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Alterra Report 619
ISSN 1566-7197

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AlterraReport 619

Alterra, Wageningen, 2008

ABSTRACT

Hendriks, R.F.A., D.J.J. Walvoort and M.H.J.L. Jeuken, 2008. *Evaluation of the applicability of the SWAP-ANIMO model for simulating nutrient loading of surface water in a peat land area. Calibration, validation, and system and scenario analysis for an experimental site in the Vlietpolder.* Wageningen, Alterra Report 619. 123 pages.; 20 figs.; 20 tables; 67 refs.

The applicability of the SWAP-ANIMO model for simulating nutrient loading of surface water in a peat land area was tested against results of an experimental plot on a peat pasture in the Vlietpolder in the West of the Netherlands. The model was calibrated against a part of these results and validated against another part. It was concluded that the model is reasonably well able to simulate nutrient loading, because it includes all major processes. It is recommended to add a second pool of dissolved organic matter, to be able to distinguish between labile (fresh) and more stable (peat) organic matter. According to the simulation results, dairy farming contributed for 25-50% to nutrient loading, depending on nutrient (N or P) and weather year.

Keywords: calibration, DOVE-veen, nutrient leaching, nutrient loading, peat soil, simulation model, submerged drains, validation

ISSN 1566-7197

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Preface

At the beginning of the first decade of the 21st century, the three DOVE projects (Diffuse belasting Oppervlaktewater door de melkVEe-houderij; diffusive (nutrient) loading of surface waters by dairy farming), DOVE-klei, DOVE-veen en DOVE-zand, were conducted in the Netherlands on clay, peat and sand soils, respectively. Objective of these projects was to study the contribution of dairy farming to the nutrient loading of surface water at experimental plots on different soil types.

As one of the financial contributors to the DOVE-projects, the Ministry of Agriculture, Fishery and Nature of the Netherlands, commissioned Alterra to test the reliability of the simulation results of the SWAP-ANIMO model against the experimental results. This model forms the core of the STONE model that is used to evaluate the Dutch fertilization legislation.

This report presents the methods and results of the evaluation of the SWAP-ANIMO model against the results of the DOVE-veen project on peat soil. This project was conducted at a peat pasture area in the Vlietpolder near Hoogmaden, close to the city of Leiden in the Western part of the Netherlands. The Vlietpolder experimental site can be considered as more or less representative for shallow, eutrophic fen peat soils in this part of the Netherlands.

The model evaluation was conducted in the period 2002-2005 by a project team consisting of ir. R.F.A. Hendriks (project leader), drs. D.J.J. Walvoort and ir. M.H.J.L. Jeuken.

Summary

Objective
Objectives of this study were to investigate whether the SWAP-ANIMO model is applicable for simulating nutrient (N and P) loading of surface waters in a peat land area and to formulate recommendations for improving the model. Therefore, the model outcome was tested against the measurement results of the DOVE-veen project (Diffuse belasting Oppervlaktewater door de melkVEe-houderij op veengrond; diffusive (nutrient) loading of surface waters by dairy farming on peat soil). This project was carried out in the period 1999-2003 in a peat pasture area in the Vlietpolder near Hoogmaden, close to the city of Leiden in the Western part of the Netherlands, by Alterra and Hoogheemraadschap (Waterboard) Rijnland. Another objective of the study at hand was to perform some system and scenario analyses with the calibrated model, of which evaluation of the contribution of dairy farming to nutrient loading of surface waters was the most.

Methods
The SWAP-ANIMO model is a process-based model that aims at dynamic simulation of nitrogen and phosphorus leaching to surface waters and groundwater from various soil types, depending on daily weather conditions and a wide range of hydrological settings and land use forms. It consists of the soil physical sub-model SWAP for simulating transport and storage of water and heat, and the nutrient sub-model ANIMO for simulation of soluble C-, N- and P-compounds on the basis of water balance terms and soil temperatures provided by SWAP. Major feature of ANIMO for simulating transformation processes in organic soils is that it contains detailed descriptions of the organic-matter/C-, N- and P-cycle and that the latter two cycles are based on the first. Furthermore, it contains a very flexible description of organic matter pools, which allows simulation of organic matter substrates of different qualities within the same soil profile. Another important feature of SWAP-ANIMO is the extensive and flexible description of boundary conditions, which counts especially for the top boundary. Therefore, it is in principle capable of simulating the basic transport and transformation processes in peat soils at the field scale.

In order to obtain realistic modelling results, the model needs site-specific input data for as well model parameters as forcing variables (boundaries). Most of these were obtained from the DOVE-veen project. Because this project basically did not focus on evaluation of or simulation with process-based models like SWAP-ANIMO, some essential input parameters were lacking. In order to obtain values for those, extra measurements were conducted. These comprised site-specific soil physical and chemical properties.

Not all model parameters can be measured. To obtain values for these immeasurable parameters, the model was calibrated and validated against measured values of (time-series of) relevant rate and state variables. In this sense, testing of the model implied calibration and validation of the model.

Conclusions

On the basis of the obtained calibration and validation results it can be concluded that SWAP is reasonably well able to simulated groundwater level behaviour and drainage to surface water in the peat pasture area of the Vlietpolder for the simulated period. Especially, the latter result is relevant because it concerns the subject of this study: nutrient loading of the surface water. ANIMO is reasonably well able to simulate the average N and P concentrations in the peat soil of the experimental field. Validation pointed out that its capability of simulating important terms of the N and P balances, i.e. N-mineralization, denitrification and annual N and P uptake by the crop, was good. But no direct information was obtained about the model's ability to correctly simulate N and P loading of the surface water.

From the combination of good results of the independent validation of discharge simulations with SWAP and the reasonable results of the ANIMO simulations of N and P concentrations, it was concluded that calibration and validation results give reason for having confidence in the results of SWAP-ANIMO simulation of N and P loading of the surface water in peat pasture areas like the Vlietpolder. Thus the conclusion was that SWAP-ANIMO is applicable for realistic simulation of nutrient loading of surface waters in peat pasture areas. However, not all aspects of the simulation of leaching of nutrients towards surface waters could be evaluated completely, as this process was not measured itself. For the ANIMO sub-model, a recommendation for improvement was derived (see: ‘Recommendations’).

Process oriented models are useful tools for analysing observed nutrient concentrations in peat pasture areas and for calculation on the basis of these observations of N and P loading of surface waters and the contribution of the main nutrient sources to this loading.

In years that are not extremely wet, the contribution of dairy farming in the form of fertilisation is not the largest contribution to the nutrient loading of the surface water of the ‘DOVE-veen’ experimental site. For N, decomposition and mineralization of the organic matter in the peat soil is the largest contributor, and for P leaching out of the P-rich soil complex in the saturated peat soil. Under wet conditions because of large precipitation surpluses, fertilisation can be the main source of nutrient loading of the surface water. Wet peat soils and (organic) fertilisers form an unfavourable combination from the point of view of nutrient leaching to surface waters.

Wetting of the peat soil of the ‘DOVE-veen’ experimental site in order to preserve the peat soil by raising ditch water level leads to increased contribution of fertilisers to nutrient loading of the surface water: fertilisers and wet peat soils are an unfavourable combination.

Contribution of the peat soil layers to nutrient loading decreases due to wetting. For N this is mainly due to decreased peat decomposition and mineralization in the smaller unsaturated zone, and for P to decreased leaching out of the soil complex of the peat layers in the permanent water saturated zone of the peat profile. For N, the increased leaching of fertilisers prevails and the overall effect of wetting of this peat soil is increase of N-loading of the surface water. For P, both processes are more or less in equilibrium and P-loading is hardly affected, but the average P-concentration of the leachate is slightly decreased.

Lowering ditch water level leads to increase of P-loading and discharge concentration, because of increase of the contribution of leaching out of the P-rich saturated peat soil. N-loading is hardly affected by this process, while N-concentration increases slightly.

For application of submerged drains it is crucial to apply the right ditch water level and corresponding drain depth. A too high level will lead to more direct draining of the by fertilisation nutrient-enriched top soil, while a too low level will cause direct drainage of nutrient rich peat soil layers. For the ‘DOVE-veen’ experimental site, the optimal ditch water level with corresponding drain depth is 0.5-0.6 m below soil surface. At that level N-loading is somewhat lower than without drains and P-loading is at most a little higher. The optimal level and depth can differ for each peat soil, depending on soil profile and hydrological conditions.

Recommendations for improving the model

From evaluating the effect of the decomposition rate of the pool of dissolved organic matter (DOM) on the concentrations of dissolved organic N in the soil solution, it is recommended to add to the ANIMO sub-model a second pool of DOM with its own properties independent of the properties of the existing pool. So that the model can cope with situations that require a labile as well as a stabile pool of DOM, like those in peat soils.

In general, it is recommended to add to the ANIMO model explicit descriptions of redox processes that affect sorption of phosphorus to the soil complex. This extension may improve simulation of phosphorus adsorption and desorption under alternating wet and dry conditions, as is the case in peat soils. For simulating the effects on phosphorus loading of strategies for wetting of peat soils in order to reduce soil surface subsidence, this can be an important improvement of the model.

Another important process that is lacking in the model is leaching of sulphate to surface waters. It is recognized nowadays that sulphate reduction can be an important process for stimulating phosphorus mobilisation from the sediment into the water column in the ditches. Especially, surface waters in peat land areas are vulnerable for this process due to organic-matter-rich sediments.

Recommendations for management of peat lands

In case of applying submerged drains for reducing soil surface subsidence, from the point view of nutrient loading it is recommended to use an optimal ditch water level and corresponding drain depth. For the Vlietpolder this level is in the range of 0.5-0.6 m below soil surface. It is expected that this range will differ only little for peat pasture areas with similar properties and conditions as the ones of the Vlietpolder.

1 Introduction

The SWAP-ANIMO model is a process-based model that aims at dynamic simulation of nitrogen and phosphorus leaching to surface waters and groundwater from various agricultural used soils, depending on daily weather conditions and a wide range of hydrological settings and land use forms (Groenendijk et al., 2005). It forms the core of the STONE model (Wolf et al., 2003), which was developed for evaluating changes in the agricultural sector (e.g. changes in fertiliser recommendations and cropping patterns) and in policy measures that restrict fertilization levels on the leaching of nitrogen (N) and phosphorus (P) to ground and surface waters on the national scale in the Netherlands (Groenendijk et al., 2005). For realistic and reliable simulation results, it is crucial that the model is evaluated against results of as many field experiments as possible.

1.1 Rational

In the period 1999-2005, three so-called DOVE projects were conducted in the Netherlands. DOVE stands for ‘Diffuse belasting Oppervlaktewater door de melkVEe-houderij’, meaning: diffusive (nutrient) loading of surface waters by dairy farming. In three field studies the contribution of dairy farming to the nutrient loading of the surface water was studied for experimental plots on clay, peat and sand soil, respectively. In these studies, relevant soil chemical, soil physical, hydrological, hydraulic and surface water parameters were measured for a period of about three years.

The study on peat soil, the ‘DOVE-veen project’, was carried out in the period 1999-2003 in a peat pasture area in the Vlietpolder near Hoogmaden, close to the city of Leiden in the Western part of the Netherlands. It was conducted by Alterra and Hoogheemraadschap (Waterboard) Rijnland. The study is extensively described by Van Beek and Oenema (2002), Van Beek et al. (2003a), Van Beek et al. (2003b), Van Beek et al. (2004a), Van Beek et al. (2004b), Van den Eertwegh and Van Beek (2004) and Van Schaik et al. (2004). In the study at hand, the experimental results of the DOVE-veen project were used to evaluate whether the SWAP-ANIMO model is capable of realistic simulating nutrient loading of surface water in peat pasture areas.

The Vlietpolder experimental site can be considered as more or less representative for shallow, eutrophic fen peat soils in this part of the Netherlands. Its non-typical properties concern the graded soil surface that resulted in a rather thick mineral top soil midway between the drains, consisting of a thick man-made soil on top of a clayey peat horizon.

1.2 Objective

Main objectives of this study were to investigate whether the SWAP-ANIMO model is applicable for realistic simulating nutrient (N and P) loading of surface waters in a peat land area and to formulate recommendations for improving the model.

Therefore, the model outcome was tested against the measurement results of the DOVE-veen project. Because it is impossible – against reasonable cost – to measure directly nutrient loading in peat areas that are drained by ditches without altering the hydrological conditions (Hendriks, 1993), this testing implied the comparing of simulation results against measured values of (time-series of) relevant rate and state variables.

In order to obtain realistic modelling results, the model needs site-specific input data for as well model parameters as forcing variables (boundaries). Most of these were obtained from the DOVE-veen project. Because this project basically did not focus on evaluation of or simulation with process-based models like SWAP-ANIMO, some essential input parameters were lacking. In order to obtain values for those, extra measurements were conducted. These comprised site-specific soil physical and chemical properties.

Not all model parameters can be measured. To obtain values for these immeasurable parameters, the model was calibrated and validated against measured values of (time-series of) relevant rate and state variables. In this sense, testing of the model implied calibration and validation of the model.

Another objective was to perform some system and scenario analyses with the calibrated model. Most important of these consisted of the main objective of the DOVE projects: evaluation of the contribution of dairy farming to nutrient loading of surface waters. Other model analyses comprised calculation of the magnitude of nutrient loading at the experimental field and evaluation of wetting strategies in order to preserve the peat soil, at that time and at the present time a major issue in the Netherlands.

1.3 Reading guide

In Chapter 2 the SWAP-ANIMO model is described. The main aspects of the model that are relevant to judge the model performance and applicability are dealt with. Chapter 3 deals with the data collection and assessment for model calibration and validation. In Chapter 4 model execution and evaluation are discussed. Results of model calibration and validation are described. System and scenario analyses with the calibrated model are dealt with in Chapter 5. Conclusions and recommendations are given in Chapter 6.

2 Model description

Aim of this study was to evaluate the applicability of the SWAP-ANIMO model for simulating nutrient loading of surface waters in peat land areas on the data from the 'DOVE-veen’ project. Therefore, the combination of the at that time (2004) most recent versions of both sub-models was used. In this chapter, a brief general description of the model is given. For more detailed descriptions, the reader should consult the literature referred to in the text below.

2.1 Modelled system

The system of interest is the peat soil profile within its atmospheric and hydrologic setting at the field scale. Especially the topsoil that will be alternately water saturated and unsaturated is of great importance for decomposition and mineralization of peat, and transformation of nutrients. Yet, also the permanent saturated, pristine peat soil is significant for anaerobic organic matter decomposition and denitrification. Furthermore, this part of the peat soil is relevant for leaching of soluble C-, N- and P-compounds to aquifers and surface waters, as it can contain large quantities of dissolved organic compounds, and ammonium and phosphate in solution and adsorbed to the soil complex (Hendriks, 1993; Van Beek et al., 2004a). Thus, the relevant modelling domain is the total peat soil profile down to the underlying mineral soil.

The internal processes in the peat soil system concern transport and storage of water, heat and solutes, and the relevant (bio)chemical and physical processes of the organic-matter-, C-, N- and P-cycle and their mutual interactions. All processes are subject to boundary conditions, of which the upper boundary at the soil surface is the most important, as it is the most dynamic due to exchange with the atmosphere, plant growth interactions and human activities (Fig. 1). For mass and heat balances, transport and leaching to drains, surface waters and deeper groundwater bodies, the lateral and bottom boundaries are relevant as well. Transport processes in the dynamic top soil and shallow groundwater are predominantly vertical. Drainage and leaching to, and subsurface infiltration from drainage systems are mainly lateral.

The SWAP-ANIMO model is in principle capable of simulating the basic transport and transformation processes in peat soils at the field scale (Fig. 1). It is a process-based model that aims at dynamic simulation of nitrogen and phosphorus leaching to surface waters and groundwater from various soil types, depending on daily weather conditions and a wide range of hydrological settings and land use forms. ANIMO, combined with hydrological model FLOCR instead of SWAP, was used for simulating N and P loading of surface waters from peat soils by Hendriks (1993, 1997b and 2003) and Hendriks et al. (1995 and 2002).

SWAP-ANIMO consists of the soil physical sub-model SWAP for simulating transport and storage of water and heat, and the nutrient sub-model ANIMO for simulation of soluble C-, N- and P-compounds on the basis of water balance terms and soil temperatures provided by SWAP (Fig. 1). The sub-models are run separately.

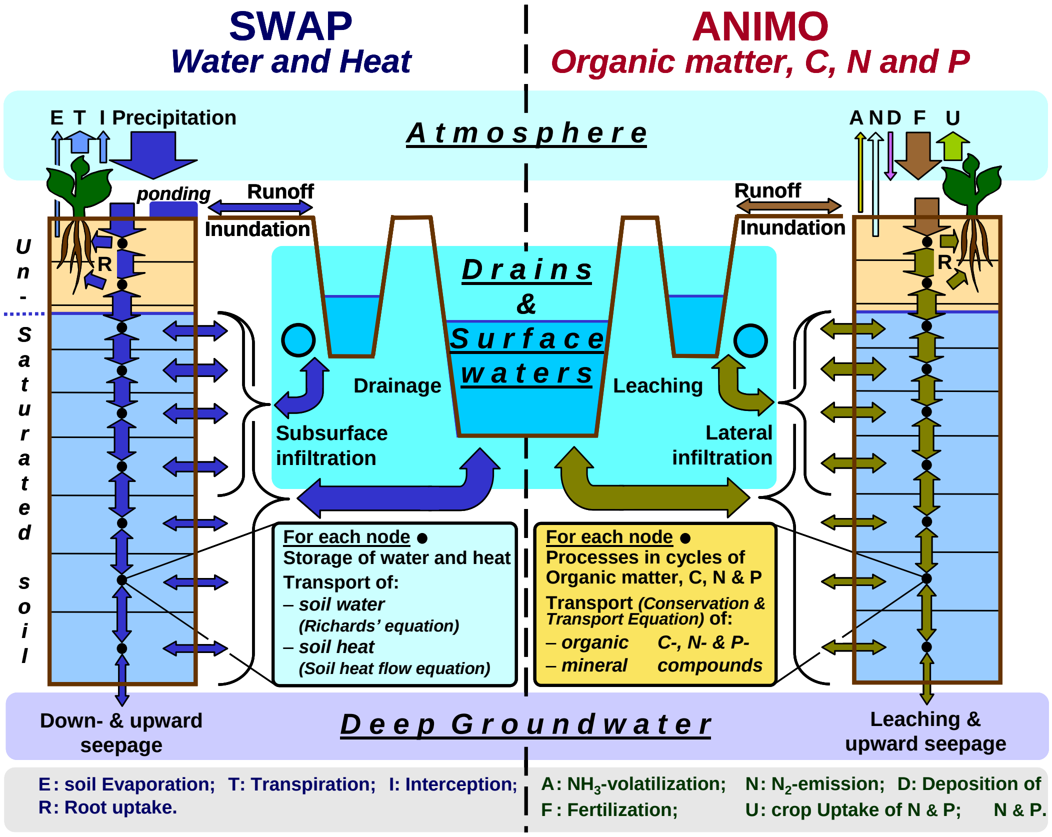

Figure 1 Schematic representation of the peat soil system at the field scale modelled with SWAP-ANIMO. ANIMO simulates processes of the carbon (C), nitrogen (N) and phosphorus (P) cycle, and transport and leaching of soluble C-, N- and P-compounds on the basis of SWAP simulations of water and heat transport and storage. Transport is predominantly vertical in a one-dimensional, unsaturated/saturated soil column; lateral transport to drains and surface water is modelled with a pseudo two-dimensional concept. Boundaries are the atmosphere at the top, pipe and open drains at the lateral side and deep groundwater in the underlying mineral soil at the bottom of the peat column.

Both are one-dimensional models: transport processes are considered in the vertical direction in a one-dimensional soil column. For performing numerical calculations, the vertical soil column is discretized into soil compartments. Discharge to and subsurface infiltration from drains and surface waters are described by a pseudo two-dimensional concept in order to ensure realistic residence times in the saturated compartments.

Major feature of ANIMO for simulating transformation processes in organic soils is that it contains detailed descriptions of the organic-matter/C-, N- and P-cycle and that the latter two cycles are based on the first. Furthermore, it contains a very flexible description of organic matter pools, which allows simulation of organic matter substrates of different qualities within the same soil profile. Another important feature of SWAP-ANIMO is the extensive and flexible description of boundary conditions, which counts especially for the top boundary (Fig. 1). These qualities provide a sound basis for a model that is applicable for analysing and predicting peat decomposition and the related process of nutrient leaching, as determined by water management and land-use.

2.2 SWAP sub-model

SWAP (Soil-Water-Atmosphere-Plant) is a comprehensive physically based model for simulating vertical transport of water, heat and solutes in various, (alternately) unsaturated and saturated soils at the field scale (Kroes et al., 2000; Van Dam et al., 2008). In this study, SWAP version 3.0.3 (Kroes and Van Dam, 2003) was used.

2.2.1 Water flow

Vertical soil water flow is calculated with the Richards' equation (Fig.1), which has a strong physical base:

$$\frac{\partial \theta}{\partial t} = \frac{\partial \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]}{\partial z} - S_{\mathrm{a}}(h) - S_{\mathrm{d}} \qquad (1)$$

where:

θ = volumetric water content ($m^3 \, m^{-3}$);
t = time (d);
K = hydraulic conductivity ($m \, d^{-1}$);
h = soil water pressure head (m);
z = vertical coordinate (m);
S_{a} = soil water extraction rate by roots ($m \, d^{-1}$);
S_{d} = rate of drainage to or infiltration from drains ($m \, d^{-1}$).

SWAP solves Richards' equation integrally for the unsaturated-saturated zone, including possible transient and perched groundwater levels. For numerical solving Eq. (1), an implicit finite difference scheme is adopted, using known relations between θ, K and h. Spatial discretisation is obtained by partitioning the vertical soil column in model compartments of thickness of one centimetre or less (top) up to several decimetres (bottom). For temporal discretisation SWAP uses a dynamic time-step, whose value ranges between 10^{-7} and 0.2 d depending on the system dynamics.

Boundary domains are the atmosphere at the top, open or pipe drains at the lateral sides and deeper groundwater, impermeable layer, unsaturated soil or open air at the bottom (Fig. 1). Top boundary conditions comprise precipitation (rain and/or snow), irrigation, interception, soil evaporation and plant transpiration. The latter is calculated from potential transpiration as related to plant growth status according to Penman-Monteith or reference evapotranspiration with crop factors, and soil moisture status to account for drought or water-logging. All concerning input data are on a daily basis; rain input can be event-based as well.

Lateral side boundary conditions encompass drainage to or subsurface infiltration from multi-level (max. 5) drainage systems including interflow through the topsoil, and surface runoff or inundation. SWAP provides several options for calculation of drainage and infiltration fluxes: drainage equations of Hooghoudt and Ernst, prescribed drainage resistance and tabulated drainage relation. Drainage base can be fixed for pipe drains or dynamic in time as surface water level in open drains. Bottom boundary conditions are Cauchy, Dirichlet or Neumann type conditions.

2.2.2 Heat flow

The soil heat flow equation used in SWAP (Fig. 1) reads:

$$C_{\mathrm{heat}} \frac{\partial T}{\partial t} = \frac{\partial \left(\lambda_{\mathrm{heat}} \frac{\partial T}{\partial z} \right)}{\partial z} \tag{2}$$

where:
T = temperature (ºC);
C_{heat} = soil heat capacity (J m^{-3} $^{\mathrm{o}}\mathrm{C}^{-1}$);
λ_{heat} = soil thermal conductivity (J m^{-1} $^{\mathrm{o}}\mathrm{C}^{-1}$ d^{-1}).

The heat flow equation is solved numerical using an implicit finite difference scheme on the basis of the same spatial and temporal discretisation used for solving Richards' equation. Both C_{heat} and λ_{heat} are calculated from soil texture and moisture content. Top boundary condition is the daily average air temperature, including a simple description for the insulating effect of a snow cover. At the bottom either prescribed temperatures or a zero heat flux can be used as boundary condition.

2.2.3 Model input

Simulation with SWAP requires input of relevant data. These data can be subdivided into the following three groups:

1. initial values of all state variables: these data comprise moisture content, pressure head and soil temperature of each model compartment;
2. values of process parameters: input data that are constant during simulations and that steer the modelled processes. Most important of these are the parameters of the Mualem-Van Genuchten functions (Van Genuchten, 1980) that describe soil water retention and soil unsaturated hydraulic conductivity, drainage resistances, resistance to vertical flow at the bottom of the system, parameters that describe actual soil evaporation and plant transpiration as related to crop growth and potential evapotranspiration, and soil textural data for assessing soil heat capacity and thermal conductivity;
3. forcing variables: values of boundaries, mostly time-series of input data that describe the atmospheric and hydrological setting of the modelled system in time. These time-series of data include precipitation and atmospheric data for calculating potential evapotranspiration for the upper boundary, surface water levels for the lateral boundary and hydraulic heads in the underlying aquifer for the bottom boundary.

2.2.4 Initialisation

Simulation with SWAP requires initialisation of state variables. In this study, these states concern moisture content, pressure head and soil temperature of each model compartment. Several options for initialisation are possible. One of them is using output from a former run to continue a simulation period. Because in general, the state variables respond relatively fast to boundary conditions, equilibrium is reached within several simulation weeks. Therefore, initialisation is a less critical aspect of simulations for SWAP than for ANIMO.

2.2.5 Model output

Model outcome comprehends a wide, user-defined selection of mass balances and time-series of rate and state variables. Relevant rate and state variables are passed on to ANIMO in a binary file. These rate variables are on a daily basis and comprise vertical water fluxes between compartments and boundary fluxes. State variables include groundwater level, possible perched groundwater level and ponding height, and per compartment moisture content, pressure head and temperature. States apply to the end of the day, except for temperature that represents a daily average.

2.3 ANIMO sub-model

ANIMO (Agricultural Nutrient Model) is a process-oriented model that aims to quantify the relation between fertilisation level, soil management and the leaching of nutrients N and P to groundwater and surface water systems for a wide range of soil types and different hydrological conditions. In this study, version 4.0 (Groenendijk et al., 2005; Renaud et al., 2005) was used.

2.3.1 Conservation and transport equation

Vertical solute transport and mass conservation are calculated with the Conservation and Transport Equation (*CTE*-equation) which in its general form reads (Groenendijk et al., 2005):

$$\frac{\partial(\theta c)}{\partial t} + \rho_{\mathrm{d}} \frac{\partial X_{\mathrm{e}}}{\partial t} + \rho_{\mathrm{d}} \frac{\partial X_{\mathrm{n}}}{\partial t} + \rho_{\mathrm{d}} \frac{\partial X_{\mathrm{p}}}{\partial t} = -\frac{\partial J_{\mathrm{s}}}{\partial z} + R_{\mathrm{p}} - R_{\mathrm{d}} - R_{\mathrm{u}} - R_{\mathrm{l}} \qquad (3)$$

where:

c = mass concentration in liquid phase (kg m^{-3});

X_{e} = content adsorbed to the solid phase in equilibrium with c (kg kg^{-1});

X_{n} = content of non-equilibrium sorption phase (kg kg^{-3});

X_{p} = content of the substance involved in precipitation reaction (kg kg^{-3});

ρ_{d} = dry bulk density (kg m^{-3});

J_{s} = vertical solute flux (kg m^{-2} d^{-1});

R_{p} = zero-order production source term (kg m^{-3} d^{-1});

R_{d} = first-order decomposition (transformation) sink term (kg m^{-3} d^{-1});

R_u = plant uptake sink term (kg m^{-3} d^{-1});
R_l = sink term for leaching to drains (kg m^{-3} d^{-1}).

ANIMO solves the *CTE*-equation numerically in an implicit finite differences scheme with a semi-analytical approach (Groenendijk et al., 2005). This approach allows large constant time-steps of 1-10 d (1 d in this study). Physical dispersion during vertical convective solute transport is accounted for by numerical dispersion. Realistic dispersion can be obtained by choosing appropriate values for the thickness of the model compartments (Groenendijk et al., 2005). Therefore, ANIMO utilises a vertical discretisation that is based on the SWAP vertical discretisation, but that is less refined in the top soil, with top compartments of 5-10 cm thick. Water balance data necessary for solving the *CTE*-equation are provided by SWAP on a daily basis. Boundaries are the same as the three SWAP boundary domains (Fig. 1).

2.3.2 Organic-matter/carbon, nitrogen and phosphorus cycle

Accumulation, transformation and transport terms in Eq. (3) are processes of the organic-matter/C-, N- and P-cycle. Organic-matter- and C-cycle are one in ANIMO, as organic matter has a fixed C content. The C-cycle is the main cycle on which transformation processes of the N- and P-cycle depend in the model. This enables simulation of leaching of dissolved organic N- and P-compounds, a major source of N- and P-loading of surface waters in peat areas (Hendriks, 1991 and 1993).

2.3.2.1 Carbon cycle

Four organic substances are distinguished (Fig. 2): 1. *fresh organic matter*, 2. *root exudates*, 3. *dissolved organic matter* and 4. *humus and living biomass*. The latter pool results from transformations of all organic substances. *Fresh organic matter* allows additions to the soil of various kinds of organic materials (up to 50; e.g. organic manure, root and crop residues). Qualities of these materials are defined by their composition of different organic classes (from 1 up to 15). These classes are characterised by user-defined values for first-order decomposition rate, assimilation efficiency and N- and P-content. Hendriks (1993) defined the bulk organic matter of peat soils as *fresh organic matter* composed of two different organic classes: a relatively fast decomposing N-rich and a slow decomposing N-poor class. This approach is generally adopted in ANIMO simulations for peat soils (Fig. 2). Qualities of the three other organic substances are defined by the user as well.

A user-defined fraction of *fresh organic matter* being decomposed, passes the soluble phase and is added to the *dissolved organic matter* pool (Fig. 2). Organic matter mineralization results into CO_2 evolution, depending on assimilation efficiency. Organic matter decomposition occurs under aerobic conditions with oxygen as electron acceptor and under anaerobic conditions with nitrate – and implicitly nitrous oxide – as electron acceptor. In the latter case, decomposition rate constants are decreased with a user-defined factor (standard: 2). Boundary conditions at the top are addition of *fresh organic matter* as organic fertilisers and crop residues, and – implicitly – emission of CO_2. Formation of crop biomass is not part of the soil C-cycle. Lateral

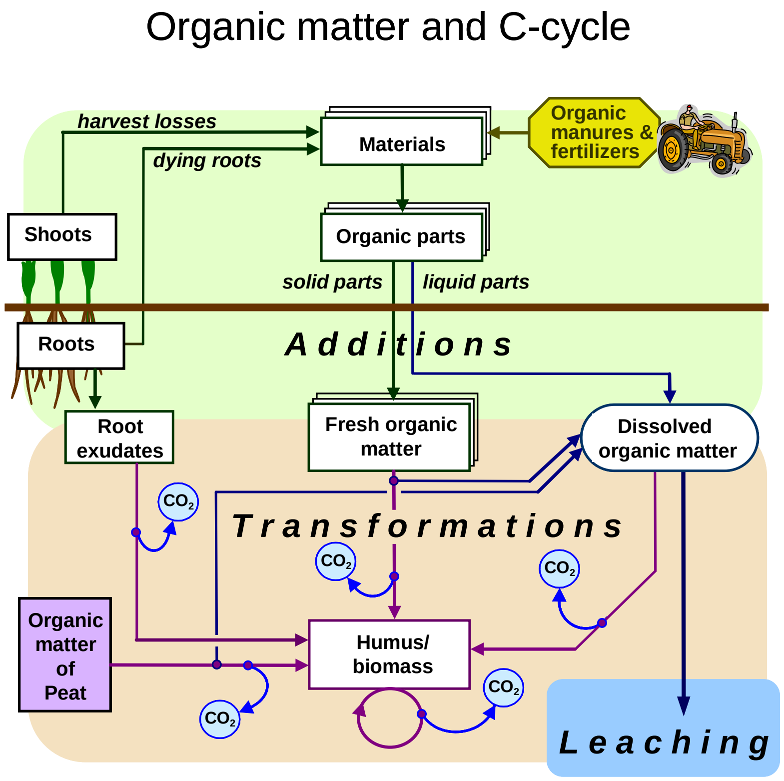

Fig. 2. Relational diagram of the organic-matter/carbon cycle in ANIMO, with transformation, accumulation and transport processes.

side and bottom boundary conditions concern leaching and infiltration of DOM (dissolved organic matter) to and from drains and deeper groundwater.

2.3.2.2 Nitrogen cycle

Transformation processes of the N-cycle in ANIMO encompass decomposition of solid organic-N into DON (dissolved organic-N), mineralization of organic-N into ammonium and reversely immobilisation, nitrification of ammonium into nitrate and denitrification of nitrate into gaseous nitrogen (Fig. 3). Decomposition and mineralization concern the same organic matter pools defined in the C-cycle; their rates are determined by the rate of organic matter decomposition. N-mineralization depends on assimilation efficiency and N-content of organic substance concerned, and on N-content of biomass/humus pool. Substrate organic-N contents too low for mineralization will result in immobilisation of ammonium. Adsorbed ammonium is in equilibrium with ammonium in the liquid phase, which is described with a linear sorption isotherm. Boundary conditions are: at the top, addition of organic- and mineral-N containing materials (e.g. fertilisers), dry and wet atmospheric deposition of ammonium and nitrate, gaseous nitrogen emission, ammonium volatilisation and crop uptake of ammonium and nitrate. At the lateral side and bottom boundary, conditions are leaching and infiltration of DON, ammonium and nitrate to and from drains and deeper groundwater.

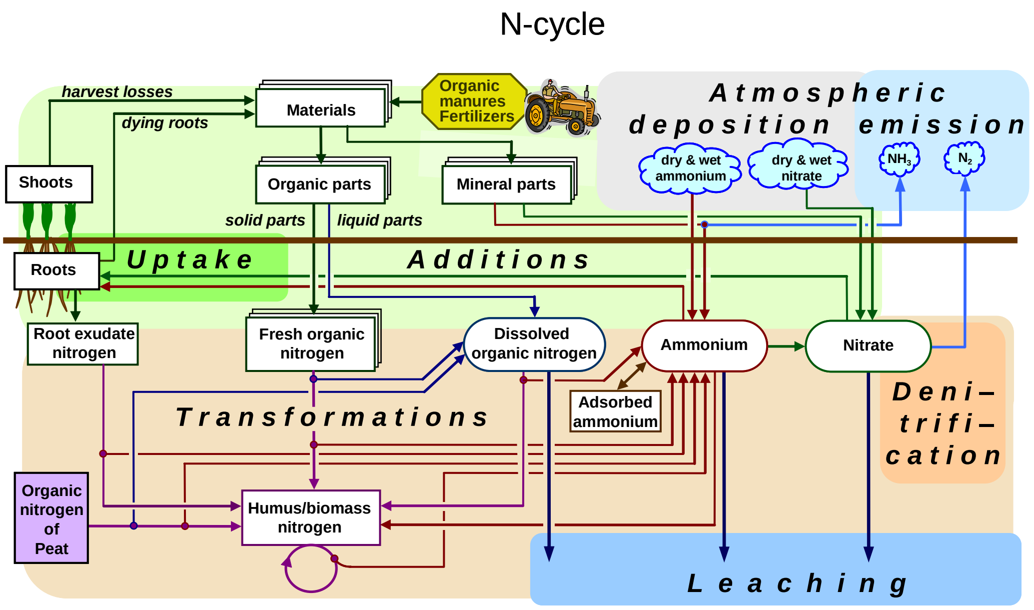

Fig. 3. Relational diagram of the nitrogen cycle in ANIMO, with transformation, accumulation and transport processes.

2.3.2.3 Phosphorus cycle

Transformation processes of the P-cycle in ANIMO comprise decomposition of solid organic-P into DOP (dissolved organic-P), mineralization of organic-P into inorganic phosphate and reversely immobilisation (Fig. 4). Descriptions of these processes are similar to descriptions for N. Accumulation of inorganic P concerns the equilibrium processes non-kinetic sorption (ad- and desorption) and chemical precipitation, and non-equilibrium process kinetic sorption. Equilibrium sorption is described with the Langmuir equation and kinetic sorption with the Freundlich equation for three separate sorption sites. Adsorption potential depends on the aluminium plus iron content of the soil, which is a good measure for peat soils as well (Schoumans, 1999). Precipitation of P is described as an instantaneous reaction with a pH depending equilibrium concentration. Effects of redox processes on phosphorus sorption due to alternating conditions of oxidation and reduction are not modelled explicitly in the model, but implicitly by choosing the right values for relevant steering parameters. Boundary conditions at the top are addition of organic- and mineral-P containing materials, and wet atmospheric deposition and crop uptake of phosphate. At the lateral side and bottom boundary, conditions are leaching and infiltration of DOP and phosphate to and from drains and deeper groundwater.

2.3.2.4 Rate response functions

In ANIMO, transformation processes in the soil are affected by the soil environmental factors aeration, moisture content, temperature and acidity (pH). The effect of each factor is described by rate response functions. Actual first order rate constants are obtained by multiplication of the potential rate constants with all response functions. Response functions for moisture and pH are fixed, while functions for aeration and temperature are described with user-defined parameters. In

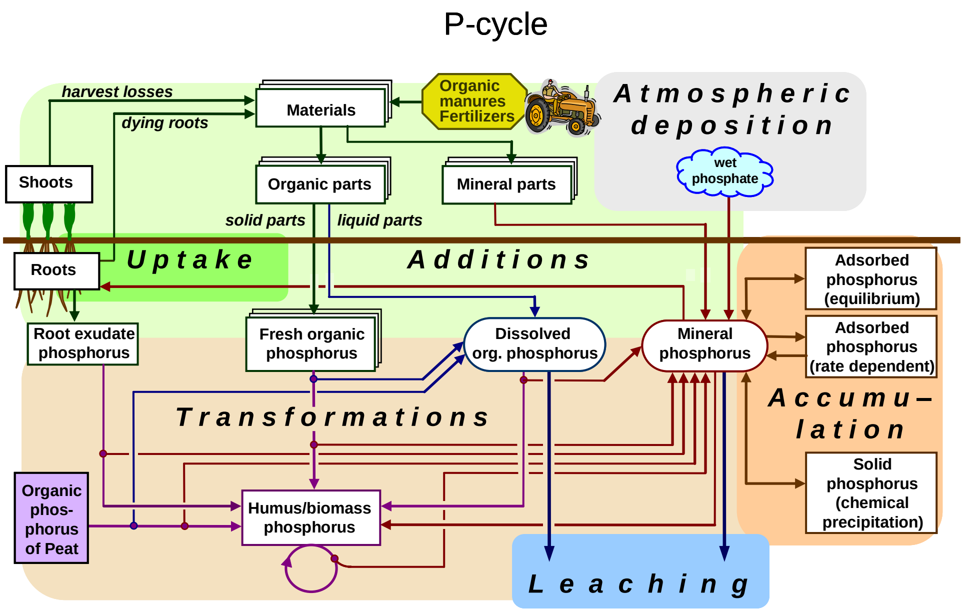

Fig. 4. Relational diagram of the phosphorus cycle in ANIMO, with transformation, accumulation and transport processes.

case of sub-optimal aeration, a partial anaerobiosis fraction is determined on the basis of calculations of oxygen diffusion in the soil gaseous phase and in soil aggregates. Oxygen diffusion coefficients are described with two user defined parameters per soil horizon. Temperature response is described with the Arrhenius equation, where the molecular activation energy is an input parameter for each soil horizon.

2.3.3 Model input

ANIMO requires a substantial amount of input data. Similar to the SWAP input data these data can be subdivided into three groups:

1. initial values of all state variables: these data comprise for all soil compartments concentration of the considered C, N and P compounds in solution, amounts of ammonium and phosphate sorped to the soil complex and amounts of organic matter per organic class;
2. values of process parameters: these data concern in general rate constants, properties of the organic classes like N and P content, soil chemical properties like pH and aluminium and iron content, parameters that steer the rate response functions and parameters that influence nutrient uptake by crops;
3. forcing variables: values of boundaries as time-series of atmospheric deposition of N and P compounds and of application of fertilisers for the upper boundary, concentrations of all dissolved C, N and P compounds in surface water for the lateral boundary and concentrations of these compounds in upward seepage water for the bottom boundary.

Besides these input data, ANIMO requires input data concerning water flow and balance provided by a model like SWAP. These data comprise rates and states as mentioned in section 2.2.5.

2.3.4 Initialisation

Initialisation of state variables is a critical aspect of ANIMO simulations. Due to the relative slow transformation and accumulation processes, the initial values for amounts of organic matter in different pools and for ammonium and phosphate content of the soil – adsorbed and in solution – have a major effect on final simulation results. Therefore, mostly a pre-run of several (usually 4-5) decades, the so-called ‘historical run’, is executed with data on historical weather, land-use and fertilisation. Model results of this historical run are used as input for the intended model runs like calibration/validation or scenario studies. Furthermore, they allow calibration of the initial values of the historical run against measured field data.

When organic matter of peat is decomposed, solid material disappears from the soil profile and the thickness of soil compartments and consequently model compartments decreases. In the model, this is accounted for by updating the soil profile at times that in reality drainage level is adjusted to soil surface subsidence (once in 10-15 years). The updating is carried out by a separate sub-model ‘PEATADDIT’. The ANIMO output file ‘Initial.out’, that contains all state variables like the amount of organic matter in all pools and classes per compartment, is updated for the original amount of organic matter in each compartment. PEATADDIT supplies as much organic matter from the underlying compartment as is needed for to reach the initial amount of the compartment. The composition of the supplied organic matter is that of the organic matter of the underlying compartment. In this way, pristine peat from the saturated zone is moved up to the soil surface, in order to simulate the moving down of the soil surface to the saturated zone with pristine peat.

2.3.5 Model output

The model generates a comprehensive, user-defined selection of material balances and time-series of rate and state variables. Material balances can be produced for up to ten balance sub-profiles and for a user-defined time interval. Selected rates and states are generated per compartment and for every time-step.

3 Data collection and assessment

The objective of this study was to investigate whether the SWAP-ANIMO model is capable of simulating nutrient (N and P) loading of surface water in peat land areas. For model testing (calibration and validation), the model outcome was compared to (time-series of) measured values of relevant rate and state variables. In order to obtain realistic modelling results, the model needs site-specific input data for as well model parameters as forcing variables (boundaries) (Section 2.2.3). In this Chapter, the collection and assessment of these input data and the data for model calibration and validation are described. Section 3.1 gives a description of the Vlietpolder and the experimental site. Section 3.2 deals with data for SWAP and Section 3.3 with data for ANIMO.

3.1 Site description

Vlietpolder

The experimental site was situated in the 'Vlietpolder' near Hoogmade, between Alphen aan de Rijn and Leiden, in the western part of The Netherlands (Figure 5). The Vlietpolder is about 200 hectares in size and its surface elevation is around two metres below mean sea level (Van Beek et al., 2004a). It is a typical Dutch fen peat pasture polder: 10% of the surface area is water and for over 90% of the land area is used for intensive dairy farming (Van den Eertwegh and Van Beek, 2004).

The soils in the Vlietpolder consist for 72% of peat soils and for 28% of riverine clay soils (Leenders, 1999). The peat soils are mainly eutrophic, woody peats classified as Terric Histosols (FAO, 1998), and according to the Dutch soil classification system, as 'Koopveengronden op bosveen' (Leenders, 1999). The peat soils in the Vlietpolder are mostly covered with a so called 'toemaakdek', a man-made A horizon that originnates from long-term application of a mixture of manure, dredging sludge, household waste from the surrounding cities (e.g. Amsterdam, Utrecht and Leiden), and sometimes dune sand (Lexmond et al., 1987). On 'Koopveengronden' these topsoils overly the clayey peat layer that originally formed the natural topsoil (Leenders, 1999).

The thickness of the peat layer is about three metres. It overlies a 6-9 m thick layer of mainly marine clay deposits on top of a sand aquifer (Leenders, 1999). The vertical flow resistance of the clay aquitard is very high: 5,000-10,000 days (Boswinkel and Cornelissen, 1980). Consequently, vertical water flow between the peat layer and aquifer, either as downward or upward seepage, is only small.

The peat soils in the polder are poorly drained. The dominant groundwater class (Gt) is IIa, implying a mean highest groundwater table less than 0.25 m below soil surface (m bss) and a mean lowest groundwater table between 0.50 and 0.80 m bss (Leenders, 1999). The soils are drained by a system of ditches at a distance of about 40-80 m. Ditches are 3-8 m wide. The polder is a pumped drainage area with target levels of 0.58 m bss for the winter half-year and 0.48 m bss for the summer half-year. The pumping station is located in the north and the water inlet in the south.

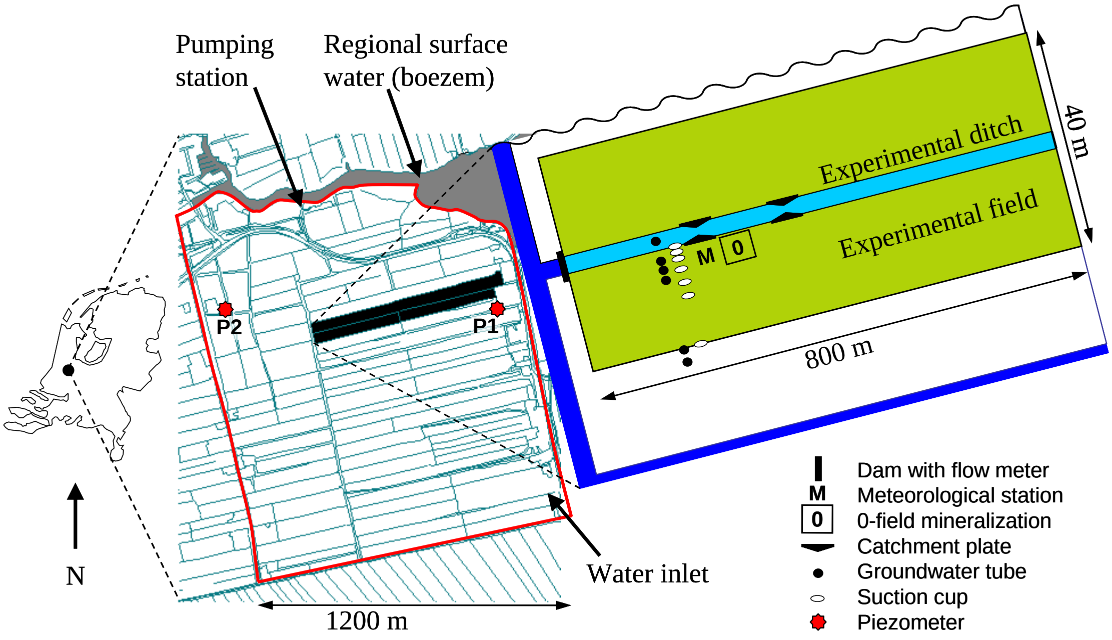

Figure 5 Location of the experimental site and setup in the Vlietpolder (after: Van Beek et al., 2004a; Van den Eertwegh and Van Beek, 2004). Not on scale.

Experimental site

For the 'DOVE-veen' research project a representative experimental site on peat soil was selected (Van Beek et al., 2004a; Van den Eertwegh and Van Beek, 2004). The site existed of the halves of two adjacent grassland fields that drained on a dead-end ditch, which itself drained on a main watercourse (Fig. 5). The dimensions of this experimental ditch were approximately 800 m long, 3-5 m wide and 0.7-0.8 m deep. The two fields were about 40 m wide so that the catchment area of the ditch amounted to approximately 3.2 ha. Occasionally, the farmer used the ditch at the dead-end for flushing a pond. The site can be considered as more or less representative for shallow, eutrophic fen peat soils in this part of the Netherlands.

The two fields were part of a dairy farm and were used for intensive grazing and hay making. They were graded to enhance surface runoff: part of the topsoil was dragged from the sides of the ditch towards the middle of the field, resulting in a convex surface with a difference in height between field sides and middle of almost 0.60 m. This is in general not a common situation and thus made the site less representative.

The southern part of the experimental side was used for conducting the field experiments and measurements (Fig. 5). A setup was installed for monitoring ground-water levels (tubes with filters), solutes concentrations in soil moisture and water (chemical-inert suction cups) and meteorologic parameters (Van Beek et al., 2004a; Van den Eertwegh and Van Beek, 2004; Van Schaik et al., 2004). In the experimental ditch, incoming and outgoing flow rates were measured and water samples were taken. Experiments were carried out in order to estimate nitrogen mineralization and denitrification rates in the peat soil, and denitrification rates in the ditch sediment and water. Within the transects of groundwater tubes and suction cups, soil samples were taken for determining physical and chemical properties of the soil. Measurements were performed by Alterra and Hoogheemraadschap (Waterboard) Rijnland. Most measurements took place in the period January 2000 until March 2003. Measurement methods and results were stored in a database (Van Schaik et al., 2004). All relevant measurements for this study are discussed in Sections 3.2 and 3.3.

Table 1 gives the distinguished soil horizons according to Leenders (1999) and some basic soil properties. The depths of the horizons refer to the average soil surface elevation of 2.09 m below mean sea level (NAP). A distinction was made between two sub-horizons in the 'Toemaakdek' on the basis of a slight difference in organic matter content. Bottom boundary of the peat layer amounted to 2.98 m bss.

Table 1 Soil horizons, texture, dry bulk density and pH. Horizon depths apply to the average soil surface elevation of -2.09 m + NAP (Dutch mean sea level). Values are averages of samples from middle and side (2 m from ditch) of the experimental field. % is by mass of solids (organic matter) or mineral parts (rest).

Horizon description (after Leenders, 1999)	Depth (m)	Organic matter (%)	Clay 0–2 μm (%)	Silt 2–50 μm (%)	Sand > 50 μm (%)	Dry bulk density (kg m^{-3})	pH–H_2O (–)
1Aap Toemaakdek 1	0.00–0.20	19.2	19.3	10.8	69.9	860	4.9
1Aap Toemaakdek 2	0.20–0.28	18.1	20.4	13.8	65.8	934	4.9
1AC Clayey peat	0.28–0.48	34.1	25.5	52.8	21.7	633	4.6
2Cu Peat, oxidised	0.48–0.78	77.7	62.7	37.3	0.0	195	5.3
2Cr Peat, reduced	0.78–2.98	76.3	59.0	41.0	0.0	155	5.4

3.2 Data for SWAP

Material and methods of data collection and assessment for SWAP are discussed in Section 3.2.1 and results are presented in Section 3.2.2. In both Sections, a distinction is made between input data and measured rates and states used for model calibration and validation. Because, compared to ANIMO, SWAP needs only a rather limited number of input data, most relevant input data are dealt with. These do not include trivial data like timing dates of simulation periods, file names, switches etc.

3.2.1 Materials and methods

3.2.1.1 Input data

Input data are categorised in the three groups distinguished in Section 2.2.3: 1. initial values of states, 2. process parameters and 3. boundaries (forcing variables).

1. Initial values of states

SWAP needs initial values of soil moisture and temperature for each model compartment. In this study, the option was used for calculating initial moisture content assuming hydrostatic equilibrium with a prescribed initial groundwater level (Table 2). This initial groundwater level was derived from the measurements of groundwater levels (Section 3.2.1.2). Initial soil temperatures must be put in as a function of depth.

Table 2 State variables of SWAP that require an initial value and the methods used to obtain them

SWAP name	Description	Requirement	Method
GWLI	Initial groundwater level	Single value	Field measurement
TSOIL	Soil temperature	Function of depth	Field measurem. & estimation

SWAP interpolates linear between given values. For the top compartment the measured daily average air temperature at the start of the simulations (January 1th 2000) was used (see this Section, ***3. Boundaries***). For deeper layers the mean annual air temperature in The Netherlands of 10 °C was taken.

2. Process parameters

The relevant process parameters that SWAP requires are listed in Table 3. SWAP needs data on soil physical properties: 1. Van Genuchten parameters to express the soil hydraulic characteristics i.e. water retention and unsaturated conductivity curves, and 2. soil texture parameters for assessing soil heat capacity and thermal conductivity. For determining these soil properties, samples were taken at different depths from two soil pits, both positioned close to the transect of groundwater tubes (Fig. 5). One was located in the middle of the field and the other at two meters from the ditch. For obtaining Van Genuchten parameters and saturated hydraulic conductivity, undisturbed samples were taken with 0.08 m high and 0.103 m wide, and with 0.10 m high and 0.20 m wide PVC cylinders, respectively. In each pit, two duplicate samples with both cylinders were taken at four depth intervals: 0.10-0.20, 0.30-0.40, 0.60-0.70 and 0.90-1.00 m below local soil surface in the pit in the middle, and at depth intervals of 0.10-0.20, 0.30-0.40, 0.50-0.60 and 0.70-0.80 m below local soil surface in the pit near the ditch. From the same depths, disturbed samples were taken for analysis of soil texture and soil chemical properties. Difference in height of the soil surface between the two sample locations was 0.29 m. On the basis of this height difference, soil texture and visual observation in the field, the samples of the two pits were attributed to the five distinguished soil horizons of Table 1 (Table 4).

Soil water retention and unsaturated hydraulic conductivity curves were measured simultaneously using the evaporation method of Wind (Stolte, 1997). Both characteristics were obtained by fitting the Van Genuchten functions (Van Genuchten, 1980) to the measured data using the RETC optimization program (Van Genuchten et al., 1991). Saturated hydraulic conductivity was measured with the constant head method (Stolte, 1997). On all samples of both measurements, dry bulk density was determined.

Soil texture was determined by Blgg Oosterbeek (Bedrijfslaboratorium voor grond- en gewasonderzoek: laboratory for soil and crop research) and additional organic matter content by Alterra. Organic matter was determined by loss on ignition with a correction for clay content of 7% of clay content as mass fraction of solids (general assumption that clay contains 7 mass-% crystal water). Mineral parts were measured with standard methods by Blgg Oosterbeek.

Because no reliable results of runoff measurements were available (Section 3.2.1.2), maximum ponding height PONDMX, threshold for generation of runoff, was estimated on the basis of visual observation and expert judgment. For the other two runoff parameters, RSRO and RSROEXP, the default values were taken.

Table 3 Relevant process parameters of SWAP and the methods used to obtain values for them

SWAP name	Description	Requirement	Method
Soil properties parameters			
1. Van Genuchten parameters			
ORES	Residual volumetric water content	Per soil horizon	Lab measurement
OSAT	Saturated volumetric water content	Per soil horizon	Lab measurement
ALFA	Shape parameter alfa of main drying curve	Per soil horizon	Lab measurement
NPAR	Shape parameter n	Per soil horizon	Lab measurement
KSAT	Saturated hydraulic conductivity	Per soil horizon	Lab measurement
LEXP	Exponent in hydraulic conductivity funct.	Per soil horizon	Lab measurement
2. Soil texture			
PSAND	Percentage sand of mineral parts	Per soil horizon	Lab measurement
PSILT	Percentage silt of mineral parts	Per soil horizon	Lab measurement
PCLAY	Percentage clay of mineral parts	Per soil horizon	Lab measurement
ORGMAT	Percentage organic matter of dry soil	Per soil horizon	Lab measurement
Drainage parameters			
PONDMX	Maximum thickness ponding water layer	Single value	Estimation
RSRO	Drainage resistance of surface runoff	Single value	Default
RSROEXP	Exponent in surface runoff relation	Single value	Default
NRLEVS	Number of drainage levels	Single value	**Calibration**
DRARES1	Drainage resistance level 1 (ditch)	Single value	**Calibration**
INFRES1	Infiltration resistance level 1 (ditch)	Single value	**Calibration**
L1	Drain spacing level 1 (ditch)	Single value	Field measurement
ZBOTDR1	Level of drain bottom level 1 (ditch)	Single value	Field measurement
ZBOTDR2	Level of bottom interflow layer	Single value	Field measurement
COFINTFLB	Coefficient for interflow relation	Single value	**Calibration**
EXPINTFLB	Exponent for interflow relation	Single value	Default
COFANI	Anisotropy factor: $K_{sat,Hor} / K_{sat,Vert}$	Per soil horizon	**Calibration**
Bottom boundary parameters			
SHAPE	Shape factor for average groundw. level	Single value	Default
HDRAIN	Mean drainage base	Single value	Dummy
RIMLAY	Vertical flow resistance of aquitard	Single value	**Calibration**
Crop parameters (see Appendix 1 for explanation)			
HLIM1	Limiting pressure head for water uptake: 1	Single value	Expert judgement
HLIM2U	Limiting pres. head for water uptake: 2U	Single value	Expert judgement
HLIM2L	Limiting pres. head for water uptake: 2L	Single value	Expert judgement
RD	Rooting depth	Single value	Field measurement

For simulating drainage to and infiltration from a ditch with known, fluctuating water level at the field scale, SWAP option 'Basic drainage, option multi-level drainage and infiltration with fixed resistances and imposed drainage levels' is the most appropriate.

Table 4 Attribution to the distinguished soil horizons (Table 1) of soil samples taken at different depth in the pits in the middle and at the side (2 m from ditch) of the experimental field

Soil horizons		Soil samples			
Average soil surface soil surface: -2.09 m + NAP		Pit in middle soil surface: –1.97 m + NAP		Pit near ditch soil surface: –2.26 m + NAP	
description	depth (m)	number	depth (m)	number	depth (m)
Toemaakdek 1	0.00–0.20	1	0.10–0.20 *(0.00-0.10)*	–	–
Toemaakdek 2	0.20–0.28	2	0.30–0.40 *(0.20-0.30)*	–	–
Clayey peat	0.28–0.48	–	–	1	0.10–0.20 *(0.29-0.39)*
Peat, oxidised	0.48–0.78	3	0.60–0.70 *(0.50-0.60)*	2	0.30–0.40 *(0.49-0.59)*
				3	0.50–0.60 *(0.69-0.79)*
Peat, reduced	0.78–2.98	4	0.90–1.00 *(0.80-0.90)*	4	0.70–0.80 *(0.89-0.99)*

(0.20-0.30) = soil sample depth in m below average soil surface

Drainage and infiltration resistances are generally calibration parameters as they cannot be measured directly. SWAP was calibrated against measured groundwater levels and drain discharges (Section 4.2.1). During the calibration it became clear from the pattern of groundwater levels above the level of the bottom of the topsoil (Toemaakdek) that, besides surface runoff and subsurface drainage to the ditch, another shallow level of drainage was relevant: lateral interflow through the top part of the soil. On the basis of measured saturated conductivities (Table 8) that show a clear decrease below the topsoil, the interflow layer was taken equal to the topsoil layer, implying that the level of the bottom of the interflow layer, ZBOTDR2, was equal to the depth of the topsoil. A linear relationship between interflow and groundwater level above ZBOTDR2 was assumed, which implies a value of one (default) for exponent EXPINTFLB. Calibration yielded values for the ditch drainage resistance and the interflow coefficient. Ditch spacing and ditch bottom level were measured in the field.

In the pseudo two-dimensional concept of SWAP for calculating residence and travel time distribution, anisotropy factors COFANI determine the distribution of drainage fluxes over the compartments in the saturated zone. COFANI's were calibrated by comparing simulated and measured Cl loads discharged from the ditch (Section 4.2.1).

As time-series of hydraulic heads were available, the bottom boundary option 'calculate bottom flux from hydraulic head in deep aquifer' was chosen. In this option the vertical flow resistance of the aquitard, RIMLAY, is required. This parameter was calibrated (Section 4.2.1).

For grass crop parameters, default values of the example case Ruurlo (grass on sandy soil; case provided on the website) were taken (Appendix 1). With exception of the limiting pressure heads for water uptake HLIM1, HLIM2U and HLIM2L. Experience has pointed out that grass on peat soil can take up water under very wet conditions. Therefore, higher values than default were used for these limiting pressure heads.

3. Boundaries (forcing variables)

Forcing variables refer to the three boundaries of the modelled system: top, lateral and bottom boundary (Fig. 1). At the top boundary, forcing variables comprise precipitation, plant interception and transpiration, and soil evaporation (irrigation was not applied), and daily average air temperature for calculating soil temperature. For calculation of potential evapotranspiration, the 'Penman-Monteith' option was chosen as this provides more realistic results for Dutch conditions then the 'reference evapotranspiration according to Makkink' option (Duineveld, 2008). The Penman-Monteith option requires time-series of the variables listed in Table 5. All of these were measured continuously with a frequency of 30 minutes at the meteorological station (Fig. 5) in the period from July 23rd 1999 through April 28th 2003, using a mobile meteorological measuring mast of Wageningen University (Moors and Stricker, 1988). Precipitation was measured using a tipping bucket. From all these data, daily values for the meteorological variables of Table 5 were calculated. In order to simulate the fast process of runoff realistic, the option was chosen to use daily precipitation duration for estimating precipitation intensity. As SWAP requires daily values, missing values were filled up by using statistical models derived from the measured data and data of other meteorological stations (Appendix 2).

At the lateral boundary, the forcing variable is the drainage base in the form of the fluctuating ditch water level (Table 5). Bi-weekly readings were performed with a water level gauge. Gaps in measurements were filled by using target levels.

At the bottom boundary, the forcing variable is the hydraulic head in the first aquifer at a depth of about 10 m bss (Table 5). Observations of two piezometers with filter in the aquifer were available: P1 with continuous and P2 with bi-weekly measurements (Fig. 5). Correlation between the two sets of results was very good, with an average difference in head of 0.42 m (P1 lower). Therefore, the results of P1 were used to calculate daily averages with a correction of + 0.21 m for the position of the experimental field half-way between the locations of the two piezometers.

Table 5 Relevant forcing variables of boundaries of SWAP and the methods used to obtain values for them

SWAP name	Description	Requirement	Method
Top boundary			
LAT	Latitude of meteo station	Single value	Map
ALT	Altitude of meteo station	Single value	Map
ALTW	Altitude of wind speed measurement	Single value	Field measurement
RAD	Solar radiation	Per day	Field measurement
Tmin	Minimum air temperature	Per day	Field measurement
Tmax	Maximum air temperature	Per day	Field measurement
HUM	Air humidity	Per day	Field measurement
WIND	Wind speed	Per day	Field measurement
RAIN	Precipitation amount	Per day	Field measurement
WET	Precipitation duration	Per day	Field measurement
Lateral boundary			
LEVEL1	Water level in ditch (drainage level1)	Function of time	Field measurement
Bottom boundary			
HAQUIF	Hydraulic head in underlying aquifer	Function of time	Field measurement

3.2.1.2 Data for model calibration and validation

Data for model calibration and validation of SWAP comprise measured time-series of rate and state variables that characterise the reactions of the modelled system to changes in the forcing variables and that are output of SWAP. For the drained peat soil system the rate variables are drainage (incl. surface runoff and interflow) and infiltration (subsurface irrigation), distribution with depth of drainage and infiltration fluxes, and seepage. The state variables are groundwater level, moisture content and/or pressure head at various depths. Of these, surface runoff, groundwater level and moisture content were measured. The latter with TDR (time domain reflectometry), but the results turned out to be unrealistic and thus unreliable. Consequently, they were not used.

In peat soils, drainage to and infiltration from the ditch, and the distribution with depth of the corresponding fluxes, can not be measured directly without disturbing the hydrological conditions. Therefore, flux densities were derived from measurements of ditch discharge and recharge, by relating measured flow rates to the catchment area of the ditch. Distribution with depth of drainage and infiltration fluxes was calibrated by using the Cl concentration gradient in the soil that inclines with depth, for calculating Cl loads in drainage water and comparing these to measured Cl loads discharged from the ditch (Section 4.2.1).

Table 6 summarises the measured rates and states and their role in the calibration and validation process in terms of the relevant object parameter(s). Groundwater level was measured along a transect of six observation wells (groundwater tubes) perpendicular to the ditch at distances of -2 (middle ditch), 2, 3, 5.5, 21 and 23 m of the ditch (Fig. 5). Length of tubes and filters were about 1.5 m and 1 m, respectively, and top of tubes was at about soil surface level. In this way, measurement of *phreatic* groundwater level was ensured. Groundwater levels were recorded bi-weekly in the period September 2000 until April 2003. The levels of the two tubes in the middle of the field correlated very well; the average of the two was used to represent the phreatic groundwater level dynamics midway between the ditches. The levels of the other tubes were used to calculate a shape factor for converting the convex or concave shaped groundwater table between the ditches into a field average groundwater table (Appendix 3). For comparing observed with simulated groundwater levels, this conversion is necessary, because up-scaling of the 1-D-soil column of SWAP to the field scale implies simulation of a groundwater level that represents a flat, field average groundwater table.

Table 6 Target variables, as measured (time-series of) rates or states, for calibration and validation of SWAP

Target rate or state variable	Function	Object parameter	Method
Groundwater level	Calibration	Drainage parameters	Field measurement
Chloride concentrations in ditch and soil water	Calibration	COFANI	Field measurement
Downward seepage	Calibration	RIMLAY	ICW, 1976
Ditch discharge & recharge	Validation	Drainage parameters	Field measurement
Surface runoff	Validation	Checking lower limit of surface runoff	Estimation by field measurement

At 190 m East of the transect, in the middle of the experimental field, a phreatic groundwater tube was measured continuously. Correlation between the levels of this tube and the levels of the tubes in the transect was weak, and consequently these measurements were not used.

Ditch discharge and recharge were measured with an electromagnetic flow meter (Magmaster) in the dam (Fig. 5). Average flow rate was stored every 5 minutes in a data logger. Analyses of the results, in cooperation with Waterboard Rijnland, pointed out that only the registration of a four month period of discharge was reliable (December 2001 until April 2002). Registered recharge and discharge in summer half-year were generally unrealistic, showing very low recharge or even discharge when the water balance in the model indicated the need of substantial recharge of water. This was due partly to flushing of a pond at the dead end of the ditch by the farmer and partly to problems with the flow meter, which is probably not suitable for surface water containing floating organic matter (A. van den Toorn pers. com., 2004). Modelling of the experimental field with Hydrus-2D revealed the same inability to simulate the result of the discharge and recharge registration, except for the mentionned four-month-discharge-period (Fig. 12 in: Droogers et al., 2005). Consequently, only this period was used for validation of discharge simulations and no data were available for validating the model for a situation of infiltration from the ditch into the soil. For comparison with model results, measured discharge was converted into drainage flux densities by dividing by the catchment area. As the exact area was not known, a maximum and a minimum area were calculated from the estimated dimensions resulting in a range with lower and upper limit of 3.0 and 3.4 ha. Using this range resulted in a range for the flux densities that was used for validation (Section 4.2.1.3).

Measurement of Cl concentrations in soil and ditch water, as used for calibration of COFANI’s in order to ascertain a realistic distribution with depth of drainage and infiltration fluxes, is discussed in Section 3.3.1.2.

Downward seepage was estimated by taking a value from literature that amounts to around 25 mm a^{-1} for the area of De Vlietpolder (ICW, 1976)

Runoff was measured with four catchment plates (Fig. 5) on a weekly basis from December 2001 till March 2002 (Van Beek et al., 2003b). However, Van den Eertwegh and Van Beek (2004) conclude that the results underestimate real runoff of the experimental field due to large spatial variation and few replicates. Therefore, these results were merely used to establish a lower limit for surface runoff.

3.2.2 Results

3.2.2.1 Input data

1. Initial values of states

Table 7 presents the initial values of the states groundwater level and soil temperature. SWAP interpolates linear between the input values of temperature in order to obtain an initial temperature for each model compartment.

Table 7 Initial values of state variables of SWAP. Levels refer to average surface elevation of –2.09 m + NAP.

SWAP name	Description	Level (m)	Value	Unit
GWLI	Initial groundwater level	–	-15.0	cm
TSOIL	Soil temperature	0.00	7.0	°C
TSOIL	Soil temperature	-0.30	10.0	°C
TSOIL	Soil temperature	-2.98	10.0	°C

2. Process parameters

Table 1 shows the results of the soil texture measurements. Values coincide reasonable well with those reported by Van Beek et al. (2004b), except for the organic matter content of the peat layers below 0.48 m bss, for which they report values of 40-45 mass-% loss on ignition. This is very low for this kind of peat and, with the clay content of 17 mass-% they report, would result in class 'clayey peat' in stead of class 'peat' in the Dutch soil classification system (Steur and Heijink, 1983). Also their very high dry bulk density of 750 kg m^{-3}, points in that direction. High clay contents as shown in Table 1 are very common in woody peats in The Netherlands.

Table 8a presents the results of the measurements and fitting of the Van Genuchten parameters and of the measurements of the saturated hydraulic conductivity. Saturated volumetric water content, OSAT, increases with depth. This is in line with increasing organic matter content and decreasing dry bulk density (Table 1). For each soil horizon, the values of these three parameters match very well. Fitted K_{sat} is much lower than measured. This is quite common, as is the large standard deviation of the latter. Large standard deviations of the measured 'hydrological K_{sat}' and larger values than those of the fitted 'soil physical K_{sat}', especially in the top soil horizons, indicate the presence of macropores. As the used versions of the models are not able to simulate saturated conditions with macropores, either explicit or implicit, the fitted K_{sat}'s were used in SWAP. Using higher, measured K_{sat} instead of fitted K_{sat} in SWAP 3.0.3, is strongly dissuaded as this will lead to (strong) overestimation of capillary rise of groundwater to the root zone.

Table 8a Values of process parameters of SWAP: Van Genuchten parameters and measured K_{sat} (saturated hydraulic conductivity). For explanation of symbols of Van Genuchten parameters, see Table 3. Depths refer to average surface elevation of –2.09 m + NAP.

Soil horizon		Van Genuchten parameters						K_{sat} measured	
ISOIL-LAY1	Depth (m)	ORES (m^3 m^{-3})	OSAT (m^3 m^{-3})	ALFA (cm^{-1})	NPAR (–)	LEXP (–)	KSAT (cm d^{-1})	average (cm d^{-1})	sd (cm d^{-1})
1	0.00–0.20	0.00	0.605	0.0241	1.122	0.000	5.000	401	480
2	0.20–0.28	0.20	0.636	0.0280	1.341	-0.876	1.880	462	450
3	0.28–0.48	0.25	0.695	0.0177	1.271	0.000	1.790	262	330
4	0.48–0.78	0.00	0.883	0.0135	1.222	-4.811	0.600	130	115
5	0.78–2.98	0.10	0.911	0.0098	1.433	-2.387	0.497	4	1.4

Note that unit *cm* for Length is unit that SWAP uses

Table 8b Values of process parameters of SWAP: drainage parameters

SWAP name	Description	Value	SWAP Unit
PONDMX	Maximum thickness ponding water layer	0.3	cm
RSRO	Drainage resistance of surface runoff	1.0	d
RSROEXP	Exponent in surface runoff relation	1.0	–
NRLEVS	Number of drainage levels	2	–
DRARES1	Drainage resistance level 1	200.0	d
INFRES1	Infiltration resistance level 1	220.0	d
L1	Drain spacing level 1	40.0	m
ZBOTDR1	Level of drain bottom level 1	-75.0	cm
ZBOTDR2	Level of bottom interflow layer	-28.0	cm
COFINTFLB	Coefficient for interflow relation	0.003	d^{-1}
EXPINTFLB	Exponent for interflow relation	1.0	–
COFANI	Anisotropy coefficient: $K_{sat,Hor} / K_{sat,Vert}$		
COFANI1:	Horizon 1, depth: 0.00-0.20 m	10.0	–
COFANI2:	Horizon 2, depth: 0.20-0.28 m	10.0	–
COFANI3:	Horizon 3, depth: 0.28-0.48 m	10.0	–
COFANI4:	Horizon 4, depth: 0.48-0.78 m	10.0	–
COFANI5:	Horizon 5, depth: 0.78-2.98 m	0.5	–

Table 8b gives values of the drainage related parameters. A system of two drainage levels is quite common in Dutch peat pastures, where traditionally a shallow (0.2-0.3 m deep) trench parallel to the ditch drains the top soil and acts as collector of surface runoff at high groundwater table and heavy rainfall. At the experimental field, the surface is graded and consequently the former trench is filled up. The graded surface enhances not only surface runoff, but also interflow through the 'toemaakdek' (Table 1), because it promotes the building up of a pressure gradient from middle to sides of the field on top of the less permeable, level clayey peat layer. In this way, interflow substitutes for drainage to the former trench. The default values for RSRO and RSROEXP imply that it takes one day to discharge all ponding water above the threshold to the ditch which seems reasonable for peat soils (Hendriks, 1993).

Drainage and infiltration resistance fall in the ranges that are reported in literature for Dutch peat pastures (e.g. ICW, 1973; Massop, 1988; Hendriks, 1993; Hendriks et al., 1994 and 2002). A 10% higher infiltration resistance than the drainage resistance is also a common condition. A value of 0.003 d^{-1} for COFINTFLB (coefficient for interflow) corresponds to a drainage resistance of 333 days. This seems high, but related to the thickness of the drained layer this resistance is six times lower than the overall drainage resistance of 200 days.

COFANI's indicate a 20 times lower value for the reduced peat layer. Transmissivities KD (COFANI · K_{sat} · D [thickness]) of the five horizons amount to 10.0, 1.5, 3.6, 1.8 and 0.6 m^2 d^{-1}, respectively. The KD's of the first two horizons, the interflow layer, SWAP uses to partition the interflow flux over these two horizons. The other KD's for partitioning the sub-surface drainage flux over the other three horizons. This implies that in a situation of a fully saturated soil 25% of the total flow through the soil to the ditch passes the interflow layer and only 7% the 2.2 m thick reduced peat layer. The latter part amounts to 9% at a groundwater level of 0.28 m bss, just below the interflow layer, and 23% at a level of 0.48 m bss. Simulated surface runoff is very high, up to 30% of the total discharge to the ditch, due to the low PONDMX value of 0.3 cm, which corresponds with the grading of the field in reality.

Table 8c Values of process parameters of SWAP: bottom boundary parameters

SWAP name	Description	Value	Unit
SHAPE	Shape factor for average groundw. level	1.0	–
HDRAIN	Mean drainage base; dummy	0.0	cm
RIMLAY	Vertical flow resistance of aquitard	18,000.0	d

Table 8c presents the bottom boundary parameters. Using the default value of 1 for SHAPE, overrules the option of converting the groundwater level into ‘a field-average level’, which is unnecessary, because the level in SWAP is per definition a field average level. The calibrated value of RIMLAY, the vertical flow resistance, of 18,000 days is high but in the same order of magnitude (5,000-10,000 days) as reported by Boswinkel and Cornelissen (1980). In combination with the average hydraulic head in the aquifer of about 1.6 m bss (Fig. 7) and an average groundwater level of around 0.45 m bss, this value results into a yearly downward seepage flux density of 25 mm a^{-1}, which was the aim (Section 3.2.1.2).

Table 8d Values of process parameters of SWAP: adjusted crop parameters

SWAP name	Description	Value	Unit
HLIM1	Limiting pressure head for water uptake: 1	0.0	cm
HLIM2U	Limiting pres. head for water uptake: 2U	–1.0	cm
HLIM2L	Limiting pres. head for water uptake: 2L	–1.0	cm
RD	Rooting depth	28.0	cm

The values of the limiting pressure heads for water uptake under wet conditions are given in Table 8d. These values are higher than the standard ones from Appendix 1, and are all equal or close to saturation (h = 0.0 cm). It is empirically found that grass on peat soil can take up water under very wet conditions (P. Rijtema pers. com., 1990).

3. Boundaries

Meteorological data, relevant for the top boundary, are shown in Figure 6 as the variables they are converted into by SWAP for use in the model: daily mean air temperature, daily sum of precipitation and daily sum of potential evapotranspiration as calculated according to ‘Penman-Monteith’. Daily mean air temperature is calculated as arithmetic mean of minimum and maximum temperature. For all years, annual mean air temperature was about 0.5 °C higher than local long-term (1971-2000) values of 9.8-10.1 °C (Sluijter and Nellestijn, 2002). Annual sums of precipitation were larger than local long-term average values of 800-850 mm a^{-1}, while potential evapotranspiration was in the local long-term average range of 555-570 mm a^{-1}. Thus, resulting precipitation surpluses were relatively high. Especially 2001 was an extremely wet year with a surplus of 671 mm, more than twice the local annual average of 300 mm a^{-1}.

Table 9 Annual mean air temperature (°C), and annual sum of precipitation, potential evapotranspiration and precipitation surplus (all in mm), for the years of the field experiment

Year	Air temp.	Precipitation P	Potential evapotranspiration E_{pot}	P – E_{pot}
2000	10.8	908	563	345
2001	10.4	1215	544	671
2002	10.7	989	570	419
2003 till April 28th	–	198	142	56

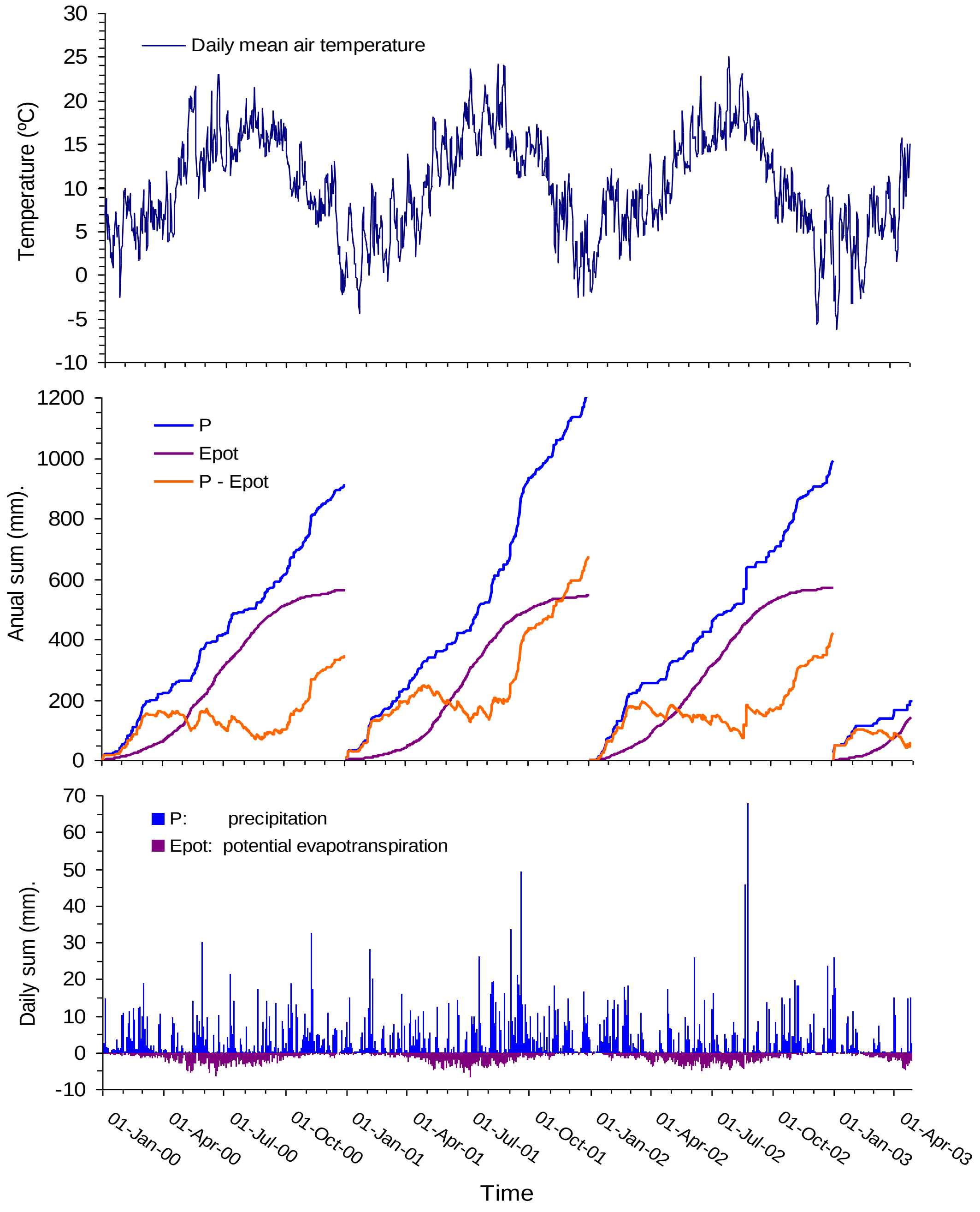

Figure 6 Daily mean air temperature, and annual and daily sum of precipitation and potential evapotranspiration, for the years of the field experiment

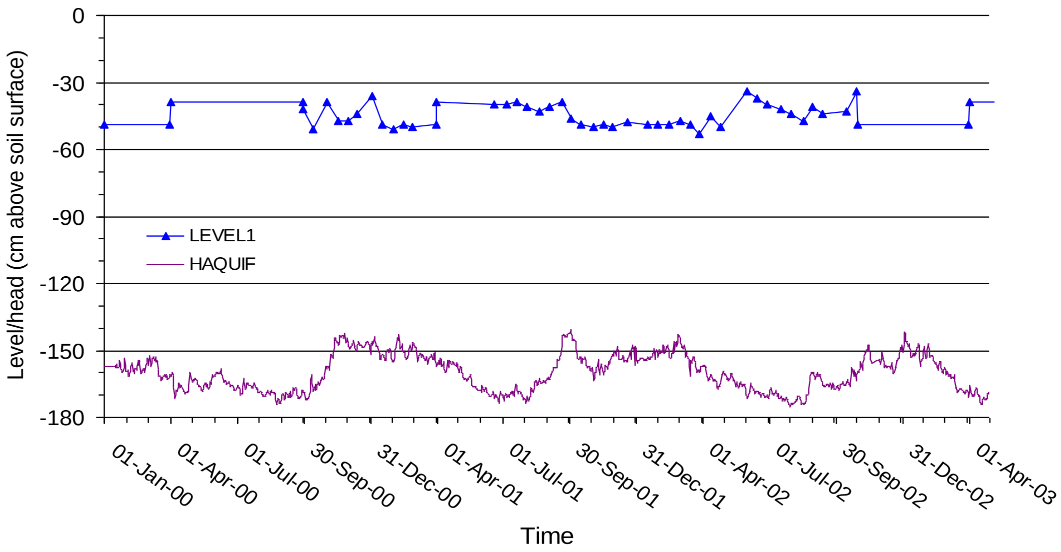

*Figure 7 Time-series of level of ditch water as drainage basis (*LEVEL1*) and hydraulic head in the aquifer (*HAQUIF*), in cm above average soil surface (–209 cm + NAP), for the years of the field*

Lateral and bottom boundaries, as time-series of ditch water level and hydraulic head in the aquifer, respectively, are shown in Figure 7. Average difference in head is about: average LEVEL1 – average HAQUIF = –44 – –160 = 116 cm. This great head difference is due to the low hydraulic head in the aquifer which is caused by draining of a neighboring polder at an elevation of about three meters deeper than the elevation of the Vlietpolder. Result is a downward seepage flow that is not negligible (25 mm a^{-1}), despite the very high vertical flow resistance.

3.2.2.2 Data for model calibration and validation

Time-series of the target variables for calibration or validation, 'groundwater level', 'drain discharge' and 'chloride loads' are presented in Figure 11 and 12 (Section 4.2.1.2) and Figure 13 (Section 4.2.1.3), respectively. The estimated groundwater table shape factor β equals 0.80 (–).Values for the average downward seepage flux density and the lower limit of surface runoff in 2001, are presented in Table 10. Even the highest value of the estimated 'lower limit of surface runoff' is quite low. According to Meinardi (2005), surface runoff generally amounts to 20% of the total discharge to the experimental ditch. As the field is graded, this percentage may be much higher. The low estimations in Table 10 are probably due to the measuring method that caused collector barrels to overflow in the time-span of a week before they were emptied. Van Beek et al. (2003b) report that 'when it (surface runoff) occurred, the collector barrels were filled at once and most often were filled completely'.

Table 10 Values of target variables for calibration and validation of SWAP

Description variable	Average value	Range	Unit
Downward seepage flux density	25	–	mm a^{-1}
Lower limit of surface runoff 2001	8	2.5–11.5	% of total discharge to ditch

3.3 Data for ANIMO

Material and methods of data collection and assessment for ANIMO are discussed in Section 3.3.1 and results are presented in Section 3.3.2. In both Sections, a distinction is made between input data and measured rates and states used for model calibration and validation. Because ANIMO requires a large number of input data and values of many of these can be obtained from example cases in the manual (Renaud et al., 2005), only input parameters whose values are not derived from the cases in the manual are dealt with. These do not include trivial data like timing dates of simulation periods, file names, switches etc.

Besides the regular input data in formatted files, ANIMO requires an unformatted file with values of process parameters and initial values and values per time-step of rates and states as provided by SWAP. Among these data is the ANIMO time-step length, which is input of SWAP. In this study the ANIMO time-step length was set to 1 day.

3.3.1 Materials and methods

3.3.1.1 Input data

All input data other than those provided by SWAP are categorised in the three groups distinguished in Section 2.2.3: 1. initial values of states, 2. process parameters and 3. boundaries (forcing variables).

1. Initial values of states

Initial values of relevant state variables are listed in Table 11. States that are not included in this table got the dummy value of 0.0, because their initial values were not determinative for their final values.

Initial amounts of organic matter and distribution over organic matter pools was obtained in an initialisation process by performing a pre-run, the so-called ‘historical run’, that covered the period 1941–1999 (see Section 2.3.4). For this run, initial values for organic matter amounts as function of depth were obtained on the basis of Table 1. In the two deepest horizons with oxidised and reduced peat, respectively, organic matter was divided over two organic classes according to Hendriks (1993) for similar eutrophic peat: 67% in a slow decomposing, nitrogen-poor class (no. 12) and 33% in a relative fast decomposing, nitrogen-richer class (no. 11). For the top horizons, initially all organic matter was put in the organic matter pool ‘humus-biomass’ (HUFROS). In a trial and error process, part of this organic matter was taken from HUFROS and added to the two peat classes until organic matter amount and nitrogen content at the end of the historical run (1st January 2000) matched the observed values of Tables 1 and 15 reasonably well.

In the historical run, also concentrations of dissolved nutrient compounds will establish under the influence of fertilisation and other sources of nutrients. Starting the historical run with zero concentrations will be sufficient for all compounds except phosphate. This does not count for the peat layers where the influence of fertiliser is

Table 11 State variables of ANIMO that require an initial value and the methods used to obtain them

ANIMO name	Description	Requirement	Method
CONH	Concentration[1] of ammonium	Per model compartment	**Calibration**
OS	Mass of organic matter in organic classes	Per model compartment per organic class	Initialisation & Hendriks, 1993
HUOS	Mass of org. matter in humus	Per model compartment	Initialisation
CODIORMA	Concentration of DOM[2]	Per model compartment	Calculated from CODIORNI
CODIORNI	Concentration of DON[2]	Per model compartment	Calculated from CONH
COPO	Concentration of phosphate	Per model compartment	**Calibration**
AMPOTO	Amount of total phosphorus	Per model compartment	Estimation
COPOEB	Background concentration of phosphate	Single value	Schoumans, pers. com.

[1] Concentration = concentration in soil moisture

[2] DOM = dissolved organic matter; DON= dissolved organic nitrogen

limited and where relative high concentrations of ammonium, phosphate, DOM (dissolved organic matter), DON (dissolved organic nitrogen) and DOP (dissolved organic phosphorus) are found. Ammonium and phosphate concentrations are in equilibrium with the peat soil complex, which implies that large amounts of these compounds are adsorped at the soil complex. The high concentrations are related to the conditions under which the peat was formed and thousands of years of slow anaerobic decomposition of the peat (Hendriks, 1991). Especially for phosphate it takes a long time to reach equilibrium. Therefore, it is crucial to put in realistic initial values for these concentrations for the historical run.

For the peat horizons (0.48 m bss and deeper; Table 1), initial concentrations in soil solution of ammonium (CONH) and phosphate (COPO) were calibrated, by taking a fixed value for the deepest soil compartment from Meinardi (2005), calibrating the value in the first (shallowest) peat soil compartment and interpolating linearly between the calibrated upper and fixed lower value (see 4.2.2.1). Initial DON concentrations were calculated from ammonium concentrations according to the observed ratio NH_4-N : DON of 1.085. Observations of DOM concentrations were not available, therefore initial DOM concentrations were calculated from DON taking a DOM : DON ratio of 12 (eutrophic peat in Vermeulen and Hendriks, 1996).

For initialisation of phosphorus concentrations, INPO = 3 was chosen, implying input of initial values for COPO, AMPOTO and COPOEB (Table 11). AMPOTO was estimated on the basis of Van Beek et al. (2003c). A value for COPOEB was obtained from O.F. Schoumans (pers. com.).

2. Process parameters

The relevant process parameters that ANIMO requires are listed in Tables 12a-12c. Properties of organic matter pools are given in Table 12a.

Table 12a Relevant process parameters of ANIMO and the methods used to obtain values for them. Input file **Material.inp***: properties of (organic) materials.*

ANIMO name	Description	Requirement	Method
FROR	Mass fraction organic matter in material	Per material[1)]	Measurement
FRNH	Mass fraction ammonium in material	Per material[1)]	Measurement
FRNI	Mass fraction nitrate in material	Per material[1)]	Measurement
FRPO	Mass fraction phosphate in material	Per material[1)]	Measurement
FR	Mass fraction of org. class in material	Per material per class[1)]	Measurement
FRCA	Mass fraction of dissolved organic matter of organic class in material	Per material per class[1)]	Measurement
ASFA	Assimilation efficiency org. classes	Per class[2)]	Hendriks, '91
RECFAV	Decomposition rate constant org. classes	Per class[2)]	Vermeulen & Hendriks, '96
NIFR	Mass fraction nitrogen in org. classes	Per class[2)]	Measurement
POFR	Mass fraction phosphorus in org. classes	Per class[2)]	Measurement
HUFROS	Mass fraction of decomposed org. mater. transformed into humus/biomass	Single value	Hendriks, '93
RECFCAAV	Decomp. rate const. dissolved org. matter	Single value	Hendriks, '93
RECFNTAV	Nitrification rate constant	Single value	Hendriks, '93
RECFDEAV	Denitrification rate constant	Single value	**Calibration**
POFRHUMA	Phosphorus content of humus/biomass	Single value	Hendriks, '93

[1)] applies to the two materials slurry and cattle droppings
[2)] applies to organic classes 11 and 12, used to describe peat

Parameters to describe fertilisers were basically taken from the example cases in the manual 'Cranendonk grass' and 'Grassland on peat' and then adjusted to meet the measured properties (see ***3. Boundaries***). Decomposition rates of the classes 11 and 12 to describe peat were not measured and therefore were taken from Vermeulen and Hendriks (1996) as their eutrophic, woody peat is similar to the peat in the Vlietpolder (e.g. for nitrogen content). Total nitrogen and phosphorus content of the soil were determined with standard methods by Blgg Oosterbeek (laboratory for soil and crop research). P in organic matter was obtained by subtracting P-oxalic from total P. For N, a correction of total N for mineral N was not necessary because of the relatively low content of mineral N compared to organic N.

Other values content of organic matter were taken from Hendriks (1993). His values for HUFROS and RECFCAAV are in between the optimal values for describing application of organic fertiliser on mineral soils (cases in the manual) and peat soil, and in this way, are a compromise. The denitrification rate constant was the only parameter that was calibrated as its value was uncertain.

Values for all parameters not listed in Table 12a were taken from example case 'Grassland on peat' except for ASFA's of organic fertilisers, that were taken as average of 'Grassland on peat' and 'Cranendonk grass', and RECFHUAV (decomposition rate constant humus/biomass pool) whose value was taken from cases 'Ruurlo grass' and 'Cranendonk grass' as the value from 'Grassland on peat' was considered too low in comparison to values commonly reported (Hendriks, 1991).

Table 12b Relevant process parameters of ANIMO and the methods used to obtain values for them. Input file **Soil.inp***: physical and chemical properties of soil.*

ANIMO name	Description	Requirement	Method
NUHO	Number of soil horizons	Single value	Table 1
HE(0)	Thickness of compartment for ponding	Single value	Table 8b
RODP	Depth initial root zone	Single value	Table 8d
PMDF1HN	Coefficient in oxygen diffusion relation	Per horizon	**Calibration**
PMDF2HN	Exponent in oxygen diffusion relation	Per horizon	**Calibration**
CDSAHN	Saturated hydraulic conductivity	Per horizon	Table 8a
RHBDHO	Dry bulk density	Per horizon	Table 1
CNRATIOHO	C/N-ratio of organic matter	Per horizon	Dummy
ACRDTEHO	Coefficient temperature rate response function for org. matter transformation and nitrification	Per horizon	Vermeulen & Hendriks, 1996
ACRDTE-DISHO	Coefficient temperature rate response function for transformation of dissolved organic matter	Per horizon	ACRDTEHO
PHHO	pH-water	Per horizon	Table 1
SOCFNHHO	Coefficient for ammonium sorption	Per horizon	Estimation
ALFEHO	Content of aluminium plus iron	Per horizon	Measurement

Process parameters concerning physical and chemical properties of the soil are given in Table 12b. Several parameters are related to SWAP input and are discussed in Section 3.2. CNRATIOHO is a dummy parameter for peat soils, since it does not affect the composition of peat soils as they are described by their own organic matter classes (Groenendijk et al., 2005). For the clay and peat horizons, values for ACRDTEHO were calculated from the Q_{10}'s reported by Vermeulen and Hendriks (1996). For the top horizon, the 'toemaakdek', default values were used, since Vermeulen and Hendriks do not provide values for this kind of sandy soil. ACRDTEDISHO was taken equal to ACRDTEHO because there was no information to decide otherwise.

Values for SOCFNHHO, the distribution coefficient for ammonium, were initially calculated as function of CEC (cation exchange capacity) according to Hoeks (pag. 48, Kroes et al., 1990), where CEC was calculated from organic matter and clay content according to Breeuwsma and Van Duivenbooden (1987). Hendriks (1993) used the same method, which was developed for sandy soils, to calculate SOCFNHHO and concluded that it yields too high values for (clayey) peat soils. He adjusted the values by calibration. His correction factors were used to obtain final values. Correction factors were 0.185 for organic matter content and 0.26 for clay content and thus a final value for SOCFNHHO, $K_{\mathrm{e,NH}_4}$ ($\mathrm{m}^3\ \mathrm{kg}^{-1}$), was calculated as:

$$K_{\mathrm{e,NH}_4} = \frac{0.185 \cdot OM + 0.26 \cdot Clay}{OM + Clay} K'_{\mathrm{e,NH}_4} \qquad (4)$$

where $K'_{\mathrm{e,NH}_4}$ is the initial, uncorrected value, OM is organic matter content (kg kg^{-1} dry soil) and $Clay$ is clay content (kg kg^{-1} mineral parts).

ALFEHO, sum of aluminium and iron content, was determined as oxalic extractable aluminium and iron with standard methods by Van Beek et al. (2003c).

The two parameters, PMDF1HN (coefficient) and PMDF2HN (exponent), to describe vertical oxygen diffusion into the soil are commonly calibrated in simulations of field experiments, as the model is quite sensitive for its values. So they were in this study for the upper three horizons: the mineral layers. For the peat horizons values from Hendriks (1993) were taken.

Parameters not presented in Table 12b got default values of example case 'Grassland on peat'

Table 12c Relevant process parameters of ANIMO and the methods used to obtain values for them. Input file **Chempar.inp**: *chemical parameters for phosphorus.*

ANIMO name	Description	Requirement	Method
PACXFAHO(2)	Max. amount Langmuir equilibrium sorption	Per horizon	Estimation
PACXFAHO(3)	Coefficient Langmuir equilibrium sorption	Per horizon	Estimation
PARKD	Coefficient Langmuir desorption	Per horizon	Estimation
PACXSLHO(1)	Coefficient linear sorption	Per horizon and per non equilibrium sorption site	Estimation
PACXSLHO(2)	Max. amount Langmuir non equil. sorption		Estimation
PACXSLHO(3)	Coefficient Langmuir non equil. sorption		Estimation
PACXSLHO(4)	Constant Freundlich non equil. sorption		Estimation
PACXSLHO(5)	Exponent Freundlich non equil. sorption		Estimation
RECFADSHO	Rate constant first order adsorption		Estimation
RECFDESHO	Rate constant first order desorption		Estimation

Parameters for describing ad/de/sorption and precipitation processes of phosphate are given in Table 12c. Values were obtained on the basis of example case 'Grassland on peat' and from Van Beek et al. (2003c). Parameters not shown in Table 12c are default values from the example case.

Dates about growing season were deducted from the recordings by the farmer on the so called 'grassland calendar', a recording of activities per field. A somewhat slighter

Table 12d Relevant process parameters of ANIMO and the methods used to obtain values for them. Input file **Plant.inp**: *parameters for grass grow and uptake.*

ANIMO name	Description	Requirement	Method
TIGRBEG	First day of growing season	Single value	Grassland calendar
TIGREND	Last day of growing season	Single value	
EFFA	Efficiency factor for gross dry matter production	Single value	P. Groenendijk
NIFRSHMI	Minimum nitrogen content of grass shoots	Single value	Measurement
NIFRROMI	Minimum nitrogen content of grass roots	Single value	Measurement
DFCFUPNIGR	Nitrate transpiration stream concentration factor of grassland (diffusive uptake)	Single value	**Calibration**
POFRSHMI	Minimum phosphorus content of grass shoots	Single value	Measurement
POFRROMI	Minimum phosphorus content of grass roots	Single value	Measurement

value for EFFA, efficiency factor for gross dry matter production, than default was obtained by personal communication of P. Groenendijk. Minimum nitrogen and phosphorus content of grass shoots and roots were derived from measurements of fresh grass samples by Blgg Oosterbeek.

Parameter DFCFUPNIGR, the nitrate transpiration stream concentration factor for diffusive uptake, was calibrated, because its default value was uncertain, and the model results turned out to be rather sensitive for its value.

Parameters not listed in Table 12d got values of example case ‘Cranendonck grass’.

3. Boundaries (forcing variables)

Forcing variables refer to the three boundaries of the modelled system: top, lateral and bottom boundary (Fig. 1). At the top boundary, forcing variables comprise atmospheric deposition (wet and dry) of N and P compounds, fertilisation as application of manure and artificial fertiliser and as cattle droppings, ammonia volatilization, gaseous nitrogen (N_2) emission and crop uptake. N_2 emission is a result of denitrification, which is steered in ANIMO by the process parameter RECFDEAV (1^{st}-order denitrification rate constant; Table 12a). Crop uptake is calculated by the model itself, as forced by harvesting and cattle grazing, which are both controlled by process parameters in file Plant.inp (Table 12d) and the latter by the annual average number of livestock-units (NRGR, Table 13b), as well.

At the lateral and bottom boundary, the forcing variables are concentrations of N and P compounds and DOM (dissolved organic matter) in infiltration and upward seepage water, respectively. As upward seepage does not occur, values of concentrations in upward seepage water are merely dummies and therefore not included in Table 13a.

Table 13a presents the forcing variables which are required in file Boundary.inp: wet and dry atmospheric deposition of N and P for the top boundary, and concentrations in infiltration water for the lateral boundary. Atmospheric deposition was obtained from RIVM (National Institute for Public Health and the Environment): wet atmospheric deposition as concentrations in precipitation water from Stolk (2001) and dry atmospheric deposition from Breugel et al. (2001). For all four simulation years (2000-2003) equal values were used. Infiltration water in polders with managed water level like The Vlietpolder concerns the ditch water in the summer-half-year. Average summer-half-year concentrations of ammonium, nitrate and phosphate (as ortho-P) in the ditch water were calculated from 42 observed concentrations per compound each, measured in the period April through September of 2001 and 2002 (Van Schaik et al., 2004). Concentrations of DON and DOP were estimated from 42 measured total-N and total-P concentrations as:

DON = total-N – ammonium-N – nitrate-N, and *DOP = total-P – ortho-P*.

DOM was estimated from DON, assuming a DOM : DON ratio of 25, a value that was found for ditch water at Zegveld, the experimental farm on peat land in the Netherlands.

Table 13b considers the forcing variables that are related to fertiliser application and that are required in file Management.inp. In general, input data were obtained from

Table 13a Relevant forcing variables of boundaries of ANIMO and methods used to obtain values for them. Input file **Boundary.inp***: boundary concentrations and depositions.*

ANIMO name	Description	Requirement	Method
Top boundary			
COPRNH[1]	Concentration of ammonium in precipitation	Per year	RIVM
COPRNI[1]	Concentration of nitrate in precipitation	Per year	RIVM
COPRPO[1]	Concentration of phosphate in precipitation	Per year	RIVM
DRDEPNH[1]	Mass of dry deposition of ammonium	Per year	RIVM
DRDEPNI[1]	Mass of dry deposition of nitrate	Per year	RIVM
Lateral boundary			
COIDNH	Concentration of ammonium in infiltration water	Single value	Measurement
COIDNI	Concentration of nitrate in infiltration water	Single value	Measurement
COIDPO	Concentration of phosphate in infiltration water	Single value	Measurement
CODIORMAID	Concentration of DOM[2] in infiltration water	Single value	Estimation
CODIORNIID	Concentration of DON[2] in infiltration water	Single value	Estimation
CODIORPOID	Concentration of DOP[2] in infiltration water	Single value	Estimation

[1] in case of the 'historical run' (Section 3.3.1.1): the STONE database (Boers et al.,1997; Willems et al., 2008)

[2] DOM, DON, DOP = dissolved organic matter, nitrogen and phosphorus, respectively

information recorded by the farmer on the grassland calendar and analyses of slurry samples by Blgg Oosterbeek. Information about cattle droppings was obtained from Van Beek and Oenema (2002). NRGR, the annual average number of livestock-units grazing on grassland must be given for each year. This variable is used in the calculation of the daily production rate of grass shoots, which is a driving force for simulation of N and P uptake by the grass crop. It was derived from registration of the number of cattle, number of days and time per day of grazing, by calculating the time-weighted average per year. Slurry was injected and thus was distributed over the top 0.10 m or the first two compartments in the model. Cattle droppings were applied on top of the first compartment. Ammonium volatilization was calculated according to Hendriks et al. (2002).

Table 13b Relevant forcing variables of boundaries of ANIMO and methods used to obtain values for them. Input file **Management.inp***: additions of fertilisers.*

ANIMO name	Description	Requirement	Method[1]
NRGR	Annual average number of livestock units	Per year	Grassland calendar
TINEAD	Time of addition event	Per event	
NUAD	Number of additions at TINEAD	Per event	Grassl. cal.
MTNU	Number of material added at TINEAD	Per event and per addition	Grassland calendar
QUMT	Mass of material added at TINEAD	idem	Grassl. cal.
WYAD	Number of compartments over which QUMT is distributed at TINEAD	idem	Estimation
FRVO	Fraction of volatilization of ammonium added at TINEAD	idem	Estimation

[1] in case of the 'historical run' (Section 3.3.1.1): the STONE database (Boers et al.,1997; Willems et al., 2008)

3.3.1.2 Data for model calibration and validation

Similar to SWAP, data for model calibration and validation of ANIMO comprise measured time-series of rate and state variables that characterise the reactions of the modelled system to changes in the forcing variables and that are output of ANIMO. In this respect, state variables are concentrations of N and P compounds in soil water and groundwater. Rate variables are N mineralization, denitrification and N and P uptake by the crop. Table 14 summarises the measured rates and states and their role in the calibration and validation of ANIMO in terms of the relevant object parameter(s).

Table 14 Target variables, as measured (time-series of) rates or states, for calibration and validation of ANIMO

Target rate or state variable	Function	Object parameter	Method
N and P concentrations in soil water	Calibration	All calibrated parameters	Field measurement
Mineralization	Validation	All calibrated param.	Field measurement
Denitrification	Validation	All calibrated N param.	Field measurement
N and P uptake by crop	Validation	All calibrated param.	Field measurement

Soil water and groundwater were sampled with suction cups placed at depths of 0.15, 0.25, 0.35, 0.50, 0.70 and 1.20 m below soil surface and at 0, 1, 2, 4, 7, 10 and 20 meters distance from the experimental ditch (Fig. 5). Suction cups were made of synthetic, chemical-inert material on which no sorption of phosphate takes place. Laboratory tests showed that sampling of soil water through this porous material was comparable to filtering water samples through 0.45 μm filters (Van den Toorn, pers. com.). From October 2001 till March 2003, every fortnight vacuum bottles (approx. -90 kPa) were connected to the suction cups in order to collect water samples. With suction cups, the mobile fraction of the soil solution is sampled (Corwin, 2002, in: Van Beek et al., 2004a). Samples were analyzed by the lab of Waterboard Rijnland for total-N, NH_4, NO_3, total-P, ortho-P, Cl and pH by continuous flow analysis (Van Beek et al., 2004a; Van Schaik et al., 2004). Interpretation of the results for use in the calibration process consisted of assigning suction cup data to a representative profile layer (Appendix 4).

Nitrogen mineralization of soil organic matter was estimated by determining the N uptake of grass in plots (Fig. 5) that were not N fertilised over a period of four years (2000-2003) (Van Beek et al., 2004a). The plots did receive phosphorus and potassium fertiliser at normal rates. Five times during the growing season all grass was harvested and soil samples were taken at three depths (0.00-0.20, 0.20-0.40, 0.40-0.60 m below soil surface) for determination of mineral N. Net N mineralization in the rooting zone was calculated as (Van Beek et al., 2004a):

Net N mineralization = N uptake + denitrification from soil – atmospheric deposition – changes in storage of soil mineral N .

N uptake in roots and stubbles was disregarded; it was assumed that this quantity equalled the N mineralization from old roots and stubbles. Denitrification was estimated with a site-specific regression equation with soil nitrate content as explaining variable (Van Beek et al., 2004b). Phosphorus mineralization was estimated from N mineralization by taking the total N : total P ratios obtained from samples taken at a depth of 50 cm below soil surface (Van Beek et al., 2004a).

Denitrification rates were measured with the ‘acetylene inhibition technique’ (Van Beek et al., 2004b). For two so called 'seasons' – 2000-2001 and 2001-2002 – every three to four weeks soil samples were taken every 10 cm from surface to the depth of groundwater table. Samples were incubated in the lab and actual denitrification rates were measured.

Nutrient uptake by the grass crop was estimated by taking samples of every grass sward in 2000-2003 (Van Schaik et al., 2004). Samples were analysed by BLGG Oosterbeek for carbon, nitrogen and phosphorus content.

3.3.2 Results

3.3.2.1 Input data

Results of the analyses of chemical properties of the soil are presented in Table 15.

Table 15 Results of analyses of chemical properties of the pet soil. For explanation of soil horizons, see Table1.

Hori-zon	Depth (m)	C, N, P in organic matter (kg kg^{-1}) C	N	P	Oxalate-extractable in soil (mmol kg^{-1}) P	Al	Fe
1	0.00-0.20	0.445	0.0418	0.00164	28.3	122	181
2	0.20-0.28	0.623	0.0491	0.00249	21.3	160	260
3	0.28-0.48	0.662	0.0486	0.00100	21.1	189	235
4	0.48-0.78	0.484	0.0338	0.00056	8.0	111	114
5	0.78-2.98	0.554	0.0344	0.00046	4.2	51	59

C content is rather low in horizons 1 and 4, suggesting the presence of relatively young organic matter. This is to be expected for the top horizon, in the form of root and crop residues and exudates, but less for the oxidised peat layer. C content is highest in the mineral soil horizons below the root zone, indicating the presence of more humified organic matter. C content of the reduced peat layer is what is commonly found in fen peats in the Netherlands (Hendriks, 1991 and 1993). This distribution with depth of C content is in line with the findings for a similar wood peat soil in the West of the Netherlands by Hendriks (1993).

N and P content are high, and C/N- and C/P-ratios consequently low, for the first three soil horizons indicating the enrichment by fertilization and creation of the ‘Toemaakdek’. N content and C/N-ratio of the peat horizons are similar to those found by Hendriks (1993) for a similar wood peat, but P content is much higher (3-4 times) and C/P-ratio much lower than this peat. Sum of oxalate-extractable Al and Fe is comparable to Hendriks (1993) except for the reduced peat horizon, which value is only half of the value of Hendriks (1993).

1. Initial values of states

Values for ammonium-N and phosphate-P at the bottom of the peat soil obtained from Meinardi (2005) amounted to 0.019 kg N m^{-3} and 0.006 kg P m^{-3}. Calibrated values at the most upper model compartment with peat were 0.005 kg N m^{-3} and 0.00135 kg P m^{-3}, respectively. In between, the values were interpolated linear. These values are very high, but of an order that is more often found in eutrophic peat soils (Hendriks, 1991 and 1993). They are results of fluvial and/or marine influence and thousands of years of slow anaerobic mineralization of the peat. They imply a substantial contribution of these permanent saturated peat layers to nutrient loading of surface waters.

2. Process parameters

Values for process parameters concerning the description of properties of (organic) materials are listed in Table 16a. Values for NIFR and POFR of organic classes 11 and 12 that describe the peat are deducted from the values of Table 15, according to the ratio between the mass of class 11 and class 12.

The value of RECFDEAV, the calibrated parameter, is 2.5 times the default value, indicating that first order denitrification in peat soils is faster than the assumption of a maximum denitrificated nitrate-fraction of 50% in 10 days for sandy soils (Renaud et al., 2005; page 83).

Table 16a Values of process parameters of ANIMO. Input file **Material.inp***: properties of materials*

ANIMO name	Description	Value		Unit
HUFROS	Mass fraction of decomposed organic matter transformed into humus/biomass.	0.75		kg kg^{-1}
RECFCAAV	Decomp. rate const. dissolved org. mat.	15.0		a^{-1}
RECFNTAV	Nitrification rate constant	100.0		a^{-1}
RECFDEAV	Denitrification rate constant	0.15		d^{-1}
POFRHUMA	Phosphorus content humus/biomass	0.0025		kg kg^{-1}
Materials as fertilisers:		**Slurry**	**Cattle drop.**	
FROR	Mass fraction organic matter in material	0.045	0.05	kg kg^{-1}
FRNH	Mass fraction ammonium in material	0.002685	0.002775	kg kg^{-1}
FRNI	Mass fraction nitrate in material	0.0	0.0	kg kg^{-1}
FRPO	Mass fraction phosphate in material	0.000488	0.000479	kg kg^{-1}
FR	Mass fraction of org. class 2 in material	0.79	0.71	kg kg^{-1}
FR	Mass fraction of org. class 3 in material	0.21	0.29	kg kg^{-1}
FRCA	Mass fract. of diss. org. mat. of class 2	0.5	0.5	kg kg^{-1}
FRCA	Mass fract. of diss. org. mat. of class 3	0.0	0.0	kg kg^{-1}
Organic classes for describing peat:		**Class 11**	**Class 12**	
ASFA	Assimilation efficiency org. classes	0.25	0.25	–
RECFAV	Decomposition rate constant org. classes	0.0447	0.001	a^{-1}
NIFR	Mass fraction nitrogen in org. classes	0.065	0.02	kg kg^{-1}
POFR	Mass fraction phosphorus in org. classes	0.0007	0.00035	kg kg^{-1}

Table 16b Values of process parameters of ANIMO. Input file **Soil.inp***: physical and chemical properties of soil. For description of parameters, see Table 12b.*

ANIMO name	Single value	Per soil horizon:					Unit
		1	2	3	4	5	
NUHO	5	–	–	–	–	–	–
HE(0)	0.003	–	–	–	–	–	m
RODP	0.28	–	–	–	–	–	m
PMDF1HN	–	0.3	0.3	0.6	0.5	0.5	_
PMDF2HN	–	1.9	1.9	1.9	1.5	1.5	_
CDSAHN	–	0.05	0.0188	0.0179	0.006	0.00497	m d^{-1}
RHBDHO	–	860.	934.	633.	195.	155.	kg m^{-3}
CNRATIOHO	–	10.	10.	10.	10.	10.	–
ACRDTEHO	–	74826	74826	88831	93824	93824	J mol^{-1}
ACRDTEDISHO	–	74826	74826	88831	93824	93824	J mol^{-1}
PHHO	–	4.9	4.9	4.6	5.3	5.4	–
SOCFNHHO	–	0.006	0.0059	0.0094	0.0182	0.0179	m^3 kg^{-1}
ALFEHO	–	302.	420.	424.	224.	224.	mmol kg^{-1}

Values for process parameters concerning the description of properties of (organic) materials are presented in Table 16b. CDSAHN's are taken from Table 8a, RHBDHO's and PHHO's from Table 1 and ALFEHO's as sum of Al and Fe for each horizon from Table 15. SOCFNHHO's are calculated with Eq. (4) on basis of the organic matter and clay contents of Table 1. The values of the calibrated parameters PMDF1HN and PMDF2HN for the upper mineral soil horizons, are in the order of the values of clayey soils with the qualification 'good' for diffusive property (Groenendijk et al., 2005).

Values of the parameters for describing ad/de/sorption and precipitation processes of phosphate are given in Appendix 5.

Values of process parameters for grass crop uptake of ammonium, nitrate and phosphate are given in Table 16c. The value of the calibrated parameter DFCFUPNIGR is 7 times the default value of 0.028, possibly indicating a strong competition between nitrate uptake by the crop and nitrate loss through denitrification.

Table 16c Values of process parameters of ANIMO. Input file **Plant.inp***: parameters for grass grow and uptake.*

ANIMO name	Description	Value	Unit
TIGRBEG	First day of growing season	60.0	d
TIGREND	Last day of growing season	274.0	d
EFFA	Efficiency factor for gross dry matter production	0.62	–
NIFRSHMI	Minimum nitrogen content of grass shoots	0.04	kg kg^{-1}
NIFRROMI	Minimum nitrogen content of grass roots	0.017	kg kg^{-1}
DFCFUPNIGR	Nitrate transpiration stream concentration factor of grassland (diffusive uptake)	0.2	d^{-1}
POFRSHMI	Minimum phosphorus content of grass shoots	0.004	kg kg^{-1}
POFRROMI	Minimum phosphorus content of grass roots	0.0024	kg kg^{-1}

3. Boundaries

Values of dry atmospheric deposition and concentrations in precipitation and infiltrating ditch water (subirrigation) are listed in Table 17a.

Table 17a Values of forcing variables for ANIMO. Input file **Boundary.inp***: boundary concentrations and depositions.*

ANIMO name	Description	Value	Unit
Top boundary			
COPRNH	Concentration of ammonium in precipitation	0.00071	kg N m^{-3}
COPRNI	Concentration of nitrate in precipitation	0.00041	kg N m^{-3}
COPRPO	Concentration of phosphate in precipitation	0.000063	kg P m^{-3}
DRDEPNH	Mass of dry deposition of ammonium	15.7	kg N ha^{-1} a^{-1}
DRDEPNI	Mass of dry deposition of nitrate	4.4	kg N ha^{-1} a^{-1}
Lateral boundary			
COIDNH	Concentration of ammonium in infiltration water	0.00027	kg N m^{-3}
COIDNI	Concentration of nitrate in infiltration water	0.00006	kg N m^{-3}
COIDPO	Concentration of phosphate in infiltration water	0.00034	kg P m^{-3}
CODIORMAID	Concentration of DOM[1] in infiltration water	0.06100	kg OM m^{-3}
CODIORNIID	Concentration of DON[1] in infiltration water	0.00245	kg N m^{-3}
CODIORPOID	Concentration of DOP[1] in infiltration water	0.00015	kg P m^{-3}

[1] DOM, DON, DOP = dissolved organic matter, nitrogen and phosphorus, respectively

Given the range of annual precipitation sum in this part of the Netherlands, total atmospheric deposition amounts to 28–34 kg N ha^{-1} a^{-1} and 0.4–0.8 kg P ha^{-1} a^{-1}, depending on the precipitation sum. Concentrations of inorganic nitrogen compounds in ditch water are very low, while phosphate concentration is over twice the Dutch target level concentration of 0.00015 kg P m^{-3}. Values of DOM and DON are in line with values more often found in ditch water in similar peat areas (Hendriks, 1991 and 1997a).

Quantities of applied fertilisers are presented in Table 17b; distribution in time of ammonium, nitrate, organic-N, phosphate and organic-P in fertilisers is presented in Figure 8. In 2003, no fertilisers were applied within the simulation period. Ammonium volatilisation was based on Hendriks et al. (2002) and amounted to 10% for slurry and 16% for cattle droppings.

The annual average number of livestock units, NRGR, amounted to 2.0, 1.8, 1.4 and 1.3 for the years 2000, 2001, 2002 and 2003, respectively.

Table 17b Values of forcing variables for ANIMO: applied fertilisers with N and P content in the years of the field experiment. Values between brackets are N values corrected for ammonium volatilisation.

Year	Kind of fertiliser	Nitrogen (kg N ha^{-1})				Phosphorus (kg P ha^{-1})		
		Org-N	NH$_4$-N	NO$_3$-N	Tot-N	Org-P	Ortho-P	Tot-P
2000	slurry	73	73 (*66*)	0	146 (*139*)	7.3	13.2	20.5
	cattle droppings	55	55 (*46*)	0	110 (*101*)	5.5	9.5	15.0
	artificial N fert.	0	104 (*102*)	104	208 (*206*)	–	–	–
	Total	128	232 (*214*)	104	**464 (*446*)**	12.8	22.7	**35.5**
2001	slurry	86	86 (*78*)	0	172 (*164*)	8.6	15.7	24.3
	cattle droppings	51	51 (*43*)	0	102 (*94*)	5.1	8.8	13.9
	artificial N fert.	0	105 (*102*)	105	210 (*207*)	–	–	–
	Total	137	242 (*223*)	105	**484 (*465*)**	13.7	24.5	**38.2**
2002	slurry	83	82 (*73*)	0	165 (*156*)	8.2	15.0	23.2
	cattle droppings	37	37 (*31*)	0	74 (*68*)	3.8	6.4	10.2
	artificial N fert.	0	80 (*78*)	80	160 (*158*)	–	–	–
	Total	120	199 (*182*)	80	**399 (*382*)**	12.0	21.4	**33.4**

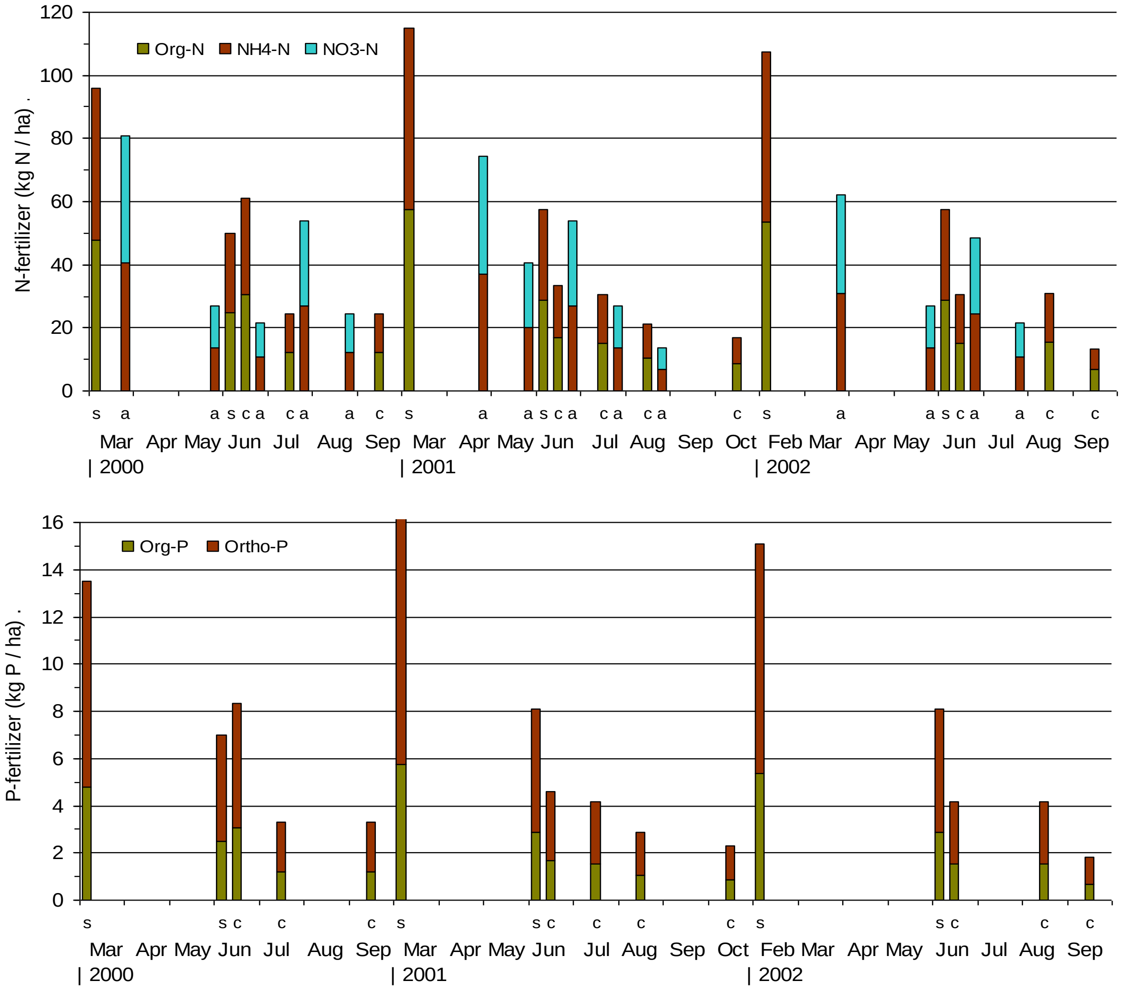

Figure 8 Distribution in time of applied N and P fertilisers for the years of the field experiment. s = slurry; c = cattle droppings; a = artificial fertiliser

3.3.2.2 Data for model calibration and validation

Concentrations of N and P compounds in soil water are given in Appendix 4.

Values of all other variables for calibration and validation of ANIMO are presented in Table 18.

Table 18 Values of target variables for calibration and validation of ANIMO

Description variable	Average value	Individual years			Unit
		2000	2001	2002	
N mineralization[1)]	263	280	232	286	kg N ha^{-1} a^{-1}
P mineralization[1)]	12	12	10	11	kg P ha^{-1} a^{-1}
Denitrification[2)]	87 (sd = 29) [4)]	–	–	–	kg N ha^{-1} a^{-1}
N uptake by crop[3)]	440	481	438	401	kg N ha^{-1} a^{-1}
P uptake by crop[3)]	44	48	43	40	kg P ha^{-1} a^{-1}

[1)] Van Beek et al., 2004a; [2)] Van Beek et al., 2004b; [3)] Van Schaik et al., 2004a;
[4)] Standard deviation

N mineralization rate is high compared to estimates for other similar eutrophic peats (values of Schothorst, 1977 in Hendriks, 1991, Schothorst, 1982; Berendse et al., 1994; Best and Jacobs, 2001). Van Beek et al. (2004a) explain this due to other sources (roots, stubbles etc.) of N than peat and the relatively warm weather in 2000 and 2002. But they state that ‘we cannot exclude some contribution of past fertilization as the zero-N plots were fenced only just in 2000’.

This last explanation is probably the most important. Limitation of the applied method is that it concerns organic matter enriched with N from long-time fertilising, and thus is not a good measure for mineralization of organic matter from peat soil. Because of its high content of organic matter, peat has a ‘strong memory’ for nutrients from fertilisation, i.e. nutrients are built-in in the organic matter. Hendriks et al. (2002) showed with ANIMO simulations for two peat soils that peaks in contribution of fertilisation to nutrient loading were 5-6 years behind peaks in fertilisation. In this present mineralization experiment, measurements were carried out over a period of four years starting directly after normal use and fertilisation. Therefore, it is concluded that it is very likely that in this way N mineralization of organic matter of peat was overestimated. Because it was estimated from N mineralization, P mineralization was very likely overestimated as well.

Denitrification rates were not available for the individual years, but only for two 'seasons' (see 3.3.1.2). Four estimations based on measurements and their average value are provided by Van Beek et al., 2004b. From these four values the mean and standard deviation as shown in Table 18 was calculated. Denitrification rate agrees reasonably well with the value of 70 kg N ha^{-1} a^{-1} reported by Koops et al. (1996) for a similar eutrophic peat pasture. About 69% of the annual N loss through denitrification originated from soil layers deeper than 0.2 m (Van Beek et al., 2004b).

4 Model execution and evaluation

In order to reach the main objective of this study – to evaluate the applicability of the SWAP-ANIMO model for simulating nutrient (N and P) loading of surface water in peat pasture areas – the model was tested against measured (time-series of) rate and state variables. The best way to test whether a model is able to simulate measured values of system variables is by building an optimal model for the modelled system, in the sense of putting into the model as much as possible known information about the system and tuning relevant unknown or uncertain model parameters against these object values. Depending on the degree of success in simulating the object values accurately, the conclusion will be that the model is more or less applicable to perform the intended simulations. Testing the optimal model against values of different but similar systems or conditions would give additional information about the models applicability.

The above described procedure is, obviously, known as calibration followed by validation of simulation models. It is adopted in this study to evaluate the applicability of SWAP-ANIMO for simulating nutrient loading of surface water in the Vlietpolder.

This Chapter explains the followed procedure. First the schematisation and discretisation of the system of the experimental site is described in Section 4.1. Then the calibration and validation of the model is discussed in Section 4.2.

4.1 Schematisation and discretisation

In order to model the system, the reality of the system must be schematised into the concept of and resulting description of reality in the model. For performing numerical calculations with the model, the modelled system must be discretized in space.

The situation of the experimental field is predominantly two-dimensional. Precipitation is collected at the soil surface and flows either vertically downwards through the vadose zone to the phreatic groundwater or laterally as surface runoff to the ditch. The difference in head between groundwater level and ditch water level is the driving force that causes drainage of groundwater towards the ditch. Streamlines are mainly perpendicular to the ditch as flow parallel to the ditch is insignificant because of relatively great distances between drains in that direction. Therefore, a two-dimensional (2-D) description of water flow through the peat soil is required for realistic simulations of leaching to the ditches.

The SWAP-ANIMO model is in principal a one-dimensional (1-D) model as it simulates flow of water and transport of solutes in the vertical direction in a 1-D soil column. Drainage or infiltration (subsurface irrigation) fluxes are basically calculated as exchange of water between the saturated soil as a whole and the drains. However, for transport of solutes it is crucial to simulate in a realistic way distribution of flow over horizontal soil layers with different properties at different depths, and residence and travel time of solutes at given depths. Therefore, in SWAP-ANIMO a pseudo 2-D concept is adopted for subdividing total drainage fluxes into sub-fluxes through each saturated soil compartment (Groenendijk et al., 2005).

In order to simulate the 2-D reality of the experimental site with the 1-D/pseudo-2-D model, the 2-D site must be schematised into a 1-D soil column that represents the vertical structure of the soil profile as given by the subdivision in different soil horizons. Therefore, average depths of horizon boundaries were established for the cross section of the field where samples were taken, including the upper boundary of the first horizon, being the soil surface. Depths of horizon boundaries in the cross section could be expected to be fairly constant regarding the relatively short distance (40 m) between the ditches and the nature of the soil deposits. This did not count for the graded soil surface, with a maximum difference in elevation of 0.6 m (see Appendix 4, fig. A4.1).

An average soil surface elevation was obtained by numerical integration of the elevation from middle to side of the field at the cross section. Boundary depths of the five distinguished soil horizons were expressed relative to the average soil surface (see Table 4). The enhancing effect of the graded soil surface on surface runoff was expressed by the small value of 3 mm for the maximum ponding height, the threshold for generation of runoff (see 3.2.1.1).

For performing numerical calculations, the vertical soil column was discretized into model compartments (Table 19 and Fig. 9). The two sub-models SWAP and ANIMO require different vertical schematisations. For correct simulation of infiltration at the soil surface, SWAP needs relatively thin (order of 0.01 m) compartments at the top of the model column (Van Dam and Feddes, 2000). ANIMO requires thicker compartments at the top, because in this model physical dispersion is accounted for by numerical dispersion, which is controlled by compartment thickness (Groenendijk et al., 2005). Experience has pointed out that compartment thicknesses of 0.05 to 0.10 m in the first meter of the model column yield realistic dispersion. For both models, compartment thickness may gradually increase with depth, as conditions become less dynamic with increasing depth.

Tabel 19 Vertical discretisation of the soil column in model compartments for SWAP and for ANIMO. Depth and thickness in m; depth refers to average soil surface.

Horizons						Compartments			
Number	Code	Description	Depth		Total thickness	SWAP		ANIMO	
			top	bottom		thickn.	number	thickn.	number
1	T1	Toemaakdek 1	0.00	–	0.05	0.01	5	0.05	1
			–	0.20	0.15	0.025	6	0.05	3
2	T2	Toemaakdek 2	0.20	0.28	0.08	0.04	2	0.08	1
3	K	Clayey peat	0.28	0.48	0.20	0.05	4	0.10	2
4	Vo	Peat, oxidised	0.48	0.78	0.30	0.05	6	0.10	3
5	Vr	Peat, reduced	0.78	–	0.20	0.10	2	0.10	2
			–	–	1.00	0.20	5	0.20	5
			–	2.98	1.00	0.25	4	0.25	4

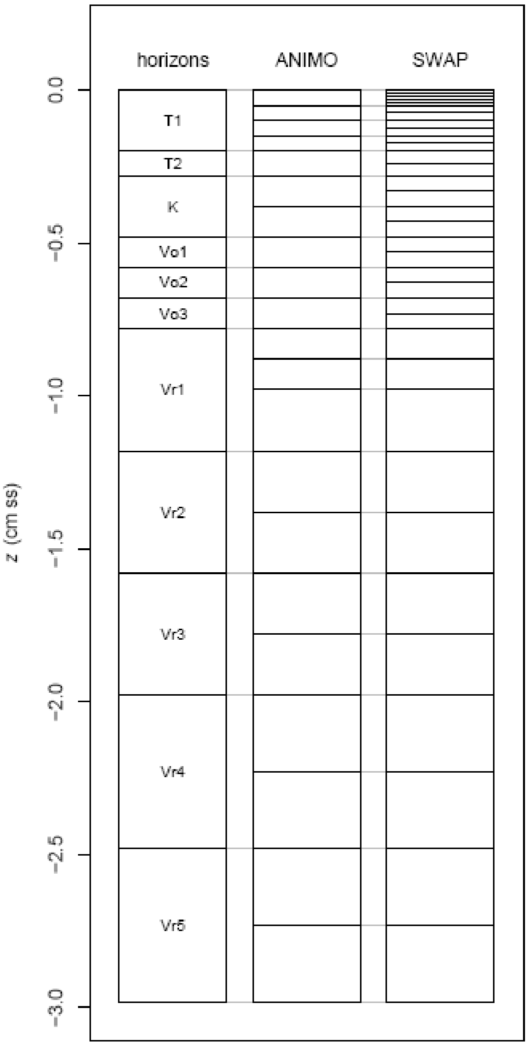

Figure 9: Soil profiles with (sub-) horizons and corresponding numeric compartments of ANIMO and SWAP

Vertical flow in the model column is governed by vertical hydraulic conductivity and pressure head gradients, while distribution of lateral flow over the compartments in the saturated zone is determined by the transmissivities of these compartments. Transmissivity is the product of compartment thickness and saturated horizontal conductivity. The latter is obtained by multiplying the saturated vertical conductivity by an anisotropy factor (COFANI; see 3.2.1.1). COFANI's were obtained in a calibration process against Cl loads discharged to the surface water (see Section 4.2.1.1).

4.2 Calibration and validation

In Chapter 3 it was shown how SWAP and ANIMO were parameterized. Values were assigned to state variables and rate parameters based on field and laboratory measurements, expert knowledge, or by adopting default, but plausible, settings. Some important parameters, however, could not be quantified this way, and had to be obtained by means of calibration. Calibration is the process of estimating model parameters given a set of observations.

During calibration, a set of parameters is modified in order to improve an objective function. An objective function quantifies the degree to which model output matches observations. An often used objective function is the sum of squared errors, i.e. the sum of the squared differences between observed and modelled quantities.

Validation is the process of evaluating the quality of the calibration. In general, the aim of validation is to establish the accuracy of the numerical solutions produced and the range over which the model is valid and appropriate to the domain of its intended use (Irving, 1988). During validation, the output of a calibrated model is compared with independent observations. As a general rule, observations that have been used for calibration should not be used for validation. This can for instance be accomplished by splitting the observation period in a calibration part and a non-overlapping validation part. Considering that only a limited amount of observations was available, collected in a relatively short time span, it was decided to use the entire observation period for calibration. As a consequence, it was not possible to validate on groundwater levels and nutrient concentrations since these model outputs were already used for calibration. Validation would then result in an unfair and overoptimistic judgment of model performance.

Although proper validation was not possible, it was possible to evaluate model performance based on model output that had not been used for calibration. In this study the model outputs were cumulative discharge for SWAP and crop uptake, denitrification and mineralization for ANIMO. Although these model outputs had not been used for calibration, they were not entirely independent. For instance, discharge is positively correlated with groundwater level. Due to this dependence, the obtained model performance evaluations were theoretically too optimistic.

To simplify calibration and validation, a stepwise procedure has been pursued. SWAP has been calibrated and validated in the first step (Section 4.2.1). In the second step, ANIMO has been calibrated and validated on the basis of hydrological input generated with the calibrated SWAP model (Section 4.2.2).

4.2.1 SWAP

Six SWAP process parameters have been calibrated (see Table 3, Section 3.2.1.1): number of drainage levels (NRLEVS), drainage resistance (DRARES1) and infiltration resistance (INFRES1), both of drainage level 1, the coefficient of interflow (COFINTFLB), the anisotropy factors for regulating distribution of drainage fluxes over saturated model compartments (COFANI), and the vertical flow resistance of the aquitard (RIMLAY). Methods and results of these calibrations are discussed below.

4.2.1.1 Calibration methods

Several methods were used to calibrate the various parameters. NRLEVS was not really calibrated but was the result of the calibration of DRARES1 and INFRES1 (see

Section 3.2.1.1 ***2. Process parameters***). RIMLAY and COFANI were calibrated by hand by running the model over and over again, adjusting the parameter values until the intended value of the object parameter was obtained. The drainage parameters DRARES1, INFRES1 and COFINTFLB were calibrated in an automatic calibration procedure.

RIMLAY

In the case of RIMLAY, the calibration procedure was applied before calibration of the other parameters, which was allowed as it was clear from literature that this resistance was very high and downward seepage was very low. Thus the exact value was not very sensitive to the values of the other parameters. The object parameter was the average annual downward seepage of 25 mm (see Section 3.2.2.1 ***2. Process parameters***).

Drainage parameters: DRARES1, INFRES1 and COFINTFLB

DRARES1, INFRES1 and COFINTFLB were calibrated simultaneously in an automatic calibration procedure. The objective function was the sum of squared errors calculated by comparing modelled and observed groundwater levels (Section 3.3.1.2). Surface water discharge was not considered as a target variable in calibration since the reliability of the observations was somewhat questionable (see Section 3.2.1.2). Therefore, surface water discharge observations were used for qualitative validation. The optimization algorithm that was used was Nelder-Mead's Down-Hill Simplex method (Press et al., 1992). To minimize the risk of ending up in a local minimum, a total of thirty randomly selected initial parameter vectors were tried.

To get an idea of the sampling space of these initial parameter vectors, the objective function value was mapped out in parameter space. An example is given in Figure 10. Note that the optimum is somewhere within the most inner ellipsis. Since many optima yielded similar results in terms of the objective function value (a.k.a. equifina-lity; Beven & Freer, 2001), the most likely parameter set was selected by means of expert judgment of the water balances.

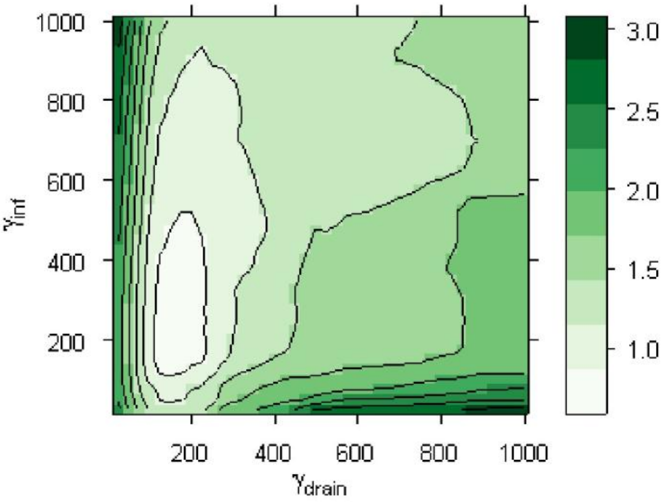

Figure 10 Objective function value as function of drainage resistance (days) and infiltration resistance (days). Lower values indicate a better calibration result.

COFANI

Simulation of solute transport to and from drains requires a realistic distribution of drainage fluxes over saturated model compartments. SWAP needs an anisotropy coefficient COFANI for each soil horizon for simulating this distribution (Table 3). Since this parameter is not required for performing regular SWAP simulations, i.e. calculation of water balance and transport in the unsaturated zone, it has only negligible effect on simulated magnitude of drainage fluxes. Therefore, COFANI can be best calibrated after calibration of the other parameters.

The object parameter was the cumulative chloride load discharged from the ditch in a drainage situation. Objective was to obtain the measured cumulative load at the end of the period under the condition of an optimal fit of the time course of the cumulative load. Measured loads were calculated from measured water discharge and Cl concentrations in ditch water. Since measured discharge was reliable only for the four month period of December 2002 until April 2003 (see Section 3.2.1.2), this period was taken for the calibration of COFANI.

Modelled chloride loads were obtained by simulation of ammonium discharge with ANIMO on the basis of SWAP calculations. By excluding all processes and other solutes except ammonium transport and storage, it was achieved that ammonium represented the conservative solute chloride. Measured Cl concentrations (Appendix 4) were used for initial concentrations in ANIMO. In the saturated deepest 2.2 m of the soil profile with reduced peat (see Table 19), chloride concentrations increased with depth from 50 mg l^{-1} to 350 mg l^{-1} (not shown in Appendix 4). These data were measured at the experimental site by (2005). These high concentrations distinguished the lower part of the profile clearly from the upper part, which provided a good basis for performing calibration of COFANI in this manner. Atmospheric deposition was included as chloride source.

Calibration was performed by hand and visual comparison of graphs. For converting the modelled loads per ha to loads for the total catchment, the mean value of 3.2 ha for the area of the experimental field and its uncertainty range from 3.0 to 3.4 ha were used (see Section 3.2.1.2).

4.2.1.2 Calibration results

Calibration results in terms of the obtained parameter values are provided in Section 3.2.2.1, Tables 8b and 8c. Results in terms of the object function and simulation of the time course of measured groundwater tables, as well as the time course of measured versus modelled chloride discharge load are presented below.

Figure 11 shows that SWAP captures the dynamic behaviour of the groundwater level in time quite well, although the timing is not always very precise. The latter is reflected in the results that represents the residuals, the difference between simulated and observed values. Figure 11 shows the plot in time of the residuals. The average value of the residuals amounted to 0.099 m while the RMSE (root mean squared error) was 0.116 m, which is a reasonably good result for this kind of models.

Figure 12 depicts the comparison between simulated and observed chloride loads discharged from the experimental ditch. Deviances in the fits are due to differences in water discharge as well as in chloride concentrations. The first is relatively small (see Fig. 13). Taking this into account, the result of the simulation is reasonable.

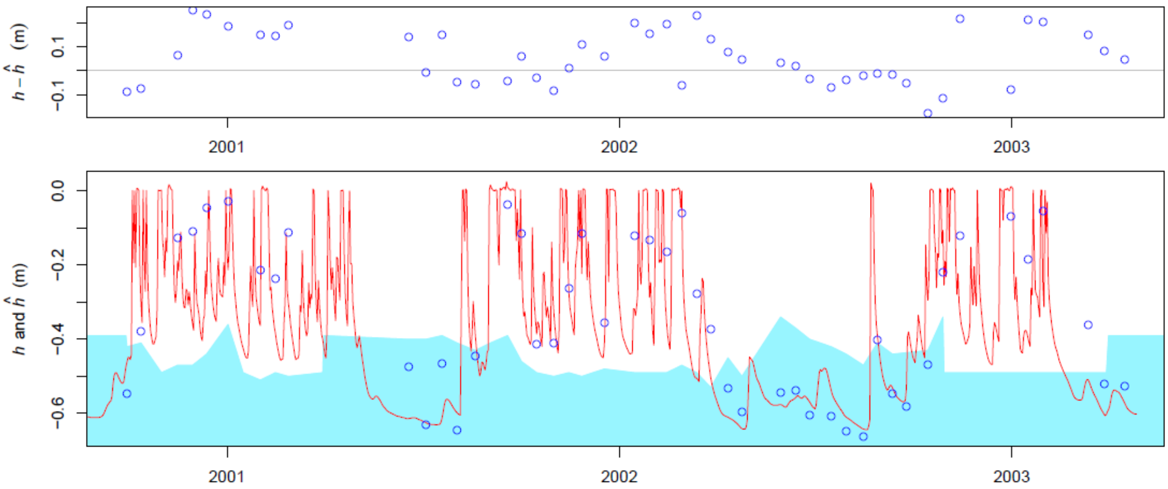

Figure 11 Bottom: simulated (ˆh) and observed (h) time-series of groundwater levels (m). Top: residual plot: h − ˆh (m). The shaded area represents corresponding surface water levels.

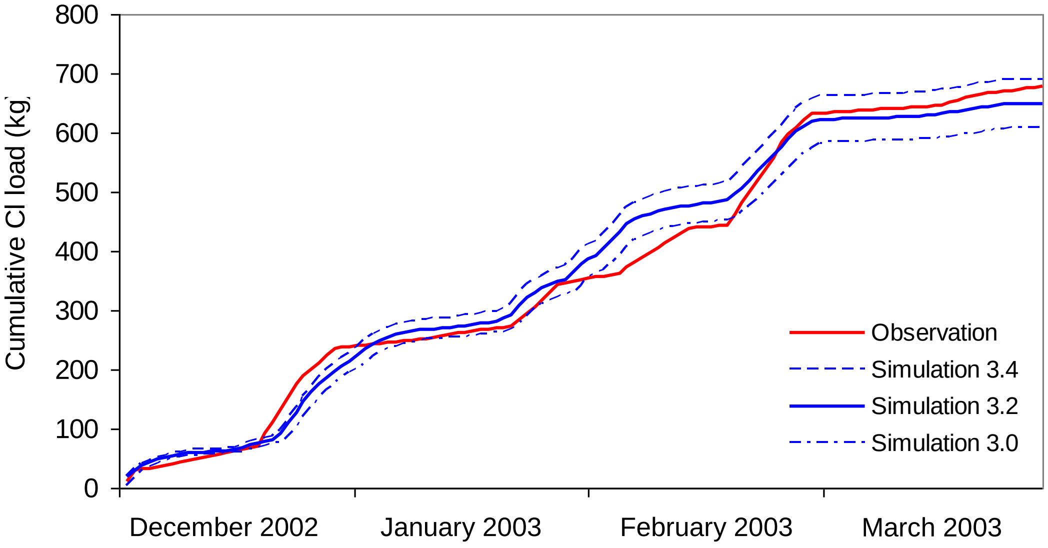

Figure 12 Simulated and observed time-series of cumulative Cl loads discharged from the experimental ditch. Simulations are for the mean catchment area of the ditch (3.2 ha) and for the lower (3.0 ha) and upper (3.4 ha) limits of the estimated range of this area.

4.2.1.3 Validation

For independent validation measured drain discharge and surface runoff were used (see Table 6). The latter, only to verify whether the lower limit of 8% of the annual drain discharge was met (see Section 3.2.1.2).

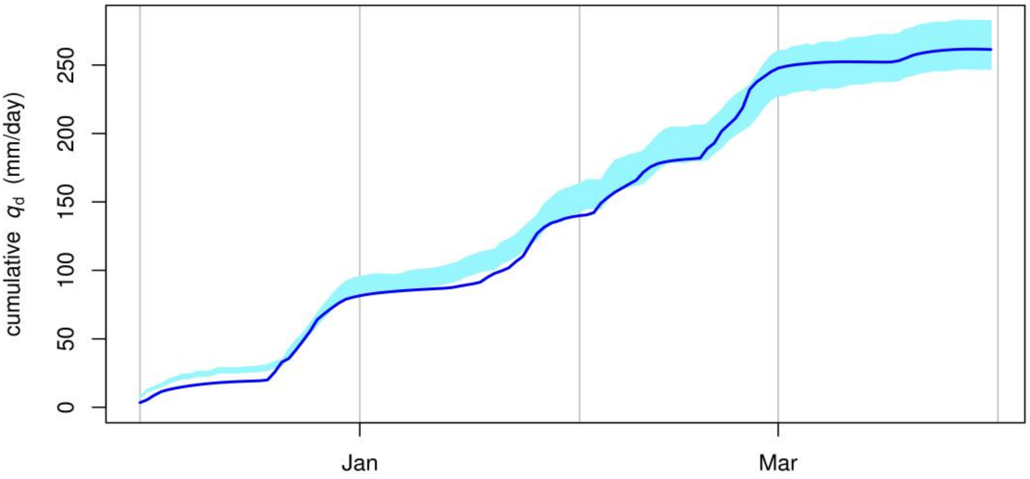

Figure 13 Simulated cumulative (blue line), versus measured discharge for the period December 2002 until April 2003. The latter is represented as a band due to uncertainty about the area that contributes to the ditch

Figure 13 presents the validation of the modelled discharge against measured discharge for the period December 2002 until April 2003. The result of this independent validation is quite good, which is an important result as discharge is the basis of nutrient loading of the surface water, the subject of this study. The main deviance in fit of the cumulative total drainage function is due to the first week of December. At the beginning of the period, the model seems to underestimate cumulative discharge. Starting at December 11 would give a much better fit. Partly due to temporal aggregation, the model matches the observations better near the end of the period.

Despite the good result, the value of this validation is only limited because of the short period of just four month. Furthermore, this validation gives no information about the periods with water recharge due to infiltration (submerged irrigation).

Runoff is with 20-35% of total discharge far above the lower limit of 8% of total discharge (see Table 10). According to Meinardi (2005) runoff in the Vlietpolder generally amounts to 20% of total discharge. This does not count exclusively for graded fields like the experimental site. Thus it may be expected that runoff is greater at graded fields. The simulated high values amount to 10-20% of precipitation. Expressed in this manner, they coincide rather well with runoff estimations for the total Vlietpolder in the range of 10-15% of precipitation reported by Michielsen and Van Schaik (2004).

4.2.1.4 Conclusions

On the basis of the obtained calibration and validation results it can be concluded that SWAP is reasonably well able to simulated groundwater level behaviour and drainage to surface water in the peat pasture area of the Vlietpolder for the simulated period.

Especially, the later result is relevant because it concerns the subject of this study: nutrient loading of the surface water. However, the relevance of this conclusion is rather limited because of the limitations of the calibration and validation results, which counts especially for the validation because of the short period. Another important limitation is that it was not able to calibrate and validate SWAP against data about moisture content or pressure head. These parameters are crucial for ANIMO simulations as they control many processes in the C, N and P cycles.

4.2.2 ANIMO

A set of six ANIMO parameters and initial conditions have been calibrated (see Section 3.3, Tables 11, 12a, 12b and 12d). These are the initial ammonium (CONH) and phosphate (COPO) concentration in the soil solution for the peat layers V0, Vr1, and Vr2 (Table 19), the parameters of the oxygen diffusion equation PMDF1HN and PMDF2HN for soil layers T1, T2 and K, the nitrate transpiration stream concentration factor for grassland (DFCFUPNIGR), and the denitrification rate (RECFDEAV). Methods and results of these calibrations are discussed below.

4.2.2.1 Calibration methods

Prior to the actual calibration, the initial conditions of the distinguished organic matter pools were tuned in a pre-run as explained in Section 3.3.1.1 ***1. Initial values of states.***

ANIMO was calibrated in an automatic calibration procedure by minimizing the difference between observed and modelled total N and phosphate – total P was not measured – concentrations in the soil solution (object function). This has been accomplished in a Bayesian setting by sampling the joint posterior parameter distribution by means of Markov Chain Monte Carlo (MCMC). The MCMC algorithm proposed by ter Braak (2006) was used. Although this algorithm provides an estimate for the entire joint parameter distribution, only a single parameter set has been selected for performing the system and scenario analyses described in Chapter 5. Selection was based on expert judgment. It was not possible to take parameter uncertainty into account during the system and scenario analyses. The reason was that no tools were readily available for performing analyses in this way. It was not possible to make these required tools within the limited time of the project.

Calibration of the initial concentrations in soil solution of ammonium (CONH) and phosphate (COPO) was performed by calibrating the concentration in the first (shallowest) peat soil compartment. With this calibrated value and a fixed value for the deepest soil compartment from Meinardi (2005), values for concentrations in the remainder of the compartments were calculated by interpolating linearly between calibrated upper and fixed lower value.

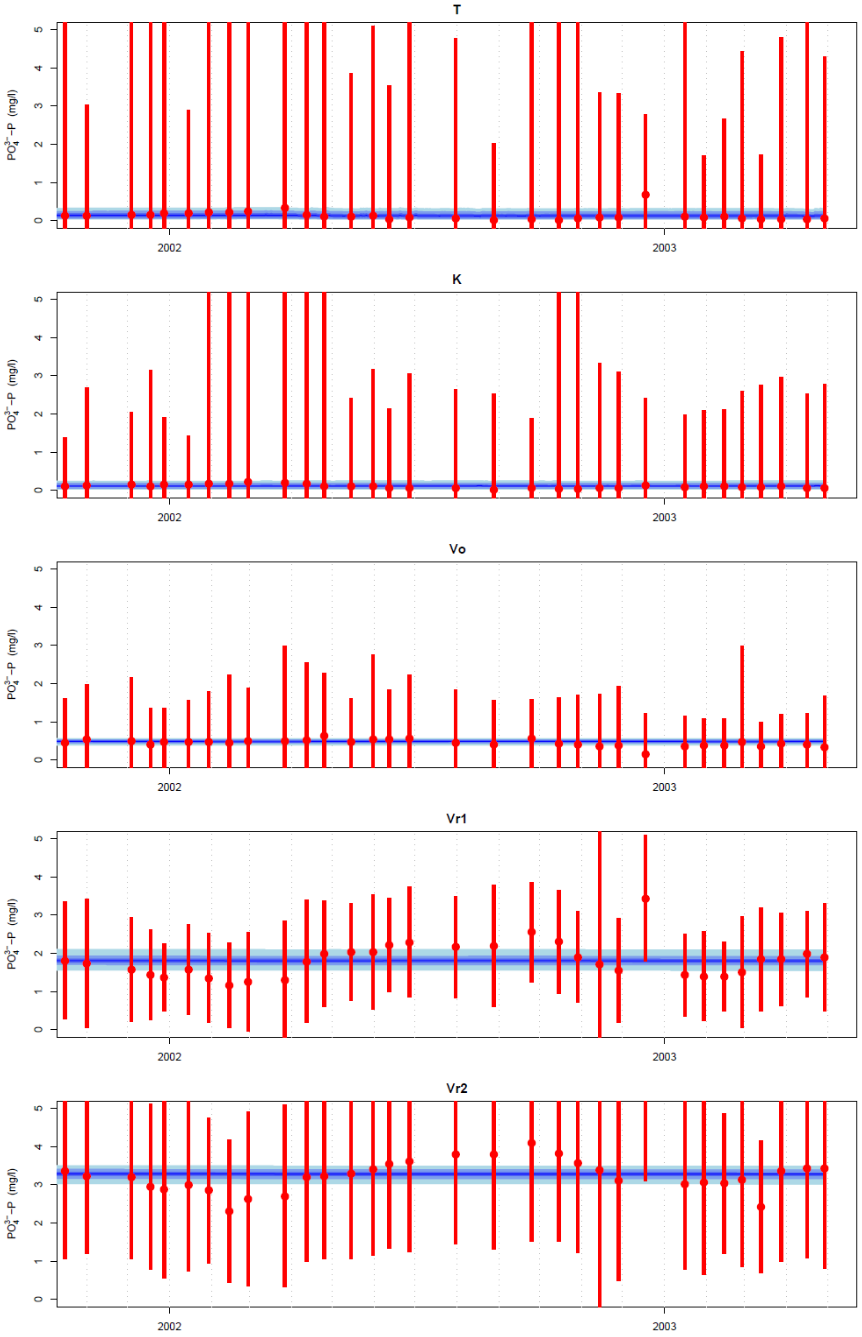

Figure 14 Calibration results for phosphate concentration (mg P l^{-1}) in soil solution, for soil horizons T, K, Vo, Vr1 and Vr2 (see Table 19). Mean observations (red dots) and standard error of the mean (red lines) corrected for missing values. The blue bands give model predictions for phosphate. The outer band is the 95% prediction interval, the inner band the 50% prediction interval and the blue line is the median prediction.

4.2.2.2 Calibration results

Calibrated values of parameter are provided in Section 3.2.2.1, Tables 16a-c. Results in terms of simulation of the time course of measured concentrations in the soil solution are presented in this Section.
The calibration results for phosphate and total N are given in Figures 14 and 15, respectively. The mean phosphate and total N concentrations (mg P or N l^{-1}) based on observations are given as red dots. The corresponding standard errors are presented as red vertical lines. These standard errors are corrected for missing values by means of the imputation procedure of Van Buuren and Oudshoorn (2000, see also Appendix 4). The model predictions are given as blue bands. These blue bands represent parameter uncertainty. The blue line is the median prediction, the outer band is the 95% prediction interval and the inner band the 50% prediction interval.

Calibration for phosphate indicates that the temporal variation of the mean observed phosphate concentration is very low with very large standard errors in the two mineral topsoil horizons. This counts less for the soil horizon Vo with oxidized peat, where standard errors are lowest. In the two reduced peat horizons Vr1 and Vr2 temporal variation is highest and also standard errors are large. Temporal variation of the corresponding model simulations for phosphate is negligible in all horizons. In addition, the systematic error is limited. Reason for the low variation in observations and simulations is the strong adsorption capacity of the soil, which is larger in the mineral soil horizons than in the peat soil horizons. In the latter horizons the fraction of irreversible adsorped phosphate was possibly overestimated. On the other hand, roughly tuning of some of these parameters did not improve simulation results in terms of more temporal variation in simulated concentrations. But in general, the model captures the mean of the observations quite well in all soil horizons.

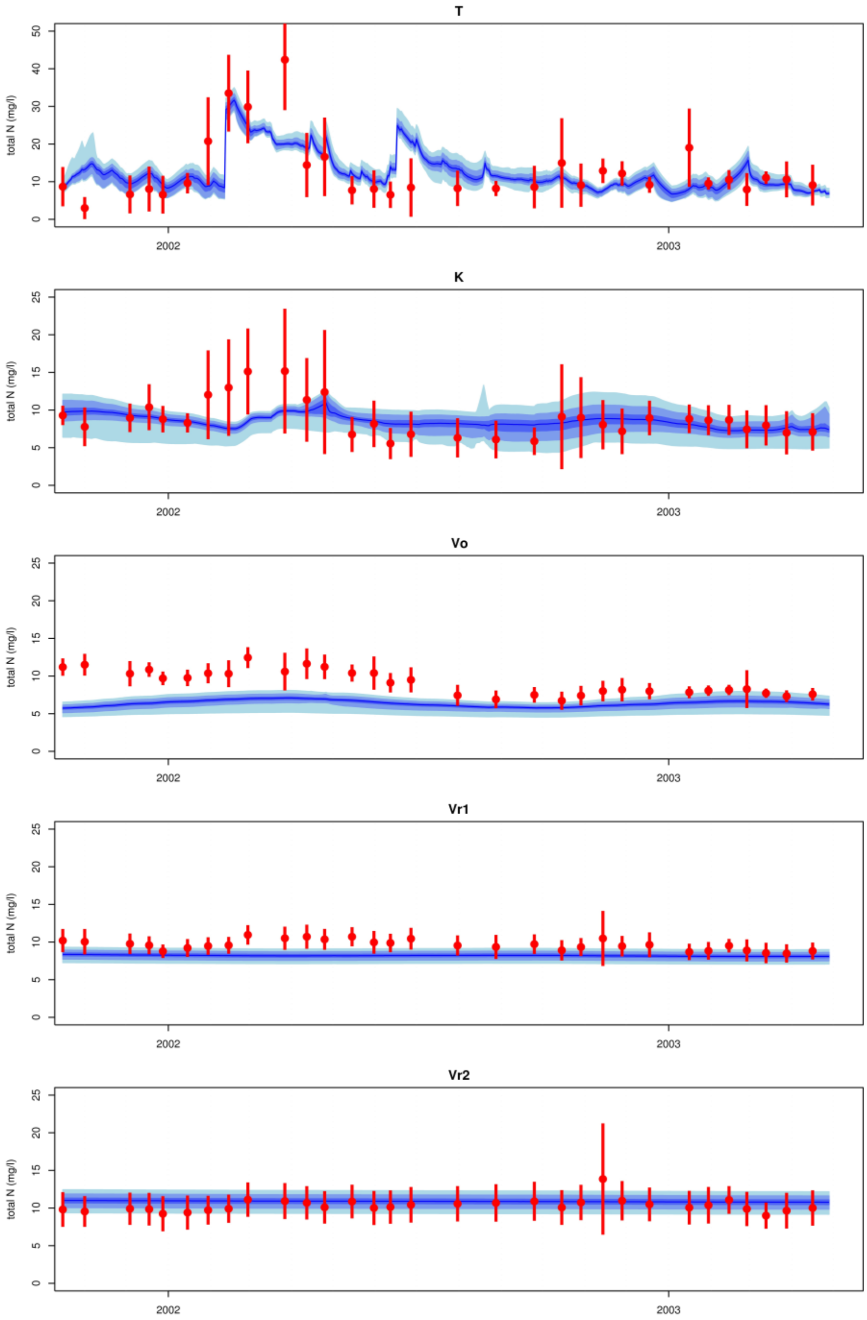

Figure 15 Calibration results for total nitrogen concentration (mg l^{-1}) in soil solution, for soil horizons T, K, Vo, Vr1 and Vr2 (see Table 19). Mean observations (red dots) and standard error of the mean (red lines) corrected for missing values. The blue bands give model predictions for total N. The outer band is the 95% prediction interval, the inner band the 50% prediction interval, and the blue line is the median prediction. Note the difference in scale of the y-axes of the T horizon!

For N, the figures clearly illustrate the uncertainty in both the average value of the observations and the model predictions. The uncertainty in the average concentrations is higher in the topsoil than in the subsoil. This clearly illustrates the more dynamic environment for N related processes in the top soil. Model simulations roughly follow the observations. In the mineral topsoil horizons T and K, the model tends to slightly overestimate the N concentrations in summer. Simulations in winter 2002-2003 are in general quite accurate in these horizons. The deviances are largest here at the end of winter 2002 after an early slurry application in February (Table 17b, Figure 8). Especially, in the K horizon the model is not able to simulate accurately the observed concentrations. In winter 2003, no fertilisers were applied.

In the reduced peat soil horizons Vr1 and Vr2, the model simulates very little temporal variation in N concentrations. This is more or less in line with the observations. In these horizons, especially in Vr2, transformation processes are extremely slow due to anaerobic conditions in these permanently saturated peat layers. Mean observations are rather well simulated, with a small underestimation for horizon Vr1. In the oxidized peat horizon Vo the model underestimates both variation and concentrations in winter 2001-2002. In the last half of the shown period the model performance is better.

The underestimation of mean concentrations in horizon Vr1 and to a lesser extend in Vo is due to underestimation of the dissolved organic N concentration (DON) by the model. ANIMO contains only one pool of dissolved organic matter (DOM). This is found before, to be a serious short coming for simulating peat soils fertilised with organic fertilisers (Hendriks, 1993). The standard value for the decomposition rate constant of DOM (RECFCAAV in Table 12a) of 30 a^{-1}, is calibrated for mineral soils fertilised with organic fertilisers (Renaud et al., 2005). Hendriks (1993) found a threefold lower value of 10 a^{-1} for unfertilised peat soils. He used a 'compromise value' of 15 a^{-1} for peat soils with organic fertilisers, which is used in the present simulations of Figure 14 as well (see Table 16a). On the basis of this knowledge, the effect of varying the value of RECFCAAV between values of 10, 15 and 30 a^{-1} on DON concentrations was investigated.

Results are presented in Figure 16. It is shown that in the mineral topsoil horizons which are influenced by organic fertilisers and other types of fresh organic matter, higher values of RECFCAAV are required than in the peat horizons with organic soil. With increasing depth, lower values are required in order to avoid underestimation of DON and consequently DOM concentrations. With the exception of the deepest horizons were hardly any decomposition of DOM takes place, so that consequently the value of RECFCAAV is irrelevant. On the other hand, too low values overestimate DON in the upper mineral soil horizons.

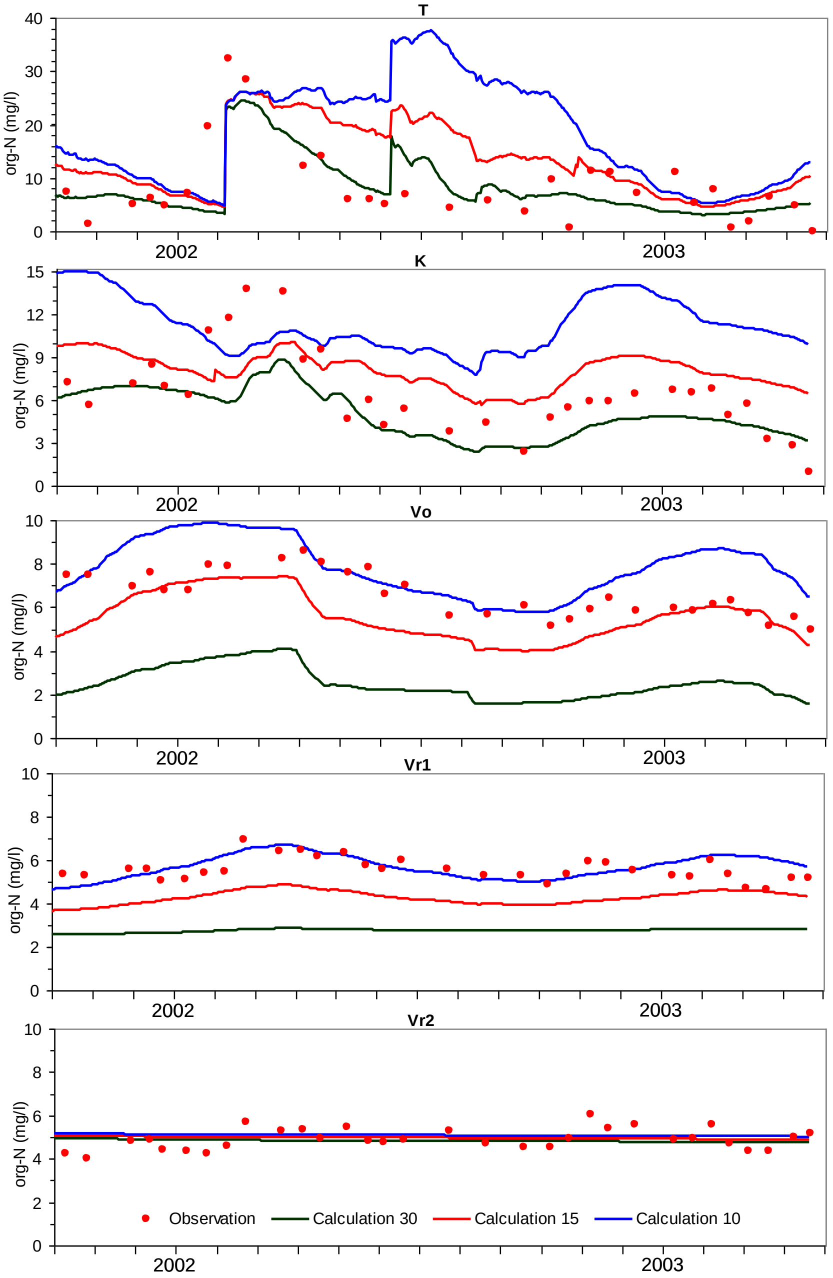

Figure 16 Observed and simulated dissolved organic N concentration (mg l-1) in soil solution for soil horizons T, K, Vo, Vr1 and Vr2 (see Table 19). Simulations are for three values of the decomposition rate constant of dissolved organic matter. Note the difference in scale of the y-axes!

These findings can be explained in terms of labile DOM originating from fresh organic matter versus more stable DOM originating from old and partly decomposed organic matter. The latter will consist of a lower fraction of DOM with high decomposition rates. After all, the easily decomposable molecules will be decomposed in soils with merely old organic matter.

This result leads again to the conclusion that a model with only one pool of DOM is not fit for simulation of nutrient leaching of organic soils fertilised with organic fertilisers. The compromise value gives too high concentrations of DON in horizons

T and K, and too low concentrations in horizons Vo and Vr1. Therefore, it is recommended to add a second, stabile pool of DOM with it's own properties independent of the properties of the existing pool.

4.2.2.3 Validation

The performance of the calibrated ANIMO model was evaluated by comparing modelled values of independed parameters to observed (measured or estimated) values. These parameters were (see Table 14): mineralization rate of peat, denitrification rate, and annual N and P uptake by the crop. The results of this validation are depicted in Table 20.

Table 20 Observed (estimated) and simulated N and P mineralization, denitrification and crop uptake of N and P. All values in kg N or P ha^{-1} a^{-1}. Values between brackets are % of observed values (mean, in case of denitrification).

Description variable	2000		2001		2002	
	Observat.	Simulat.	Observat.	Simulat.	Observat.	Simulat.
N mineralization	280	160 (57)	232	144 (62)	286	135 (47)
P mineralization	12	9 (75)	10	7 (70)	11	6 (55)
Denitrification	87 ± 29	89 (102)	87 ± 29	111 (127)	87 ± 29	75 (87)
N uptake by crop	481	468 (97)	438	407 (93)	401	414 (103)
P uptake by crop	48	47 (97)	43	39 (90)	40	42 (105)

All results are very good, in the sense of comparing observed and simulated values, with the exception of mineralization rates for which simulations were much – N: 38-53%, P: 25-45% – lower than the estimated values. As discussed in Section 3.3.2.2, these estimations are high compared to other findings for similar eutrophic peat soils. The simulated values for N are all in the range of N-mineralization rates estimated by Hendriks (1991) as function of ditch water level, through interpolation between measured values reported by Schothorst (1977) for similar Dutch eutrophic fen peats with various ditch water levels. Thus it was concluded that the simulations are more reliable than the estimations for reasons given in the discussion in Section 3.3.2.2. Consequently, the results of this aspect of the validations are quite good as well.

Simulated denitrification rates are all in the range of the mean value ± the standard deviation (see Table 18). Results for annual N uptake and, to a somewhat lesser extend, P uptake are especially good. Simulated N and P uptake are in the range of 93-103% and 90-105% of measured values, respectively.

Despite the good results, the value of this validation is only limited, because contrary to the validation of SWAP, it provides no information about the model performance concerning the subject of this study: the correct simulation of the N and P loading of the surface water. Nevertheless, the good results are encouraging, because possible results indicating that the model is not able to correctly simulate N and P loading are lacking as well.

4.2.2.4 Conclusions and recommendation

On the basis of the obtained calibration and validation results it can be concluded that ANIMO is reasonably well able to simulate the average N and P concentrations in the peat soil of the experimental field, and that the model is well able to simulate the important terms of the N and P balance: N- and P-mineralization, denitrification and annual N and P uptake by the crop. But no direct information was obtained about the model's ability to correctly simulate N and P loading of the surface water. Nevertheless, the combination of good results of the validation of discharge simulations with SWAP and the reasonable results of the ANIMO simulations of N and P concentrations, gives reason for having confidence in the results of SWAP-ANIMO simulation of N and P loading of the surface water in peat pasture areas like the Vlietpolder.

From evaluating the effect of the decomposition rate of the pool of dissolved organic matter (DOM) on the concentrations of dissolved organic N in the soil solution, it is recommended to add a second pool of DOM with its own properties independent of the properties of the existing pool. The present pool can then be used as it generally is, for more labile DOM originating from (fresh) organic matter in the topsoil, while the second pool can be deployed for simulation of more stable DOM originating from old organic matter like peat.

5 System and scenario analyses with the calibrated model

Calibrated and validated models can be powerful tools for analysing the system for which they are calibrated and validated. For the purpose of gaining insight in detailed processes that are hard to study by experimental methods or for to derive immeasurable parameters from measured state and/or rate variables, models can be vital instruments as they contain (mostly) all of our knowledge about the system in a dense and formal way, readily for execution. Furthermore, calibrated and validated models can be used for performing scenario analyses in order to predict the behaviour of the system under different conditions than the ones experimentally studied. Mostly in the way of investigating the effects of changes in the driving forces, like climatic changes, effects of different fertilisation levels, changing the drainage basis by rising or lowering ditch water level etc. Boundary condition for both applications is that the model should not be used beyond the limits for which it was calibrated and validated.

Section 5.1 deals with the system analyses and Section 5.2 with the scenario analyses that are carried out with the calibrated and validated model.

5.1 System analyses

The main objective of the ‘DOVE’ projects was to study the contribution of dairy farming to the nutrient loading of surface waters for clay, peat and sandy soils. This implied assessment of as well the total loading as the contribution of the agricultural use. The nutrient loading of surface waters from soils is only directly measurable if the bottom boundary is impermeable and drainage occurs via drain pipes that are well measurable and sampleable. This situation is rarely to be found in peat pastures in The Netherlands and did not exist in the experimental site in The Vlietpolder.

In these cases, nutrient loading must be assessed by interpreting parameters that can be measured with the best knowledge about the system that we have. These parameters concern for instance the course in time of groundwater level and concentrations of chloride, nitrogen and phosphorus compounds in soil, groundwater and surface water, in relation to the discharge of the ditch. Such an interpretation is a model of reality that will be more complex as more information is taken into account. Several models are applied in the ‘DOVE-veen’ project (e.g.Van Beek et al., 2004a), among which SWAP-ANIMO. The advantage of this model is its process-oriented nature that allows analysis of system processes and model prediction.

This section discusses the calculation with the model of the magnitude of the actual nutrient loading of the surface water (5.1.1) and the analysis of the contribution of the main nutrient sources to this loading (5.1.2).

5.1.1 Actual loading of surface water

The nitrogen and phosphorus loads to the surface water as calculated by the calibrated SWAP-ANIMO model differ strongly between the various years (Fig. 18): for nitrogen from 26 to 48 kg per ha per year and for phosphorus from 3.1 to 5.4 kg per ha per year. The cause of this is the great variety in precipitation and more precise precipitation surplus in the considered years: 908 and 297 mm respectively in the year 2000, 1215 and 633 mm in 2001, and 989 and 375 mm in 2002. In 2001, the nitrogen and phosphorus loads are exceptionally high because of the extreme weather conditions.

The year averaged drainage water concentrations, calculated as annual nutrient loads divided by annual water loads, differ substantially less between the considered years than the loads (Fig. 18): 6.6-7.6 mg N per litre and 0.79-0.87 mg P per litre, respectively. Remarkable is that in 2001 N and P loads are highest but concentrations are intermediate, while in 2002 N and P concentrations are highest and loads are intermediate. This is caused by runoff of large amounts of precipitation during heavy rainstorms at times that little remains of fertilisers are present at the soil surface, resulting in relatively low N and P concentrations in drainage water. In 2000, both loads and concentrations are lowest. In this driest year, N and P from fertilisers are better utilised by the grass crop than in the wetter years.

Loads and especially concentrations are in the same order of magnitude as those calculated by SWAP-ANIMO for similar peat pastures in De Alblasserwaard, De Krimpenerwaard and De Lopikerwaard in The Netherlands (Hendriks, 1993; Hendriks, 1997b; Hendriks et al., 2002; Hendriks, 2003). All loads are within the broad ranges for N and P loads of 29-61 kg N ha^{-1} a^{-1} and 2.8-8.8 kg P ha^{-1} a^{-1} respectively, as calculated for 2000-2002 by Van Beek et al. (2004a). Their means and medians for the three years-period are substantially lower than the arithmetic averages of the ranges of the present study.

5.1.2 Contribution of sources

The calibrated SWAP-ANIMO model was used to analyse the contribution of the main nutrient sources to the surface water loading: 1. fertilisation, 2. atmospheric deposition (wet and dry), 3. infiltration of ditch water, 4. decomposition and mineralization of organic matter (mostly, but not only peat) and 5. leaching out of the N and P rich peat in the saturated zone of the peat soil. For this purpose, all five sources were one by one excluded from the simulations including the ‘historical’ pre-run. The difference between results of simulations with and without the concerning source were compared to calculate the contribution of that source. Contributions of the five individual sources were summed up and the sum was compared to the loads of the regular runs. Differences were within 10% of the regular loads. These differences were distributed over the five sources according to their relative contribution.

In the extremely wet years 2001 and 2002, fertilisation provides the highest contribution (50%) to the phosphorus loading and an equal contribution (40%) to the

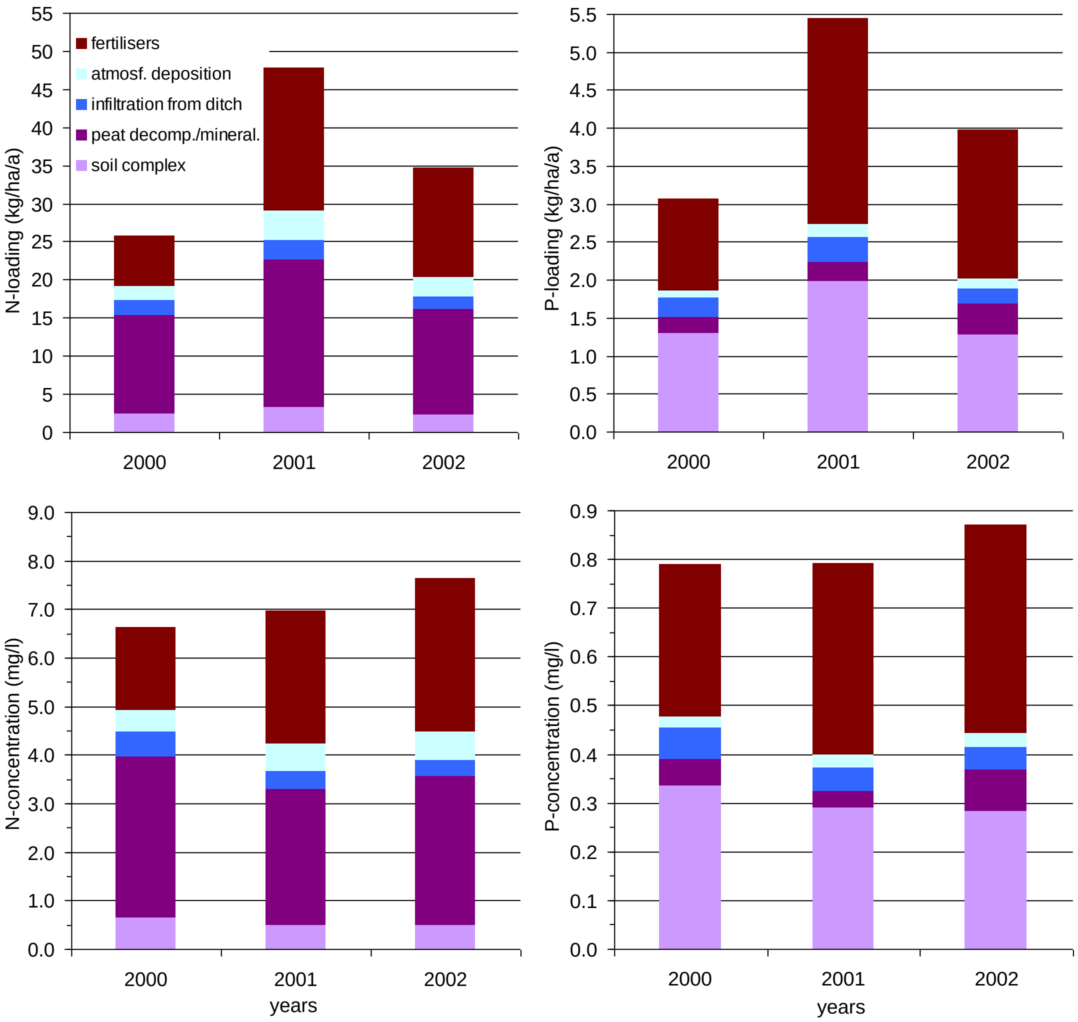

Figure 18 Loading of the surface water (top) and average discharge concentration (bottom) for Nitrogen (left) and Phosphorus (right), divided into contribution of relevant sources, as simulated with SWAP-ANIMO

nitrogen loading as decomposition and mineralization of organic matter, which mostly but not exclusively consists of peat. In all years, the flow paths are shallow due to the large contribution to total drainage of surface runoff and interflow through the top layer of the soil. Consequently, N and P from fertilisers are vulnerable for leaching to surface waters, especially under wet conditions. Wet conditions imply suboptimal conditions for oxygen diffusion into the topsoil and consequently for oxygen depending processes like organic matter decomposition, mineralization of N and P and nitrification. In wet peat soils with their abundance of organic matter, application of organic fertilisers as manure leads to competition for oxygen between peat and fertiliser. Because of this, less organic N and P from fertilisers is converted into nitrate and phosphate, substances that leach less to surface waters from drained peat soils than the organic forms; the first because it is quickly denitrified in the organic rich peat soil and the latter because it is adsorped on the topsoil complex under dry conditions (Hendriks, 1993). Wet peat soils and (organic) fertilisers are a bad combination from the point of view of nutrient leaching to surface waters.

In the dryer year 2000, the leaching of nutrients from fertilisers is considerably less. Then, fertilisation is the largest but one source of N (25%) and P (40%) leaching. Largest source under drier conditions is decomposition and mineralization for N (50%) and leaching out of the P-rich peat soil complex for P (43%). For N, leaching out of the peat soil complex is but a small contributor (6-10%). For P, this counts for decomposition and mineralization (4-10%), as the organic matter of peat contains little organic bound P.

Atmospheric deposition is the smallest source of P loading, followed by infiltration from ditch water as the smallest but one source. For N, this is the other way around. Remarkably, the relative contribution of infiltration of ditch water is largest in the driest year 2000, when precipitation deficit in the dry season is largest. Consequently, in this year infiltration of N and P containing ditch water in the summer half-year is greatest. In winter, these nutrients partly leach back into the ditch.

In some parts of the Western peat pasture area in The Netherlands, upward nutrient rich seepage is another major source of nutrient loading of the surface water (Hendriks, 1993; Hendriks et al., 2002; Hendriks, 2003). At the experimental site and in most of the Vlietpolder, merely downward seepage takes place.

5.1.3 Conclusions

Process oriented models are useful tools for analysing observed nutrient concentrations in peat pasture areas, and for calculation on the basis of these observations of N and P loading of surface waters and the contribution of the main nutrient sources to this loading.

In years that are not extremely wet, the contribution of dairy farming in the form of fertilisation is not the largest contribution to the nutrient loading of the surface water of the ‘DOVE-veen’ experimental site. For N, decomposition and mineralization of the organic matter in the peat soil is the largest contributor and for P leaching out of the P-rich soil complex in the saturated peat soil. Under wet conditions because of large precipitation surpluses, fertilisation can be the main source of nutrient loading of the surface water. Wet peat soils and (organic) fertilisers form an unfavourable combination from the point of view of nutrient leaching to surface waters.

5.2 Scenario analyses

In The Netherlands, wetting of peat soils is considered to be the most effective and practical way to conserve peat soils and slow down subsidence of the soil surface and emission of greenhouse gasses into the air. Drainage of peat soils promotes oxygen diffusion into the soil, resulting in aerobic microbial decomposition (oxidation) of peat organic matter and consequently disappearing of the peat soil itself as carbon dioxide and nitrous oxide, both greenhouse gasses, into the air. Wetting reduces oxygen diffusion and thus oxidation of peat organic matter.

Reducing drainage by raising the drainage basis through raising the ditch water level is the obvious way to wet drained peat soils. Disadvantage of this method is unfavourable conditions for crop growing, grazing and trafficability in wet periods, leading to deterioration of grass species, poaching by cattle and damaging of the top soil by heavy machinery. About 90% of peat oxidation takes place in the summer half year as a result of highest temperatures and driest conditions due to crop transpiration. Effectiveness of raising summer ditch water level for wetting of the peat soil is mostly rather limited because of high resistance to infiltration due to low permeability of these soils. Therefore, in The Netherlands submerged drains are studied and promoted as an alternative to ditch water level raising for enhancing wetting of peat soils. Those pipe drains are situated about 0.15 m below the expected lowest target ditch water level at distances of 6-8 m perpendicular to the ditch. In this way, they increase infiltration in dry periods as well as drainage in wet periods and thus combine two goals: conservation of peat soil and practising of profitable agriculture. They even allow higher ditch water levels than acceptable with no drains without hampering conditions for cost-effective farming (Hoving et al., 2008).

One of the questions connected to application of submerged drains is whether and how they affect the leaching of nutrients from the peat soil to the surface water in comparison to merely ditch water level raising. Therefore, the effects of the wetting scenarios ‘ditch water level raising’ and ‘submerged drains’ on nutrient loading of the surface water were studied with the calibrated SWAP-ANIMO model.

5.2.1 Methods

Seven different ditch water level scenarios were simulated with the calibrated model: present level and six levels around present level. Each level was simulated without and with submerged drains at 0.15 m below that level. Levels were: present target level which is 0.5 m below soil surface (m bss) in winter half-year and 0,4 m bss in summer half-year, and six constant levels of 0.3, 0.4, 0.5, 0.6, 0.7 and 0.8 m bss the year round. This range of levels amply represents the target levels of the Western agriculturally used peat pastures in the Netherlands, which are commonly between 0,4 and 0,6 m bss.

For the other forcing variables at the bottom and lateral boundary, present values from the calibration runs were used: bottom boundary condition in SWAP, atmospheric deposition and concentrations of N- and P-compounds in infiltration (ditch) water in ANIMO. Forcing variables at the top boundary are the most crucial for the modelled system: precipitation surplus determines strongly the magnitude of nutrient loading of the surface water as well as the conditions for soil chemical processes and fertilisation is an important source of nutrients (see 5.1). In order to get a realistic impression of the average behaviour of the system concerning the wetting scenarios, simulations were performed for a real series of 15 weather years (1986-2000) and annual averages of the model outcomes were analysed and studied. As input for fertilisation, the input of the years 2000 and 2001 alternating were used.

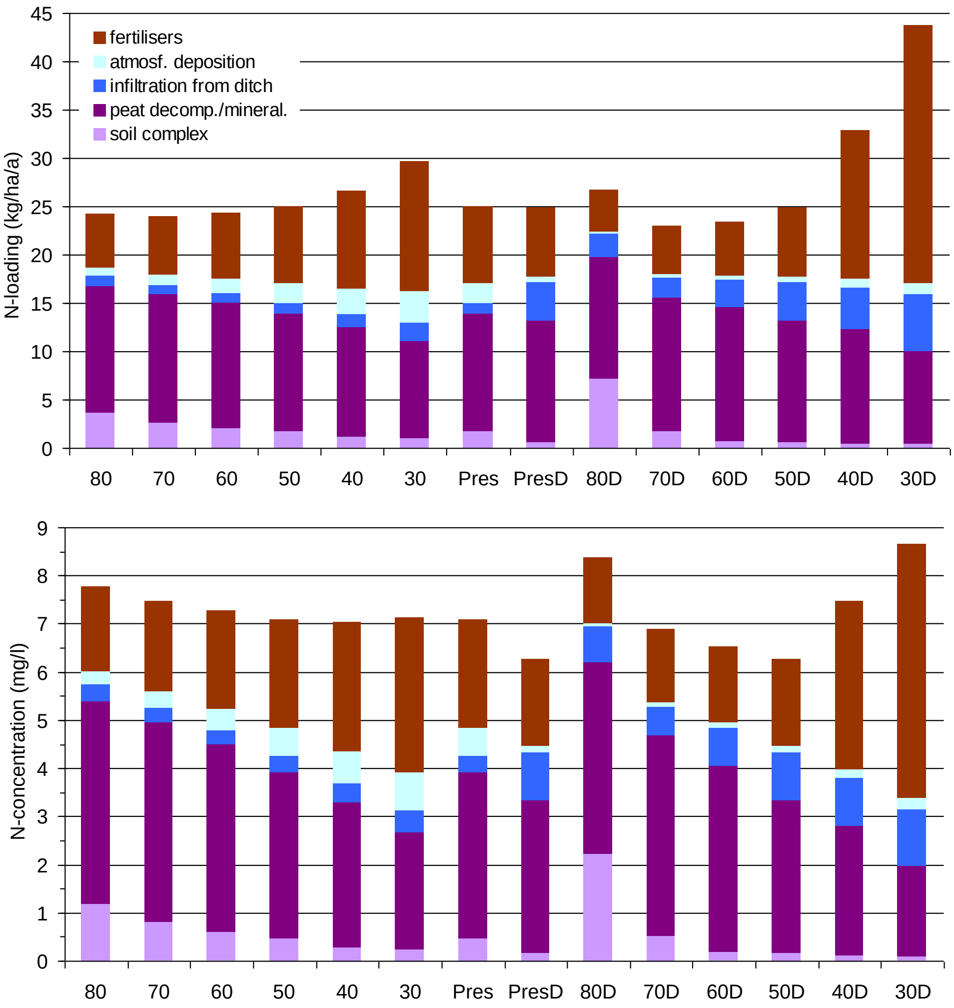

Figure 19 Results of wetting scenarios for Nitrogen as loading (top) and average discharge concentra-tion (bottom) divided into contributions of relevant sources. 80 = target level in cm below soil surface (bss); Pres = present target level (50 cm bss in winter, 40 cm bss in summer); D = submerged drain.

5.2.2 Results

Ditch water level has a great impact on nutrient loading of the surface water, as well in situations with as in situations without submerged drains (Fig. 19 and 20):

1. raising ditch water level promotes leaching of nutrients from fertilisation and atmospheric deposition: wet peat soils and fertilisation do not go well together, considering nutrient leaching to surface waters (see also 5.1.2). Lowering ditch water level compared to present level of 0.5 m bss, reduces contribution of both sources, but only slightly. Contribution of atmospheric deposition to P leaching is only very moderate;
2. raising ditch water level implies more infiltration from ditch water, due to increase of downward seepage over the bottom boundary. Consequently, contribution of this nutrient source increases, as part of the infiltrated nutrients leach back from the soil into the ditch. This effect is more pronounced for the situation with drains;

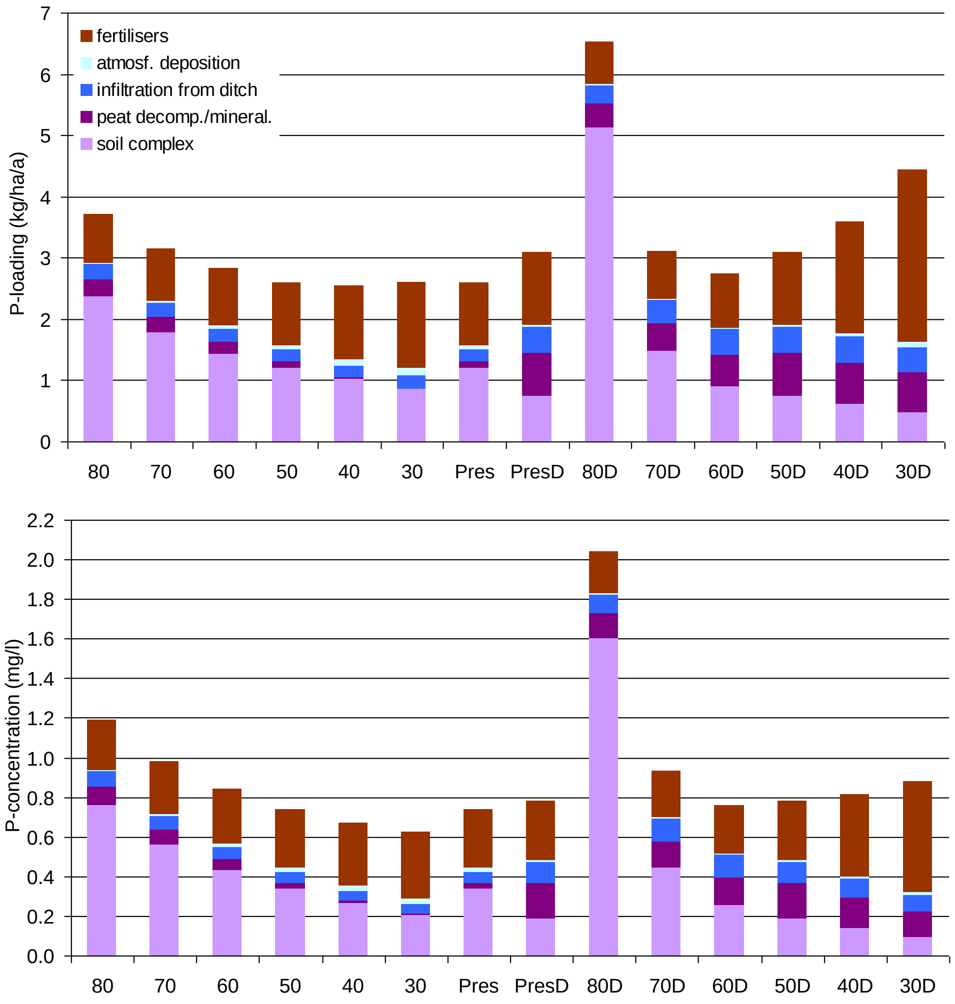

Figure 20 Results of wetting scenarios for Phosphorus as loading (top) and average discharge concentration (bottom) divided into contributions of relevant sources. 80 = target level in cm below soil surface (bss); Pres = present target level (50 cm bss in winter, 40 cm bss in summer); D = submerged drain.

3. lowering ditch water level increases contribution of the peat soil to the nutrient loading. For N, this is mainly due to decomposition and N-mineralization of the organic matter of peat, as leaching out of the peat soil complex gives but a relatively small contributor to N leaching. Enhanced drainage promotes aerobic decomposition and mineralization of peat. As the organic matter of peat contains little organic bound P, increased decomposition and mineralization of peat have but a limited effect on P-leaching. For P, leaching out of the P-rich peat soil complex is strongly increased by lowering of the water level, as this leads to deeper streamlines and thus more water flow through the P-rich peat soil.

The overall effect of raising ditch water level in the situation without drains is an increase of N-loads and hardly any effect on P-loads. Lowering ditch water level has the opposite effect: increase of P-loads and no effect on N-loads. This does not count for average discharge concentrations: for N the effect is opposite to the effect on the loads, but less pronounced, and for P the effect is a consistent decline of concentrations with higher ditch water levels. The consequence of this on the N- and P-concentrations in the surface water can not be derived from these results, but should be investigated with surface water quality model that considers the total water and nutrient balance of the surface water system.

Submerged drains enlarge the effects of changing ditch water level, especially for the extremer levels:

1. at the highest levels leaching of nutrients from fertilisation is extreme. At these levels and drain depths, submerged drains create a shortcut between the fertilised topsoil and the surface water. For N this effect is equally strong for loads and concentrations; for P it is only strong for loads;
2. the effect of raising water level on infiltration of ditch water, is much more clear in the case with drains. In fact, this demonstrates the functioning of the drains as promoters of infiltration;
3. at the lowest level, increase of leaching out of the N- and P-rich peat soil is most extreme, especially for P with an extreme loading of 6.5 kg per ha per year at a level of 0.8 m bss, of which 80% leaching out of the peat soil complex. In this case, drains are situated in and close to peat layers with high concentrations of ammonium, DON, phosphate and DOP, so that a shortcut is created between this source of nutrients and the surface water.

For N, effects of drains on loads and on concentrations are quite similar at higher levels, while at lower levels effects are more extreme for concentrations. For P, this is the other way round; at highest levels effects on loads are more extreme.

The by far most important result of the scenarios is that from the point of view of nutrient loading, in the case of drains there appears to be an optimal level: 0.5 m bss for N and 0.6 m bss for P. In the range 0.5-0.6 m bss in the case of drains compared to no drains, N loads and concentrations are somewhat lower (max. 10%), and P loads and concentrations are somewhat lower or only slightly higher for 0.5 m bss. The latter is important, because from the point of view of peat conservation 0.5 m bss is a more effective level than 0.6 m bss.

5.2.3 Conclusions

Wetting of the peat soil of the ‘DOVE-veen’ experimental site by raising ditch water level leads to increased contribution of fertilisers to nutrient loading of the surface water: fertilisers and wet peat soils are an unfavourable combination.

Contribution of the peat soil to nutrient loading decreases due to wetting. For N this is mainly due to decreased peat decomposition and mineralization, and for P to decreased leaching out of the soil complex.

For N, the increased leaching of fertilisers prevails and the overall effect of wetting of this peat soil is increase of N-loading of the surface water. For P, both processes are more or less in equilibrium and P-loading is hardly affected, but P-concentration is slightly decreased.

Lowering ditch water level leads to increase of P-loading and discharge concentration, because of increase of the contribution of leaching out of the P-rich saturated peat soil. N-loading is hardly affected by this process, while N-concentration increases slightly.

For application of submerged drains it is crucial to use the, from the point view of nutrient loading, optimal ditch water level and corresponding drain depth. A too high level will lead to more direct draining of the by fertilisation nutrient-enriched top soil, while a too low level will cause direct drainage of nutrient rich peat soil layers. For the ‘DOVE-veen’ experimental site, the optimal ditch water level with corresponding drain depth is 0.5-0.6 m bss. At that level N-loading is somewhat lower than without drains and P-loading is at most a little higher. The optimal level and depth can differ for each peat soil, depending on soil profile and hydrological conditions.

6 Conclusions and recommendations

6.1 Model evaluation

6.1.1 Conclusions

On the basis of the obtained calibration and validation results it can be concluded that SWAP is reasonably well able to simulated groundwater level behaviour and drainage to surface water in the peat pasture area of the Vlietpolder for the simulated period. Especially, the later result is relevant because it concerns the subject of this study: nutrient loading of the surface water. However, the relevance of this conclusion is rather limited because of the limitations of the calibration and validation results, which counts especially for the validation because of the short period. Another important limitation is that it was not able to calibrate and validate SWAP against data about moisture content or pressure head. These parameters are crucial for ANIMO simulations as they control many processes in the C, N and P cycles.

On the basis of the obtained calibration and validation results it can be concluded that ANIMO is reasonably well able to simulate the average N and P concentrations in the peat soil of the experimental field, and that the model is well able to simulate the important terms of the N and P balance N-mineralization, denitrification and annual N and P uptake by the crop. But no direct information was obtained about the model's ability to correctly simulate N and P loading of the surface water. Nevertheless, the combination of good results of the validation of discharge simulations with SWAP and the reasonable results of the ANIMO simulations of N and P concentrations, gives reason for having confidence in the results of SWAP-ANIMO simulation of N and P loading of the surface water in peat pasture areas like the Vlietpolder. Thus the conclusion was that SWAP-ANIMO is applicable for simulation of nutrient loading of surface waters in peat pasture areas. However, not all aspects of the simulation of leaching of nutrients towards surface waters could be evaluated completely, because this process was not measured itself. A recommendations for improvement of the ANIMO sub-model was derived.

6.1.2 Recommendations

From evaluating the effect of the decomposition rate of the pool of dissolved organic matter (DOM) on the concentrations of dissolved organic N in the soil solution, it is recommended to add a second pool of DOM with its own properties independent of the properties of the existing pool.

From evaluating the effect of the decomposition rate of the pool of dissolved organic matter (DOM) on the concentrations of dissolved organic N in the soil solution, it is recommended to add to the ANIMO sub-model a second pool of DOM with its own properties independent of the properties of the existing pool. So that the model can cope with situations that require a labile as well as a stabile pool of DOM, like peat soils.

In general, it is recommended to add to the ANIMO model explicit descriptions of redox processes that affect sorption of phosphorus to the soil complex. This extension may improve simulation of phosphorus adsorption and desorption under alternating wet and dry conditions, as is the case in peat soils. For simulating the effects on phosphorus loading of strategies for wetting of peat soils in order to reduce soil surface subsidence, this can be an important improvement of the model.

Another important process that is lacking in the model is leaching of sulphate to surface waters. It is recognized nowadays that sulphate reduction can be an important process for stimulating phosphorus mobilisation from the sediment into the water column in the ditches. Especially, surface waters in peat land areas are vulnerable for this process due to organic-matter-rich sediments.

6.2 Model analyses

6.2.1 System

Process oriented models are useful tools for analysing observed nutrient concentrations in peat pasture areas, and for calculation on the basis of these observations of N and P loading of surface waters and the contribution of the main nutrient sources to this loading.

In years that are not extremely wet, the contribution of dairy farming in the form of fertilisation is not the largest contribution to the nutrient loading of the surface water of the ‘DOVE-veen’ experimental site. For N, decomposition and mineralization of the organic matter in the peat soil is the largest source and for P leaching out of the P-rich soil complex in the saturated peat soil. Under wet conditions because of large precipitation surpluses, fertilisation can be the main source of nutrient loading of the surface water. Wet peat soils and (organic) fertilisers form an unfavourable combination from the point of view of nutrient leaching to surface waters.

6.2.2 Scenarios

Wetting of the peat soil of the ‘DOVE-veen’ experimental site in order to preserve the peat soil by raising ditch water level leads to increased contribution of fertilisers to nutrient loading of the surface water: fertilisers and wet peat soils are an unfavourable combination.

Contribution of the peat soil layers to nutrient loading decreases due to wetting. For N this is mainly due to decreased peat decomposition and mineralization in the smaller unsaturated zone, and for P to decreased leaching out of the soil complex of the peat layers in the permanent water saturated zone of the peat profile. For N, the increased leaching of fertilisers prevails and the overall effect of wetting of this peat soil is increase of N-loading of the surface water. For P, both processes are more or less in equilibrium and P-loading is hardly affected, but the average P-concentration of the leachate is slightly decreased.

Lowering ditch water level leads to increase of P-loading and discharge concentration, because of increase of the contribution of leaching out of the P-rich saturated peat soil. N-loading is hardly affected by this process, while N concentration increases slightly.

For application of submerged drains it is crucial to use the, from the point view of nutrient loading, optimal ditch water level and corresponding drain depth. A too high level will lead to more direct draining of the by fertilisation nutrient-enriched top soil, while a too low level will cause direct drainage of nutrient rich peat soil layers. For the ‘DOVE-veen’ experimental site, the optimal ditch water level with corresponding drain depth is 0.5-0.6 m bss. At that level N-loading is somewhat lower than without drains and P-loading is at most a little higher. The optimal level and depth can differ for each peat soil, depending on soil profile and hydrological conditions.

6.2.3 Recommendations

In case of applying submerged drains for reducing soil surface subsidence, it is from the point view of nutrient loading recommended to use an optimal ditch water level and corresponding drain depth. For the Vlietpolder this level is in the range of 0.5-0.6 m below soil surface. It is expected that this range will differ only little for peat pasture areas with similar properties and conditions as the ones of the Vlietpolder.

In general, it is recommended to add to the ANIMO model explicit descriptions of redox processes that affect sorption of phosphorus to the soil complex. This extension may improve simulation of phosphorus adsorption and desorption under alternating wet and dry conditions, as is the case in peat soils. For simulating the effects on phosphorus loading of strategies for wetting of peat soils in order to reduce soil surface subsidence, this can be an important improvement of the model.

Another important process that is lacking in the model is leaching of sulphate to surface waters. It is recognized nowadays that sulphate reduction can be an important process for stimulating phosphorus mobilisation from the sediment into the water column in the ditches. Especially, surface waters in peat land areas are vulnerable for this process due to organic-matter-rich sediments.

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Van Schaik, F.H., F. Douwsma, C.L. Van Beek en D. Oudendag, 2004. *Database Vlietpolder: een beschrijving van een Access database ontworpen voor het Vlietpolder project.* Deelrapport Veenweideproject fase 1. Hoogheemraadschap van Rijnland, Leiden.

Appendix 1 Default grass crop input file of SWAP

Default values of a grass crop input file for the SWAP simple crop model.
Case Ruurlo grass. Provided on: www.swap.alterra.nl, Downloads, download Swap32.
Only relevant options are shown. Irrigation was not practiced and thus not relevant.

```
***********************************************************************************************
* Filename: GrassS.CRP
* Contents: SWAP 3.0 - Crop data of simple model; case Ruurlo grass
***********************************************************************************************
*** PLANT GROWTH SECTION ***
***********************************************************************************************
* Part 1: Crop development
  IDEV = 1 ! length of growth period: 1 = fixed, 2 = variable
* If fixed growth period (IDEV = 1), specify:
  LCC  =   366 ! Length of the crop cycle [1..366 days, I]
***********************************************************************************************
* Part 2: Light extinction
  KDIF   =     0.75 ! Extinction coefficient for diffuse visible light [0..2 -, R]
  KDIR   =     0.75 ! Extinction coefficient for direct visible light  [0..2 -, R]
***********************************************************************************************
* Part 3: Leaf area index or soil cover fraction
  SWGC = 1 ! choice between LAI [=1] or soil cover fraction [=2]
* If SWGC = 1, list leaf area index [0..12 ha/ha, R],    as function of dev. stage [0..2 -,R]:
* If SWGC = 2, list soil cover fraction [0..1 m2/m2, R], as function of dev. stage [0..2 -,R]:
*        DVS   LAI or SCF  ( maximum 36 records)
  GCTB =
        0.00   3.0
        2.00   3.0
* End of table
***********************************************************************************************
* Part 4: crop factor or crop height
  SWCF = 2 ! choice between crop factor [=1] or crop height [=2]
* If SWCF = 1, list crop factor [0.5..1.5, R],   as function of dev. stage [0..2 -,R]:
* If SWCF = 2, list crop height [0..1000 cm, R], as function of dev. stage [0..2 -,R]:
*        DVS   CF or CH   (maximum 36 records)
  CFTB = 0.0    12.0
         2.0    12.0
* End of table
***********************************************************************************************
* Part 5: rooting depth
* List rooting depth [0..1000 cm, R], as a function of development stage [0..2 -,R]:
*        DVS   RD    (maximum 36 records)
  RDTB =
        0.0   30.00
        2.0   30.00
* End of table
***********************************************************************************************
* Part 6: yield response
* List yield response factor [0..5 -,R], as function of development stage [0..2 -,R]:
*        DVS   KY   (maximum 36 records)
  KYTB =
        0.00   1.00
        2.00   1.00
* End of table
***********************************************************************************************
```

```
**********************************************************************************************
* Part 7: soil water extraction by plant roots
  HLIM1  =   -10.0 ! No water extraction at higher pressure heads, [-100..100 cm, R]
  HLIM2U =   -25.0 ! h below which optim. water uptake starts for top layer, [-1000..100 cm, R]
  HLIM2L =   -25.0 ! h below which optim water uptake starts for sub layer, [-1000..100 cm, R]
  HLIM3H =  -200.0 ! h below which water upt. reduct. starts at high Tpot, [-10000..100 cm, R]
  HLIM3L =  -800.0 ! h below which water uptake reduct. starts at low Tpot, [-10000..100 cm, R]
  HLIM4  = -8000.0 ! Wilting point, no water extract. at lower pres. heads, [-16000..100 cm, R]
  RSC    =    70.0 ! Minimum canopy resistance used for potent. transpiration, [0..1000 s/m, R]
  ADCRH  =     0.5 ! Level of high atmospheric demand, [0..5 cm/d, R]
  ADCRL  =     0.1 ! Level of low atmospheric demand,  [0..5 cm/d, R]
**********************************************************************************************
* Part 9: interception
  SWINTER =  1  ! Switch for rainfall interception method:
                ! 0 = No interception calculated
                ! 1 = Agricultural crops (Von Hoyningen-Hune and Braden)
                ! 2 = Trees and forests (Gash)
* In case of interception method for agricultural crops (SWINTER = 1) specify:
  COFAB  =      0.25 ! Interception coefficient Von Hoyningen-Hune and Braden, [0..1 cm, R]
**********************************************************************************************
* Part 10: Root density distribution and root growth
* List relative root density [0..1 -, R], as function of relative rooting depth [0..1 -, R]:
*    Rdepth Rdensity  (maximum 11 records)
  RDCTB =
       0.00     1.00
       1.00     1.00
* End of table
**********************************************************************************************
* End of simple crop input file .CRP!
**********************************************************************************************
```

Appendix 2 Filling up missing values in the meteorological time series of De Vlietpolder

A2.1 Introduction

Meteorological time series of the Vlietpolder contain several gaps. In order to run SWAP, these missing values have to be substituted by proper predictions. The aim of this study is therefore to fill up these time series by using auxiliary data and statistical models. All analyses have been performed by means of the R-program *meteoVlietpolder.R*.

A2.2 Available data

Meteorological data for the Vlietpolder were obtained from table *qryMeteoTabel* residing in the *Vlietpolder-eigendatabase.mdb* database. The following time series are of interest for SWAP (see Table 5, Section 3.2.1.1 main text):

‘RAD’ ‘Tmin’ ‘Tmax’ ‘HUM’ ‘WIND’ ‘RAIN’ ‘WET’

The time series cover the period from July 23rd 1999 through April 28th 2003 and have an observation frequency of 30 minutes. In order to use these time series as SWAP input, the observations have been aggregated to daily averages and daily totals. Each daily observation is therefore based on 48 observations. The resulting time series are given in Figure A2.1. The WET time series is the duration of each daily rainfall event. Pairwise scatter plots and distributions are given in Figure A2.2. The number of missing values (in days) per time series are shown in Table A2.1. This has been visualized in Figure A2.3.

Table A2.1 Number of missing values per time-series

RAD	Tmin	Tmax	HUM	WIND	RAIN	WET
133	128	128	174	154	59	59

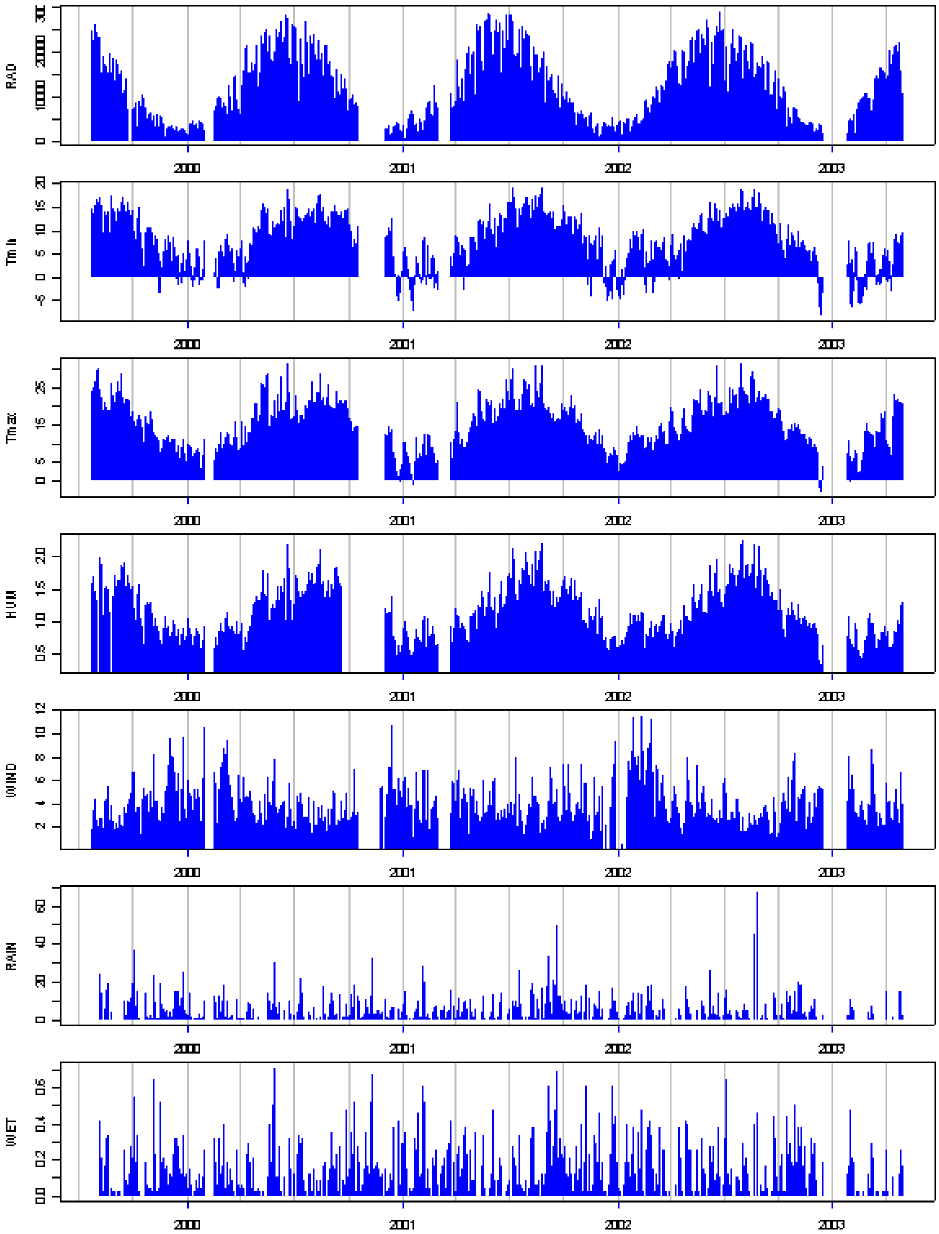


Figure A2.1 Time series of meteorologic data of the Vlietpolder

In order to fill up missing values, external information has been used. The following external time series were available:

- main meteorological station De Bilt (KNMI 260):
  - DDVEC: prevailing wind direction in degrees (360=North, 0=calm/variable);
  - FG: daily mean windspeed (m/s);
  - FHX: maximum hourly mean windspeed (m/s);
  - FX: maximum wind gust (m/s);
  - TG: daily mean temperature (°C);
  - TN: minimum temperature (°C);
  - TX: maximum temperature (°C);
  - SQ: sunshine duration (h);

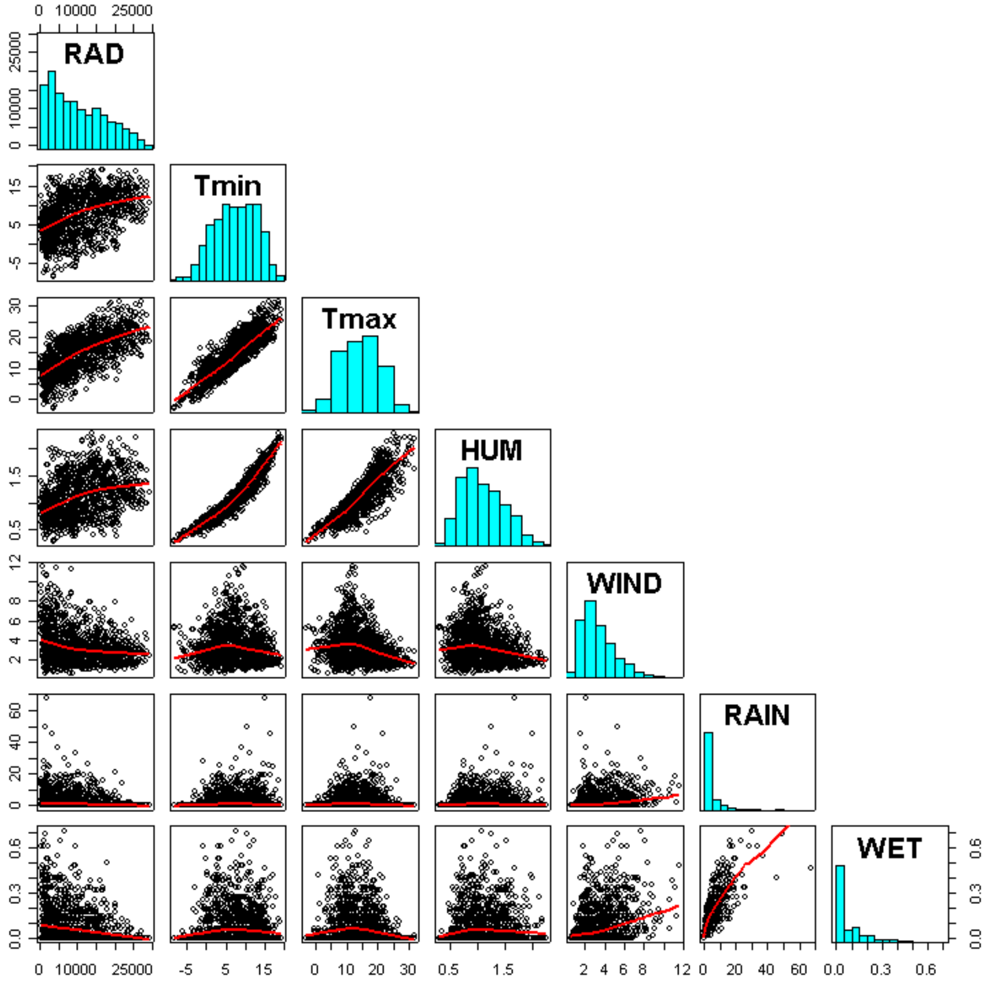


Figure A2.2 Pair plots and distributions of meteorological time series

  - SP: percentage of maximum possible sunshine duration (%);
  - DR: precipitation duration (h);
  - RH: daily precipitation amount (mm);
  - PG: daily mean surface air pressure in (hPa);
  - VVN: minimum visibility (-);
  - NG: cloud cover in octants (9=sky invisible).
- local meteorological station ‘wageningen’: daily rainfall (mm);
- local meteorological station ‘rijnland’: daily rainfall (mm);
- meteorological station Leiden: daily rainfall (mm);
- meteorological station Boskoop: daily rainfall (mm);
- meteorological station Zoetermeer: daily rainfall (mm).

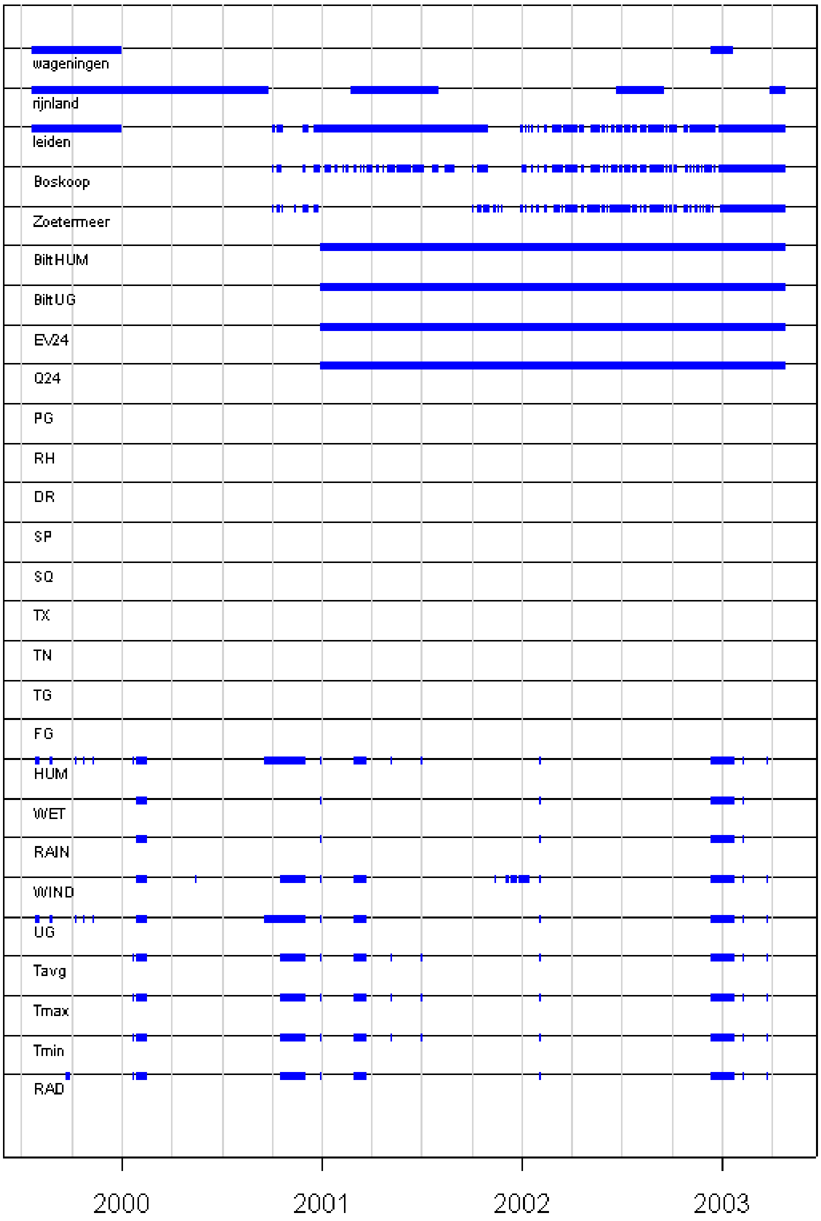


Figure A2.3 Missing values (vertical lines) as function of time for each time

A2.3 Prediction of missing values

In the following sections, the models are described that have been used to fill up the gaps in the time-series. For each time-series, it has been assumed that one model is sufficient to fill up missing values.

A2.3.1 Rainfall

For the prediction of rainfall, only the RH time-series of de Bilt fully covered all ’missing values’ periods of the RAIN time-series at Vlietpolder (Figure A2.3). Unfortunately, the relation between RH and RAIN is rather weak (Figure A2.4). Therefore, an extended version of the the ‘wageningen’ time-series has been used. In this so called ‘wagrijn’ series, missing values in the ‘wageningen’ time-series have been replaced by observations of the ‘rijnland’ time-series. The model for completion of the RAIN time series is:

$$\text{RAIN} \sim -1 + \text{wagrijn}$$

The regression is significant and $R^2_{adj} = 0.99$. The resulting time series are given in Figure A2.5.

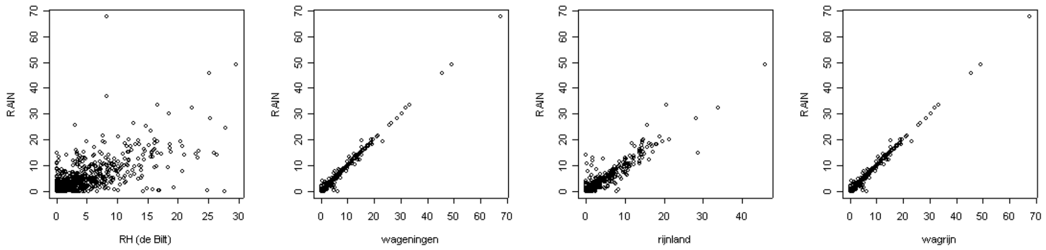


Figure A2.4 Regression of daily rainfall at the Vlietpolder site versus daily rainfall at other locations

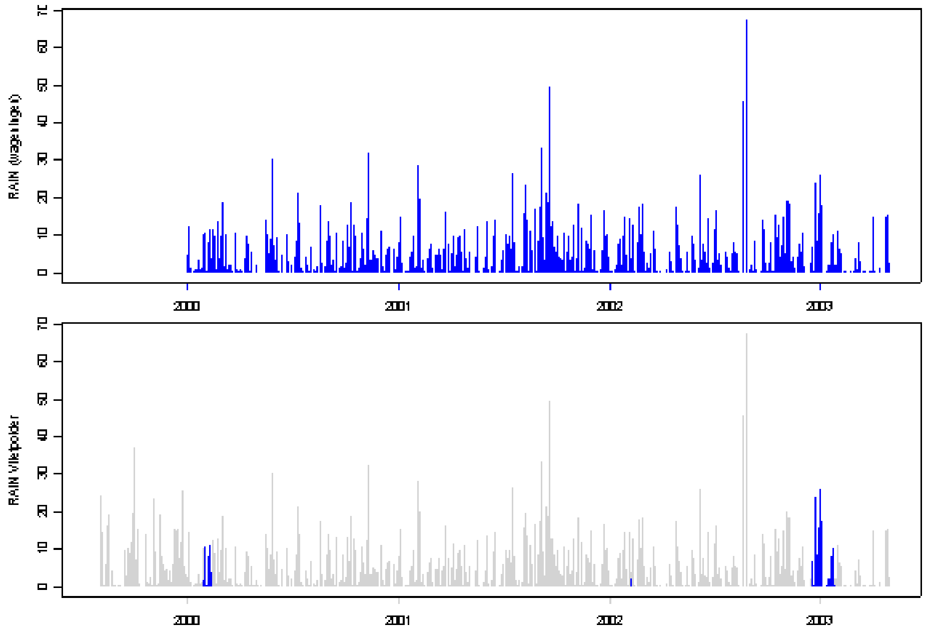


Figure A2.5 The time series of ‘wageningen’ and the filled up time series at Vlietpolder (gray: original, blue: predicted)

A2.3.2 Rainfall duration

Rainfall duration has been predicted by means of:

WET ~ –1 + RAIN + DR + quarter

where quarter is a qualitative variable representing the four quarters of the year. This relation was obtained by means of stepwise linear regression, with the AIC (Akaike Information Criterion) as selection criterion. The relation is significant and R^2_{adj} = 0.89. Plots are given in Figures A2.6 and A2.7.

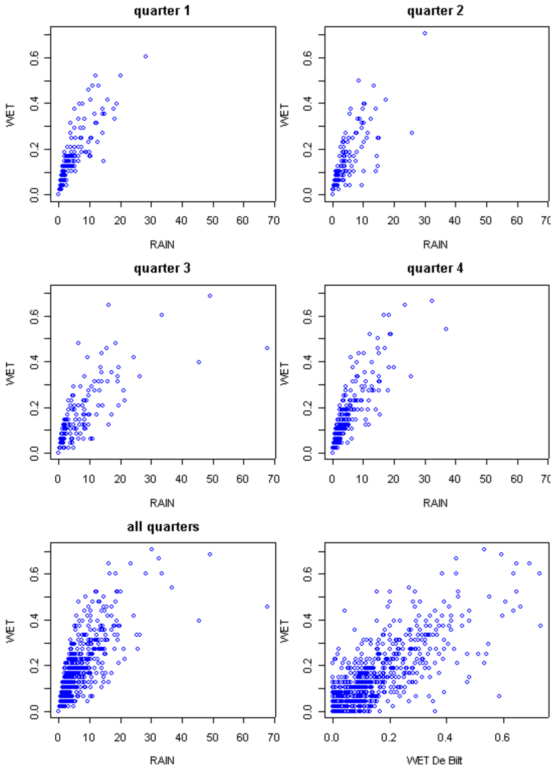


Figure A2.6 Rainfall duration as function of rainfall amount and quarter

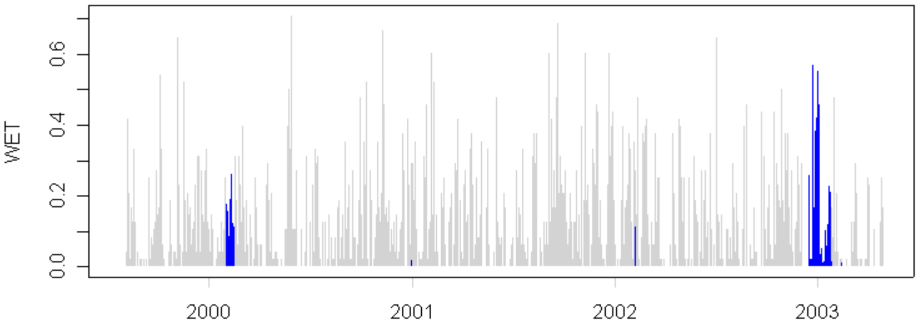


Figure A2.7 The WET time series of Vlietpolder (gray: original, blue: predicted)

A2.3.3 Maximum temperature

Maximum temperature has been predicted by means of:

Tmax ~ TX

The relation is significant and R^2_{adj} = 0.98. Results are given in Figures A2.8 and A2.9.

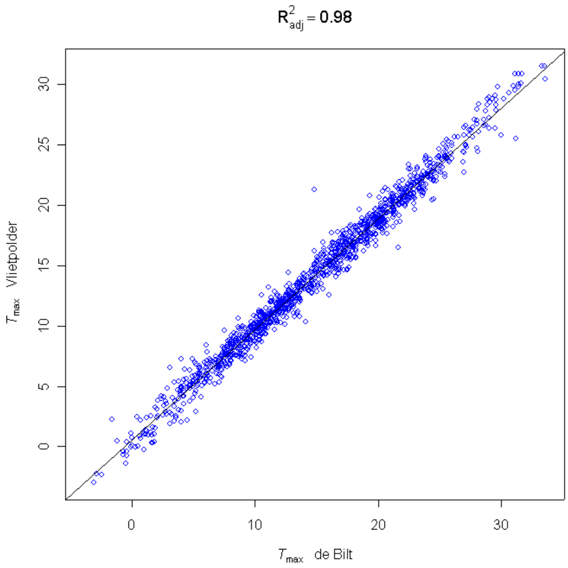


Figure A2.8 Maximum daily temperature at Vlietpolder as function of maximum daily temperature at de Bilt

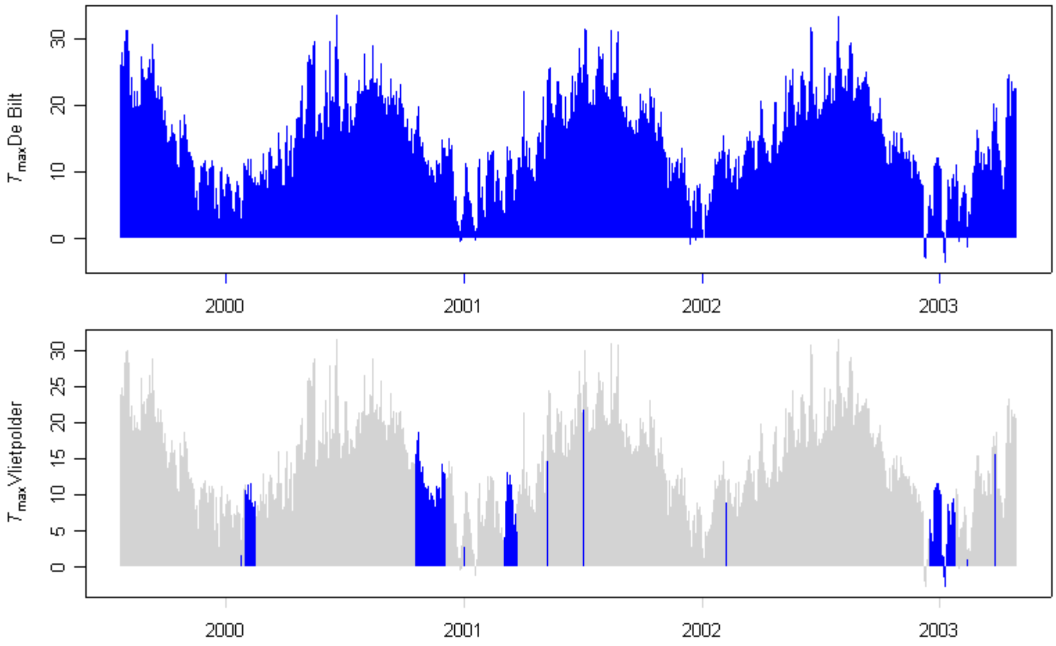


Figure A2.9 The Tmax time series of De Bilt and Vlietpolder (gray: original, blue: predicted)

A2.3.4 Minimum temperature

Minimum temperature has been predicted by means of:

Tmin ~ TN

The relation is significant and $R^2_{adj} = 0.96$. Results are given in Figures A2.10 and A2.11.

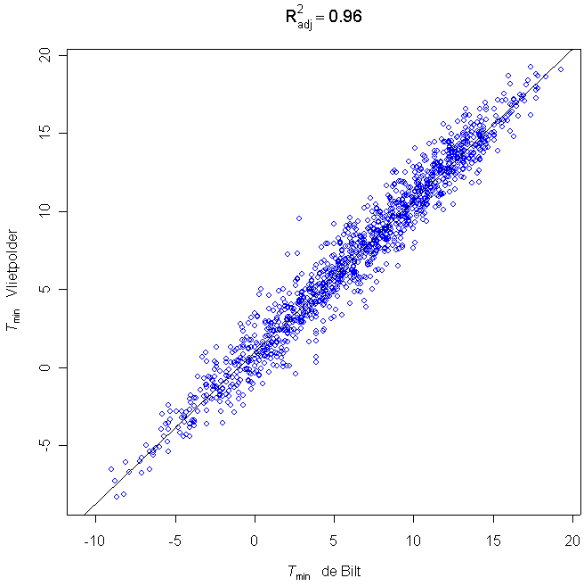


Figure A2.10 Minimum daily temperature at Vlietpolder as function of minimum daily temperature at de Bilt

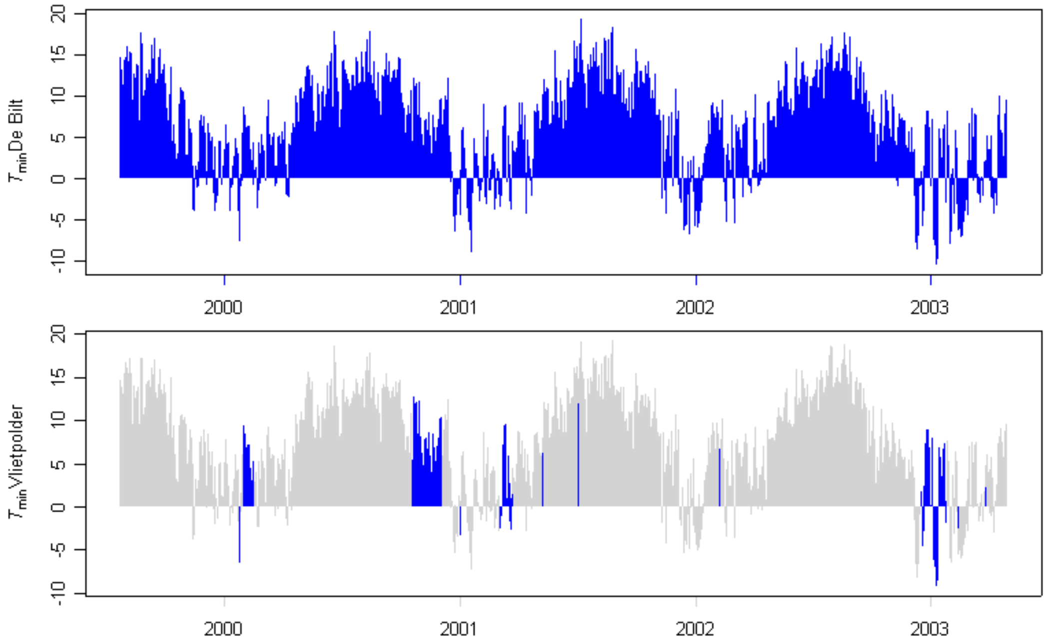


Figure A2.11 The Tmin time series of De Bilt and Vlietpolder (gray: original, blue: predicted)

A2.3.5 Average temperature

The average temperature has been predicted by means of:

Tavg ~ TG

The relation is significant and $R^2_{adj} = 0.99$. Results are given in Figures A2.12 and A2.13.

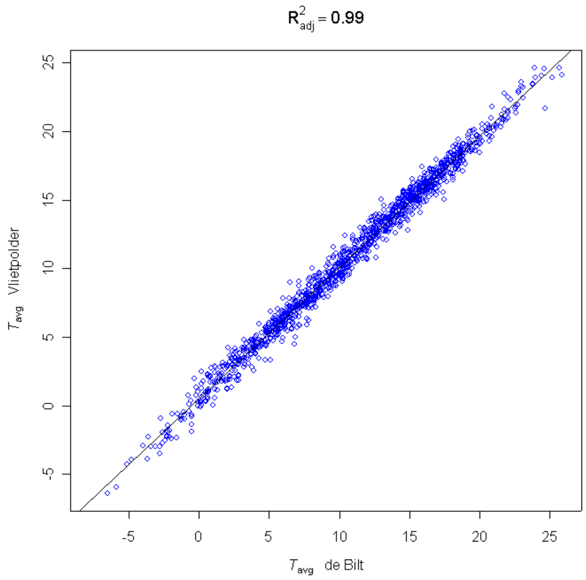


Figure A2.12 Daily mean temperature at Vlietpolder as function of daily mean temperature at de Bilt

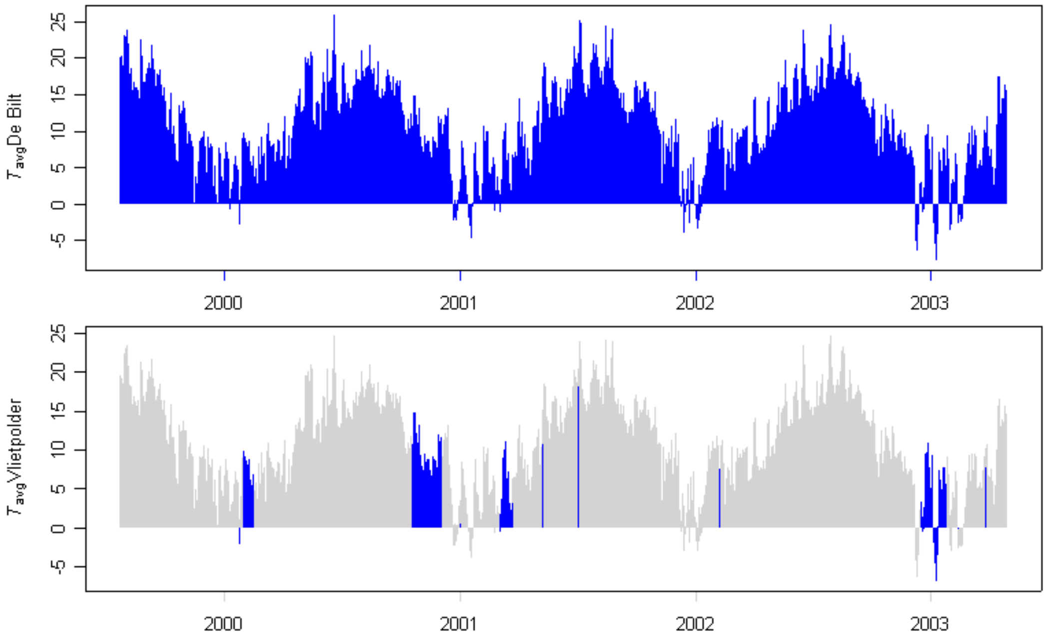


Figure A2.13 The Tavg time series of De Bilt and Vlietpolder (gray: original, blue: predicted)

A2.3.6 Windspeed

Windspeed has been predicted by means of:

WIND ~ FG

The relation is significant and $R^2_{adj} = 0.90$. Results are given in Figures A2.14 and A2.15.

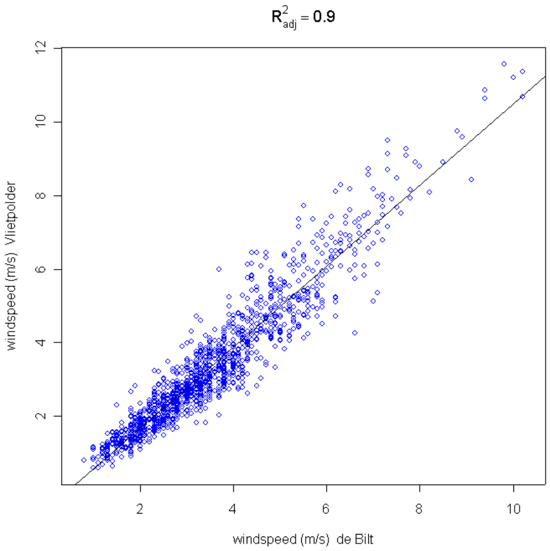


Figure A2.14 Windspeed at Vlietpolder as function of windspeed at de Bilt

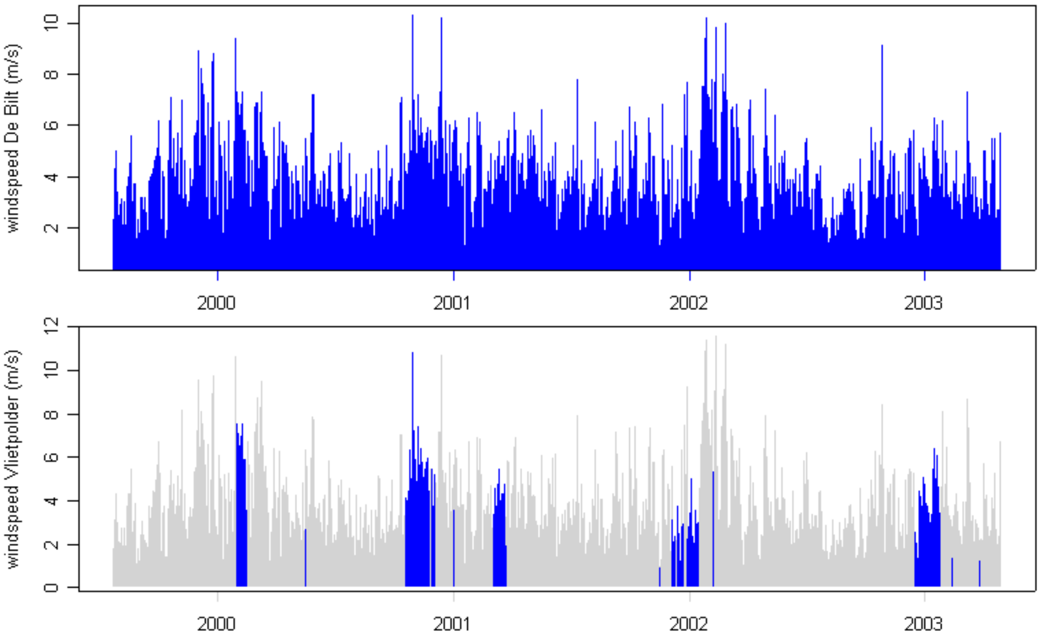


Figure A2.15 Windspeed at De Bilt and Vlietpolder (gray: original, blue: predicted)

A2.3.7 Humidity

Humidity has been predicted by means of:

$$\log(HUM) \sim Tmin$$

The relation is significant and $R^2_{adj} = 0.93$. Results are given in Figures A2.16 and A2.17.

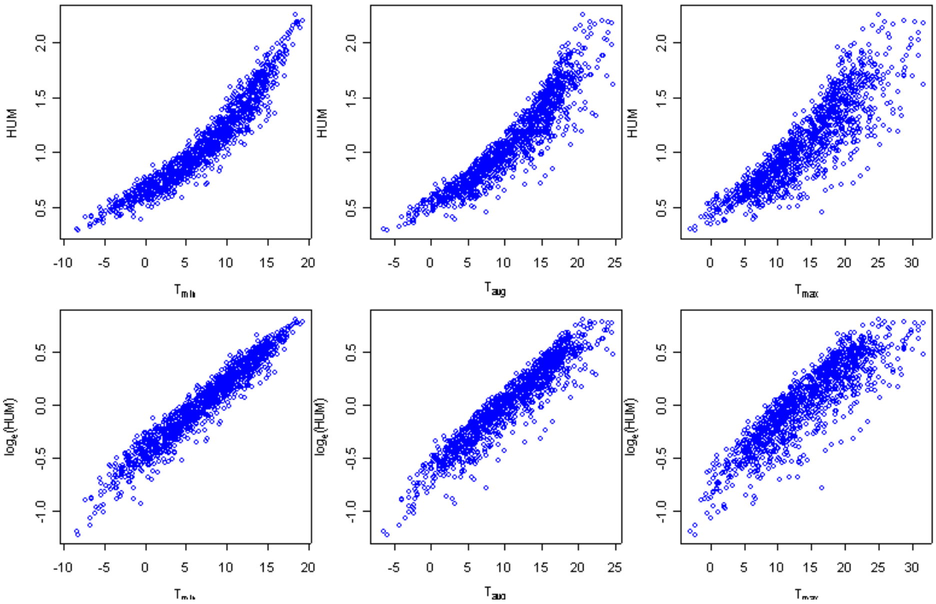


Figure A2.16 Humidity at Vlietpolder as function of temperature

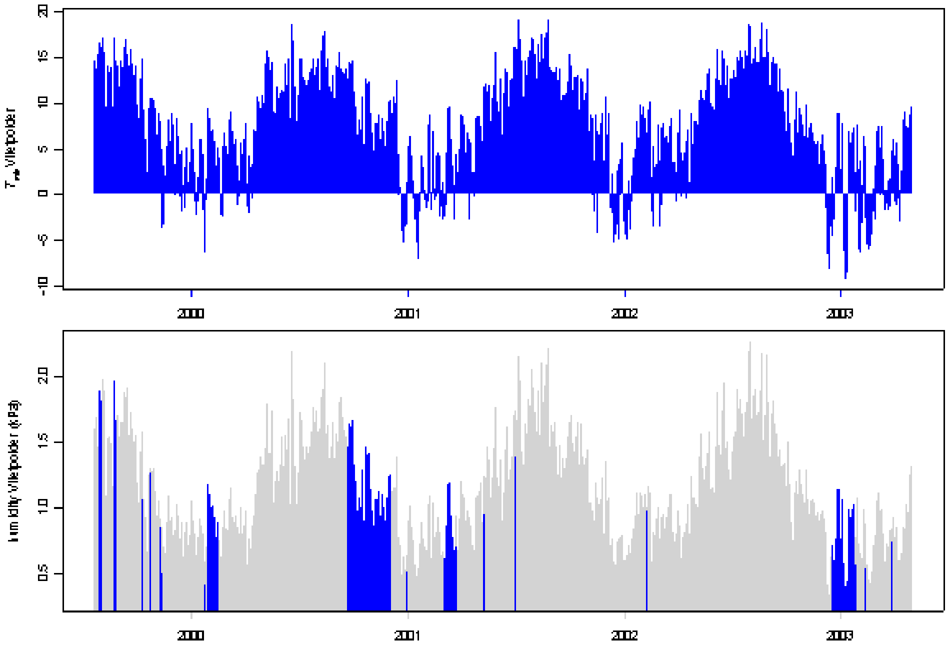


Figure A2.17 Minimum temperature and humidity at Vlietpolder (gray: original, blue: predicted)

A2.3.8 Radiation

Radiation has been predicted by means of stepwise multiple linear regression with the AIC (Akaike Information Criterion) as selection criterion. The selected parsimonious model is:

RAD ~ Tmax + SQ + SP

The relation is significant and $R^2_{adj} = 0.87$. Results are given in Figures A2.18 and A2.19.

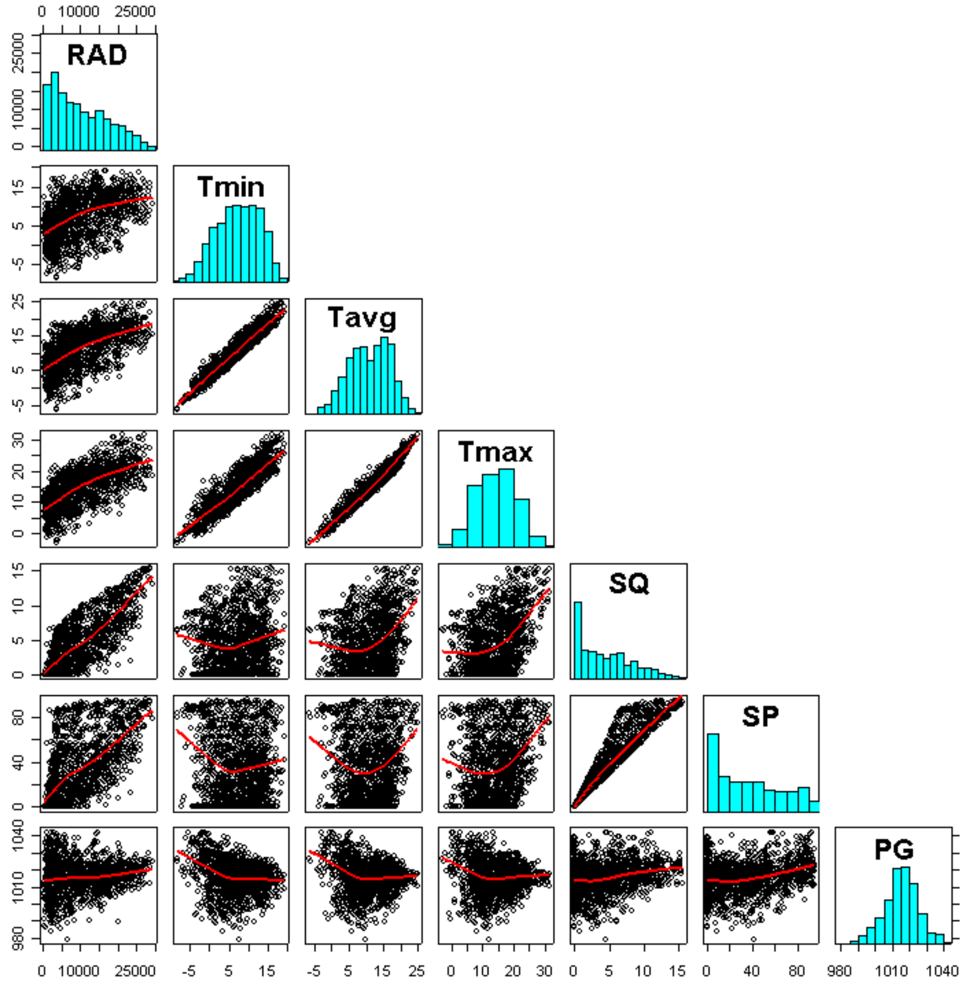


Figure A2.18 Pair plots and distributions of radiation related data

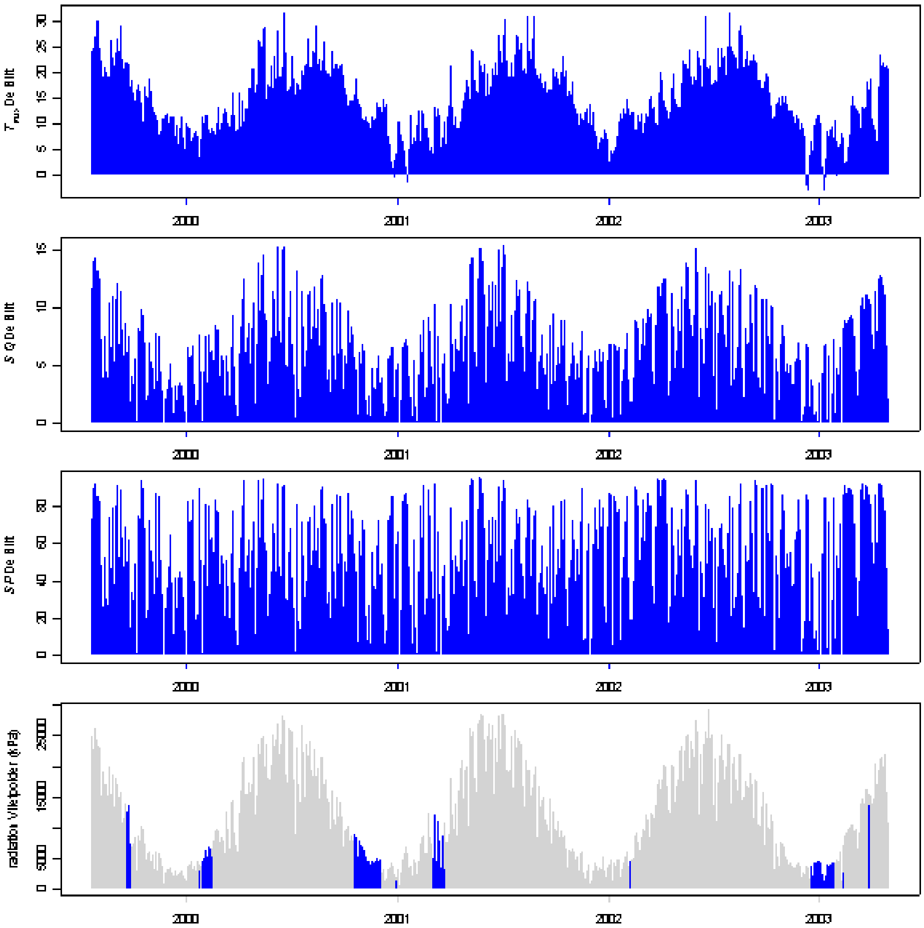


Figure A2.19 Tmax, SQ and SP at de Bilt and radiation at Vlietpolder (gray: original, blue: predicted)

Appendix 3 Estimation of the groundwater table shape factor β

Upscaling of the 1-D-soil column of SWAP to the field scale implies simulation of a groundwater level that represents a flat, field average groundwater table. Consequently, for comparing simulated groundwater levels to observed, the observed convex or concave shaped groundwater table between the ditches in the field must be converted into a field average groundwater table (Section 3.2.1.2). This conversion requires the groundwater table shape factor β to be known for estimating the average phreatic head (groundwater level):

$$h_{\mathrm{avg}} = h_{\mathrm{ditch}} + \beta\, h_{\mathrm{diff}} \qquad \text{with} \quad h_{\mathrm{diff}} = h_{\mathrm{obs,m}} - h_{\mathrm{ditch}}$$

where h_{avg} is the average phreatic head [L], h_{ditch} the hydraulic head of the ditch [L], h_{diff} the differential head (in Dutch: opbolling) [L], $h_{\mathrm{obs,m}}$ the observed phreatic hydraulic head midway between the two ditches [L] and β the groundwater table shape factor [–].

The Vlietpolder database contains profiles of phreatic heads (h_{obs}) measured along a 23 m transect of five groundwater level tubes perpendicular to the ditch (Fig. 5, Section 3.1, main text). These profiles have been visualised in Figure A3.1. Groundwater table shape factor β has been estimated by means of the following procedure:

1. estimate h_{avg} for each profile from $h_{\mathrm{obs},i}$ of each observation point *i*. Note that the observations are not taken at equidistant intervals so that each observation point *i* has to be weighted by a factor related to its distance from the ditch side. This weighing factor equals the distance from its left neighboring point *i*-1 to its right neighboring point *i*+1 relative to twice the total distance (2 x length of 'effective' transect = 44 m). In this way, for the five relevant observation points of Fig. A3.1, at distance 0, 2, 3, 5.5 and 22 m from the ditch side, the weighing factors amount to 0.045, 0.068, 0.080, 0.432 and 0.375, respectively (0 = ditch water level and 22 = average of the two points in the middle at distance 21 and 23). It is better to compute h_{avg} for estimating β that in turn will be used to estimate h_{avg} instead of using h_{avg} directly, for β is invariant in time, whereas h_{avg} has only been measured at a limited number of time steps. Aim is to find an average value for β that can be used to convert each measured h_{diff} into a h_{avg};
2. estimate groundwater shape factor β by means of linear regression of ($h_{\mathrm{avg}} - h_{\mathrm{ditch}}$) versus h_{diff} . De regression results are given in Figure A3.2.

The estimated groundwater table shape factor β equals 0.80 (−). The high value of R^2_{adj} of 0.997 is due to the fact that the intercept has been excluded from the regression equation. Hence, the degrees of freedom for computing the residual variance increased from $n - 2$ to $n - 1$, where n is the number of observations. A lower residual variance results in a higher R^2_{adj}.

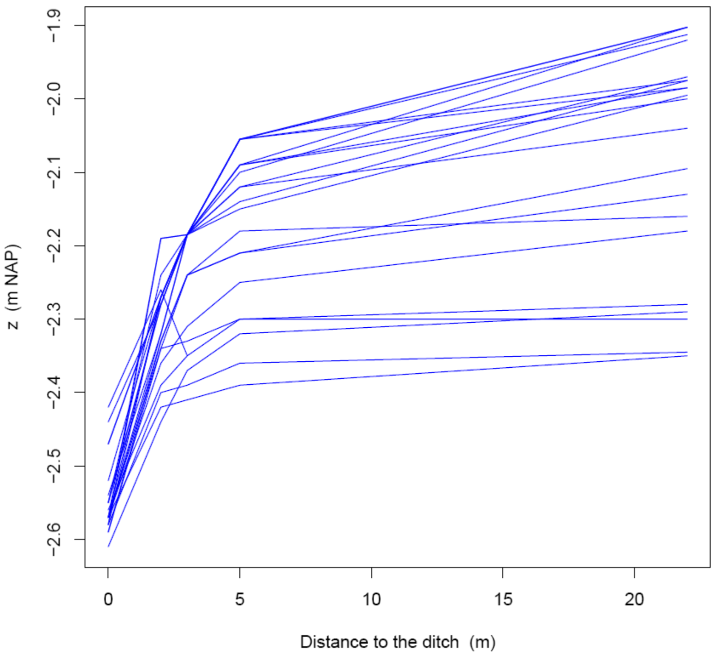


Figure A3.1 Profiles of phreatic heads, $h_{\mathrm{obs},i}$*, along a 22 m transect perpendicular to the ditch.* z *is elevation relative to mean sea level (NAP).*

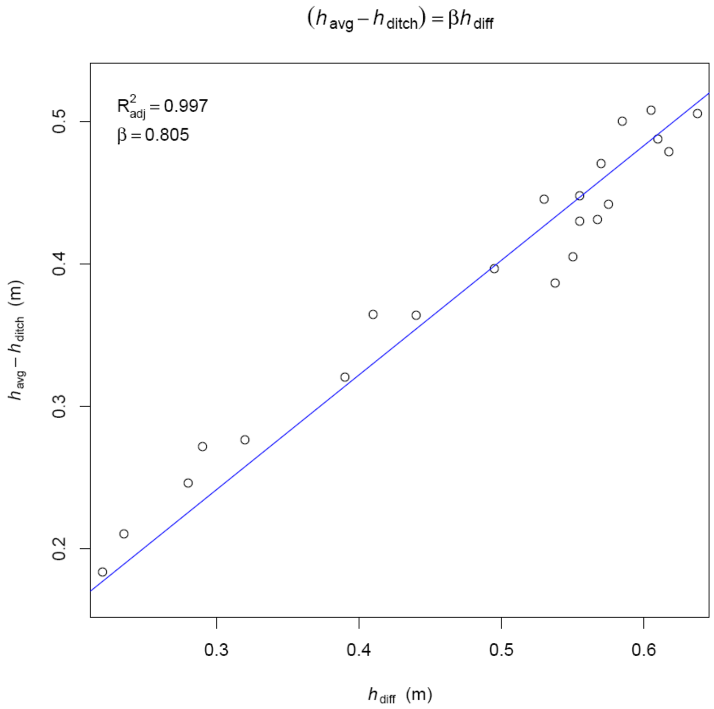


Figure A3.2 Regression for estimating groundwater table shape factor β *(corresponds to slope of regression line)*

Appendix 4 Assigning suction cup data to a representative profile

A4.1 Introduction

At the study site, the following soil horizons can be discerned:

Table A4.1 Distinguished horizons and sub-horizons (see Section 3.1 for explanation horizons)

Horizons & sub-horizons		Depth (m − average soil surface)		Elevation (m + NAP*)	
symbol	description	top	bottom	top	bottom
T1	Toemaakdek 1	0.00	0.20	-2.09	-2.29
T2	Toemaakdek 2	0.20	0.28	-2.29	-2.37
K	Clayey peat	0.28	0.48	-2.37	-2.57
Vo1	Peat, oxidised	0.48	0.58	-2.57	-2.67
Vo2	Peat, oxidised	0.58	0.68	-2.67	-2.77
Vo3	Peat, oxidised	0.68	0.78	-2.77	-2.87
Vr1	Peat, reduced	0.78	1.18	-2.87	-3.27
Vr2	Peat, reduced	1.18	1.58	-3.27	-3.67
Vr3	Peat, reduced	1.58	1.98	-3.67	-4.07
Vr4	Peat, reduced	1.98	2.48	-4.07	-4.57
Vr5	Peat, reduced	2.48	2.98	-4.57	-5.07

*NAP = Normaal Amsterdams Peil (Normal Amsterdam Level) ~ mean sea level

T1 and T2 are of anthropogenic origin. T1 is the root zone. K is a clayey peat layer, Vo is an oxidized peat layer and Vr1..5 are reduced peat layers. The column names refer to the top and bottom of each horizon with respect to the average soil surface and Normal Amsterdam Level (*NAP).

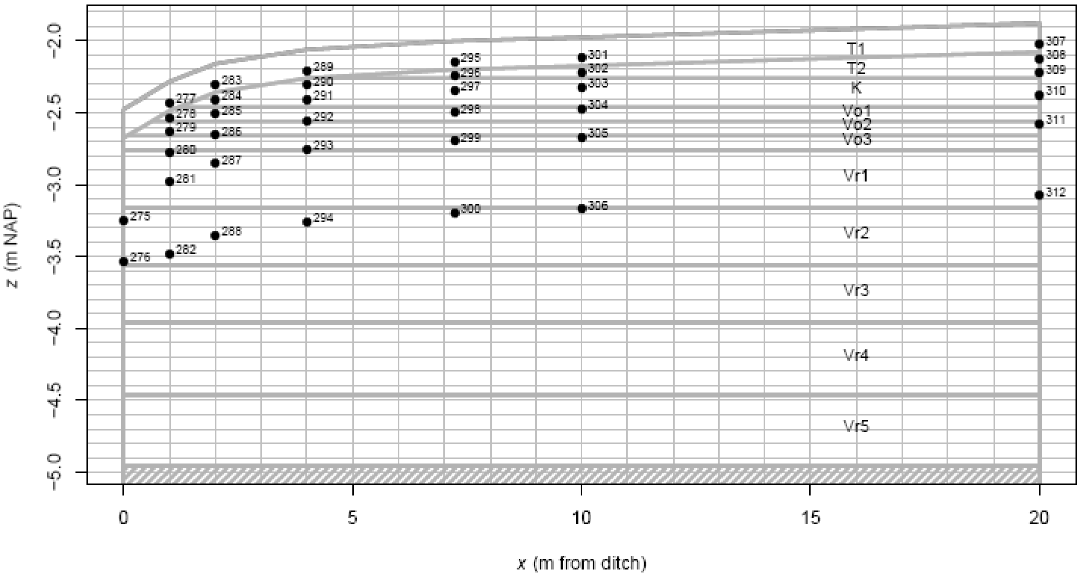


Figure A4.1: Cross section of the study area at the Vlietpolder. The representative soil horizons are given by thick gray lines, the points indicate the positions of the ceramic cups, the labels at the right of these circles the cup indices. The layer at the bottom (hatched) is an impermeable clay layer representing the bottom boundary of the model system.

The soil profile is assumed to be representative for a cross section of the study area at Vlietpolder and has been schematised in Figure A4.1. Cups positions are denoted by dots. At 32 occasions during the period from 2001–10–16 to 2003–04–29, soil moisture samples were extracted from each suction cup. These samples were analysed for Cl^-, NH_4^+-N, NO_3^--N, N, PO_4^{3-}-P, P and SO_4^{2-}. All solutes are expressed in mg/l.

As can be seen in Fig. A4.2, each soil horizon is divided into one or more numerical layers for ANIMO and SWAP. The numeric compartments of SWAP are nested in those of ANIMO which in turn are nested in the soil horizons. In order to initialise, calibrate and validate ANIMO, representative solute concentrations have to be assigned to each numerical ANIMO layer for each sampling date. In this report, a method will be developed for this purpose. In addition, it will also take the uncertainty of the suction cup data into account.

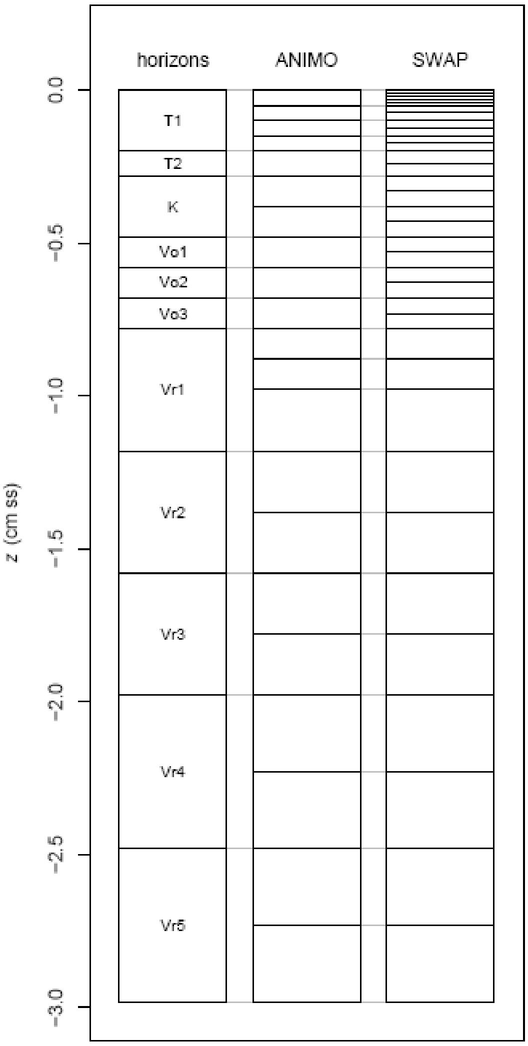


Figure A4.2: Soil profiles with (sub-) horizons and corresponding numeric compartments of ANIMO and SWAP

A4.2 Method

The following issues have to be considered:

1. Soil moisture samples have been extracted from 38 cups at 32 dates. Two cups, with ids 275 and 276 have been excluded from analysis as they were not part of the soil system. These cups were placed in the ditch and have been reported missing after a dredging campaign in September 2002;

2. Soil moisture samples have been analysed for the following solutes: Cl^-, NH_4^+-N, NO_3^--N, N, PO_4^{3-}-P, P and SO_4^{2-}. All solutes are expressed in mg/l. In this report, only solutes that contain nitrogen and phosphorus will be considered;

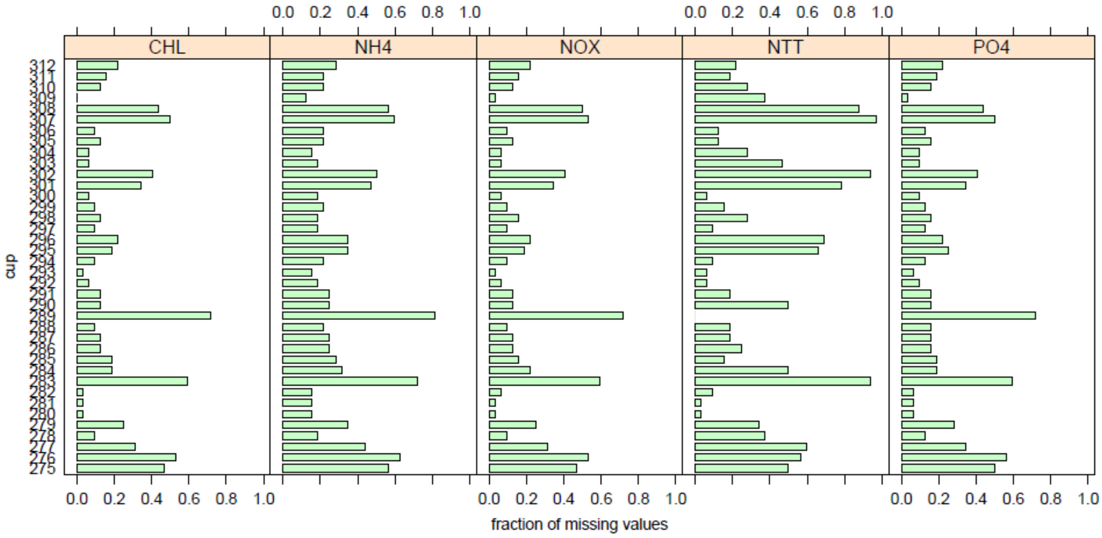


Figure A4.3: Fraction of missing values per solute

3. Assigning Cups tend to be spatially clustered. Cup density is increasing in the direction of the ditch (Fig. A4.1);

4. Depending on the solute, the number of missing values can be considerable (Fig. A4.3).

A4.2.2 Possible approaches

In this section, methodologies will be given for estimating representative solute concentrations. All methodologies will produce some kind of average solute concentration for each horizon, based on suction cups along the entire profile. One may argue that it is more appropriate to only consider cups that are close to the ditch because these cups resemble emission concentrations to the surface water system most. However, computing average solute concentrations based on all cups seems to be legitimate because:

1. Being a pseudo 2–D model, animo also computes average solute concentrations for each numerical layer. Average concentrations will generally be greater than emission concentrations due to N and P retention in the soil system, e.g., denitrification of N, sorption of P, and crop uptake. Estimating some kind of average solute concentration for each numerical layer will therefore be more consistent with the process model itself;

2. Interpretation of suction cup data is hard. Not only due to measurement error, but also because the origin of the extracted soil moisture is often not clear. It is highly affected by pore size distribution (in particular macropores), and the suction applied to the cup. Moreover, the exact locations of the suction cups is not exactly known either. Averaging all cup data will decrease these sources of uncertainty.

1. Simple ('naive') averaging

A simple method is to average solute concentrations in each horizon for each date. Although its simplicity is appealing, naive averaging of solute concentrations will implicitly give more weight to cups near the ditch. Hence, estimates based on this method will be biased.

2. Spatial interpolation

Alternatively, average solute concentrations can be obtained by means of spatial interpolation for each date (e.g. Isaaks and Srivastava, 1989; Goovaerts, 1997). Block-based variants of inverse distance weighting and ordinary kriging seem to be interesting in this respect. However, the first might give biased estimates in case of clustered data configurations, whereas the latter requires estimation of spatial structure. The number of observations may not be large enough to yield reliable estimates of spatial structure. Moreover, even in case of sufficient observations, spatial analysis for all available dates (32) is time consuming.

3. Space–time interpolation

Space-time interpolation not only takes spatial structure into account, but also relations between variables in time. Unfortunately, the number of data is insufficient to perform space–time analysis.

4. Imputation followed by declustering

An interesting alternative is multiple imputation followed by declustering. This procedure tackles both the missing data problem (Fig. A4.3) and the clustering of cups. This method will be described in more detail in the following section.

A4.2.3 Multiple Imputation followed by declustering

Imputation is the practice of 'filling in' missing data with plausible values (Schafer, 1999). In this report, multiple imputation has been performed by means of the mice–package (Van Buuren and Oudshoorn, 2000, 2005). The basic idea is that missing values are substituted by plausible values that are derived from the joint probability distribution of the observed data.

Multiple imputation is basically a three–step process (Rubin, 1987; Schafer, 1999; Van Buuren and Oudshoorn, 2000; Horton and Lipsitz, 2001):
1. simulate sets of plausible values to replace missing values;
2. analyse each set by 'complete–data' methods;
3. combine ('pool') the results.

So, usually not one, but several imputations are generated. In this way, the additional uncertainty due to imputation can be taken into account.

1. Simulation of imputations

The first step is to complete our data by imputation. This has been done by a procedure called 'predictive mean matching' (see the online help in Van Buuren and Oudshoorn (2005) for more details). A total of m = 10 independent imputations have been obtained by means of Gibbs sampling (Gilks et al., 1996; Van Buuren and Oudshoorn, 2000, Appendix A). This number is in agreement with recommendations found in literature, i.e., five to ten imputations (Schafer, 1999). More imputations have little or no practical benifit (but won't hurt either). The total number of iterations of the Gibbs sampling algorithm was set to ten. This is in agreement with findings of Van Buuren and Oudshoorn (2000). Log–transformation has been applied prior to imputation, and only cups at the same distance to the ditch as the cup that has to be imputed were taken as predictors.

2. Analyses of imputations

Having obtained m = 10 imputations, the next thing to do is to apply a 'complete–data' method to each imputation. In our case, the 'complete-data' method is to apply a weighted mean. The aim is to obtain average solute concentrations for each horizon at each date while taking the clustering of cups into account. This comes down to assigning proper declustering weights to the cups. The weights are computed as follows:

1. Construct a Voronoi tessellation given the locations of the cups (Fig. A4.4);

2. Compute the intersection between the soil horizon boundaries and the Voronoi tessellation. The areas of the resulting polygons are denoted by A_{ij}, i.e., the area of influence of cup i in horizon j;

3. Weight λ_{ij} for cup i and horizon j is a function of A_{ij}. Clustered cups have smaller A_{ij} and therefore receive smaller weights:
$$\lambda_{ij} = \frac{A_{ij}}{\sum_i A_{ij}} = \frac{A_{ij}}{\bar{A}_j} \tag{A4.1}$$
where denominator $\bar{A}_j = \sum_i A_{ij}$ represents the total area of horizon j.

This procedure is often referred to as 'polygonal declustering' (Isaaks and Srivastava, 1989). Weights λ_{ij} as function of cup i and horizon j are given in Fig. A4.5. Note that $\sum_i \lambda_{ij} = 1 \forall j$.

After having computed the declustering weights, the (weighted) mean solute concentration for horizon j and imputation $\ell = 1, \ldots, m$ can be estimated by:

$$\bar{C}_j^{(\ell)} = \sum_{i=1}^{n} \lambda_{ij} C_i^{(\ell)} \tag{A4.2}$$

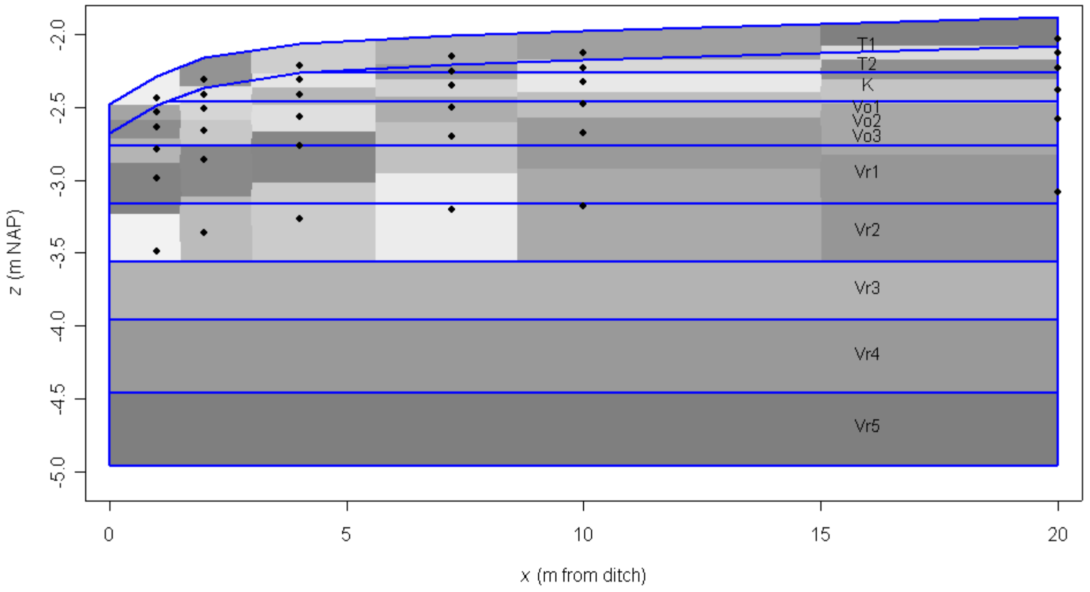


Figure A4.5: Cross section of the study area at the Vlietpolder. Each cup has been plotted in its area of interest.

where $C_i^{(\ell)}$ is the imputed solute concentration for cup i, and n is the total number of cups. Note that $\sum_i^n \lambda_{ij} = 1$.

Its (weighted) squared standard error[1] is given by:

$$U_j^{(\ell)} = \frac{1}{n-1} \sum_{i=1}^{n} \lambda_i \left(C_i^{(\ell)} - \bar{C}_j^{(\ell)} \right)^2 \qquad \text{(A4.3)}$$

where $\sum_i^n \lambda_{ij} = 1$.

3. Pooling of imputations

Following Schafer (1999), the overall mean solute concentration for horizon j is simply:

$$\bar{C}_j = \frac{1}{m} \sum_{\ell=1}^{m} \bar{C}_j^{(\ell)} \qquad \text{(A4.4)}$$

---

[1] The weighted squared standard error is equal to the weighted variance $\frac{n}{n-1} \sum_{i=1}^{n} \lambda_i \left(C_i^{(\ell)} - \bar{C}_j^{(\ell)} \right)^2$ divided by n.

The uncertainty in $\bar{C}_j$ consists of two components, i.e., the average within–imputation variance $\bar{U}_j$ and the between–imputations variance B_j. The first can be obtained by pooling the squared standard errors for all m imputations:

$$\bar{U}_j = \frac{1}{m}\sum_{\ell=1}^{m} U_j^{(\ell)} \qquad \text{(A4.5)}$$

The between–imputations variance is given by:

$$B_j = \frac{1}{m-1}\sum_{\ell=1}^{m}\left(\bar{C}_j^{(\ell)} - \bar{C}_j\right)^2 \qquad \text{(A4.6)}$$

The overall squared standard error is then given by:

$$B_j = \frac{1}{m-1}\sum_{\ell=1}^{m}\left(\bar{C}_j^{(\ell)} - \bar{C}_j\right)^2 \qquad \text{(A4.6)}$$

See Schafer (1999) or Schafer and Graham (2002) for a description in more general terms.

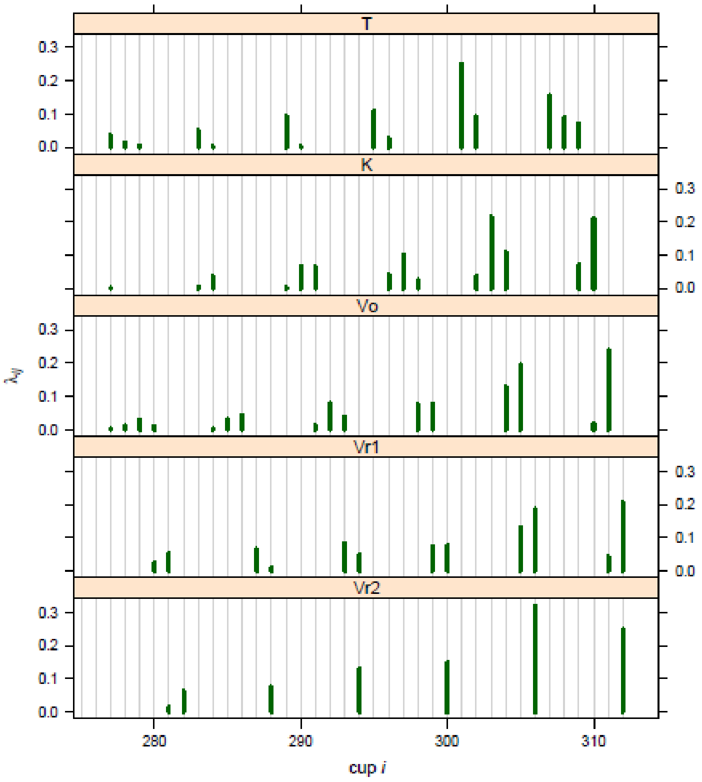


Figure A4.6: Trellis plots of declustering weights λ_{ij} as function of cup i and soil horizon j. Soil horizons T1 and T2 have been taken together as horizon T.

A4.3 Results

A4.3.1 Validation of multiple imputation algorithm

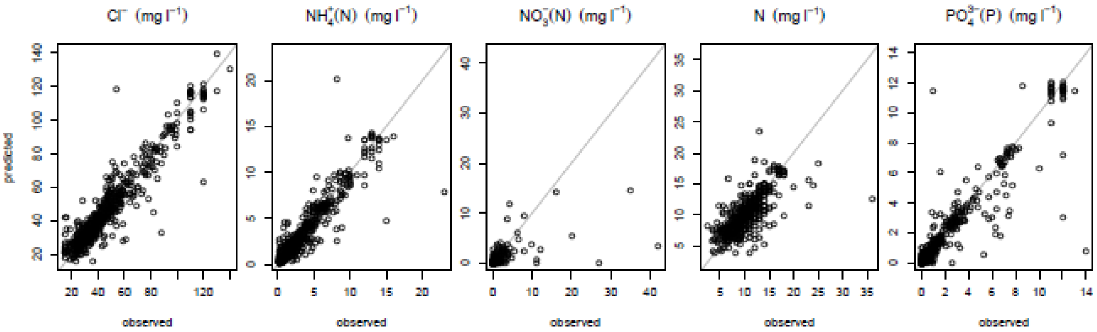


Figure A4.7: Predicted versus observed solute concentrations based on leave–one–out cross–validation of the MICE procedure. Validation statistics for chloride: ME = 0.30 and RMSE = 46; for ammonium–N: ME = 0.10 and RMSE = 1.45; for nitrate–N: ME = 0.19 and RMSE = 4.06; for total nitrogen: ME = 0.14 and RMSE = 4.87; for phosphate–P: ME = 0.09 and RMSE = 0.83. All units are in mg/l. MICE settings: 10 imputations, 10 iterations, maximum fraction of missing values allowed for predictor variables is 0.4.

A4.3.2 Results for substances concerned

Figures A4.8-A4.15 give the results of the applied method for the substances concerned: chloride, ammonium, nitrate, total nitrogen, ortho-phosphate, total phosphorus and sulphate.

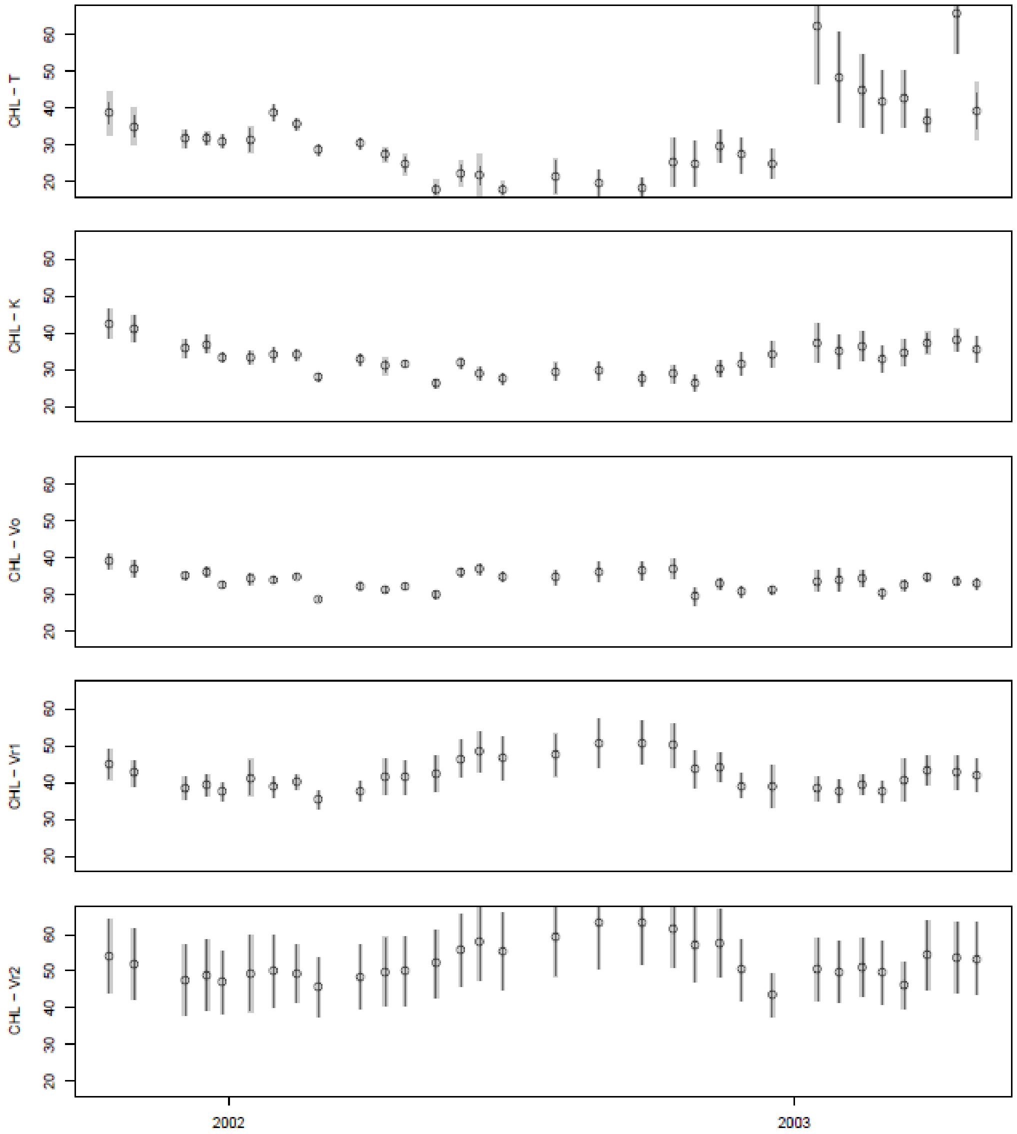


Figure A4.8: Time-series of ***Chloride (mg L^{-1})*** *for each soil horizon. The dots represent average observations, the thick gray bars are standard errors corrected for the uncertainty of missing values, the thin black lines are within-imputation standard errors. The difference between the standard errors is due to the occurrence of missing values.*

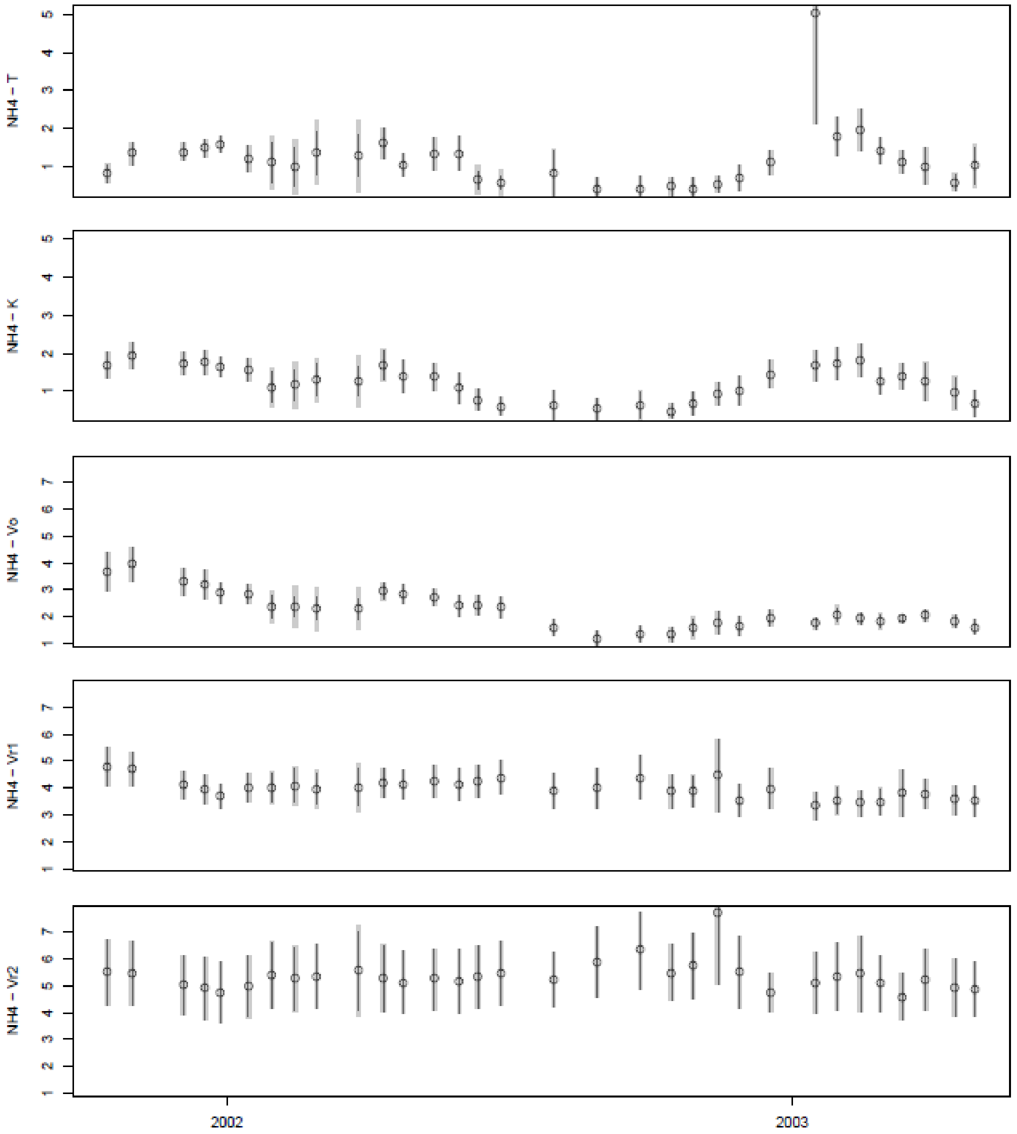


Figure A4.9: Time-series of **Ammonium (mg N L^{-1})** *for each soil horizon. The dots represent average observations, the thick gray bars are standard errors corrected for the uncertainty of missing values, the thin black lines are within-imputation standard errors. The difference between the standard errors is due to the occurrence of missing values. Note differences in scale.*

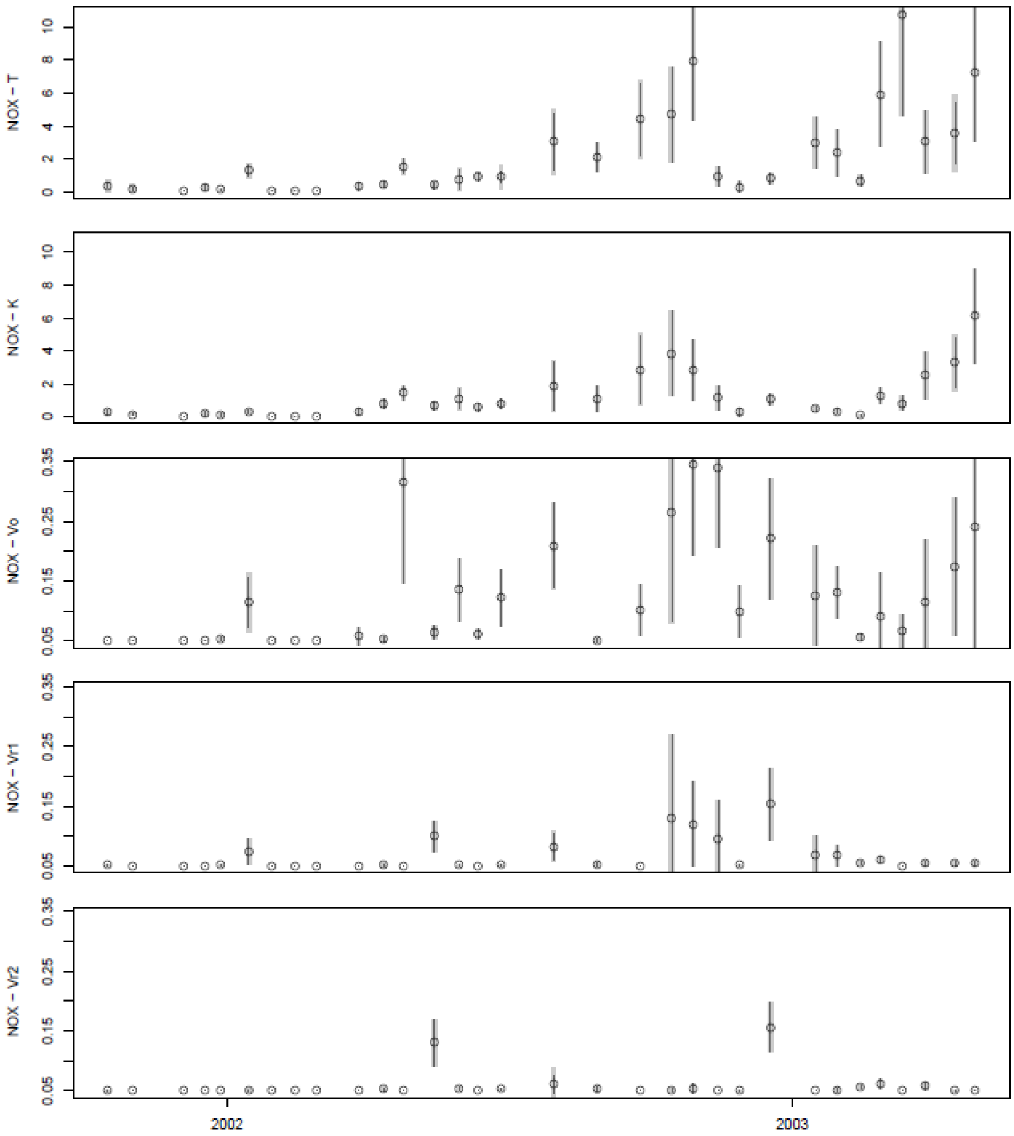


Figure A4.10: Time-series of ***Nitrate (mg N L^{-1})*** *for each soil horizon. The dots represent average observations, the thick gray bars are standard errors corrected for the uncertainty of missing values, the thin black lines are within-imputation standard errors. The difference between the standard errors is due to the occurrence of missing values. Note differences in scale.*

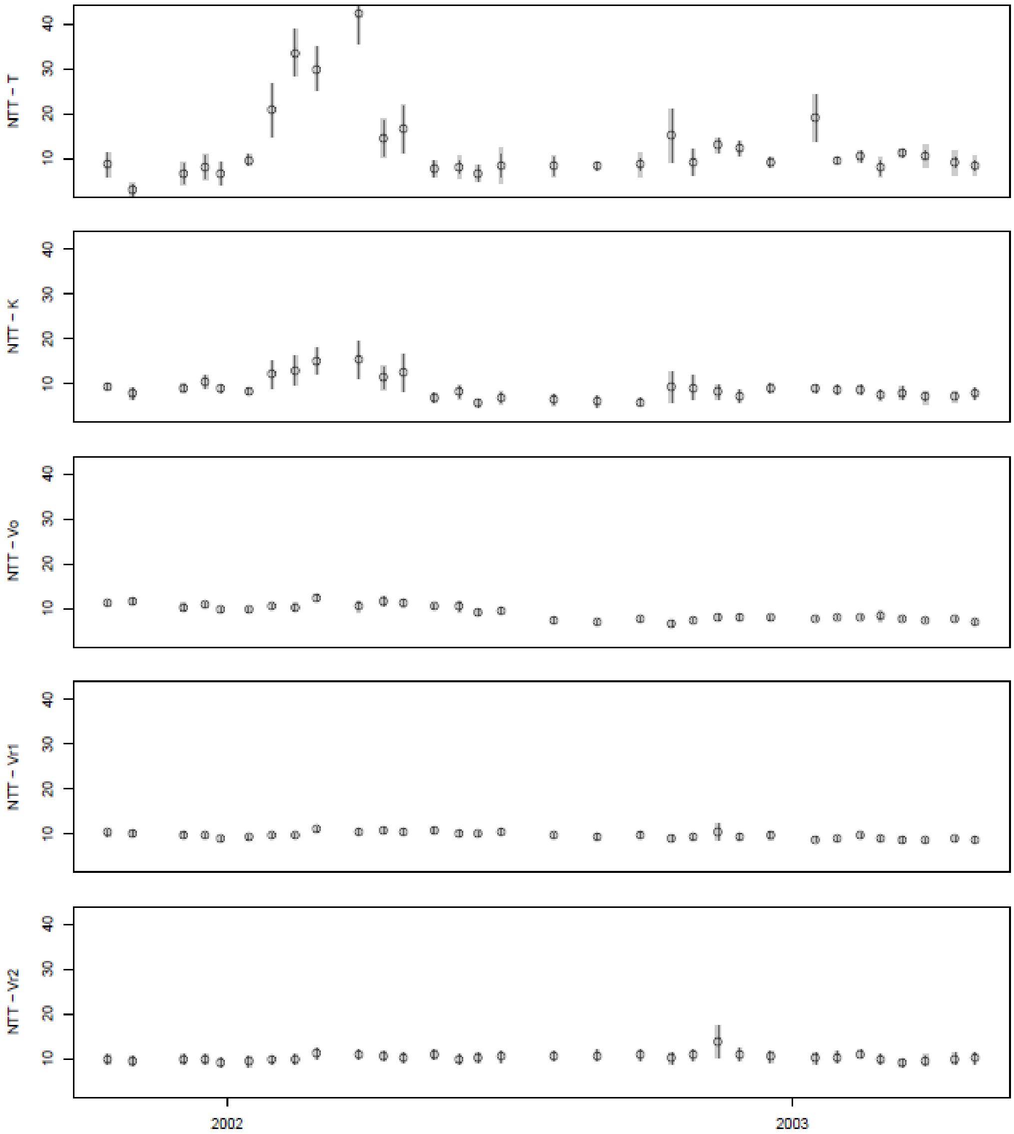


Figure A4.11: Time-series of ***Total nitrogen (mg N L^{-1})*** *for each soil horizon. The dots represent average observations, the thick gray bars are standard errors corrected for the uncertainty of missing values, the thin black lines are within-imputation standard errors. The difference between the standard errors is due to the occurrence of missing values.*

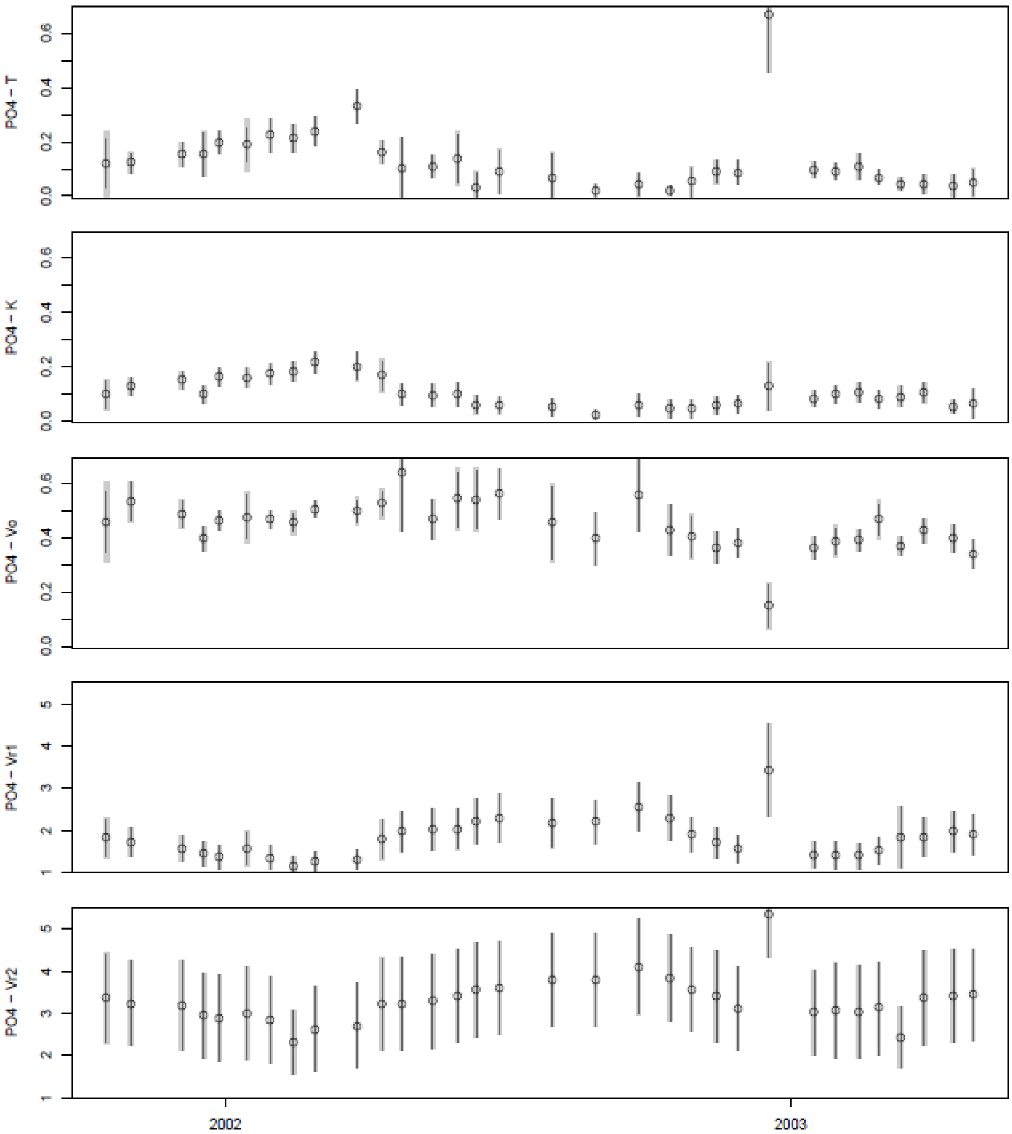


Figure A4.13: Time-series of **Ortho phosphate (mg P L^{-1})** *for each soil horizon. The dots represent average observations, the thick gray bars are standard errors corrected for the uncertainty of missing values, the thin black lines are within-imputation standard errors. The difference between the standard errors is due to the occurrence of missing values. Note differences in scale.*

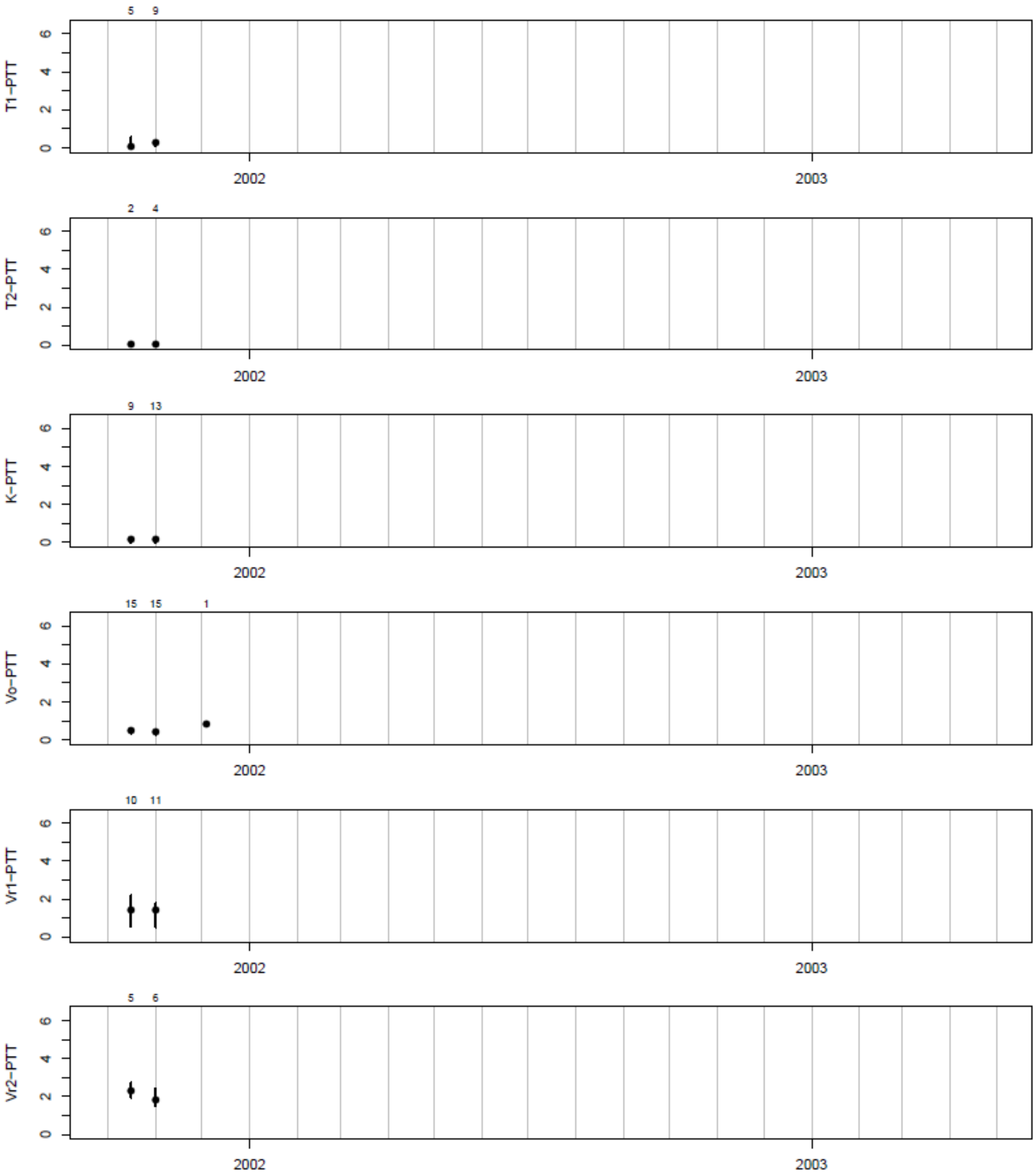


Figure A4.14: Time-series of **Total phosphorus (mg P L^{-1})** *for each soil horizon. The dots represent median observations whereas the bars give interquartile distances. Fifty percent of the observations at specific date are within this interval. The numbers at the top margins represent the number of values on which the statistics are based.*

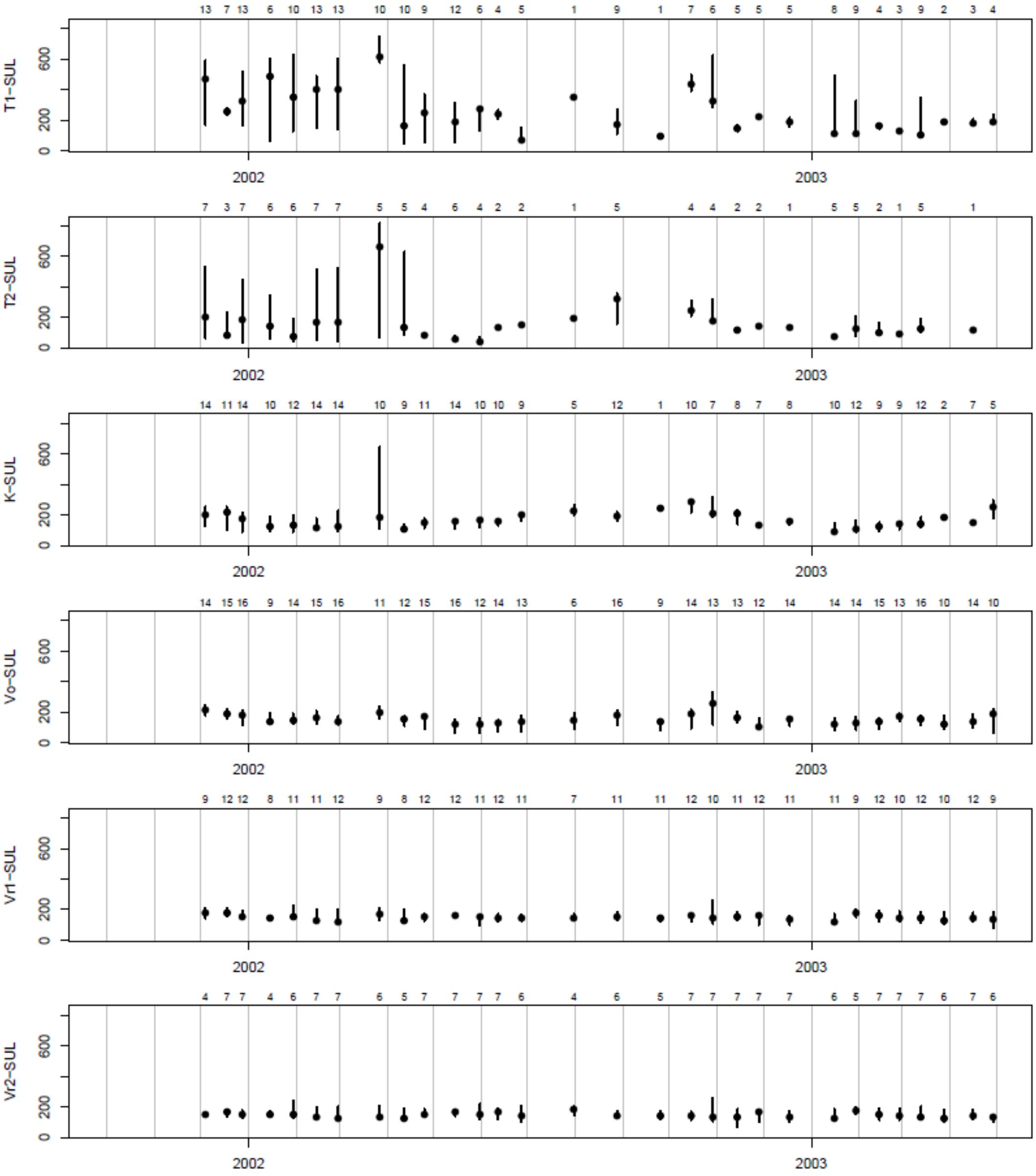
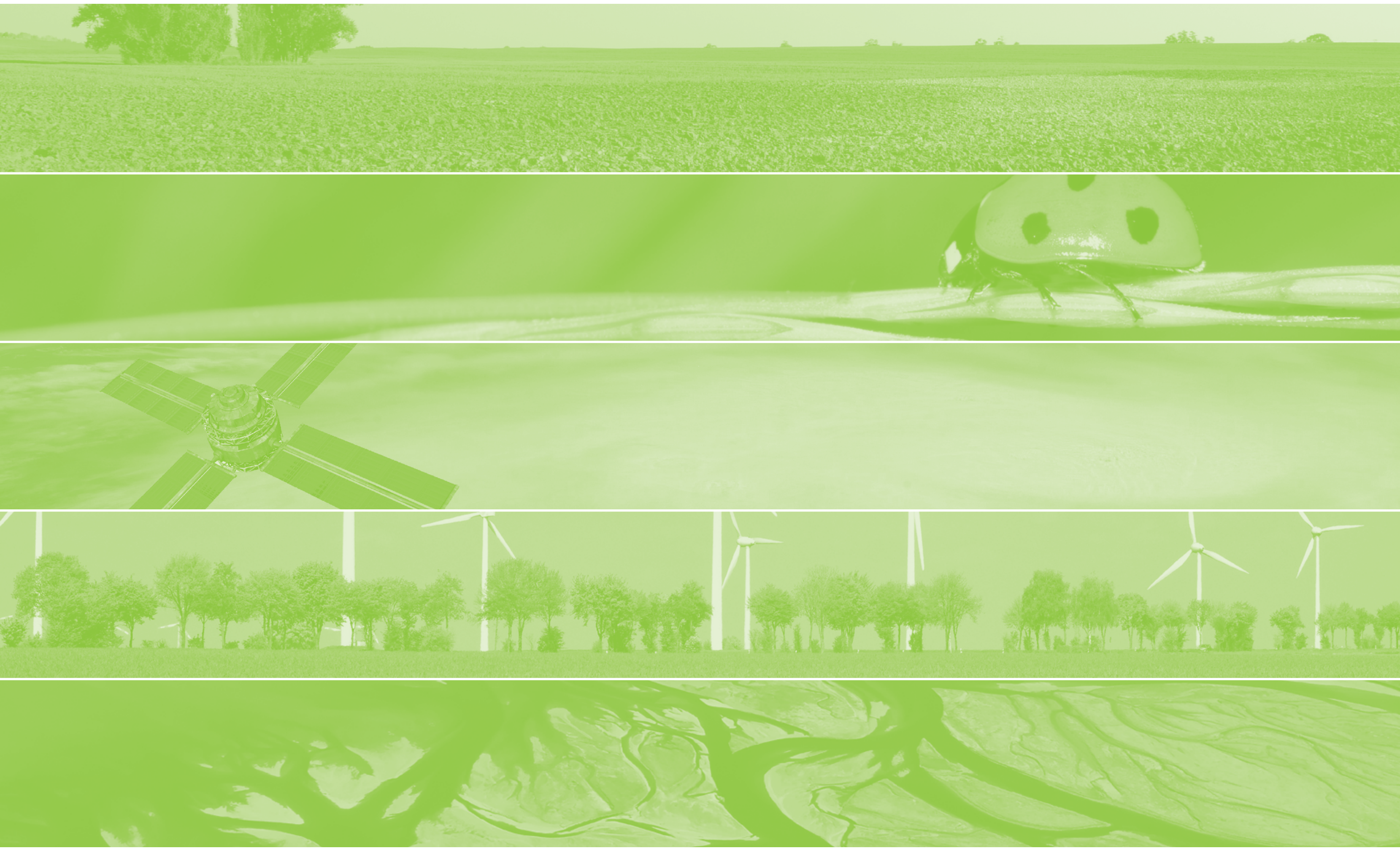


Figure A4.15: Time-series of ***Sulphate (mg SO_4^{2-} L^{-1})*** *for each soil horizon. The dots represent median observations whereas the bars give interquartile distances. Fifty percent of the observations at specific date are within this interval. The numbers at the top margins represent the number of values on which the statistics are based.*

Appendix 5 Input file Chempar.inp

```
Filename:  CHEMPAR.INP

Content:   Input for ANIMO-version 4.0: Vlietpolder

>chedef: ----------------- definition of chemical system ---------------
 2       ! optcxfa: langmuir
 1       ! ncxfa:   1 equilibrium sorption site
 3       ! optcxsl: freundlich
 3       ! ncxsl:   3 non equilibrium sorption site
 0       ! optpr:   non equilibrium precipitation

>chesor: ----------------- sorption variables --------------------------
 2
       0.00E+00      2.79E-06      4.00E+02      0.00E+00      0.00E+00
       3.00E-01
       0.00E+00      0.00E+00      0.00E+00      1.06E-05      2.10E-01
       1.21E+00      1.21E-02
       0.00E+00      0.00E+00      0.00E+00      8.93E-07      1.80E-02
       1.51E-01      1.51E-03
       0.00E+00      0.00E+00      0.00E+00      2.67E-06      2.54E-01
       1.63E-02      1.63E-04
       0.00E+00      3.41E-06      4.00E+02      0.00E+00      0.00E+00
       3.00E-01
       0.00E+00      0.00E+00      0.00E+00      9.55E-06      7.18E-01
       4.97E+00      4.97E-02
       0.00E+00      0.00E+00      0.00E+00      3.79E-06      1.48E-01
       6.12E-01      6.12E-03
       0.00E+00      0.00E+00      0.00E+00      1.07E-04      4.32E-01
       1.33E-04      1.33E-06
       0.00E+00      4.65E-06      4.00E+02      0.00E+00      0.00E+00
       3.00E-01
       0.00E+00      0.00E+00      0.00E+00      6.84E-06      2.21E-01
       8.37E-01      8.37E-03
       0.00E+00      0.00E+00      0.00E+00      1.08E-06      7.85E-02
       1.52E-02      1.52E-04
       0.00E+00      0.00E+00      0.00E+00      0.00E+00      1.00E-03
       1.00E-03      1.00E-05
       0.00E+00      7.75E-06      5.00E+01      0.00E+00      0.00E+00
       3.00E-01
       0.00E+00      0.00E+00      0.00E+00      2.39E-06      1.30E-01
       4.96E-01      4.96E-03
       0.00E+00      0.00E+00      0.00E+00      1.33E-05      8.39E-01
       9.84E-03      9.84E-05
       0.00E+00      0.00E+00      0.00E+00      0.00E+00      1.00E-03
       1.00E-03      1.00E-05
       0.00E+00      9.92E-06      5.00E+01      0.00E+00      0.00E+00
       3.00E-01
       0.00E+00      0.00E+00      0.00E+00      5.11E-07      9.70E-02
       4.26E-01      4.26E-03
       0.00E+00      0.00E+00      0.00E+00      5.39E-07      2.38E-01
       5.73E-03      5.73E-05
       0.00E+00      0.00E+00      0.00E+00      0.00E+00      1.00E-03
       1.00E-03      1.00E-05


>chepre: ----------------- precipitation variables ---------------------
 0.01     ! recfpr

>chebuf: ----------------- buffer concentration ------------------------
 0        ! optcobu : cobuho calculated in subr. INICALC_P with given pH
 0.05     ! cobuho(1)
```



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