3}B$)
Co = dissolved oxygen concentration ($g\ m^{-3}$ water)
Cp = total inorganic phosphate concentration ($g\ P\ m^{-3}$ bottom)
Cpd_0 = detritus phosphorus concentration in the overlying water ($gP\ m^{-3}$)
Cpd_b = amount of detritus phoshorus in the boundary layer ($gP\ m^{-2}$)
Cpd = detritus phosphorus concentration ($gP\ m^{-3}B$)
Cpp = precipitated phosphate concentration ($g\ P\ m^{-3}$ bottom)
Cr = amount of reduced substances ($gO_2\ m^{-2}$)
Cs = concentration dissolved silicate ($g\ Si\ m^{-3}$ water)
Cs_s = saturation concentration ($g\ Si\ m^{-3}$ pore water)
Cxd_0 = slow decomposing detritus (OOC) concentration in the overlying water ($g\ m^{-3}$)
Cxn_0 = slow decomposing detritus nitrogen (OON) concentration in overlying water ($gN\ m^{-3}$)
Cxp_0 = slow decomposing detritus phosphorus (OOP) concentration overlying water ($gP\ m^{-3}$)
d = thickness of the "active" bottom layer (m)
d_1 = thickness of the aerobic layer (m)
d_2 = thickness of the denitrifying layer (m)
d_3 = thickness of the upper reduced layer (m)

d_4 = thickness of the lower reduced layer (m)
D = dispersion coefficient (m^2 d^{-1})
Db = bioturbation dispersion coefficient (m^2 d^{-1})
dh = thickness of the upper layer (m)
dl = thickness of the lower layer (m)
Dm = molecular diffusion coefficient (m^2 d^{-1})
do = thickness of the oxidized layer (m)
do_m = minimal thickness of the oxidized layer in SWITCH (m)
fa = correction factor for organic nitrogen degradation rate (-)
Fa = dispersive ammonium flux between layers (g N m^{-2} d^{-1})
Fa_0 = dispersive ammonium return flux to overlying water (g N m^{-2} d^{-1})
Fa_b = ammonification flux from the boundary layer (g N m^{-2} d^{-1})
fac = empirical factor linking up the adsorption capacity with layer thickness (-)
fap = adsorbed phosphate fraction (-)
Fas = seepage flux of ammonium between layers (g N m^{-2} d^{-1})
Fb = burial flux based on bottom volume (m^3 m^{-2} d^{-1})
Fd = bioturbation flux of detritus (g C m^{-2} d^{-1})
Fd_b = flux of detritus incorporated in the upper layer (g C m^{-2} d^{-1})
Fd_s = flux of detritus settled from overlying water (g C m^{-2} d^{-1})
fdp = dissolved phosphate fraction (-)
fm = fraction of precipitated phosphorus stored in the stable mineral (-)
fmp = stable mineral phosphate fraction (-)
Fn_0 = dispersive nitrate return flux to overlying water (g N m^{-2} d^{-1})
Fn_1 = nitrate flux to the denitrifying layer (g N m^{-2} d^{-1})
Fnd = bioturbation flux organic nitrogen (gN m^{-2} d^{-1})
Fnd_b = flux of detritus nitrogen incorporated in the upper layer (gN m^{-2} d^{-1})
Fnd_s = flux of detritus nitrogen settled from the overlying water (gN m^{-2} d^{-1})
fo = correction factor for the oxygen concentration (-)
Fo_b = oxygen consumption flux in the boundary layer (g O_2 m^{-2} d^{-1})
Fo_c = chemical oxygen demand (g O_2 m^{-2} d^{-1})
fp = correction factor for organic phosphorus degradation rate (-)
Fp = dispersive phosphate flux between layers (g P m^{-2} d^{-1})
Fp_0 = dispersive phosphate return flux to overlying water (g P m^2 d^{-1})
Fp_b = phosphate release flux from the boundary layer (g P m^{-2} d^{-1})
Fp_s = sedimentation flux of adsorbed phosphate (g P m^2 d^{-1})
Fpd = bioturbation flux organic phosphorus or inorganic phosphate between layers (g P m^{-2} d^{-1})
Fpd_b = flux of detritus phosphorus incorporated in the upper layer (gP m^{-2} d^{-1})
Fpd_s = flux of detritus phosphorus settled from the overlying water (gP m^{-2} d^{-1})
fpp = vivianite phosphate fraction (-)
Fpp = bioturbation flux between layers (g P m^{-2} d^{-1})
Fps = seepage flux of phosphate between layers (g P m^{-2} d^{-1})
frf = factor for the conversion of detritus into refractory organic matter (-)
Fr = resuspension flux based on bottom volume (m^3 m^{-2} d^{-1})
fro = fraction reduced substances permanently removed or fixed (-)
Fs = sedimentation flux based on displaced bottom volume (m^{3}B m^{-2} d^{-1})
Fs_b = dissolution flux of silicate in the boundary layer (g Si m^{-2} d^{-1})
Fs_0 = dispersive silicate return flux to overlying water (g Si m^{-2} d^{-1})
Fss = seepage flux of silicate between layers (g Si m^{-2} d^{-1})

Fxd_s = flux of slow decomposing detritus (OOC) incorporated in the sediment 77 ($gC\ m^{-2}\ d^{-1}$)
Fxn_s = flux of slow decomposing detritus nitrogen (OON) incorp. in sediment ($gN\ m^{-2}\ d^{-1}$)
Fxp_s = flux of slow decomp. detritus phosphorus (OOP) incorp. in sediment ($gP\ m^{-2}\ d^{-1}$)
k^{20} = process rate at 20 ^0C (d^{-1})/
kc = degradation rate of detritus in the bottom (d^{-1})
kc_b = degradation rate of detritus in the boundary layer (d^{-1})
kd = denitrification rate (d^{-1})
kdis = the (second order) dissolution rate constant ($m^3\ gFe^{-1}\ d^{-1}$)
kdp = dissolution rate ($m^{-2.01}\ gP^{0.67}\ d^{-1}$)
kn = nitrification rate (d^{-1})
knd_b = degradation rate of detritus nitrogen in the boundary layer (d^{-1})
ko = chemical oxidation rate (d^{-1})
kob = chemical oxidation rate related to bioturbation (d^{-1})
kop = chemical oxidation rate related to oxygen penetration (d^{-1})
kp = phosphate precipitation rate (d^{-1})
kpd_b = degradation rate of detritus phosphorus in the boundary layer (d^{-1})
ks = silicate dissolution rate (d^{-1})
Ks = half saturation phosphate concentration ($g\ P\ m^{-3}$ pore water)
kt = temperature coefficient in process rates (-)
l = thickness of the water boundary layer (m)
L_s = solubility product of vivianite
p = porosity (-)
pa = average porosity (-)
rc = rate of detritus incorporation in the sediments (d^{-1})
Rdis = the dissolution rate ($gP\ m^{-3}\ d^{-1}$)
Ro = oxygen consumption rate ($g\ m^3$ bottom d^{-1})
sc = sedimentation rate for detritus ($m\ d^{-1}$)
t = time (d)
T = temperature (^0C)
tlag = time between day 1 and the day at which ko is maximal (d)
vs = seepage velocity ($m\ d^{-1}$)
Ws = specific weight of the sediments ($kg\ m^{-3}$)
z = sediment depth (m)

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