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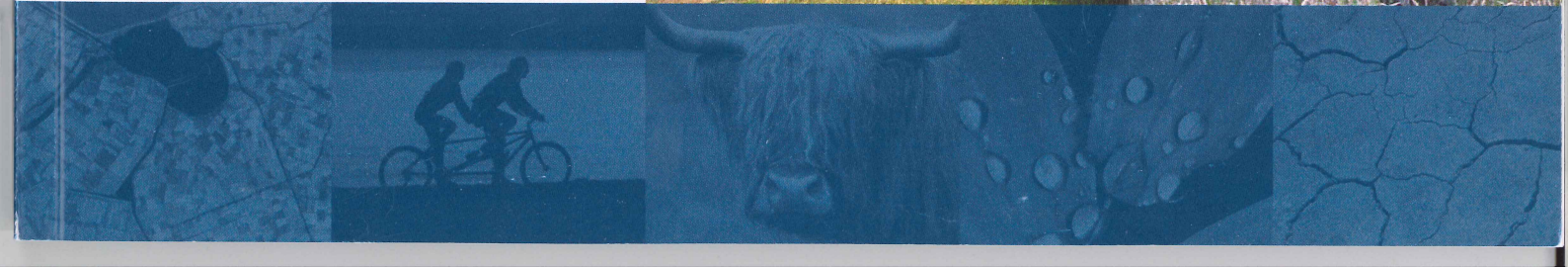
Prediction of Nitrogen and Phosphorus leaching to groundwater and surface waters

Process descriptions of the Animo4.0 model

P. Groenendijk
L.V. Renaud
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ABSTRACT

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The fertilization reduction policy intended to pursue environmental objects and regional water management strategies to meet Water Framework Directive objectives justify a thorough evaluation of the effectiveness of measures and reconnaissance of adverse impacts. The model aims at the evaluation and prediction of nutrient leaching to groundwater and surface water systems under the influence of fertilization, land use and land management, water management and soil properties. Since the release of ANIMO version 3.5 some new model formulations have been implemented regarding the influence of soil moisture content on mineralization and denitrification. Also the input of daily nutrient uptake rates as simulation results of external crop models is facilitated. A concise description is presented of the process descriptions as have been implemented in version 4.0 of the ANIMO model.

Keywords: eutrophication, fertilization, nitrate leaching, nutrient management, simulation model, soil processes, surface water pollution, water management

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Preface

This report gives an account of the simulation model ANIMO (Agricultural Nutrient Model) version 4.0. An extensive description of the theoretical background of earlier versions is given by [Groenendijk and Kroes \(1999\)](#) and [Rijtema *et al.* \(1999\)](#).

The ANIMO model was originally developed in 1985 by the Institute for Land and Water management Research. The first version of the model was operational in 1985 and ever since its development has continued until the present version. Version 4.0 of the model ANIMO is integrated into the model instrument STONE (Samen Te Ontwikkelen Nutrinten Emissiemodel). STONE is a tool for analyzing the impacts of fertilization scenarios on nutrient leaching to groundwater and surface water systems on the Dutch national scale. For analysis of the nutrient leaching at field scale and at sub-catchment scale, the model ANIMO will be available as a stand-alone model or as a model to be integrated into other comprehensive modeling systems.

DWK-research programme 398-III has taken the responsibility for the maintenance of the model and software implementation. For questions about the model formulations, the reader is referred to Mr. P. Groenendijk (piet.groenendijk@wur.nl). Information on the programme code or availability of the ANIMO model is obtainable by contacting Mr. L.V. Renaud (leo.renaud@wur.nl).

Wageningen, August 2005
Piet Groenendijk

Summary

The ANIMO model aims to quantify the relation between fertilization level, soil management and the leaching of nutrients to groundwater and surface water systems for a wide range of soil types and different hydrological conditions. The model comprises a large number of simplified process formulations.

This report presents an update of the ANIMO model. The ANIMO model has been incorporated in the model chain STONE which aims at evaluation of the effects of change in the agricultural sector and policy measures on the leaching of N and P to groundwater and surface waters. Since the last release of the ANIMO description, some new options have been implemented. The new options aim at:

- reach agreement among scientists with respect to process formulations. Simplified relations for the response of soil moisture on process rates have been adopted from the SONICG-model.
- tailor the crop uptake to measured data and agricultural census data by creating the ability to input pre-processed nutrient uptake data. Within the STONE model chain these data are supplied by the QUAD-MOD model.
- make use of recent developments in the supporting hydrological model SWAP. Some subjects have been refined in the SWAP model: simulation of soil temperatures, simulation of a snow layer and frost conditions with accompanying water balance items.
- provide information on modeled P-pools in terms of the agronomical concept *Pw-number*
- improve the applicability of the model on regional scale

A concise description of the process formulations implemented in ANIMO version 4.0 is presented. These include:

- Addition of organic materials and nutrients to the soil system by fertilization, root residues and harvest losses and the redistribution of these materials by tillage.
- Accumulation and decomposition of soil organic matter in relation to the quality and composition of different organic materials.
- Crop uptake of nitrogen and phosphorus in relation to the nutrient status of arable crops and grassland. Dry matter production of grassland is simulated by a dynamic sub-model. Another option is to input data concerning N and P uptake and crop residues per day.
- Sorption of ammonium to the solid soil phase.
- Accumulation of phosphate in soil. Four mineral phosphorus pools are distinguished: 1) aqueous phase; 2) adsorption phase described by a Langmuir

sorption isotherm; 3) diffusion-precipitation of phosphate described by a multi-site rate dependent sorption equation and 4) chemical precipitation when the solubility product has been exceeded. The model has an option to calculate the *Pw-number* per soil compartment.

- Nitrification and denitrification as a function of the oxygen demand of transformation processes and the diffusive properties of the soil.
- Volatilization of ammonium and atmospheric supply by dry and wet deposition.
- Influence of environmental factors (*pH*, temperature, aeration and drought condition) on the transformation rates. The newly implemented option uses the *water filled pore space* as a controlling factor.
- Leaching of different nitrogen and phosphorus species: ammonium, nitrate, dissolved organic nitrogen, mineral phosphate and dissolved organic phosphorus.

The model generates material balances as well as time series of all relevant state variables for a user defined number of soil compartments and a user defined time interval. The initialization demands special attention for regional scale applications. The assignment of initial values to the organic matter and phosphate pools has a major influence on the final simulation results. Even the results of long-term scenario studies may be affected by the initial estimates of the organic matter pools and the phosphate state variables. In the framework of the STONE-model an initialization pre-run is conducted with assumed land use and fertilizations rates between 1941 and 1985 or between 1941 and 2000. The resulting contents of the organic matter pools and phosphate pools is used as an input for further model analysis for the period thereafter. The results of these historical simulation runs allow verification to measured field data and provide insight in the overall model performance.

Although the data acquisition requires considerable efforts and required skills to apply the model instrument is high, the model has proven to be a useful tool in scenario analysis and decision making.

1 Introduction

Management of land and water resources has resulted in an increased need for information on the environmental impacts of fertilization strategies, land use changes and water management policies. Application of animal manure and artificial fertilizers to mineral soils has resulted in an increased leaching of nutrients to groundwater (Fraters *et al.*, 1998) and surface water systems (van der Molen *et al.*, 1998; Willems and Boers, 2004). In many cases the sorption capacity of iron and aluminium minerals has been utilized to fix phosphates to such a degree that leaching of soluble phosphate to surface waters can be expected. Legislation measures to control fertilizer applications have been implemented at regional, national and international levels). The EU nitrate directive (European Commission, 1991) sets goals for reducing the pollution of groundwater by agricultural sources (Henkens and van Keulen, 2001).

In the Netherlands policy measures were implemented from 1984 onwards to limit the negative consequences of the intensification of Dutch agriculture. From 1995, an N and P accounting system (MINAS) at the farm level was implemented. The accounting system aimed at more than 50% lowering (compared to 1985) of all N and P emissions from agriculture, including the emissions into surface waters (Oenema and Roest, 1998; Oenema *et al.*, 1998). Until now, most of the measures are based on rough risk assessments with regard to nitrate leaching. It is not always clear what the short and long term effects of regulative measures will be.

The aim of integrated water management is to develop sustainable policies that reconcile competing functions within catchments. Interaction between processes make this a difficult task. The EU Framework Water Directive (European Commission, 1997) provides a legal status to water management policies by defining constraints based on local conditions. Member States shall protect, enhance and restore all surface water bodies with the aim of achieving a good surface water status. This requires an EU-wide inventory of local water conditions, including an analysis of the pressures and the driving forces of eutrophication. Models provide assistance to help foresee the likely outcomes of different options.

There is a need to quantify the sources of nutrients which contaminate groundwater systems and lead to eutrophication of surface waters. Quantification and evaluation of strategies requires various climatic conditions, soil types, water management alternatives, cropping patterns and agricultural technologies. A thorough understanding of the transfer and transformation principles which lead to contamination and eutrophication requires a comprehensive knowledge of processes governing the changes in the soil-water-plant system. Due to the development of simulation models, the interactions of different processes as influenced by farming strategies and soil and water management can be studied. A simulation model enables the integration of knowledge of different disciplines and the analysis of short and long term impacts of changes in farming strategy, climate and water management on the environment.

In scenario studies, models can be used to identify feasible targets (e.g. water quality level) and to compare the efficacy of various possible policy measures, for example, in reducing nutrient emissions to ground and surface waters. There is usually no alternative to simulation model applications, as the effects of policy measures and the resulting environmental changes gradually occur over a long time span (e.g. 30

years). A clear advantage of process-based simulation models [e.g. WHNSIM (Huwe and van der Ploeg, 1991; Huwe, 1992); MIKE SHE (Refsgaard *et al.*, 1999) and NTT (Nikolaides *et al.*, 1998)] for such policy evaluations is the possibility to take into account the interactions between various ecosystem elements (e.g. soil, water and atmosphere) and management and measures. Such approach can support and may improve decision making. More simple, often empirical nutrient emission models [MAGPIE (Lord and Anthony, 2000); INITIATOR (de Vries *et al.*, 2001); POLFLOW (de Wit, 2001) and the model of Johnes (1996)] appeared often to be sufficient for analyzing specific purposes at large spatial and temporal scales, but do not give information on the spatial and temporal variation in output data, do not describe the soil and transport processes, do not give output from intermediate variables, and may overlook certain factors.

Detailed mechanistic leaching models require detailed hydrological information with respect to soil water balances, the interaction between soil water and deep groundwater and the interaction between soil water and surface waters. Most hydrological modeling approaches addressing the interaction between soil water or shallow groundwater and surface water systems have used one-dimensional or two-dimensional models. Analysis and simulation of the three dimensional nature of the problem is needed for a better understanding of these interactions. As computation capacity increases every year, recent modeling efforts attempt to describe the comprehensive unsaturated/saturated soil water and overland flow and surface water system fully integrated. InHM is a physically based, spatially distributed, finite element, integrated surface water and groundwater model developed by VanderKwaak (1999). The MikeShe/Mike11 modeling system (Refsgaard *et al.*, 1995; Abbott *et al.*, 1986) is a physically-based, spatially-distributed, finite difference, integrated surface water and groundwater model. WASH123 (WATERShed systems of 1D Stream, 2D Overland and 3D subsurface Media) is capable of simulating Surface water-Groundwater interactions and overland flow in a finite-element framework (Yeh *et al.*, 1998), based on FEMWATER (Lin *et al.*, 1997). However, most models operating at a regional scale today are still not well equipped to deal with local phenomena related to flow near domain boundaries [e.g. MODFLOW (McDonald and Harbaugh, 1988)].

The coherence between water quantity and water quality issues could be guaranteed by using two- or three dimensional groundwater models. However, these type of models could not be applied at national or supra-regional scale for assessment of water quality parameters. Up-scaling of groundwater flow descriptions and conceptualization of the relations involved has resulted to a feasible approach. The SWAP model (Kroes *et al.*, 2000; van Dam, 2000; Kroes and van Dam, 2003) is a comprehensive one-dimensional physically based mode for simulating the vertical transport of water, heat and solutes in the saturated and unsaturated top-soil compartments. The soil water transport module is based on the well-known Richards' equation. The top boundary is the soil surface, which can be with or without a crop. The infiltration of water from precipitation and irrigation and the water losses by plant evaporation, soil evaporation and surface runoff are simulated here. The bottom boundary should be defined by the model user and determines the vertical flux to or from deeper soil compartments. In the Dutch national application with STONE (Wolf *et al.*, 2003) of the SWAP model the lower boundary is chosen at 13 m depth. The lateral boundary is used to simulate the interaction (discharge or infiltration) with surface water systems.

The STONE model (Wolf *et al.*, 2003) was developed for evaluating the effects of

changes in the agricultural sector (e.g. changes in fertilizer recommendations and cropping patterns) and in policy measures that restrict fertilization levels on the leaching of N and P to ground water and surface waters. The system was in particular developed for evaluations at the national scale, and may also be applied at the regional scale. STONE consists of a chain of models, which are applied to spatial units that represent the biophysical conditions in the Netherlands (e.g. land use and soil type). Calculations are carried out successively using the different components of the model chain. First, various policy measures to reduce nutrient emissions to ground water and surface waters are specified and translated into data on the number of various farm animals and their manure excretion by the CLEAN model ([van Tol *et al.*, 2001](#)). This module computes the N and P input into the soil from application of manure and inorganic fertilizer and the ammonia emission from agriculture. Next, the OPS/SRM model ([van Jaarsveld, 1990](#)) is applied for calculating the N deposition from the atmosphere. N and P uptake by crops and input to the soil by crop residues is calculated using the QUAD-MOD model ([ten Berge *et al.*, 2000](#)). Finally the ANIMO model, wrapped into a geographical oriented software shell ([Boogaard and Kroes, 1997](#)), is used for calculating the organic matter and nutrient cycling in the soil and the N and P transport to the groundwater and surface water systems. Within this system the results can be presented as maps of, for example, crop uptake rates, N and P accumulation in soils, nitrate concentrations in groundwater, phosphate contents of topsoils and the N and P transport to surface waters.

The ANIMO model is a software package maintained by the Alterra institute for Green World Research. It aims for field and regional assessments with respect to groundwater and surface water pollution by nitrogen and phosphorus, originating from soil with agricultural land use. General characteristics are:

- process oriented, but each process simply described
- complete description of organic matter, nitrogen and phosphorus cycle
- dynamic, with internal computation time steps of one or ten days, but total simulation length of time may amount more than 100 years
- one dimensional solute transport, but the discharge to surface water has been based on a pseudo two-dimensional concept

The model has been described by [Groenendijk and Kroes \(1999\)](#) and has been applied in a large number of research projects. Recently new options have been implemented. The new options aim at:

- reach agreement among scientists with respect to process formulations. Simplified relations for the response of soil moisture on process rates have been adopted from the SONICG-model ([Bril *et al.*, 1994](#)).
- tailor the crop uptake to measured data and agricultural census data by creating the ability to input pre-processed nutrient uptake data. Within the STONE model chain these data are supplied by the QUAD-MOD model.
- make use of recent developments in the supporting hydrological model SWAP. Some subjects have been refined in the SWAP model: simulation of soil temperatures, simulation of a snow layer and frost conditions with accompanying water balance items.

- provide information on modeled P-pools in terms of the agronomical concept *Pw-number*
- improve the applicability of the model on regional scale

In most applications ANIMO uses the results generated by the SWAP model as hydrological input. In the STONE model chain the ANIMO is one of the primary links. The model has been tested and the overall performance has been validated for a number of field plots. A sensitivity analysis of the model parameters and a tentative uncertainty analysis have been carried out by [Groenenberg *et al.* \(1996\)](#).

The underlying report gives an account of the process descriptions implemented in the ANIMO model. Chapter two provides a brief description of the land management aspects which can be handled by the model. Chapter three presents the pre-supposed hydrological schematization and in chapter four a discussion on the numerical elaboration of the *conservation and transport equation* is given. Crop production and nutrient uptake are described in chapter five. Model assumptions and rate equations concerning the organic matter cycle, the nitrogen cycle and the phosphorus are given in resp. chapter six, seven and eight. Chapter nine gives an account of the way environmental factors as moisture content, temperature and acidity have an influence on process rates. Finally some aspects with respect to the initialization of the organic matter pools and the mineral phosphate pools are summarized in chapter ten.

For user guidelines and modelers instructions, the reader is referred to [Renaud *et al.* \(2005\)](#). More detailed information on the results of research projects for which the model was used can be found in a number of reports and publications ([Drent *et al.*, 1988](#); [Kroes *et al.*, 1990](#); [van der Bolt *et al.*, 1990](#); [Hendriks *et al.*, 1994](#); [Schoumans and Kruijne, 1995](#); [Hack-ten Broeke and Dijkstra, 1995](#); [van der Bolt *et al.*, 1996](#); [Groenendijk and van der Bolt, 1996](#); [Kruijne *et al.*, 1996](#); [Boers *et al.*, 1997](#); [Groenendijk and Boers, 1999](#); [Vinten, 1999](#); [van der Salm and Schoumans, 2000](#); [Roelsma, 2001](#); [Overbeek *et al.*, 2001a,b](#); [Milieu- en Natuurplanbureau, 2002](#); [Schoumans *et al.*, 2002](#); [Milieu- en Natuurplanbureau, 2004](#); [Schoumans *et al.*, 2004a](#); [ten Berge, 2002](#); [van Middelkoop *et al.*, 2004](#); [Schoumans *et al.*, 2004b](#)). The model has been subjected to a number of reviews and model comparisons ([Reiniger and Vereecken, 1990](#); [de Willigen, 1991](#); [Wu and McGechan, 1998](#); [Lewis and McGechan, 2002](#); [McGechan and Lewis, 2002](#); [McGechan, 2002](#); [Silgram and Schoumans, 2004](#)).

2 Land management

2.1 Fertilization

One of the original aims for the development of the ANIMO model was to analyze the nutrient leaching for different soil types and for different hydrological regimes as a result of a broad spectrum of agricultural activities. These activities may lead to the addition of several materials of different quality (e.g. types of manure, fertilizers, crop residues, compost, treated waste water residues, etc.) to the soil. The ANIMO model has the ability to handle a wide range of materials. The user should specify the number of materials to be considered in model simulations as well as a number of characteristics. The organic compounds of the materials are sub-divided into a number of classes, each with its own properties. This provides the user the flexibility to specify the decomposition and mineralization of the organic compounds in accordance with measured time series. The characterization of organic materials as well as a method to relate the decay constants to empirical approaches is discussed in Par. 6.1. An overview of the schematization of the materials and the accompanying parameters is given in Table 2.1.

Table 2.1: Definition of materials in the ANIMO model

Material	Mineral substances			Organic substances				
	f^{NH_4N}	f^{NO_3N}	f^{PO_4P}	f^O	Classes			
					1	2	·	n_f
					k_1	k_2	·	k_{n_f}
					a_1	a_2	·	a_{n_f}
					f_1^N	f_2^N	·	$f_{n_f}^N$
					f_1^P	f_2^P	·	$f_{n_f}^P$
1	$f_1^{NH_4N}$	$f_1^{NO_3N}$	$f_1^{PO_4P}$	f_1^O	$f_{1,1}$	$f_{1,2}$	·	f_{1,n_f}
2	$f_2^{NH_4N}$	$f_2^{NO_3N}$	$f_2^{PO_4P}$	f_2^O	$f_{2,1}$	$f_{2,2}$	·	f_{2,n_f}
·	·	·	·	·	·	·	·	·
nm	$f_{nm}^{NH_4N}$	$f_{nm}^{NO_3N}$	$f_{nm}^{PO_4P}$	f_{nm}^O	$f_{nm,1}$	$f_{nm,2}$	·	f_{nm,n_f}

where:

nm	: number of materials	(-)
n_f	: number of organic classes	(-)
f^O	: organic weight fraction of a material	($kg\ kg^{-1}$)
f^{NH_4N}	: ammonium-N content of a material	($kg\ kg^{-1}$)
f^{NO_3N}	: nitrate-N content of a material	($kg\ kg^{-1}$)
f^{PO_4P}	: phosphate-P content of a material	($kg\ kg^{-1}$)
$k_1 \dots k_{n_f}$: first order decomposition rate constant of an organic class	(a^{-1})
$a_1 \dots a_{n_f}$: assimilation ratio of an organic class	(-)
$f_1^N \dots f_{n_f}^N$: nitrogen weight fraction of an organic class	($kg\ kg^{-1}$)
$f_1^P \dots f_{n_f}^P$: phosphorus weight fraction of an organic class	($kg\ kg^{-1}$)

Imposing a fertilization event should provide information on:

- the material type as it corresponds to a material number in the definition of Table 2.1.
- the quantity of the dosage.
- the timing. The ANIMO model allows multi-day simulation time steps. If a specified application does not coincide with the start of a simulation time step, the materials will nevertheless be applied at the start of the time step involved.
- the depth. Materials may be added on to the soil surface or incorporated into a user specified number of soil compartments. Organic parts of an addition on to the surface are incorporated in the first soil compartment.
- the fraction of the ammonium-N part of the addition that volatilizes.

2.2 Cropping pattern

The ability of defining a cropping pattern is one way of the ANIMO model to satisfy the needs to translate the agricultural practise into model events. A crop type can be specified for each year by referring to a crop number for which the parameters are given in the input. It should be noted that the relation between meteorological data and crop production should be described in a supporting model. The ANIMO model acquires its hydrological input information from the output of a supporting model hydrological (see Par. 3). This information comprises also the distribution with depth of the root extraction for plant evaporation. The annual crop type specification in the ANIMO model should coincide with the cropping pattern in the hydrological model.

The original crop modules of the ANIMO3.5 version as described by [Groenendijk and Kroes \(1999\)](#) have been maintained and an extra option has been implemented to input information concerning crop uptake and crop residues to be incorporated in the soil (Par. 5.3).

Crop modules implemented in ANIMO3.5

- Arable crops
 - The process descriptions are given in Par. 5.1. The user should specify a number of parameters for each annual arable crop:
 - assignment of the material number of crop residues
 - depth of incorporation of died plant roots into the soil. Since the root system develops during the growing season, this input variable should be specified as a function of time
 - the ANIMO model distinguishes root exudates as a special organic matter pool for arable crops (see Chap. 6). The exudate formation is related to gross root biomass production. The modeler should specify the dry matter biomass weight of root system as a function of time

- sowing date, harvesting date and the transition date between two growing stages
 - long term averaged plant-evaporation and N- & P-uptake for the 1st and 2nd growing stage
 - if on a certain day the simulated nutrient uptake lags behind to the expected uptake more than a certain percentage of the expected quantity, it is assumed that the uptake deficit can not be recovered completely and a part of the total yield is damaged. The modeler should specify a *damage recovery factor* (see Fig. 5.1)
- Perennial grassland and natural vegetation

The process descriptions concerning biomass growth and nutrient uptake of grassland are given in Par. 5.2. In regional applications of the ANIMO model, nutrient dynamics in natural terrestrial ecosystems have been simulated as unfertilized soils covered by grassland (Kroes *et al.*, 1990; Hendriks *et al.*, 1994; Boers *et al.*, 1997; Overbeek *et al.*, 2001a; Hendriks *et al.*, 2002; Schoumans *et al.*, 2002, 2004a) The user should specify a number of parameters:

 - timing: start and end of growing season
 - the grassland sub-model comprises a biomass growth description as a function of light intensity. Therefore the relative sunshine duration should be imposed
 - efficiency of light absorption related to shoot biomass
 - respiration and efficiency factors concerning the relation photosynthesis and biomass production
 - partitioning of assimilates between shoots and roots
 - turn-over rate constant with respect to root biomass
 - minimum and maximum N- and P-content of shoots and roots
 - it is assumed that beside Fickian nitrate and ammonium transport to plant roots also an active uptake process may occur governed by the plant nitrogen status and the soil nitrogen status. The user should specify some parameters (see Par. 5.2.2)
 - livestock density
 - grazing and harvest losses

To meet the request for accurately simulation of recorded crop yields the ability was implemented in ANIMO4.0 to read information per time step with respect to crop

uptake and crop losses by stubble and root residues (see Par.5.3). This information can be derived from actual field measurements or from the simulation results of a supporting crop uptake model. While using such a supporting uptake model the cropping pattern is implicitly defined by results of this external crop module. The user should take care of consistency between the supporting hydrological model, the supporting crop uptake model and the definitions of the ANIMO model.

2.3 Soil tillage

Agricultural tillage practises may have an impact on nutrient leaching and surface water eutrophication. Phosphate transport in topsoils to surface water is governed by the soil P-status and the occurrence of high groundwater levels. Mixing of soil compartments by ploughing may accelerate the downward phosphate transport and may yield an increased P-content in the deeper layers. During periods with relatively high groundwater levels phosphate arrived in a certain compartment by soil mixing may be transported to surface water. To analyze the eventual impact of tillage practises on leaching, the ANIMO model comprises a module to describe ploughing and other mixing interventions. Dissolved and solid compounds are mixed, however an eventual user defined stratification of the dry bulk density in the mixing zone is preserved. The user should specify the timing and the numbers of soil compartments involved in the mixing.

3 Hydrological schematization

3.1 Water flow

The ANIMO model requires data delivered by a water quantity model. Dependent on the scale of available information and the scale of model application, a hydrological field model (e.g. SWAP; Kroes and van Dam (2003)) or a regional groundwater model (e.g. SIMGRO; van Walsum *et al.* (2004)) must be applied in advance. The hydrological model generates information with respect to water balance items and state variables for a freely chosen number of compartments. In the ANIMO model the same calculation grid definition is applied for simulation of transport, transformation and accumulation processes. A schematic representation of the water balances for an arbitrary number of compartments is depicted in Fig. 3.1 The ANIMO model has some

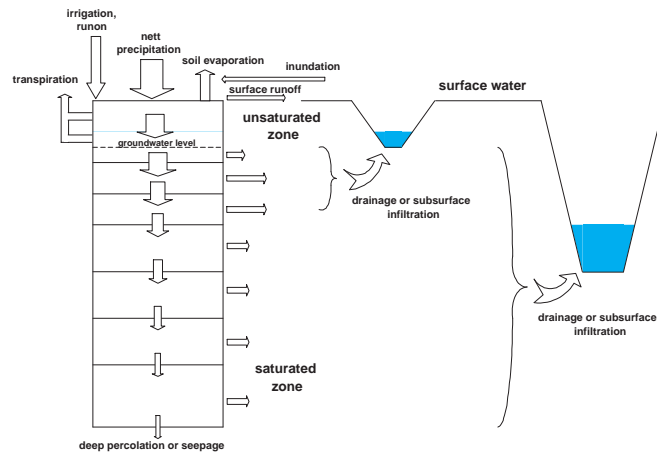


Figure 3.1: *Definition of a soil profile and the main terms of the water balance*

features for down-scaling of the aggregated water balance information obtained from a two-layered hydrological model WATBAL (Berghuijs-van Dijk, 1985; Vinten, 1999). A complete water balance for a soil-water-crop system can be formulated as:

$$\frac{\Delta V}{\Delta t} = q_p^n + q_{irr} + q_{ro} + q_{inu} + q_{me} + q_s - q_{es} - q_{ep} - q_{eow} - q_{per} - q_{ru} - \sum_{k=1}^{ndr} q_{dr,k} \quad (3.1)$$

where:

$\frac{\Delta V}{\Delta t}$: change of areal water volume per time step	$(m d^{-1})$
q_p^n	: net precipitation	$(m d^{-1})$
q_{irr}	: irrigation	$(m d^{-1})$
q_{ro}	: run-on from adjacent fields	$(m d^{-1})$
q_{inu}	: inundation from adjacent watercourses	$(m d^{-1})$
q_{me}	: snow melt	$(m d^{-1})$
q_s	: upward seepage at lower boundary	$(m d^{-1})$
q_{es}	: soil evaporation	$(m d^{-1})$
q_{ep}	: plant evaporation	$(m d^{-1})$
q_{eow}	: evaporation from ponded water layer	$(m d^{-1})$
q_{per}	: percolation at lower boundary	$(m d^{-1})$
q_{ru}	: runoff	$(m d^{-1})$
$\sum_{k=1}^{n_{dr}} q_{dr,k}$: drainage to multiple drainage systems	$(m d^{-1})$
n_{dr}	: number of drainage systems considered	$(-)$

The net precipitation is calculated by subtracting both the snow fall and crop canopy interception from the gross precipitation. The drainage fluxes can have both positive and negative values. A negative value indicates subsurface infiltration.

3.2 Surface reservoir

The SWAP3.0 model (van Dam, 2000; Kroes and van Dam, 2003) comprises a description of water storage in a so called ponding reservoir. The *inflow* and *outflow* items of the water balance to be considered are depicted in Fig. 3.2.// Surface runoff

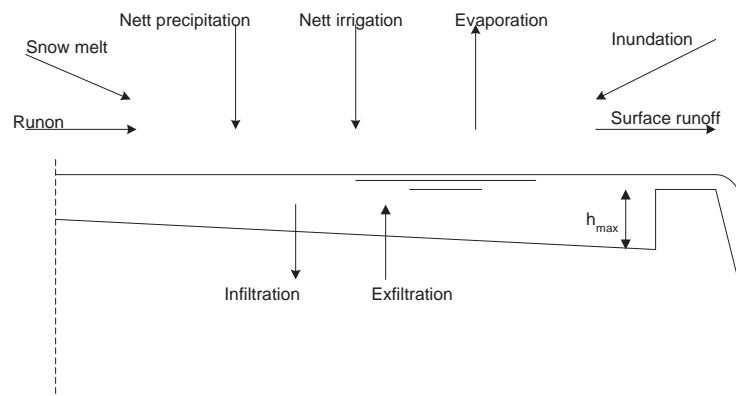


Figure 3.2: Balance items of the surface water reservoir

can be the result of exceeding the infiltration capacity by the incoming flux intensity at the soil surface and a complete saturation of the soil profile. The incoming flux may consist of precipitation, snow melt, run-on from adjacent fields and inundation from adjacent water courses. When the *frozen soil option* in SWAP3.0 is active, during spring time the discharge of defrosted soil compartments can be impeded by frozen soil compartments at a greater depth. Then, the limited storage capacity of the upper soil compartments can be rapidly exceeded. The specific storage of this

reservoir should be specified by the user as a function of ponding height h_{pond} .

$$\mu(h_{pond}) \frac{\Delta h_{pond}}{\Delta t} = inflow - outflow \quad (3.2)$$

where $\mu(h_{pond})$ is a ponding storage coefficient as a function of ponding height. The redistribution and delaying mechanisms in the ANIMO model are characterized by differentiation between the different sources of surface runoff and the delayed penetration of ammonium, nitrate, phosphate and dissolved organic N and P by temporal storage in an artificial reservoir.

3.2.1 Partitioning of surface runoff

Three pathways are considered: a direct route to which the precipitation concentration is attributed, a route through the ponded water layer and a route where the runoff water has been in close contact with the upper soil. This type of runoff water passes through the upper soil compartment and the liquid solute concentration of this compartment is assigned to this route. This may be of special importance in situations where fertilizers are broadcasted or animal manure is applied by old fashioned methods on top of the soil surface. The substance will only enter the soil by infiltration of rainwater coming after a fertilization event. During such surface runoff events the discharging water may contain high doses of the substance applied.

The load on surface water equals the sum of three different fluxes:

$$J_{s,r} = q_{ru} \{ f_{po} c_{po} + f_1 c_1 + (1 - f_{po} - f_1) c_{pr} \} \quad (3.3)$$

where:

$J_{s,r}$: surface runoff transport to surface waters	$(kg\ m^{-2}\ d^{-1})$
q_{ru}	: areal surface runoff water flux	$(m\ d^{-1})$
f_{po}	: fraction to which c_{po} is assigned	(-)
f_1	: fraction to which c_1 is assigned	(-)
c_{pr}	: weighted concentration of hydrological entry routes (Fig.3.3)	$(kg\ m^{-3})$
c_{po}	: time averaged concentration of ponded water	$(kg\ m^{-3})$
c_1	: time averaged concentration of the upper compartment	$(kg\ m^{-3})$

The surface runoff pathway to surface water systems is depicted in Fig. 3.3 The concentration of the ponded water layer results from solving the conservation and transport equation of this particular compartment. Hydrology driven routes are the most important pathways for entering substances to the ponded water layer. Although direct fertilization of the ponded water layer is not realistic, such a situation could occur when the timing of fertilization events are not attuned to the results of the supporting hydrological model.

3.2.2 Precipitation driven penetration

Animal manure and fertilizers can be applied to soil at any time. Most of the added nutrients will be transported into the soil profile by percolation of rain water. It thus depends on the rainfall pattern whether and when the fertilization will be available for plant roots. To account for this phenomenon, an imaginary storage reservoir has been formulated at the soil surface in which all additions are immediately dissolve.

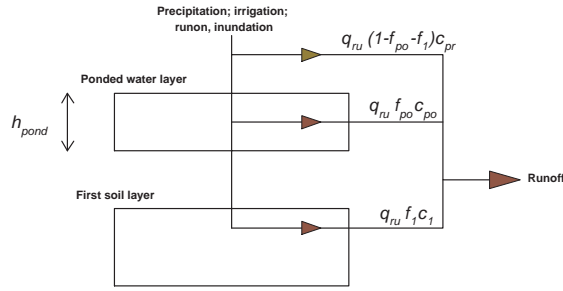


Figure 3.3: Schematization of surface water contamination by surface runoff

The solute migration within this reservoir is described as a piston flow. The total quantity of added material in stock will be depleted after a precipitation volume which equals the reservoir volume. The store of materials in this artificial reservoir is evaluated each time interval by means of book keeping. When the front of the piston flow breaks through at the bottom of the reservoir within a certain time interval, the average input concentration to the first soil compartment is calculated as a time weighted average of old and new concentrations in the surface reservoir. The release rate can be manipulated by the choice of an appropriate thickness Z_{surf} of the reservoir. The amount released after a rain shower is calculated according to:

$$M_r = M \frac{\sum q_p \Delta t}{Z_{surf}} \quad (3.4)$$

where:

M_r	: fertilizer released from surface reservoir	$(kg\ m^{-2})$
M	: fertilizer added to surface reservoir	$(kg\ m^{-2})$
$\sum q_p \Delta t$: cumulative precipitation since addition	(m)
Z_{surf}	: user specified thickness of surface reservoir	(m)

When a ponding event occurs, the total quantity of material stored in the artificial reservoir is added to the pondered water layer.

3.3 Lateral drainage sink term

The drainage fluxes are considered as lateral sink-terms R_{dr} (d^{-1}) in the water balance. The distribution of lateral-drainage sink terms with depth can be derived from the vertical flux (q_y) relation with depth according to:

$$\frac{dq_y}{dy} = -R_{dr} \quad (3.5)$$

The vertical flux with depth determines implicitly the travel time distribution of exfiltrating groundwater. A point model however considers only one dimension. An accurate projection of the two- or three-dimensional flow field on the vertical axis can be found by defining an up-scaled vertical flux as a function of height $\bar{q}_y(y)$ for

which the travel time is defined by:

$$t_1 - t_0 = \int_{y_0}^{y_1} \frac{\varepsilon dy}{\bar{q}_y(y)} \quad (3.6)$$

In a two-dimensional flow field streamlines are mathematically described by the streamfunction $\Psi(x, y)$ ($m^2 d^{-1}$). For a given value $\Psi(x, y) = \Psi_0$ streamlines can be constructed from the points (x, y) for which the streamfunction equals Ψ_0 . Let Q_d be the total discharge ($m^2 d^{-1}$) of a cross section between $x = 0$ and the water divide midway between the drains at $x = \frac{L}{2}$. L is the distance between the drains. A streamline for which holds $\Psi(x, y) = \Psi_0$ separates the flow field into two zones. Through the first zone a discharge equal to Ψ_0 is conveyed and the other zone drains the remaining part of the total discharge ($Q_d - \Psi_0$). For each streamline the deepest point can be found. The deepest point of each streamline for which holds that a certain part of the total discharge which will never pass that depth. This rule can

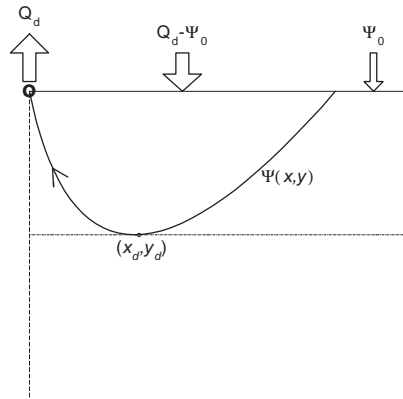


Figure 3.4: Separation of two-dimensional flow field by a stream line into two zones

be used to determine the x -coordinate at a certain depth for which the vertical flux intensity on a streamline equals zero. For the deepest point of each streamline at depth y_d holds:

$$q_y(x_d, y_d) = 0 \quad (3.7)$$

This generally yields an expression for x_d as a function of y_d and Ψ for the flow domain considered. The total recharge can be divided into a part passing through the plane at y_d and the remaining part that has left the soil profile already before reaching the plane at y_d . Let the part of the drain discharge which will never pass through level y_d amount to $\Psi(x_d, y_d)$. In the schematized vertical soil column the remaining part $Q_d - \Psi(x_d, y_d)$ passes the plane at y_d as vertical flow. The average vertical flux at depth y_d is then found by substitution of x_d and y_d in the streamfunction relation and division by the half drain spacing:

$$\bar{q}_y(y_d) = \frac{Q_d - \Psi(x_d, y_d)}{\frac{L}{2}} \quad (3.8)$$

Groundwater flow in an aquifer drained by fully penetrating drainage canals can be described by:

$$\Phi = \frac{R}{2H}(z - z_0)^2 \quad (3.9)$$

where H (m) is the thickness of the aquifer, R ($m d^{-1}$) is the recharge of the aquifer drained by drains at distance L (m) and z_0 is given by: $z_0 = \frac{L}{2} - iH$. Expressions for the streamfunction and the vertical flux density can be derived:

$$\Psi(x, y) = \frac{R}{H} \left(x - \frac{L}{2}\right)(y + H) \quad (3.10)$$

and:

$$q_y(x, y) = \frac{R}{H}(y + H) \quad (3.11)$$

The deepest point on each streamline is found at the outflow boundary at $x = 0$. Consequently $x_d = 0$. For the total discharge for the area between the drain and midway between the drains holds: $Q_d = R\frac{L}{2}$. Substitution of $x_d = 0$, the discharge and Eq. 3.10 into Eq. 3.8 yields the following relation for the one-dimensional vertical flux:

$$\bar{q}_y = R \frac{H + y}{H} \quad (3.12)$$

Up-scaling the relation between the residence time distribution and the determination of key parameters to assess the regional response of changed inputs on drainage water quality has been reported by several authors (Groenendijk and Roest, 1996; Luther and Haitjema, 1998; van den Eertwegh, 2002). The approach most widely applied is to consider a region as a collection of independent fields and to calculate the drainage water quality as a flow weighted average. The interdependency between flow patterns which may arise when nested flow systems occur is often not accounted for in lumped models which describe the solute breakthrough of exfiltrating groundwater as a mixing process in a linear reservoir (van der Molen and van Ommen, 1988). The hierarchical distribution of exfiltrating streamlines as well as the influence of bio-chemical reactions on the concentrations necessitates to distinguish between the hydraulic and chemical properties of different soil compartments. The SWAP model (Kroes and van Dam, 2003) has the ability to calculate lateral sink terms for a multi-level drainage system. The flow pattern is schematized to a uni-lateral flow to perfect drains ignoring radial flow components in the vicinity of the drains.

In the drainage model describing the discharge to parallel equidistant water courses, the discharge flow $Q_{d,i}$ is defined as:

$$Q_{d,i} = q_{d,i} \frac{A}{\sum l_i} \quad (3.13)$$

where $q_{d,i}$ is the drainage flux density of system i ; A is the catchment area and $\sum l_i$ is the total length of drainage system i . An essential assumption made in the SWAP model (Kroes and van Dam, 2003) is the proportionality of the ratio between the occupied flow volumes V_i and the ratio between the discharge rates $Q_{d,i}$

$$\frac{V_i}{V_{i-1}} = \frac{Q_{d,i}}{Q_{d,i-1}} \quad (3.14)$$

The classification of the lines drains and the compilation of the hierarchy allows for the superposition of drainage fluxes. First order drains act also as second and higher order drains. Fig. 3.5 depicts the schematization of the regional groundwater flow, including the occupied flow volumes for nested drain systems. The volume V_i consists

of summed rectangles $L_i H_i$ of superposed drains, where H_i is the thickness (m) of discharge layer i . The method employed has been based on the assumption that the groundwater volume occupied between the upper boundary and the zones indicated by H_1 and H_2 can be neglected. This assumption is rather questionable. If

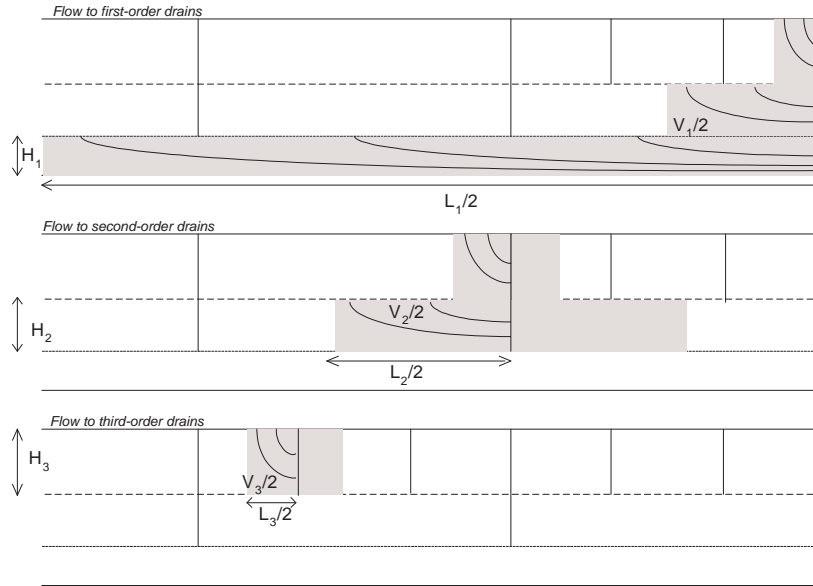


Figure 3.5: Schematization of groundwater flow to three different types of lines drains

n is the total number of drainage classes, the flow volume V_i assigned to a drainage system i is related to drain distances L_j and thickness H_j of the discharge layers i to n :

$$V_i = \sum_{j=i}^n L_j H_j \quad (3.15)$$

Using the proportionality between occupied volumes and flow discharges and rearranging of Eq. 3.15 yields:

$$L_1 H_1 : L_2 H_2 : L_3 H_3 = (q_{d,1} \frac{A}{\sum l_1} - q_{d,2} \frac{A}{\sum l_2}) : (q_{d,2} \frac{A}{\sum l_2} - q_{d,3} \frac{A}{\sum l_3}) : q_{d,3} \frac{A}{\sum l_3} \quad (3.16)$$

If the horizontal conductivities exhibit a stratified constitution, the heterogeneity can be taken into account by substituting transmissivities T for layer thicknesses. The thickness of a certain layer can be derived by considering the vertical cumulative transmissivity relation with depth as shown in Fig. 3.6. The lateral flux relation per unit soil depth shows a uniform distribution. Lateral drainage fluxes $q_{d,i,k}$ to drainage system i multiplied by the ratio between the transmissivity of nodal compartment k and the total transmissivity of the discharge layer with depth H_i . The average concentration in the discharge water to a line drain results from flux weighted ($q_{d,i,k}$) averaging the nodal concentrations.

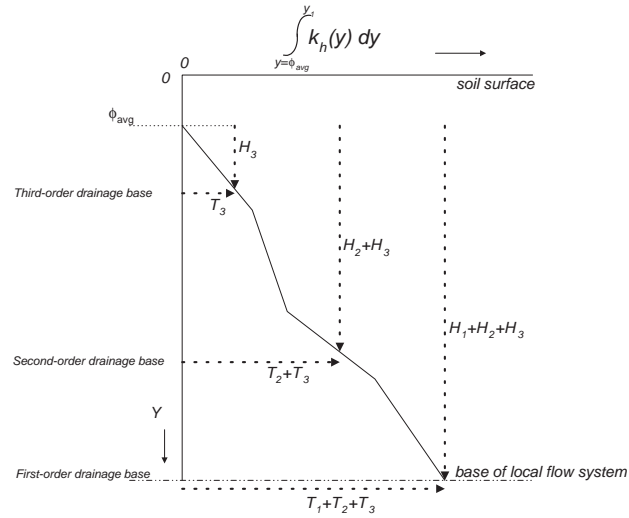


Figure 3.6: Discharge layer thickness H_i as a function of transmissivity T_i in a stratified soil profile

3.4 Seepage at lower boundary

Upward seepage at the lower boundary may cause an extra source for eutrophication of surface waters. On the other hand the concentrations in upward seepage water can be of importance for assessment of the initial concentration profile. It is expected that P-concentrations in upward seepage water determine the phosphorus contents in soil compartments at greater depth. For regional applications of the ANIMO model in the Netherlands an average depth of the *seepage surface* has been estimated from long term hydrological simulation results. The dependency of the *seepage surface* position is depicted in Fig. 3.7. Below the *seepage surface* the soil P-content is assumed to be in equilibrium with the seepage concentration. The P-content of compartments between the root zone and the *seepage surface* is in equilibrium with a user defined background concentration. A map has been compiled on the basis of monitoring results of the *Landelijk Grondwater Meetnet* (Bronswijk *et al.*, 1998; Reijnders *et al.*, 1998) and additional information reported by Griffioen *et al.* (2002). Missing values and concentrations deeper than 20 m below soil surface were excluded. For each monitoring location the values were calculated as an time averaged value. Extreme P-concentrations have been cut-off to a level of 10 mg l^{-1} . The resulting values were interpolated to a $250 \times 250 \text{ m}$ grid based map by weighted linear interpolation. The inverse distances of max. adjacent points were used as weighing factors. The result of this grid map was clustered to the spatial STONE schematization (Kroon *et al.*, 2001).

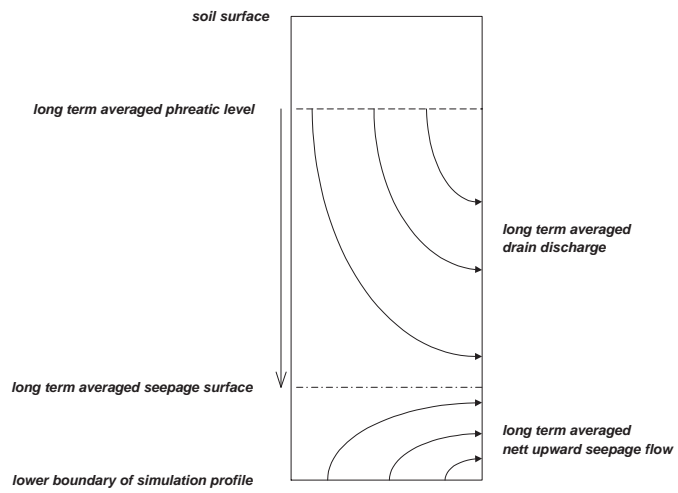


Figure 3.7: *Estimation of the position of the seepage surface*

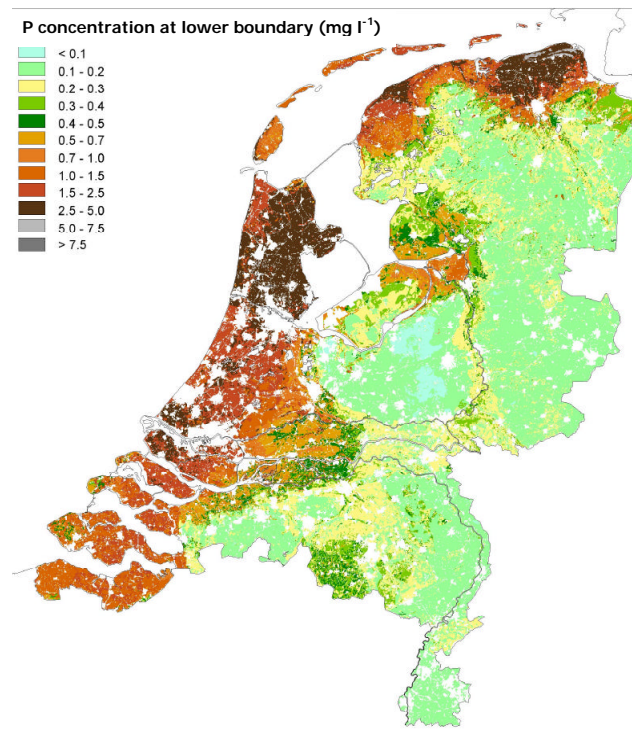


Figure 3.8: *P-concentrations at the lower boundary in the national STONE schematization*

4 Transport processes

4.1 Mass conservation

The general formulation of the mass conservation and transport equation reads as follows:

$$\frac{\partial c^*}{\partial t} = -\frac{\partial J_s}{\partial z} + R_p - R_d - R_u - R_x \quad (4.1)$$

where:

c^*	: mass concentration	$(kg\ m^{-3})$
J_s	: vertical solute flux	$(kg\ m^{-2}\ d^{-1})$
R_p	: production source term	$(kg\ m^{-3}\ d^{-1})$
R_d	: decomposition sink term	$(kg\ m^{-3}\ d^{-1})$
R_u	: plant uptake sink term	$(kg\ m^{-3}\ d^{-1})$
R_x	: drainage sink term	$(kg\ m^{-3}\ d^{-1})$

The mass concentration of a substance in a soil system equals the sum of the concentrations present in the liquid phase and in the solid phases:

$$c^* = \theta c + \rho_d X_e + \rho_d X_n + \rho_d X_p \quad (4.2)$$

where:

c	: mass concentration in the 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	$(kg\ kg^{-1})$
X_p	: content of the substance involved in precipitation reaction	$(kg\ kg^{-1})$
θ	: volume moisture fraction	$(m^3\ m^{-3})$
ρ_d	: dry bulk density	$(kg\ m^{-3})$

By combining the Eq.4.1 and Eq.4.2 a general conservation and transport equation (*CTE*-equation) is obtained:

$$\frac{\partial(\theta c)}{\partial t} + \rho_d \frac{\partial X_e}{\partial t} + \rho_d \frac{\partial X_n}{\partial t} + \rho_d \frac{\partial X_p}{\partial t} = -\frac{\partial J_s}{\partial z} + R_p - R_d - R_u - R_x \quad (4.3)$$

From this equation the resulting concentration c has to be found. Due to the second order partial differential there are only a few analytical solutions available for a limited set of boundary conditions. Therefore this type of *CTE*-equations is mostly solved by numerical approximation methods such as finite differences. The *CTE*-equation is then rewritten as an equation with finite differences and a numerical solution scheme (explicit/implicit) is used to solve sets of (linear) difference equations. The ANIMO model utilizes a semi-analytical solution of the *CTE*-equation.

4.2 Linearized solute transport equation

Assuming the incoming and outgoing water fluxes constant within a time interval, the soil moisture content varies linear with time according to: $\theta(t) = \theta_0 + \frac{\Delta\theta}{\Delta t}t$. The rate of change of the quantity within the aqueous phase is then expressed by:

$$\frac{\partial(\theta c)}{\partial t} = \left(\theta_0 + \frac{\Delta\theta}{\Delta t}t\right) \frac{\partial c}{\partial t} + \frac{\Delta\theta}{\Delta t}c \quad (4.4)$$

The expression of the equilibrium sorption can be incorporated into the conservation equation by elaborating the differential quotient $\frac{\partial X_e}{\partial t}$:

$$\rho_d \frac{\partial X_e}{\partial t} = \rho_d \left(\frac{dX_e}{dc} \right) \frac{\partial c}{\partial t} = \rho_d K_d(c) \frac{\partial c}{\partial t} \quad (4.5)$$

where $K_d(c)$ is the differential sorption coefficient ($m^3 kg^{-1}$). The differential adsorption coefficient is approximated by the average value $\bar{K}_d(c)$. This value is assessed by calculating the slope of the chord of the adsorption isotherm:

$$\bar{K}_d(c) = \frac{1}{c(t) - c(t_0)} \int_{t_0}^t \left(\frac{dX_e}{dc} \right) dc = \frac{X_e(t) - X_e(t_0)}{c(t) - c(t_0)} \quad (4.6)$$

Although $\bar{K}_d(c)$ is a function of the concentration, its average value is assumed to be constant during the time step.

The transport term is approximated by:

$$- \frac{\partial J_s}{\partial z} \approx \frac{q_{i-\frac{1}{2}}}{\Delta z} \bar{c}_{i-1} - \frac{q_{i+\frac{1}{2}}}{\Delta z} c_i \quad (4.7)$$

where $q_{i-\frac{1}{2}}$ and $q_{i+\frac{1}{2}}$ the inflowing resp. the out-flowing water fluxes, Δz is the thickness of a soil compartment (m) and c_{i-1} is the concentration in an adjacent upstream soil compartment. The implications of these assumptions with respect to the mathematical dispersion and numerical stability are discussed in Par. 4.3.

All transformation processes such as the decomposition of organic compounds and the nitrification of ammonium have been described by first order rate kinetics. The liquid concentration or the solid contents of the substances itself are the rate limiting factors of these processes. An exception on the description of transformation by first order rate processes has been made for the decomposition of nitrate by denitrification (see Par. 7.2 and 9.2.2). The general formulation for decomposition reads:

$$R_d = k_1 \theta_i c_i \quad (4.8)$$

where k_1 is a first order rate coefficient (a^{-1}).

Crop uptake of nutrients is described proportional to the liquid concentration of the soil water phase and the plant evaporation flux q_{ep} towards plant roots. A multiplication factor has been introduced to account for preferential uptake when the nutrient availability is not sufficient to fulfill the crop requirement by passive uptake with the water flow. The general equation reads:

$$R_u = \sigma \frac{q_{ep}}{\Delta z} c_i \quad (4.9)$$

where σ is the selectivity factor to account for specific deficit or surplus situations. The assessment of this parameter is given for arable crops in Par. 5.1 and perennial grassland in Par. 5.2.

Sources are described as zero-order terms. In the carbon cycle, formation of dissolved organic carbon from the solubilization of fresh organic matter and the formation of the humus/biomass pool is described by zero-order kinetics. These processes

have also been described in the nitrogen and phosphorus cycle . The formation of ammonium and mineral phosphate is considered as a zero-order process when one considers the ammonium and the mineral phosphate balance respectively. Looking in detail to the nitrate balance, the formation of nitrate through nitrification has been described as a zero-order term.

The conservation equation can be developed as follows when the expressions for the average differential sorption coefficient and the first order rate sorption are substituted:

$$\left\{ \theta_0 + \frac{\Delta\theta}{\Delta t} t + \rho_d \bar{K}_d \right\} \frac{dc_i}{dt} \approx - \left\{ \frac{q_{i+\frac{1}{2}}}{\Delta z} + \frac{\Delta\theta}{\Delta t} + \frac{\sigma q_{ep}}{\Delta z} + R_x + k_1 \theta_i \right\} c_i + \frac{q_{i-\frac{1}{2}} c_{i-1}}{\Delta z} + R_p \quad (4.10)$$

When precipitated chemicals are absent at low concentration levels the conservation and transport equation can be rewritten as follows:

$$\frac{dc_i}{dt} + \frac{A}{\theta_0 + \rho_d \bar{K}_d + \left(\frac{\Delta\theta}{\Delta t}\right) t} c_i = \frac{B}{\theta_0 + \rho_d \bar{K}_d + \left(\frac{\Delta\theta}{\Delta t}\right) t} \quad (4.11)$$

where

$$A = \frac{q_{i+\frac{1}{2}}}{\Delta z} + \frac{\Delta\theta}{\Delta t} + \frac{\sigma q_{ep}}{\Delta z} + R_x + k_1 \bar{\theta}_i$$

and

$$B = \frac{q_{i-\frac{1}{2}} c_{i-1}}{\Delta z} + R_p$$

The moisture fraction θ in the decomposition rate term of Eq. 4.10 is approximated by the average moisture content. The general solution to this differential equation reads:

$$c_i(t) = \xi_1(t) c_i(t_0) + \xi_2(t) B \quad (4.12)$$

where $\xi_1(t)$ (-) and $\xi_2(t)$ (d) are model coefficients for which the calculation procedure is given below. An expression for the time averaged concentration \bar{c} can be obtained by integration of $c_i(t)$ over the time variable between t_0 and t and dividing by the time interval:

$$\bar{c}_i = \zeta_1(t) c_i(t_0) + \zeta_2(t) B \quad (4.13)$$

where $\zeta_1(t)$ (-) and $\zeta_2(t)$ (d) are also model coefficients. The coefficients $\xi_1(t)$, $\xi_2(t)$, $\zeta_1(t)$ and $\zeta_2(t)$ are defined as follows:

- If $\frac{\Delta\theta}{\Delta t} \neq 0$ and $A \neq 0$:

$$\xi_1(t) = \left(\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\theta_0 + \rho_d \bar{K}_d(c)} \right)^{-\frac{A t}{\Delta\theta}} \quad \text{and} \quad \xi_2(t) = \frac{1 - \xi_1(t)}{A}$$

- If $\frac{\Delta\theta}{\Delta t} \neq A$

$$\zeta_1(t) = \frac{\theta_0 + \rho_d \bar{K}_d(c)}{\left(\frac{\Delta\theta}{\Delta t} - A\right) t} \left[\left(\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\theta_0 + \rho_d \bar{K}_d(c)} \right)^{\frac{\Delta\theta - A \Delta t}{\Delta\theta}} - 1 \right] \quad \text{and} \quad \zeta_2(t) = \frac{1 - \zeta_1(t)}{A}$$

- If $\frac{\Delta\theta}{\Delta t} = A$

$$\zeta_1(c, t) = \frac{\theta_0 + \rho_d \bar{K}_d(c)}{\frac{\Delta\theta}{\Delta t} t} \ln \left(\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\theta_0 + \rho_d \bar{K}_d(c)} \right) \quad \text{and} \quad \zeta_2(t) = \frac{1 - \zeta_1(t)}{A}$$

- If $\frac{\Delta\theta}{\Delta t} = 0$ and $A \neq 0$:
 $\xi_1(t) = e^{-\frac{A}{\theta_0 + \rho_d \bar{K}_d(c)} t}$ and $\xi_2(t) = \frac{1 - \xi_1(t)}{A}$
 $\zeta_1(t) = \frac{\theta_0 + \rho_d \bar{K}_d(c)}{At} \left(1 - e^{-\frac{A t}{\theta_0 + \rho_d \bar{K}_d(c)}} \right)$ and $\zeta_2(t) = \frac{1 - \zeta_1(t)}{A}$
- If $\frac{\Delta\theta}{\Delta t} \neq 0$ and $A = 0$:
 $\xi_1(t) = 1$ and $\xi_2(t) = \frac{\Delta t}{\Delta\theta} \ln \left(\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\theta_0 + \rho_d \bar{K}_d(c)} \right)$
 $\zeta_1(t) = 1$ and $\zeta_2(t) = \frac{\Delta t}{\Delta\theta} \left[\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\frac{\Delta\theta}{\Delta t} t} \ln \left(\frac{\theta_0 + \rho_d \bar{K}_d(c) + \frac{\Delta\theta}{\Delta t} t}{\theta_0 + \rho_d \bar{K}_d(c)} \right) - 1 \right]$
- If $\frac{\Delta\theta}{\Delta t} = 0$ and $A = 0$:
 $\xi_1(t) = 1$ and $\xi_2(t) = \frac{t}{\theta_0 + \rho_d \bar{K}_d(c)}$
 $\zeta_1(t) = 1$ and $\zeta_2(t) = \frac{t}{2(\theta_0 + \rho_d \bar{K}_d(c))}$

4.3 Numerical elaboration

The up-scaled one dimensional solute flux J_s of an inert substance through the aquifer is the sum of an advection flux and a dispersive flux attributed to the combination of molecular diffusion and dispersive mixing:

$$J_s = \bar{q}_z c - \theta D \frac{\partial c}{\partial z} \quad (4.14)$$

where D is the dispersion coefficient ($m^2 d^{-1}$). The dispersion coefficient is assumed linear proportional to the water velocity according to $D = \lambda \frac{\bar{q}_z}{\theta}$ where λ is the dispersion length (m). Relating solute flux to mass conservation gives:

$$-\frac{\partial J_s}{\partial z} = -\frac{\partial}{\partial z} (\bar{q}_z c - \theta D \frac{\partial c}{\partial z}) - R_x c = -\frac{\partial}{\partial z} \bar{q}_z (c - \lambda \frac{\partial c}{\partial z}) - R_x c \quad (4.15)$$

Taylor expansion is used to derive a finite difference expression where second and higher order terms are ignored. The concentrations are defined at the center of each compartment and have the subscript i . The inflowing and out-flowing water flux are considered at resp. the top and the bottom of compartment i and are defined as resp. $\bar{q}_{i-\frac{1}{2}}$, and $\bar{q}_{i+\frac{1}{2}}$. The concentration at the interface between compartments $i-1$ and i is calculated as the weighted average of c_{i-1} and c_i . For steady state flow conditions the partial derivative for transport can be developed as follows:

$$\begin{aligned} -\frac{\partial J_s}{\partial z} &\approx -\frac{\bar{q}_{i+\frac{1}{2}}}{\Delta y_i} \left(\frac{\Delta z_i - 2\lambda}{\Delta z_i + \Delta z_{i+1}} \right) c_{i+1} + \\ &\quad \left\{ \frac{\bar{q}_{i+\frac{1}{2}}}{\Delta z_i} \left(\frac{\Delta z_{i+1} - 2\lambda}{\Delta z_i + \Delta z_{i+1}} \right) - \frac{\bar{q}_{i-\frac{1}{2}}}{\Delta z_i} \left(\frac{\Delta z_{i-1} + 2\lambda}{\Delta z_i + \Delta z_{i-1}} \right) - R_{dr} \right\} c_i + \\ &\quad \frac{\bar{q}_{i-\frac{1}{2}}}{\Delta z_i} \left(\frac{\Delta z_i + 2\lambda}{\Delta z_{i-1} + \Delta z_i} \right) c_{i-1} \end{aligned} \quad (4.16)$$

Diffusion/dispersion can be described by choosing an appropriate value of the vertical compartment thickness. When thickness of the compartments are taken identical the dispersion length λ is set to half of the compartment thickness the expression reduces to:

$$-\frac{\partial J_s}{\partial z} \approx -\left(\frac{\bar{q}_{i-\frac{1}{2}}}{\Delta z_i} + R_{dr}\right) c_i + \frac{\bar{q}_{i-\frac{1}{2}}}{\Delta z_i} c_{i-1} \quad (4.17)$$

The natural dispersion term resulting from physical processes in Eq. 4.14 is replaced by a dispersion term which accounts for the mathematical dispersion. Neglecting sink and source terms and focusing on the concentration in the liquid phase results in the following equation:

$$\frac{\partial c}{\partial t} = -\frac{q}{\theta} \frac{\partial c}{\partial z} + D_n \frac{\partial^2 c}{\partial z^2} \quad (4.18)$$

where D_n is the mathematical dispersion coefficient ($m^2 d^{-1}$). The convection / dispersion equation is solved by means of a pseudo-analytical method. The computation scheme yields the following sources of numerical dispersion:

- as a result of spatial discretization;
- as a result of temporal discretization and the assumption of time averaged constant concentration values within a time interval.

The numerical dispersion resulting from the discretization scheme can be quantified under restricted circumstances. An expression for the numerical dispersion coefficient D_n is derived, allowing manipulation of model variables such as time interval and thickness of soil compartments to achieve agreement between physical and numerical dispersion. Steady state soil moisture flow conditions are assumed and the soil profile is schematized to compartments with equal thickness. The spatial term ∂z expresses a discretization to finite increments with thickness Δz . In first instance, the dispersion term is ignored since the computation algorithm introduces a numerical dispersion, which is utilized to describe physical dispersion. Both the concentration in the liquid phase of compartment i and of the adjacent upstream compartment $i-1$ are defined as a function of time. This function $c_{i-1}(t)$ is replaced by the time averaged concentration in the inflowing soil water from an upstream compartment to facilitate the solution of the differential equation. This results in the differential equation for compartment i :

$$\frac{dc_i}{dt} = \frac{q}{\theta \Delta z} \bar{c}_{i-1} - \frac{q}{\theta \Delta z} c_i(t) \quad (4.19)$$

where Δz is the compartment thickness and the subscripts i and $i-1$ denote the compartment numbers. The averaged concentration is determined by calculating the integral and dividing by the length of the time interval considered:

$$\bar{c}_{i-1} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} c_{i-1}(t) dt \quad (4.20)$$

The introduction of the time averaged constant value obeys to the mass conservation law. Subject to the initial condition $c_i = c_i(t_0)$ at $t = t_0$, the solution to this differential equation reads:

$$c_i = c_i(t_0) e^{-\frac{q}{\theta \Delta z} t} + \bar{c}_{i-1} (1 - e^{-\frac{q}{\theta \Delta z} t}) \quad (4.21)$$

At small values of Δt , the resulting concentration c_i will be determined nearly completely by the initial value of the concentration. At large values of Δt , the resulting concentration will approach the value of the forcing function c_{i-1} . This solution can be considered as a combination of an explicit and an implicit numerical solution to a finite difference computation scheme. The measure of dependency of the initial value and the value of the forcing function is determined by the exponential function $e^{-\frac{q}{\theta\Delta z}t}$.

The residence time of the soil moisture (t_{res}) in the compartment considered can be defined as:

$$t_{res} = \frac{\theta\Delta z}{q} \quad (4.22)$$

After some algebraic manipulations, an expression for the numerical dispersion coefficient can be obtained:

$$D_n = \frac{(\Delta z)^2}{t_{res}} \left(\frac{\frac{\Delta t}{t_{res}}}{1 - e^{-\frac{\Delta t}{t_{res}}}} - \frac{1}{2} \left(1 + \frac{\Delta t}{t_{res}} \right) \right) \quad (4.23)$$

As long as the computation order proceeds in the flow direction, the mathematical solution is always stable. The ANIMO model comprises a module for the determination of the computation sequence dependent on the flow conditions per time step.

5 Crop production and nutrient uptake

5.1 Annual crops

Crop production of arable crops is assumed to be controlled by plant evaporation. Therefore, the daily plant evaporation as results from a supporting agro-hydrological model is used as a driving force to describe nutrient uptake. For arable crops, no explicit biomass production module has been formulated.

The growing season is divided into two periods. During each period the N or P concentration in the plant evaporation flow resulting to optimum crop production conditions is defined as:

$$c_{opt,1} = \frac{U_1^*}{\sum_{t_p}^{t_c} q_{ep}} \quad c_{opt,2} = \frac{U_2^*}{\sum_{t_c}^{t_h} q_{ep}} \quad (5.1)$$

where:

$c_{opt,1}; c_{opt,2}$: optimal N or P concentrations in plant evaporation flow during resp. 1 st and 2 nd growing stage	($kg\ m^{-3}$)
$U_1^*; U_2^*$: long term averaged cumulative uptake during resp. 1 st and 2 nd growing stage	($kg\ m^{-2}$)
$\sum_{t_p}^{t_c} q_{ep}$: long term averaged plant evaporation during 1 st stage	(m)
$\sum_{t_c}^{t_h} q_{ep}$: long term averaged plant evaporation during 2 nd stage	(m)
t_p	: planting date	(-)
t_c	: transition date between both growing periods	(-)
t_h	: harvesting date	(-)

The expected optimal cumulative uptake and cumulative plant evaporation flow are defined by the user in the model input files. For years with higher or lower plant evaporation rates, the total crop uptake will increase or decrease proportionally. Under optimal circumstances, the *transpiration concentration stream factors* as used in the conservation and transport equation (Par. 4.2) σ_{NO_3} , σ_{NH_4} and σ_{PO_4} are defined as the ratio between the optimum concentration and the actual concentration:

$$\sigma_{NO_3} = \frac{c_{opt,NO_3,j}}{c_{NO_3}} \quad \text{and} \quad \sigma_{NH_4} = \frac{c_{opt,NH_4,j}}{c_{NH_4}} \quad \text{and} \quad \sigma_{PO_4} = \frac{c_{opt,PO_4,j}}{c_{PO_4}} \quad (5.2)$$

where the subscript j denotes the growing stage number. Under sub-optimal conditions (excessive supply or uptake deficit), the parameters are adjusted assuming that the actual crop uptake depends on two driving forces: the soil availability and the crop requirement.

5.1.1 Nitrogen uptake

For establishing the ammonium and nitrate uptake parameters three types of nitrogen requirement are distinguished:

1. Nitrogen uptake deficit of previous time steps:

$$\Omega_N^{def} = c_{opt,j} \sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} q_{ep,i} \Delta t - \sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} (\sigma_{NH_4} \bar{c}_{NH_4,i} + \sigma_{NO_3} \bar{c}_{NO_3,i}) q_{ep,i} \Delta t \quad (5.3)$$

2. Demand for nitrogen due to biomass growth during the current time step:

$$\Omega_N^{gr} = c_{opt,j} \sum_{i=1}^{N_r} q_{ep,i} \Delta t \quad (5.4)$$

3. Luxurious consumption of nitrogen, when excessive supply conditions occurs:

$$\Omega_N^{lux} = f_N^{lux} \left(\sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t + \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t \right) \quad (5.5)$$

with:

$$f_N^{lux} = \left(\frac{\sum_{i=1}^{N_r} \Delta z_i ((\theta_i + \rho_d K_e) c_{NH_4,i} + \theta_i c_{NO_3,i})}{\sum_{i=1}^{N_r} \Delta z_i \theta_i} \right) \frac{1}{1000} \frac{1 - f_{ds}}{f r_N} \frac{1 - f_{ds}}{f_{ds}} \quad (5.6)$$

where:

N_r	: number of soil compartments in the root zone	
Ω_N^{def}	: Nitrogen uptake deficit	(kg m ⁻²)
Ω_N^{gr}	: Nitrogen uptake demand	(kg m ⁻²)
Ω_N^{lux}	: Nitrogen luxurious consumption	(kg m ⁻²)
f_N^{lux}	: factor related to the ratio between the supply potential	
	: of the soil expressed and the nitrogen status of the plant	(-)
$f r_N$: nitrogen content of biomass dry matter	(-)
f_{ds}	: dry matter fraction of fresh biomass	(-)

A reasonable estimate for $\frac{1}{1000} \frac{1 - f_{ds}}{f r_N} \frac{1 - f_{ds}}{f_{ds}}$ amounts to 0.25. The concentrations $\bar{c}_{NH_4,i}$ and $\bar{c}_{NO_3,i}$ refer to time averaged concentrations during previous time steps and for $c_{NO_3,i}$ and $c_{NH_4,i}$ resulting values of the previous time step are used.

Nutrient uptake is also determined by the soil availability. Based on the mass preservation law and the electro-neutrality preservation rule a preference for nitrate uptake to the disadvantage of ammonium has been assumed. The nutrient availability Φ_{NH_4} and Φ_{NO_3} (kg m⁻²) is defined by:

$$\begin{aligned} \Phi_{NH_4} &= \sum_{i=1}^{N_r} \left(1 + \frac{\rho_d K_e}{\theta_i} \right) c_{NH_4,i,t_0} q_{ep,i} \Delta t \\ \Phi_{NO_3} &= \sum_{i=1}^{N_r} c_{NO_3,i,t_0} q_{ep,i} \Delta t \end{aligned} \quad (5.7)$$

Depending on the plant nutrient status as expressed by the requirement parameters and the soil availability, the *transpiration concentration stream factors* are set to a certain value (Table 5.1)

Table 5.1: *Transpiration concentration stream factors for ammonium and nitrate*

Condition	σ_{NH_4}	σ_{NO_3}
$\Omega_N^{def} + \Omega_N^{gr} + \Omega_N^{lux} < \Phi_{NO_3}$	0	$\frac{\Omega_N^{def} + \Omega_N^{gr} + \Omega_N^{lux}}{\Phi_{NO_3}}$
$\Omega_N^{def} + \Omega_N^{gr} < \Phi_{NO_3} < \Omega_N^{def} + \Omega_N^{gr} + \Omega_N^{lux}$	0	$\frac{\Omega_N^{def} + \Omega_N^{gr}}{\Phi_{NO_3}}$
$\sigma_N^{max} \Phi_{NO_3} < \Omega_N^{def} + \Omega_N^{gr} < \sigma_N^{max} \Phi_{NO_3} + \Phi_{NH_4}$	$\frac{\Omega_N^{def} + \Omega_N^{gr} - \sigma_N^{max} \Phi_{NO_3}}{\Phi_{NH_4}}$	σ_N^{max}
$\sigma_N^{max} (\Phi_{NO_3} + \Phi_{NH_4}) < \Omega_N^{def} + \Omega_N^{gr}$	σ_N^{max}	σ_N^{max}

The *transpiration concentration stream factor* is bounded to a maximum value σ_N^{max} in cases where the requirement exceeds a maximum soil availability value. In a number of regional applications of the ANIMO model σ_N^{max} was set to 5.0 (-).

Crop damage due to an unfavorable mineral nitrogen status of the soil is assumed when the actual realized cumulative uptake is less than a certain fraction of the cumulative uptake for optimum growth. The permitting nitrogen deficit is bounded to a maximum by defining a *recoverable uptake deficit*, expressed by the parameter f_{def} . If the crop damage, expressed by the uptake deficit, is greater than a certain fraction of the expected optimal cumulative uptake, the crop can only recover partially from its damage. In the remaining part of the growing season the relation for optimum uptake does not apply anymore and is adjusted to a lower level. This adaptation takes place at the time of on occurring deficit exceeding and is formulated as:

$$\left(\sum_{t=t_p}^{t_0+\Delta t} \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t \right)^* = (1 - f_{def}) \sum_{t=t_p}^{t_0+\Delta t} \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t + \sum_{t=t_p}^{t_0+\Delta t} \sum_{i=1}^{N_r} \bar{c}_i q_{ep,i} \Delta t \quad (5.8)$$

The reduction of the optimum uptake curve is illustrated in Fig. 5.1 In a number of regional model applications f_{def} was set to 0.9.

5.1.2 Phosphorus uptake

P-uptake by arable crops has been described similarly to the nitrogen uptake. The *transpiration concentration stream factor* σ_P is defined as the ratio between the optimal uptake concentration and the current liquid concentration in the root zone. An unfavorable phosphate status can thus lead to an increased value of this parameter. The σ_P is bounded to a maximum as may be caused by a limited soil availability.

Similarly to the nitrogen uptake three types of crop demand have been identified: demand induced by an uptake deficit, growth and maintenance demand and a luxurious demand:

1. Phosphate uptake deficit of previous time steps:

$$\Omega_P^{def} = \sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t - \sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} \sigma_{PO_4} \bar{c}_{PO_4,i} q_{ep,i} \Delta t \quad (5.9)$$

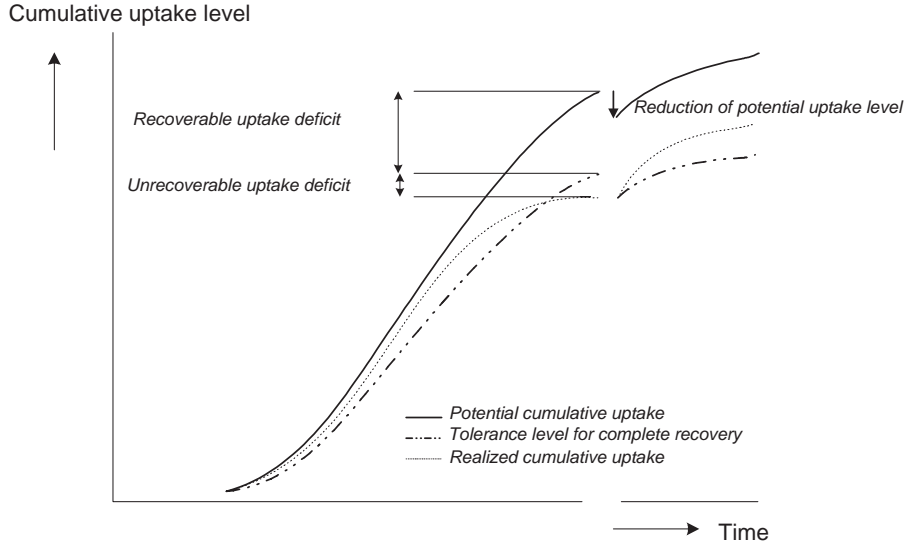


Figure 5.1: Reduction of the potential uptake level when the uptake deficit exceeds a defined tolerance level

2. Demand due to biomass growth during the current time step:

$$\Omega_P^{gr} = c_{opt,j} \sum_{i=1}^{N_r} q_{ep,i} \Delta t \quad (5.10)$$

3. Luxurious consumption, when excessive supply conditions occurs:

$$\Omega_P^{lux} = f_P^{lux} \left(\sum_{t=t_p}^{t_0} \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t + \sum_{i=1}^{N_r} c_{opt,j} q_{ep,i} \Delta t \right) \quad (5.11)$$

with the ratio between the supply potential of the soil and the P-status of the plant system expressed as phosphorus concentration in plant liquids:

$$f_P^{lux} = \left(\frac{\sum_{i=1}^{N_r} \Delta z_i ((\theta_i + \rho_d K_e^{app}) c_{PO_4,i})}{\sum_{i=1}^{N_r} \Delta z_i \theta_i} \right) \frac{1}{1000} \frac{1 - f_{ds}}{f_{rP} f_{ds}} \quad (5.12)$$

where f_{rP} is the phosphorus fraction in dry matter of productive parts and K_e^{app} is the apparent linear sorption coefficient which has been defined as:

$$K_e^{app} = \frac{X_P^{eq.s} + X_P^{prec}}{c_{PO_4,i,t_0}} \quad (5.13)$$

where $X_P^{eq.s}$ and X_P^{prec} are resp. the adsorbed phosphorus content of the equilibrium sorption pool and the precipitated phosphorus content and $c_{PO_4,i}$ is the mineral phosphorus concentration of soil moisture at the start of the timestep. Based on the crop requirement and the soil availability, the *transpiration concentration stream factor* for phosphorus is calculated according to the expression given in Table 5.2. In all other situations, the factor σ_P takes the maximum value σ_P^{max} . Crop damage

Table 5.2: *Transpiration concentration stream factors for mineral phosphorus*

Condition	σ_P
$\Phi_P > \Omega_P^{def} + \Omega_P^{gr} + \Omega_P^{lux}$	$\frac{\Omega_P^{def} + \Omega_P^{gr} + \Omega_P^{lux}}{\Phi_P}$
$\Omega_P^{def} + \Omega_P^{gr} < \Phi_P < \Omega_P^{def} + \Omega_P^{gr} + \Omega_P^{lux}$	1
$\frac{\Omega_P^{def} + \Omega_P^{gr}}{\sigma_P^{max}} < \Phi_P < \Omega_P^{def} + \Omega_P^{gr}$	$\frac{\Omega_P^{def} + \Omega_P^{gr}}{\Phi_P}$

due to limited P-availability is estimated similarly to the crop response to a mineral nitrogen deficit of the root zone. If a certain threshold value for phosphorus deficit is exceeded, the expected optimal cumulative uptake is decreased. Some part of the uptake deficit can not be recovered during the remaining part of the growing season. The ratio between the new value of the optimal phosphorus uptake and the value before adjustment is also applied to the nitrogen uptake curve.

5.2 Perennial grassland

Land management, grazing by cattle and harvesting of grass shoots plays an important role in nutrient dynamics of soil covered by perennial grassland. Moreover, the dynamics of grassland roots is another important factor since the total biomass turnover by died roots exceeds most of the time the carbon supply by additional sources. A simple biomass production module has been implemented to account for the shoot and root dynamics as a function of climate, soil moisture conditions, soil nutrient status and land management.

5.2.1 Biomass production

The nutrient demand of the crop is derived from a regionalized dry matter production model, assuming unconstrained nitrogen and phosphorus conditions. The actual daily production rate of grass shoots is given by the expression:

$$\frac{dQ_s(t)}{dt} = \chi_o \chi_p f_{NP} f_{sh} \frac{\sum_{i=1}^{N_r} q_{ep,i}}{q_{ep}^{pot}} P_{st}(t) \left(1 - e^{-\kappa \frac{Q_s(t)}{Q_{s,ref}}} \right) - W \quad (5.14)$$

where:

$Q_s(t)$: shoot dry matter amount as a function of time	$(kg\ m^{-2})$
κ	: coefficient related to light absorption by shoot biomass	$(-)$
$Q_{s,ref}$: reference value Q_s related to κ	$(kg\ m^{-2})$
$P_{st}(t)$: gross photosynthesis under standard conditions	$(kg\ m^{-2})$
$\sum_{i=1}^{N_r} q_{ep,i}$: actual plant evaporation rate during the current time step	$(m\ d^{-1})$
q_{ep}^{pot}	: potential plant evaporation	$(m\ d^{-1})$
f_{NP}	: reduction factor for nutrient limitation	$(-)$
χ_o	: grass biomass growth efficiency factor (optimal conditions)	$(-)$
χ_p	: grass biomass growth efficiency under practical farm conditions relative to optimal conditions	$(-)$
f_{sh}	: shoot fraction	$(-)$
W	: grass intake rate by grazing cattle	$(kg\ m^{-2}\ d^{-1})$

For Dutch weather conditions, this equation holds within the period 10th April - 20th Nov. Net shoot production is neglected between 20th Nov. and 10th April. The standard gross dry matter production $P_{st}(t)$ is calculated from a sinusoidal wave function which is based on empirical data of [de Wit \(1965\)](#):

$$P_{st}(t) = 0.0161 + 0.0159 f_{cl} + (0.0118 + 0.0092 f_{cl}) \sin\left(2\pi \frac{t + 284}{365}\right) \quad (5.15)$$

where f_{cl} is the cloudiness factor. The sink function for grazing W is expressed by:

$$W = \frac{1}{10\,000} \frac{14}{1 - f_{gr,loss}} N_{lsu} \quad (5.16)$$

where N_{lsu} is the average number of live stock units per hectare during the growing season and $f_{gr,loss}$ is the fraction of grazing losses. In most of the regional model applications, N_{lsu} has been taken as a regional seasonal average value. The daily herbage intake per cow is set at 14 ($kg\ d^{-1}\ cow^{-1}$) and the factor $\frac{1}{10000}$ accounts for the number of live stock units per m^2 . During spring, when the shoot production is insufficient to allow grazing, W is set to zero. The starting date for grazing is determined by the model when a threshold level of $Q_s = 0.25\ (kg\ m^{-2})$ is exceeded. When this criterium has not been reached before 10th of May, grazing will start at this date. The sward will be cut when a threshold level of 0.4 ($kg\ m^{-2}$) has been exceeded. A part of this yield is considered as a loss and remains at the field ($f_{ha,loss}$). At the end of the growing season (20th Nov.), the standing sward is cut and applied to the first soil compartment. In this regionalized approach, the swards always increase between two cuttings, due to the low regional and seasonal mean value of live stock units.

The gross increase in root dry matter due to partitioning of assimilates is proportional to the gross production of shoot dry matter:

$$\frac{dQ_r(t)}{dt} = \frac{1 - f_{sh}}{f_{sh}} \left(\frac{dQ_s(t)}{dt} + W \right) \quad (5.17)$$

A first order process is assumed for the dying of roots. The decrease rate is assumed proportional to the actual quantity of roots. The net increase of the dry matter weight of living roots:

$$\frac{dQ_r(t)}{dt} = \frac{1 - f_{sh}}{f_{sh}} \left(\frac{dQ_s(t)}{dt} + W \right) - k_{gr,decease} Q_r(t) \quad (5.18)$$

where $k_{gr,decease}$ is a first order rate constant for living root turn-over (d^{-1}). Died roots and grazing losses are applied to the soil continuously. Harvest losses are incorporated in the upper soil compartment when a harvest event occurs. Table 5.3 denotes the set of parameters which has been used for Dutch climatic conditions .

Table 5.3: *Parametrization of grassland related parameters in the ANIMO model*

Parameter	Value	Unit
$Q_{s,ref}$	0.35	($kg\ m^{-2}$)
κ	2.3	(-)
f_{cl}	0.321	(-)
f_{sh}	0.725	(-)
χ_o	0.62	(-)
χ_p	0.8 – 1.0	(-)
$k_{gr,decease}$	0.0055	(d^{-1})
$f_{gr,loss}$	0.2	(-)
$f_{ha,loss}$	0.2	(-)
threshold level of Q_s for harvesting	0.4	($kg\ m^{-2}$)
remaining shoot quantity after harvest		
— non-grazed pastures	0.075	($kg\ m^{-2}$)
— grazed pastures	0.165	($kg\ m^{-2}$)
$k_{gr,dif}$	0.03	(d^{-1})
$f_{N,s}^{min}$	0.019	(-)
$f_{N,r}^{min}$	0.0076	(-)
$f_{N,s}^{max}$	0.05	(-)
$f_{N,r}^{max}$	0.02	(-)
$f_{P,s}^{min}$	0.003	(-)
$f_{P,r}^{min}$	0.0018	(-)
$f_{P,s}^{max}$	0.0054	(-)
$f_{P,r}^{max}$	0.0032	(-)
f_{ds}	0.2	(-)

5.2.2 Nutrient uptake

Nutrient uptake by grassland is described by a two-compartment model considering a soil compartment and a plant compartment. This concept accounts for the internal transport of nutrients from the root system to the shoots. The nitrate concentration in grass shoot liquids can be considered as the internal concentration of the plant (c_{pl}). Plant uptake is calculated by balancing the demand of the crop and the soil supply.

The total nitrogen fraction $f_{pl,N_{tot}}$ of the shoots is calculated according to:

$$f_{pl,N_{tot}} = \frac{U(t)}{Q_s(t)} \quad (5.19)$$

where:

- $U(t)$: nitrogen quantity present in grass shoot system ($kg\ m^{-2}$)
- $Q_s(t)$: biomass present in grass shoot system ($kg\ m^{-2}$)

The amount of nitrogen present in the shoot system can be found from the remaining quantity after the last cutting and the nitrogen quantity extracted from the soil partitioned to the shoots. The biomass present in the grass shoot system is simulated by the simple grassland production module.

Nitrate uptake

The concept of supply potential is based on the assumption that total uptake is equivalent to the sum of convective transport and diffusive transport to plant roots.

$$R_{u,NO_3} = R_{u,c} + R_{u,d} \quad (5.20)$$

where the subscripts c and d denote resp. the convective and diffusive transport. The convective uptake transport of dissolved nutrients is described as Fickian transport:

$$R_{u,c} = \frac{q_{ep}}{\Delta z} \bar{c}_{NO_3} \quad (5.21)$$

where:

$$\begin{aligned} q_{ep,i} & : \text{ plant evaporation flux of compartment } i & (m \text{ d}^{-1}) \\ \Delta z_i & : \text{ thickness of compartment } i & (m) \\ \bar{c}_{NO_3,i} & : \text{ time averaged nitrate concentration in compartment } i & (kg \text{ m}^{-3}) \end{aligned}$$

When the soil nitrate concentration exceeds the nitrate concentration of root liquids, the diffusive nitrate uptake is determined by:

$$R_{u,d} = \theta k_{gr,dif} \left(\bar{c}_{NO_3} - \frac{f_{N,r}^{min}}{f_{N,s}^{min}} c_{pl} \right) \quad (5.22)$$

where the diffusion rate is proportional to a first order rate constant $k_{gr,dif}$ (d^{-1}) and the difference between the nitrate concentration in soil moisture and in plant roots. The internal concentration in plant roots has been assumed proportional to the concentration in plant shoots and the ratio between the nitrogen fractions in plant roots and plant shoots.

In numerical computation schemes, the soil system is schematized to homogeneous compartments with thickness Δz_i . The nitrate uptake in compartment i is then determined by:

$$R_{u,i} = \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO_3,i} + \theta_i k_{gr,dif} \left(\bar{c}_{NO_3,i} - \frac{f_{N,r}^{min}}{f_{N,s}^{min}} c_{pl} \right) \quad (5.23)$$

The uptake process has been incorporated in the conservation and transport equation by defining the *transpiration concentration stream factors* $\sigma_{NO_3,i}$ per soil compartment i and adding an extra term to zero-production term k_{0,NO_3} . When the nitrogen accumulation has not lead to nitrogen contents above a defined threshold level, the uptake parameters are defined by:

$$\begin{aligned} \sigma_{NO_3,i} & = 1 + \theta_i k_{gr,dif} \frac{\Delta z_i}{q_{ep,i}} \\ k_{0,NO_3,i}^* & = k_{0,NO_3,i} + \theta_i k_{gr,dif} \frac{f_{N,r}^{min}}{f_{N,s}^{min}} c_{pl} \end{aligned} \quad (5.24)$$

The internal concentration in grass shoots c_{pl} ($kg\ m^{-3}$) is calculated from a relation between the concentration and the N-fraction in the shoots, based on experimental data. The internal plant concentration is assumed to be proportional to the nitrate fraction of the shoots (f_{pl,NO_3}):

$$c_{pl} = \frac{f_{ds}}{1 - f_{ds}} 1000 f_{pl,NO_3} \quad (5.25)$$

where f_{ds} is the dry matter content of the biomass. The nitrate fraction in the shoots is related to the total nitrogen fraction. In an analysis of experimental field data of Ruurlo (Fonck, 1982b,a), both the NO_3 -N concentrations ($kg\ m^{-3}$) and the total nitrogen fractions have been calculated as a annual average values, based on 7 cuttings per field plot (5.2).

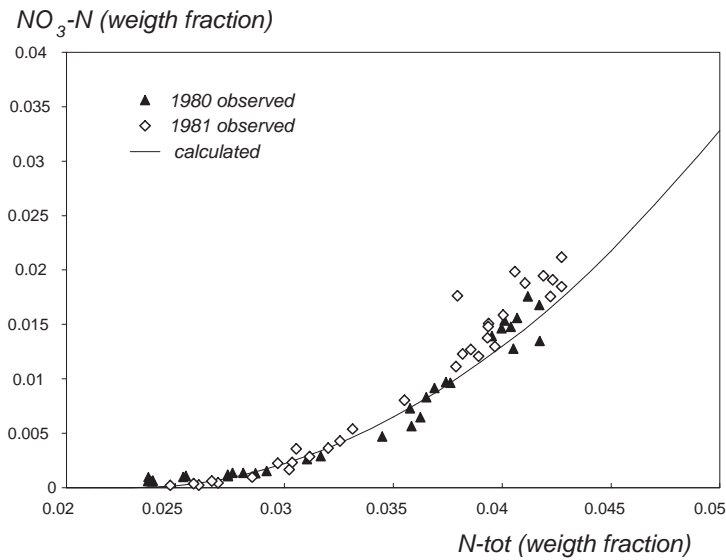


Figure 5.2: Nitrate-N weight fraction (f_{pl,NO_3}) as a function of total nitrogen weight fraction ($f_{pl,N_{tot}}$) in grass shoots

The nitrate weight fraction f_{pl,NO_3} is related to the total nitrogen fraction $f_{pl,N_{tot}}$ according to a fitted relation:

$$\begin{aligned} f_{pl,N_{tot}} \leq 0.023 & \quad f_{pl,NO_3} = 0 \\ 0.023 < f_{pl,N_{tot}} \leq 0.04 & \quad f_{pl,NO_3} = 45(f_{pl,N_{tot}} - 0.023)^2 \\ f_{pl,N_{tot}} > 0.04 & \quad f_{pl,NO_3} = \frac{0.06561}{1 + e^{-140f_{pl,N_{tot}} + 7}} \end{aligned} \quad (5.26)$$

Ammonium uptake

The ammonium uptake is based on convective transport (*concentration* \times *water flow*) and takes account for the quantity adsorbed to soil particles:

$$R_{u,NH_4} = \left(1 + \frac{\rho_d}{\theta} K_{e,NH_4}\right) \frac{q_{ep}}{\Delta z} \bar{c}_{NH_4} \quad (5.27)$$

where:

$$\begin{aligned} K_{e,NH_4} & : \text{ linear adsorption coefficient of ammonium} & (m^3 kg^{-1}) \\ \bar{c}_{NH_4,i} & : \text{ time averaged ammonium concentration of soil moisture} & (kg m^{-3}) \end{aligned}$$

The ammonium uptake per soil compartment for a certain time step reads:

$$R_{u,i} = \left(1 + \frac{\rho_d}{\theta_i} K_{e,NH_4} \right) \frac{q_{ep,i} \bar{c}_{NH_4,i}}{\Delta z_i} \quad (5.28)$$

The uptake process has been incorporated in the conservation and transport equation by defining the *transpiration concentration stream factors* $\sigma_{NH_4,i}$ per soil compartment i . When the nitrogen accumulation has not lead to nitrogen contents above a defined threshold level, the uptake parameters are defined by:

$$\sigma_{NH_4,i} = 1 + \frac{\rho_d}{\theta_i} K_{e,NH_4} \quad (5.29)$$

When the soil mineral nitrogen availability exceeds the crop requirement, the uptake parameter σ_{NH_4} will be adjusted on the basis of a defined maximum requirement. Due to electro-neutrality considerations, a preference for nitrate uptake is assumed. Nitrate and ammonium soil availabilities (Φ_{NO_3} and Φ_{NH_4}) are defined according to Eq. 5.7. Maximum uptake requirement Ω_N^{max} and the mean uptake requirement Ω_N^{mean} variables are introduced:

$$\Omega_N^{max} = Q_s(t) f_{N,s}^{max} + Q_r(t) f_{N,r}^{max} - U(t_0) \quad (5.30)$$

$$\Omega_N^{mean} = Q_s(t) \frac{f_{N,s}^{max} + f_{N,s}^{min}}{2} + Q_r(t) \frac{f_{N,r}^{max} + f_{N,r}^{min}}{2} - U(t_0) \quad (5.31)$$

Based on these defined uptake requirements and the availability of nitrogen, the ammonium uptake factor is determined. If the nitrate availability exceeds the maximum requirement, no ammonium will be taken up:

$$\Phi_{NO_3} > \Omega_N^{max} \Rightarrow \sigma_{NH_4} = 0 \quad (5.32)$$

If the nitrate availability is less than the maximum nitrogen requirement, but the sum of nitrate and ammonium availability is greater than the maximum requirement, the uptake parameter is calculated by:

$$\Phi_{NO_3} < \Omega_N^{max} < \Phi_{NO_3} + \Phi_{NH_4} \Rightarrow \sigma_{NH_4} = \frac{\Omega_N^{max} - \Phi_{NO_3}}{\Phi_{NH_4}} \quad (5.33)$$

When the sum of nitrate and ammonium availability is less than the maximum nitrogen requirement, but greater than the mean nitrogen requirement:

$$\Omega_N^{mean} < \Phi_{NO_3} + \Phi_{NH_4} < \Omega_N^{max} \Rightarrow \sigma_{NH_4} = 1 \quad (5.34)$$

In all other situations the *transpiration concentration stream factor* for ammonium σ_{NH_4} takes the maximum value ($\sigma_{NH_4}^{max}$).

Phosphorus uptake

Uptake of mineral phosphate by plant roots has been described closely related to the nitrogen uptake. However, for phosphorus no accumulation for future growth has been assumed.

$$R_{u,P} = \sigma_P \frac{q_{ep}}{\Delta z} c_{PO_4}(t) \quad (5.35)$$

The uptake factor σ_P is defined on the basis of soil availability and crop requirement. Soil availability of phosphate is calculated as the sum of the amounts present in the liquid phase, the fast sorption pool $X_P^{eq,s}$ (equilibrium) and the precipitation pool X_P^{prec} . The phosphorus uptake under unconstrained conditions equals the mineral P availability:

$$U(t_0 + \Delta t) = U(t_0) + \Phi_{PO_4} \quad (5.36)$$

where the mineral phosphorus availability is approximated by:

$$\Phi_{PO_4} = \sum_{i=1}^{N_r} \left(1 + \frac{\rho_d K_e^{app}}{\theta_i} \right) q_{ep,i} c_{PO_4,i} \Delta t \quad (5.37)$$

with K_e^{app} as the apparent linear sorption coefficient defined by Eq. 5.13. The phosphate requirement for plant growth is defined as the gross dry matter production multiplied by the actual phosphorus content of shoots and roots. The P-fractions relate to the total N-fractions according to:

$$\begin{aligned} f_{P,s} &= \frac{f_{P,s}^{min} + f_{P,s}^{max}}{f_{N,s}^{min} + f_{N,s}^{max}} (f_{pl,N_{tot}} - f_{pl,NO_3}) \\ f_{P,r} &= \frac{f_{P,r}^{min} + f_{P,r}^{max}}{f_{N,r}^{min} + f_{N,r}^{max}} \frac{f_{N,r}^{min}}{f_{N,s}^{min}} (f_{pl,N_{tot}} - f_{pl,NO_3}) \end{aligned} \quad (5.38)$$

Based on the demand and the availability, the plant uptake parameter σ_P is defined by:

$$\begin{aligned} \Phi_P > \Omega_P &\Rightarrow \sigma_P = \frac{\Omega_P}{\Phi_P} \\ \Omega_P > \sigma_P^{max} \Phi_P &\Rightarrow \sigma_P = \sigma_{P,max} \end{aligned} \quad (5.39)$$

The maximum value of the plant parameter (σ_P^{max}) has been set to one in a number of regional model applications.

5.2.3 Nutrient limitation of biomass production

The nitrogen uptake under unconstrained conditions is identical to the mineral nitrogen availability:

$$\begin{aligned} U(t_0 + \Delta t) &= U(t_0) + \sum_{i=1}^{N_r} q_{ep,i} \Delta t \left(1 + \frac{\rho_d K_{e,NH_4}}{\theta_i} \right) \bar{c}_{NH_4,i} \\ &+ \sum_{i=1}^{N_r} \Delta t \left(q_{ep,i} \bar{c}_{NO_3,i} + k_{gr,d} \theta_i \Delta z_i \left(\bar{c}_{NO_3,i} - \frac{f_{N,r}^{min}}{f_{N,s}^{min}} c_{pl} \right) \right) \end{aligned} \quad (5.40)$$

The nitrogen requirement for plant growth is defined as the gross dry matter production multiplied by the actual nitrogen content of shoots and roots, resp $f_{N,s}$ and $f_{N,r}$:

$$\Omega_N = f_{N,s} \int_{t_0}^{t_0+\Delta t} \left(\frac{dQ_s(t)}{dt} + W \right) dt + f_{N,r} \int_{t_0}^{t_0+\Delta t} \left(\frac{dQ_r(t)}{dt} + k_{gr,decease} \right) dt \quad (5.41)$$

where the actual nitrogen contents are determined by:

$$\begin{aligned} f_{N,s} &= f_{N,s}^{\min} \max \left(1, \frac{U(t)}{f_{N,s}^{\min} Q_s(t) + f_{N,r}^{\min} Q_r(t)} \right) \\ f_{N,r} &= f_{N,r}^{\min} \max \left(1, \frac{U(t)}{f_{N,s}^{\min} Q_s(t) + f_{N,r}^{\min} Q_r(t)} \right) \end{aligned} \quad (5.42)$$

When the nitrogen demand can not be fulfilled by the potential soil supply, the reduction of crop growth is assumed proportional to the shortage. Under optimal conditions, the factor for nutrient limitation f_{NP} is set to one, but when the ratio between $U(t)$ and the minimum accumulation level in shoots and roots ($f_{N,s}^{\min} Q_s(t) + f_{N,r}^{\min} Q_r(t)$) tends to value less than unity, the value one for this ratio is maintained and crop production will be reduced by taking f_{NP} a value less than one according to:

$$f_{NP} = \frac{U(t) - f_{N,s}^{\min} Q_s(t_0) - f_{N,r}^{\min} Q_r(t_0)}{f_{N,s}^{\min} \Delta Q_{s,gr} + f_{N,r}^{\min} \Delta Q_{r,gr}} \quad (5.43)$$

where $\Delta Q_{s,gr}$ and $\Delta Q_{r,gr}$ are the gross quantities of produced shoot and root material f_{NP} within the time increment under unconstrained conditions. The numerator is an expression for the uptake during the timestep plus the accumulated surplus from previous time steps. The denominator is an expression for the required nitrogen supply for growth of shoots and roots.

5.3 External crop model

5.3.1 The quadmod module

Information per time step with respect to crop uptake and crop losses by stubble and root residues can be read by the ANIMO model from an input file. The ANIMO model is able to reproduce the *forced* input with high accuracy. The data flow of a model chain with a separate crop uptake model and its dependency from a fertilization model is depicted in Fig. 5.3. This diagram applies to the STONE version 2.0 as was reported by Wolf *et al.* (2003) where the QUADMOD model (ten Berge *et al.*, 2000) was used to simulate crop uptake and crop residue release rates.

The static QUADMOD approach expresses the relations between the nitrogen application rate, the crop N-yield and the crop biomass yield. Additional descriptions in the QUADMOD model deals with partitioning of biomass, nitrogen and phosphorus over plant parts, the time of N and P uptake and the *release* of crop residues. The response of total seasonal nitrogen yield U_N ($kg\ ha^{-1}$) to the total applied nitrogen dose A_N ($kg\ ha^{-1}$) is determined by crop and soil characteristics, weather, general crop management and nutrient management. QUADMOD quantifies the response of crop yield Y to N-input A_N on the basis of the partial responses of crop yield Y to N-uptake U_N , $Y(U_N)$, and of N-uptake U_N to N-input A_N , $U_N(A_N)$ (Fig. 5.4). In the STONE framework, QUADMOD parameter sets have been estimated for grass, maize, wheat, sugar beet and potato (ten Berge *et al.*, 2000). Annual yield estimates from agricultural census as reported in LEI/CBS (1995) were used to calibrate the maximum crop yields to practical farm conditions.

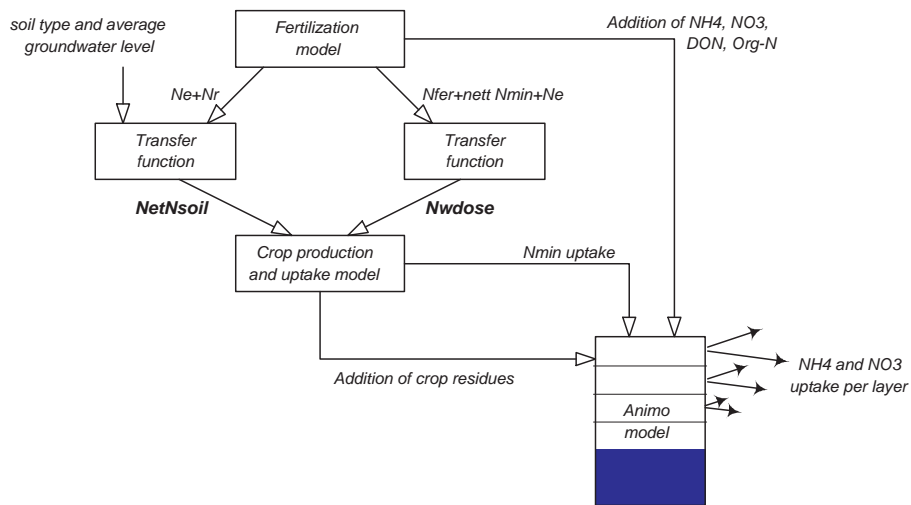


Figure 5.3: *Linked model chain in national model application of the STONE model (Wolf et al., 2003)*

The QUADMOD model uses annual information concerning two driving forces which should be supplied by the model user: the effective nitrogen dosage (N_{wdose}) and the soil nitrogen supply ($netN_{soil}$). This information can be derived from fertilization, soil type and land use information as has been depicted schematically in Fig. 5.3.

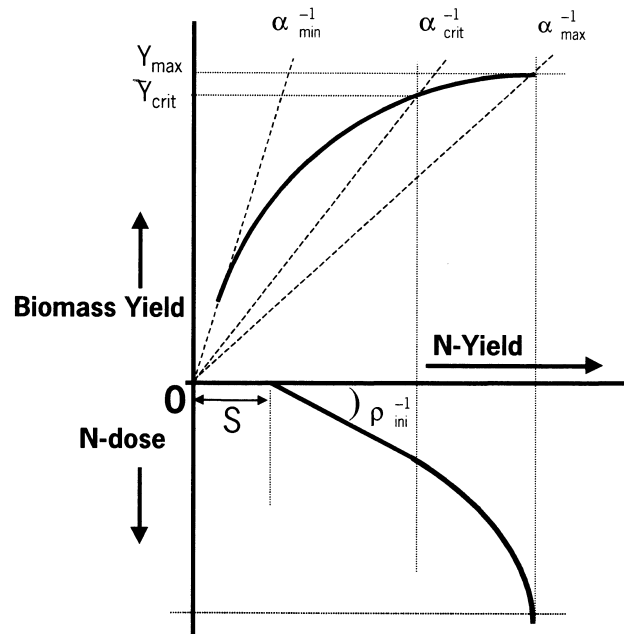


Figure 5.4: *Relations between N-dose, N-yield and biomass yield described by the QUADMOD model (ten Berge et al., 2000)*

5.3.2 Effective nitrogen dosage

The effective nitrogen dosage (N_{dose}) is an input variable to the QUADMOM model and is calculated from the annual supply of artificial and organic fertilizers. The excretion produced by grazing cattle during their outdoor periods is neglected. This type of manures may contribute to some extent to grass production but is assumed to cause some damage in and around manure paths. The total net impact of outdoor produced manure was originally set to zero, but nowadays with decreasing fertilization rates, an effectiveness is attributed to the outdoor produced manure. The N_{dose} variable is calculated as follows:

$$N_{dose} = N_{fertilizer} + N_{min}^{om} - NH_3 \uparrow + f_{Ne} \cdot N_e \quad (5.44)$$

in which:

$N_{fertilizer}$: annual N dose by artificial fertilizers	$(kg\ ha^{-1})$
N_{min}^{om}	: annual N dose by manure and slurry	$(kg\ ha^{-1})$
$NH_3 \uparrow$: ammonia volatilization	$(kg\ ha^{-1})$
N_e	: readily available organic N in manure and slurry	$(kg\ ha^{-1})$
f_{Ne}	: factor expressing the contribution of N_e to N_{dose}	(-)

Note that the excretion of grazing cattle has been disregarded for the determination of N_{dose} . In most animal manure types the organic part amounts to 0.5 of the total dose. Setting f_{Ne} to 0.6 results to an efficiency of 0.3. Additional assumptions regarding the volatilization ratio and the efficiency of mineral nitrogen in animal manure (N_{min}^{om}) results to an overall efficiency of 0.65 of the total organic N dose which is considered a reasonable estimate for Dutch agricultural practises (Noij and Westhoek, 1992).

5.3.3 Soil nitrogen supply

The *soil nitrogen supply* indicated as $NetN_{Soil}$ should theoretically be derived from simulation results of the soil nitrogen cycle. The variable should represent the net annual mineralization. Although deposition of nitrogen compounds from the atmosphere is entirely unrelated to the net mineralization, it should be included in the *soil nitrogen supply* variable. For reasons of independency of eventual weaknesses and errors of ANIMO simulation results concerning nitrogen mineralization, an alternative approach has been chosen in the STONE framework (Wolf *et al.*, 2003) to determine $NetN_{Soil}$.

The *soil nitrogen supply* in the QUADMOM model is defined as the amount of nitrogen captured by a crop on a soil in its first year of non-fertilization (Ruitenber *et al.*, 1991). This definition accounts for the crop uptake definition and the farm management practise in the preceding years to the time one wants to determine the soil nitrogen supply. Residual organic nitrogen originating from crop manure residues and can influence the mineralization rates for a number of years afterwards. Although mineralization rates are simulated by the ANIMO model, the model is not able to produce such a seasonal figure since it would require an annual pre-run with fertilization set to zero. In the STONE framework (Wolf *et al.*, 2003), the *soil nitrogen supply* values that serve as input to the QUADMOM (N_{dose}) model are calculated by a transfer function based on results of simulation experiments and soil data interpretations as reported by Ruitenber *et al.* (1991). The transfer function makes use of data concerning soil type, mean highest average groundwater level and annual addition of organic nitrogen (N_{org}).

Table 5.4: Transfer function for assessment of soil nitrogen supply as a function of organic N addition, soil type and mean highest groundwater level (MHG)

No	Description	MHG	Grassland	Maize and arable crops
1	Decomposed clayey peat over eutrophic peat: peat soil with decomposed topsoil (hVb, hVc)	> 25 cm	$0.2 \cdot (N_{org-175}) + 350$ $0.2 \cdot (N_{org-175}) + 250$	$0.16 \cdot (N_{org-125}) + 350$ $0.16 \cdot (N_{org-125}) + 250$
2	Decomposed meso-trophic peat over a coarse textured, sandy subsoil: peat soil with decomposed topsoil (aVz, hVz)	< 25 cm < 25 cm	$0.2 \cdot (N_{org-175}) + 350$ $0.2 \cdot (N_{org-175}) + 250$	$0.16 \cdot (N_{org-125}) + 350$ $0.16 \cdot (N_{org-125}) + 250$
3	Humic very fine textured, clay topsoil over eutrophic peat: peat soil with a clay cover (pVb, kVb)	> 25 cm	$0.2 \cdot (N_{org-175}) + 200$	$0.16 \cdot (N_{org-125}) + 200$
4	Humic very fine textured, clay topsoil over coarse textured, sandy subsoil: peat soil with a clay cover (kVz)		$0.2 \cdot (N_{org-175}) + 200$	$0.16 \cdot (N_{org-125}) + 200$
5	Humic, medium textured, sandy topsoil over coarse textured, sandy subsoil: peat soil with sand cover (iWz, iWp)		$0.2 \cdot (N_{org-175}) + 200$	$0.16 \cdot (N_{org-125}) + 200$
6	Decomposed clayey peat over unripened clay: peat soil with decomposed topsoil (W0)		$0.2 \cdot (N_{org-175}) + 250$	$0.16 \cdot (N_{org-125}) + 250$
7	Eolian, coarse textured sandy soil: sandy soil (Zd20, Zd21)		$0.2 \cdot (N_{org-200}) + 75$	$0.18 \cdot (N_{org-125}) + 75$
8	Podzolic, coarse textured sandy soil: sandy soil (Hd21)		$0.2 \cdot (N_{org-200}) + 100$	$0.18 \cdot (N_{org-125}) + 100$
9	Podzolic, medium textured sandy soil: sandy soil (Hn21)		$0.2 \cdot (N_{org-200}) + 125$	$0.18 \cdot (N_{org-125}) + 125$
10	Podzolic, medium textured sandy soil over coarse textured sand: sandy soil (Hn21g)		$0.2 \cdot (N_{org-200}) + 100$	$0.18 \cdot (N_{org-125}) + 100$
11	Podzolic, medium textured sandy soil over boulder clay: sandy soil (Hn23x)		$0.2 \cdot (N_{org-200}) + 125$	$0.18 \cdot (N_{org-125}) + 125$
12	Plaggen, coarse textured sandy soil: sandy soil (zEZ21)		$0.2 \cdot (N_{org-200}) + 150$	$0.18 \cdot (N_{org-125}) + 150$
13	Humic gleysol, coarse textured sandy soil: sandy soil (pZg23)		$0.2 \cdot (N_{org-175}) + 200$	$0.18 \cdot (N_{org-125}) + 200$
14	Podzolic, coarse textured sandy soil: sandy soil (gHd30)		$0.2 \cdot (N_{org-200}) + 100$	$0.18 \cdot (N_{org-125}) + 100$
15	Calcareous, medium textured, clay soil: alluvial soil (Mn25A)		$0.2 \cdot (N_{org-165}) + 150$	$0.14 \cdot (N_{org-125}) + 150$
16	Medium textured clay soil: alluvial soil (Mn35A, Rd90A, Rd90C)		$0.2 \cdot (N_{org-165}) + 150$	$0.14 \cdot (N_{org-125}) + 150$
17	Fine textured clay soil: alluvial soil (Rn44C, gMn83C, kMn48C, Rn47C)		$0.2 \cdot (N_{org-165}) + 125$	$0.14 \cdot (N_{org-125}) + 125$
18	Fine textured clay over meso-trophic peat: alluvial soil (RvO1C, Mv41C)		$0.2 \cdot (N_{org-165}) + 125$	$0.14 \cdot (N_{org-125}) + 125$
19	Medium textured clay over sand: alluvial soil (Mn22A)		$0.2 \cdot (N_{org-165}) + 125$	$0.14 \cdot (N_{org-125}) + 125$
20	Medium textured clay over coarse textured sand: alluvial soil (n52A)		$0.2 \cdot (N_{org-165}) + 125$	$0.14 \cdot (N_{org-125}) + 125$
21	Eolian, medium textured loam: lss soil (BLd6)		$0.2 \cdot (N_{org-165}) + 150$	$0.14 \cdot (N_{org-125}) + 150$

The variable N_{org} is determined as the total organic nitrogen flow to a field including the excretion of grazing cattle.

6 Organic matter cycle

Leaching of dissolved organic matter results from additions and dissolution processes in the organic matter cycle (Fig. 6.1). Four organic substances are distinguished:

- *Fresh organic matter* consists mainly of root and other crop residues after harvesting and of the organic parts of manure. These are materials that come available at clearly defined points in time. Also the bulk of organic (peat) soils is considered as fresh organic matter. Fresh organic matter may be subdivided into a number of fractions. Each fraction is characterized by a first order decomposition rate and a N- and P-content.
- *Root exudates* are organic compounds excreted by living roots and dead root cells discarded by plants. These products are added to the soil continuously as long as living roots are present.
- *Dissolved organic matter* is applied as the liquid fraction of organic manure and can be produced as a spin-off of fresh organic matter transformations.
- *Humus and living biomass* consists of dead organic soil material and living biomass. This pool results from the transformations of fresh organic matter, root exudates and dissolved organic matter.

Decomposition of fresh organic materials results to dissimilation of organic carbon, solubilization and transformation to the humus/biomass pool. Decomposition of dissolved organic compounds results in dissimilation and transformation to the humus/biomass pool. The humus/biomass pool decomposes to a residual fraction, accompanied by partial dissimilation of these residues. This residual material has been lumped with the humus/biomass pool, so only nett dissimilation of this pool has been taken into consideration. A new feature in ANIMO version 4.0, is the possibility to specify an assimilation/dissimilation ratio for each fresh organic fraction (a_{fn}), for dissolved organic matter (a_{dom}) and for the root exudate pool (a_{ex}). When a certain amount of organic material has been introduced into the soil system, only the state variables of a limited number of classes are simulated, because the schematization of organic materials into certain defined classes follows a linear approach.

6.1 Characterization of fresh organic materials

The fresh organic materials can be applied to the soil system and can optionally be mixed with the present organic materials in one or more top compartments. These materials can vary strongly in quality. Each kind of material is considered to exist of one or more classes; each class with its own decomposition rate and nitrogen and phosphorus contents. The model requires a definition of the organic and mineral (anorganic) fractions of the introduced materials. The decomposition of each class is assumed to follow first order rate kinetics. The sub-division of a material over different classes:

$$M(t) = \sum_{n=1}^{nf} OM_n(t) \quad (6.1)$$

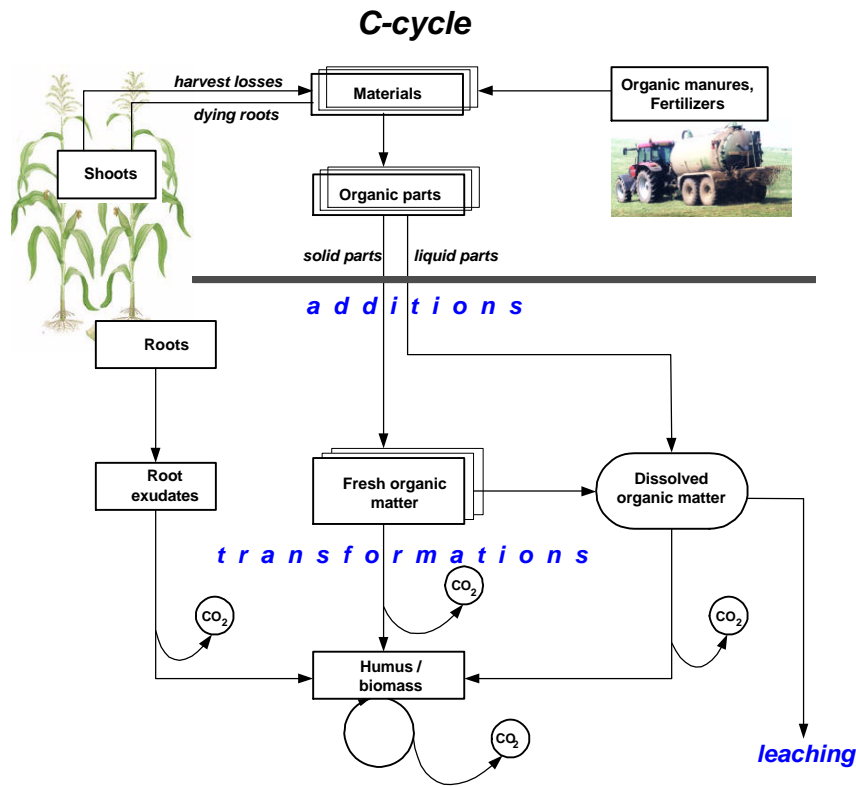


Figure 6.1: Relational diagram of the organic matter cycle

First order rate decomposition of an organic class:

$$\frac{dOM_n}{dt} = -k_n OM_n \rightarrow OM_n(t) = OM_n(t_0) e^{-k_n(t-t_0)} \quad (6.2)$$

thus:

$$\frac{dOM_n}{dt} = -k_n OM_n(t_0) e^{-k_n(t-t_0)} \quad (6.3)$$

For a material, the decomposition rate reads as:

$$\frac{dM(t)}{dt} = \sum_{n=1}^{nf} -k_n OM_n(t_0) e^{-k_n(t-t_0)} \quad (6.4)$$

where M expresses the material, $OM_n(t)$ is the organic class and k_n is the rate constant.

The possibility to define a number of a number classes to represent a material allows the mathematical simulation of empirical decomposition curves as given by [Kolenbrander \(1969\)](#) or [Janssen \(1986\)](#). He derived a time dependent decomposition rate of peat and other organic materials using the data published by [Kolenbrander \(1969, 1974\)](#). He introduced the so-called apparent age concept for different organic materials, and concluded from the experimental data that the initial decomposition rate was equal to $2.82\tau_a^{-1.6}$. Substitution of the relationship between decomposition

rate and time and integration for the quantity of organic material present yields the following expression:

$$OM(t) = OM(t_0)e^{4.7((\tau_a+t)^{-0.6}-\tau_a^{-0.6})} \quad (6.5)$$

in which:

- $OM(t)$: quantity organic material present at time t ($kg\ m^{-3}$)
- $OM(t_0)$: quantity organic material present at time t_0 ($kg\ m^{-3}$)
- τ_a : apparent age of the organic material (a)

The *Janssen*-model suggests that a certain organic material transfers into another type of material, as related to the decomposition rate. The essence of this model is the use of one general relationship between $\log(k)$ and $\log(t)$ for all organic materials. In the long run this agrees with the conclusions of Allison (1973), that from different organic materials after a period of decomposition, products are formed with a similar chemical composition. Although the model of *Janssen* has the advantage of being a one parameter time dependent model it appears from the formulation in Eq. 6.5 that after a long period of decomposition, with $t \rightarrow \infty$, the remaining quantity of inert organic material depends on the apparent age τ_a ($\frac{OM(\infty)}{OM(t_0)} \rightarrow e^{-4.7\tau_a^{-0.6}}$). And that is not realistic.

When appropriate parameter sets are chosen for combination of class-fractions and first order rate constants of a certain organic material, the ANIMO concept is able to reproduce equivalent relations to the empirical approach of Janssen (1986). When one wants derive a parameter set for a certain material on the basis of an empirical relation, it should be kept in mind that most of these relations describe the overall decay. The capabilities of the ANIMO-concept to reproduce the *Janssen*-relation is illustrated in Fig. 6.2. In the ANIMO model the decomposition rate constant of the

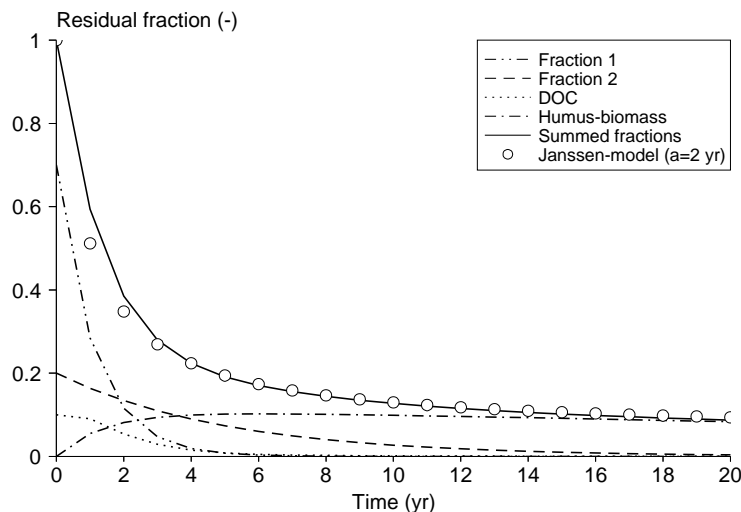


Figure 6.2: Simulation of the *Janssen* decay relation by an appropriate choice of parameters

dissolved organic matter pool has values which are more than ten times higher than the rate constants of the solid pools. The rate limiting step in the transformation chain *Solid fresh organic matter* \rightarrow *Dissolved organic matter* \rightarrow *Humus / biomass* is the first step.

Considering the dosage of one ($kg\ m^{-3}$) organic matter in a soil which is subdivided into two fractions solid *Fresh organic material*, the rate equations for class 1 and 2 and humus/biomass read:

$$\begin{aligned}\frac{dOM_1}{dt} &= -k_1OM_1(t); & OM_1(t_0) &= f_{i,1} \\ \frac{dOM_2}{dt} &= -k_2OM_2(t); & OM_2(t_0) &= f_{i,2} \\ \frac{dHU}{dt} &= a_1k_1OM_1(t) + a_2k_2OM_2(t) - k_{hu}HU(t); & HU(t_0) &= 0\end{aligned}\quad (6.6)$$

After solving these differential equations, the simplified course with time of the material can be written as:

$$\begin{aligned}M_i(t) &= OM_1(t) + OM_2(t) + HU(t) \\ &= f_{i,1} \left(1 - \frac{a_1k_1}{k_1 - k_{hu}}\right) e^{-k_1t} + f_{i,2} \left(1 - \frac{a_2k_2}{k_2 - k_{hu}}\right) e^{-k_2t} \\ &\quad + \left(f_{i,1} \frac{a_1k_1}{k_1 - k_{hu}} + f_{i,2} \frac{a_2k_2}{k_2 - k_{hu}}\right) e^{-k_{hu}t}\end{aligned}\quad (6.7)$$

Since only two fractions are considered, the relation $f_{i,1} + f_{i,2} = 1$ holds. Substitution and introducing of new parameters yields:

$$\frac{M_i(t)}{M_i(t_0)} = \eta_1 e^{-k_1t} + \eta_2 e^{-k_2t} + \eta_3 e^{-k_{hu}t}\quad (6.8)$$

where:

$$\begin{aligned}\eta_1 &= f_{i,1} \left(1 - \frac{a_1k_1}{k_1 - k_{hu}}\right) \\ \eta_2 &= (1 - f_{i,1}) \left(1 - \frac{a_2k_2}{k_2 - k_{hu}}\right) \\ \eta_3 &= f_{i,1} \frac{a_1k_1}{k_1 - k_{hu}} + (1 - f_{i,1}) \frac{a_2k_2}{k_2 - k_{hu}}\end{aligned}\quad (6.9)$$

Utilizing the *Janssen* model for a certain apparent age results to series of $(t, M_i(t))$ data pairs. Optimal values of η_1 , η_2 and η_3 can be obtained by assuming values for k_1 , k_2 and k_{hu} and employing a least square fitting to these data pairs. Results of the fitting are given in Table 6.1 for the combination $k_1=2$, $k_2=0.2$ and $k_{hu} = 0.02$ (a^{-1}). Since the expression given in Eq. 6.9 are mathematically dependent ($\eta_1 + \eta_2 + \eta_3 = 1$) it is possible to find expressions for $f_{i,1}$, a_1 and a_2 for only two parameters. Assuming a_1 identical to a_2 , values for f_1 and a_1 as could be obtained from η_1 , η_2 and η_3 as given in Table 6.1 have been listed in Table 6.2. Apparently the assimilation/dissimilation ratio ranges from 0.025 to 0.40. This range agrees with data from literature (van Rijn, 1998; Yang, 1996). Organic materials of young apparent age will mostly dissimilate and decomposition of older materials will contribute to the humus/biomass pool much more.

Results given in Table 6.2 have been fitted against the apparent age τ_a , where $\tau_a \leq 5$ (a):

$$\begin{aligned}f_1 &= -0.0105\tau_a^3 + 0.1394\tau_a^2 - 0.6904\tau_a + 1.4767 \\ a_1 &= -0.0066\tau_a^3 + 0.0673\tau_a^2 - 0.1096\tau_a + 0.0705\end{aligned}\quad (6.10)$$

Table 6.1: Derivation of intermediate organic matter related parameters from the Janssen relation

τ_a (yr)	η_1 (-)	η_2 (-)	η_3 (-)
1.0	0.900	0.074	0.026
1.5	0.690	0.278	0.032
2.0	0.530	0.400	0.070
2.5	0.408	0.467	0.125
3.0	0.317	0.497	0.186
3.5	0.248	0.503	0.249
4.0	0.195	0.495	0.310
4.5	0.155	0.478	0.367
5.0	0.123	0.455	0.422

Table 6.2: Derivation of ANIMO organic matter parameters from intermediate parameters

τ_a (yr)	f_1 (-)	$a_1=a_2$ (-)
1.0	0.92	0.025
1.5	0.71	0.030
2.0	0.57	0.066
2.5	0.46	0.117
3.0	0.38	0.174
3.5	0.32	0.231
4.0	0.27	0.286
4.5	0.23	0.338
5.0	0.20	0.387

Remaining organic matter quantities calculated with the ANIMO pool-subdivision and parameterized with Eq. 6.10 are in close agreement with quantities calculated with the *Janssen* model.

6.2 Additions

6.2.1 Fresh organic materials

During fertilization events fresh organic materials and dissolved organic matter are applied as instantaneous pulse-type doses. The organic part of the applied substance is divided over fresh organic matter and dissolved organic matter.

The amount of fresh organic matter at the start of the time step is calculated by totalizing the initial quantity and the dose applied:

$$OM_{fn}(t + \tau) = OM_{fn}(t) + (f_{i,fn} - f_{i,fn}^L) \frac{f_i^O M_i}{\Delta z} \quad (6.11)$$

where:

$OM_{fn}(t + \tau)$: volumic mass of organic matter class fn after addition	$(kg\ m^{-3})$
$OM_{fn}(t)$: volumic mass of organic matter class fn before addition	$(kg\ m^{-3})$
$f_{i,fn}$: fraction of the fn^{th} class as a part of material applied	$(-)$
$f_{i,fn}^L$: liquid fraction of the fn^{th} class as a part of material applied	$(-)$
f_i^O	: organic fraction of the applied material	$(-)$
M_i	: areic mass of applied material	$(kg\ m^{-2})$
τ	: infinite small time increment	(d)

6.2.2 Dissolved organic matter

The impact of fertilization or other additions on liquid concentration of dissolved organic matter is calculated according to:

$$c_{dom}(t + \tau) = c_{dom}(t) + \sum_{fn=1}^{nf} f_{i,fn}^L f_i^O \frac{M_i}{\theta \Delta z} \quad (6.12)$$

where:

$c_{dom}(t + \tau)$: concentration dissolved organic matter after addition	$(kg\ m^{-3})$
$c_{dom}(t)$: concentration dissolved organic matter before fertilization	$(kg\ m^{-3})$
nf	: number of organic matter classes	$(-)$

6.2.3 Root residues

The decease of grassland roots is described by a dynamic sub-model (see Par. 5.2.1). Root material died during the previous time step is added to the root zone at the beginning of the current time step. Dead roots are considered as a composition of two classes of fresh organic material. The first class has a high nutrient content and the second is characterized by a low nutrient fraction. The dead roots are divided over these two materials subject to the condition that the nutrient content of the mixture is in accordance with the nutrient fraction calculated by the dynamic sub-model. Since the decease rate has been modeled proportional to the root mass, information is available to distribute the materials with depth. Grazing losses and harvest losses of grass shoots are treated in a similar way, but are added to the top compartment only.

Residual root materials of arable crops (*exudates*) are applied to the soil compartments of the root zone at the end of the growing season. During the growing season, the growth and maintenance of the root system produces dead root cells and hair roots. These materials are defined as root exudates which are described by a separate pool. The ANIMO model comprises a sub-model for dry matter production and nutrient uptake of grassland. In this sub-model grassroots die continuously throughout the year. These dead grass roots are added to the soil system as one of the defined fresh organic materials during each simulation time step. These dead grass roots are distributed in the root zone linearly decreasing with depth.

Dry matter production of arable crops is defined as input to the model. No specific nutrient balances of roots or shoots have been formulated. Spin-off products of root growth are described as root exudates with fixed user defined nitrogen and phosphorus contents. At harvest, the root material is added to the root zone as a fresh organic material. The nutrient contents are calculated from the realized

dry matter production and the cumulative nutrient uptake. The addition of dead roots and dead over-ground parts are treated in a similar way as grass roots. They are considered as a composition of two classes organic material and the division over these materials is calculated from the defined nutrient fractions and the actual nitrogen fractions of the remaining plant parts.

6.3 Transformations

Organic substances can be transformed from one species into another with production as a source and decomposition as a sink term in the general mass conservation and transport equation. These terms will be given for the four organic substances: fresh organic matter, dissolved organic matter, humus/biomass and exudates. R_d and R_p stand for resp. the decomposition rate and the production rate and are elaborated in the subsequent paragraphs

Fresh organic matter

The introduction of fresh organic matter occurs by additions of manure, root materials, grazing and harvest losses and any other organic materials defined in the input files. Decomposition of fresh organic matter into humus/biomass is described by first order kinetics:

$$R_{d,OM \rightarrow HU} = \sum_{fn=1}^{nf} \left(-\frac{dOM_{fn}}{dt} \right) = f_{hu} \sum_{fn=1}^{nf} k_{fn} OM_{fn} \quad (6.13)$$

where:

$$\begin{aligned} f_{hu} &: \text{fraction of fresh organic matter directly transformed to humus/biomass} & (-) \\ k_{fn} &: \text{first order rate constant of organic class } fn & (d^{-1}) \end{aligned}$$

Transformation into dissolved organic matter is described as:

$$R_{d,OM \rightarrow DOM} = - \sum_{fn=1}^{nf} \frac{dOM_{fn}}{dt} = (1 - f_{hu}) \sum_{fn=1}^{nf} k_{fn} OM_{fn} \quad (6.14)$$

where $(1 - f_{hu})$ is fraction fresh organic matter subject to solubilization $(-)$.

Dissolved organic matter

Formation of dissolved organic matter results from the decomposition of the different fresh organic matter classes and is formulated as:

$$R_{p,DOM} = \frac{d\theta c_{dom}}{dt} = (1 - f_{hu}) \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} \sum_{fn=1}^{nf} k_{fn} OM_{fn} dt \quad (6.15)$$

Decomposition of dissolved organic matter is described as a first order process:

$$R_{d,DOM} = - \frac{d\theta c_{dom}}{dt} = k_{dom} \theta c_{dom} \quad (6.16)$$

where k_{dom} is the rate constant for decomposition of dissolved organic matter (d^{-1}) .

Exudates

Production of exudates is considered for arable crops only. The ANIMO model comprises a sub-model for grassland for simulation of dry matter production of shoots and roots as well as the turn-over of roots. For arable crops, the exudate production has been formulated proportionally to the root mass increase. The root growth characteristic has to be defined as model input and from these data, the model calculates the increase of root mass during the simulation time step. Within the simulation time step, the root growth is assumed constant. On the basis of scarce literature data Berghuijs-van Dijk *et al.* (1985) derived an exudate production rate of 41% of the gross dry matter production of roots. Hence, it follows:

$$R_{p,EX} = \frac{dEX}{dt} = 0.41 \frac{R_{t_0+\Delta t} - R_{t_0}}{\Delta t} \quad (6.17)$$

Decomposition of exudates into humus is described as a first order process:

$$R_{d,EX} = - \frac{dEX}{dt} = k_{ex} EX \quad (6.18)$$

where k_{ex} (d^{-1}) is the first order rate constant for decomposition of exudates.

Humus/biomass

Production of humus/biomass results from the decomposition of fresh organic matter, dissolved organic matter, exudates and an internal turnover of humus. The assimilation process is accompanied by a dissimilation which requires most of the organic material for energy supply of the living biomass. Production of humus/biomass as a result of the decomposition of fresh organic matter is given by the following equation:

$$R_{p,OM \rightarrow HU} = \frac{dHU}{dt} = f_h \sum_{fn=1}^{nf} a_{fn} k_{fn} OM_{fn} \quad (6.19)$$

Production of humus/biomass as a result of the decomposition of dissolved organic matter:

$$R_{p,DOM \rightarrow HU} = \frac{dHU}{dt} = \frac{a_{dom}}{\Delta t} \int_{t_0}^{t_0+\Delta t} k_{dom} \theta c_{dom} dt \quad (6.20)$$

Production of humus/biomass as a result from the decomposition of exudates:

$$R_{p,EX \rightarrow HU} = \frac{dHU}{dt} = a_{ex} k_{ex} EX \quad (6.21)$$

In the ANIMO model, no separate production of humus/biomass as a result of humus/biomass turnover has been formulated explicitly, because the newly formed humus/biomass material has been lumped with the total humus/biomass pool and the rate constant has been formulated for the nett decomposition. The gross decomposition rate and the formation rate of humus biomass can be written as:

$$\begin{aligned} \left(\frac{dHU}{dt} \right)_{decomp} &= \frac{1}{1 - a_{hu}} k_{hu} HU \\ \left(\frac{dHU}{dt} \right)_{form} &= \frac{a_{hu}}{1 - a_{hu}} k_{hu} HU \end{aligned} \quad (6.22)$$

The nett decomposition rate:

$$R_{d,HU} = -k_{hu} HU \quad (6.23)$$

7 Nitrogen cycle

7.1 Mineralization and immobilization

As a result of organic matter dissimilation, part of the organic nitrogen is transformed into the mineral status (Fig. 7.1). Another part of the organic nitrogen remains in the organic status in dead humic components. On the other hand, part

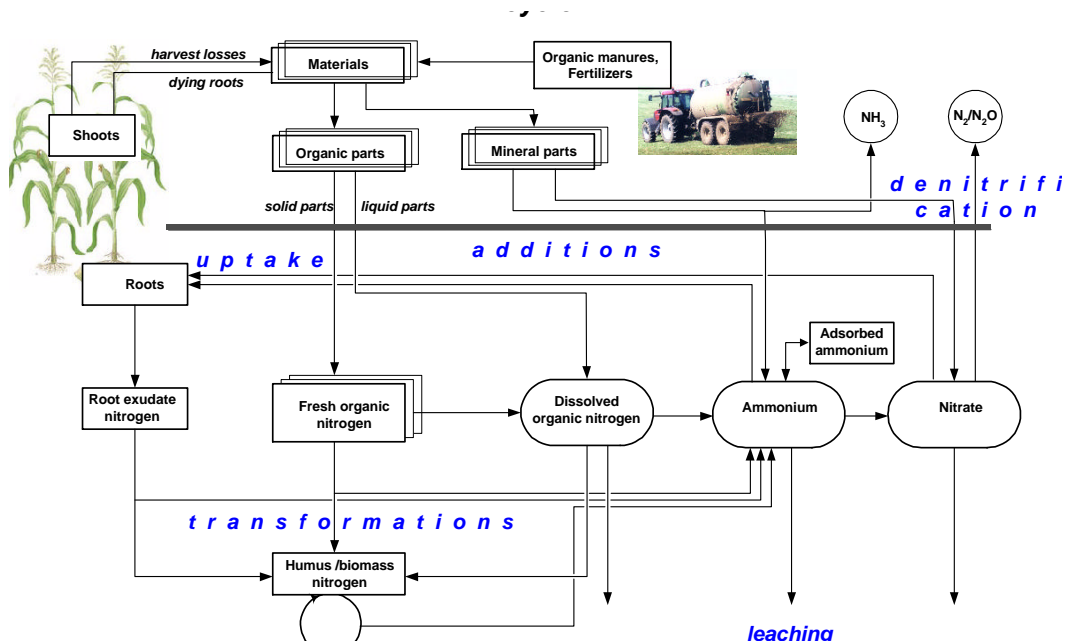


Figure 7.1: Nitrogen transformation-, accumulation- and transport processes considered in the ANIMO model

of the mineral nitrogen can be immobilized through the biomass-synthesis in the living biomass. Depending on the assimilation ratio and the ratio between nitrogen content in parent fresh organic material and the nitrogen weight fraction of the humus/biomass pool, the transformation yields or requires mineral N. The net mineralization has been formulated as a zero-order term in the *conservation and*

transport equation of ammonium, defined by:

$$\begin{aligned}
R_{p,NH_4} &= \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left(\sum_{fn=1}^{nf} (f_N^{fn} - a_{fn} f_N^{hu}) f_{hu} k_{fn} OM_{fn}(t) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left(k_{dom} \theta (c_{doN}(t) - a_{dom} f_N^{hu} c_{dom}(t)) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left((f_N^{ex} - a_{ex} f_N^{hu}) k_{ex} EX(t) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} f_N^{hu} k_{hu} HU(t) dt
\end{aligned} \tag{7.1}$$

where f_N^{hu} is the nitrogen weight fraction of humus/biomass (–) and $c_{doN}(t)$ is the concentration dissolved organic nitrogen ($kg\ m^{-3}$).

When the right hand side of the equation takes a negative value, ammonium is immobilized. No immobilization of nitrate has been assumed. When the initial quantity of ammonium at the beginning of the time step is not sufficient to cover the total immobilization requirement, the assimilation ratio is decreased and less humus/biomass will be formed. In case of nitrogen shortage, the transformation occurs less efficient. ? reviewed mineralization processes in peat soils and concluded that the reduction of the assimilation ratio is not according to literature data. However, no alternative formulation for the influence of nitrogen limitation on the organic matter decomposition have become available.

7.2 Nitrification and denitrification

Under (partial) aerobic conditions in the soil system, ammonium is oxidized to nitrate. The production rate of nitrate is assumed proportional to the liquid concentration of ammonium. In the ammonium *conservation and transport equation* nitrification has been described by first order rate kinetics:

$$R_{d,NH_4} = k_{nit} \theta c_{NH_4} \tag{7.2}$$

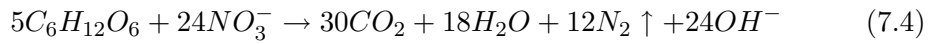
where k_{nit} is the first order rate constant. Under complete aeration and favorable soil conditions (pH), this constant equals the reference value as must be specified by the model user. When the moisture condition in soil leads to (partial) anaerobiosis, this constant is adapted by a response factor for incomplete aeration f_{ae} . At complete aeration f_{ae} takes the value one, at complete anaerobiosis f_{ae} equals zero. The numeric value of f_{ae} is calculated in a sub-model which optionally describes the aeration process on the basis of oxygen diffusion in air filled soil pores and in saturated soil aggregates (original ANIMO concept) or describes the response factor as a function of air filled pore volume (adjusted SONICG concept, see Par.9.2.3).

In the *conservation and transport equation* of nitrate, the production rate R_p equals

the average decomposition rate of ammonium given by the expression:

$$R_{p,NO_3} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} k_{nit} \theta_{c_{NH_4}}(t) dt \quad (7.3)$$

Decomposition of organic materials under anaerobic conditions can proceed if sufficient nitrate-oxygen is available to meet the oxygen demand. At high nitrate concentrations, the oxygen requirement of organic decomposition processes is the rate limiting factor. At low nitrate contents, the NO_3 concentration can be the rate limiting factor for anaerobic decomposition. In the ANIMO model, it is assumed that denitrification is governed by:



The oxidation of one mol carbon requires 24/30 mol NO_3^- and the weight ratio between nitrogen and carbon reads 14/12. If the carbon content of organic material is taken as 58% on dry weight basis, it follows that the nitrate demand for denitrification can be expressed by a zero-order consumption term:

$$R_{p,den} = -0.58 \frac{24}{30} \frac{14}{12} f_{hetero} \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left[\sum_{fn=1}^{nf} (1 - a_{fn}) f_{hu} k_{fn} OM_{fn}(t) + (1 - a_{dom}) k_{dom} (\theta_{c_{dom}}) + (1 - a_{ex}) k_{ex} EX(t) + k_{hu} HU(t) \right] dt \quad (7.5)$$

The factor f_{hetero} has been introduced to account for the reduced organic matter transformation rates when only nitrate oxygen is available. In many field validations and regional applications, a value 0.5 has been assumed for f_{hetero} . In case the nitrate concentration limits the decomposition of organic materials under anaerobic conditions, the following first order rate expression has been defined:

$$R_{d,den} = k_{den} \theta_{c_{NO_3}}(t) \quad (7.6)$$

where k_{den} is the first order rate constant to be defined as model input (d^{-1}). Determination of the rate limiting process is conducted by first computing both alternatives. The process leading to the highest nitrate concentration at the end of the time interval is subsequently selected by the model.

7.3 Ammonium sorption

Ammonium may be adsorbed to the soil complex, consisting of the negative surfaces of clay particles and humic compounds. The sorption process results to an equilibrium between ammonium in liquid and adsorbed phase, an equilibrium which is described by a linear sorption isotherm:

$$X_{e,NH_4} = K_{e,NH_4} c_{NH_4} \quad (7.7)$$

where X_{e,NH_4} is the adsorbed ammonium content ($kg\ kg^{-1}$) and K_{e,NH_4} is the ammonium adsorption or partitioning coefficient ($m^3\ kg^{-1}$). [Hoeks *et al.* \(1979\)](#) showed the influence of the clay content on the adsorption affinity of ammonium. Exploring the theory of cation exchange in multi-component systems, a relation

can be derived between the linear adsorption coefficient and the Cation Exchange Capacity (CEC). The Gapon equation for $NH_4^+ \rightleftharpoons Ca^{2+}$ exchange:

$$\frac{\Gamma_{NH_4}}{\Gamma_{Ca}} = K_G \frac{(NH_4^+)}{\sqrt{(Ca^{2+})}} \quad (7.8)$$

where:

$$\begin{array}{ll} \Gamma_{NH_4}, \Gamma_{Ca} & : \text{ ammonium, calcium complex occupation} \quad (meq (100g)^{-1}) \\ (NH_4^+), (Ca^{2+}) & : \text{ molar concentrations of ammonium, calcium} \quad (mol l^{-1}) \\ K_G & : \text{ Gapon exchange coefficient} \quad (mol^{-\frac{1}{2}} l^{\frac{1}{2}}) \end{array}$$

When constant levels of Γ_{Ca} and (Ca^{2+}) are assumed, the Gapon equation describes the linear ammonium sorption, where the linear sorption coefficient K_{e,NH_4} is related to the Gapon coefficient according to:

$$K_{e,NH_4} = 10^{-5} K_G \frac{\Gamma_{Ca}}{\sqrt{(Ca^{2+})}} \quad (7.9)$$

Values of the Gapon coefficient are reported by e.g. [Bruggenwert and Kamphorst \(1982\)](#) and [Appelo \(1988\)](#). From their data, a value of 0.5 (range: 0.3-0.7) was established as a good approximation. In most soils having favorable pH-values for agricultural production, calcium occupies the greatest part of the exchange complex (0.5-0.9). The ammonium concentrations only changes this occupation to a slight extent.

$$K_{e,NH_4} = 10^{-5} K_G \frac{f_{Ca} CEC}{\sqrt{(Ca^{2+})}} \quad (7.10)$$

Where f_{Ca} is the calcium fraction of the total adsorbed cationic composition. The fraction shows a range from 0.5 to 0.9 and is highly dependent on pH . Inserting a CEC-value of 5 ($meq (100g)^{-1}$), a calcium occupation fraction of 0.7 and a calcium concentration of 3 ($mmol l^{-1}$) yields a K_{e,NH_4} -value of $3 \cdot 10^{-4}$ ($m^3 kg^{-1}$). When only data on CEC-values are available, the relation $K_{e,NH_4} = 6 \cdot 10^{-5} \cdot CEC$ can be used as a first approximation.

8 Phosphorus cycle

8.1 Mineralization and immobilization

Mineralization of organic phosphorous and immobilization of mineral phosphorus compounds is formulated similarly to nitrogen mineralization and immobilization (Fig. 8.1).

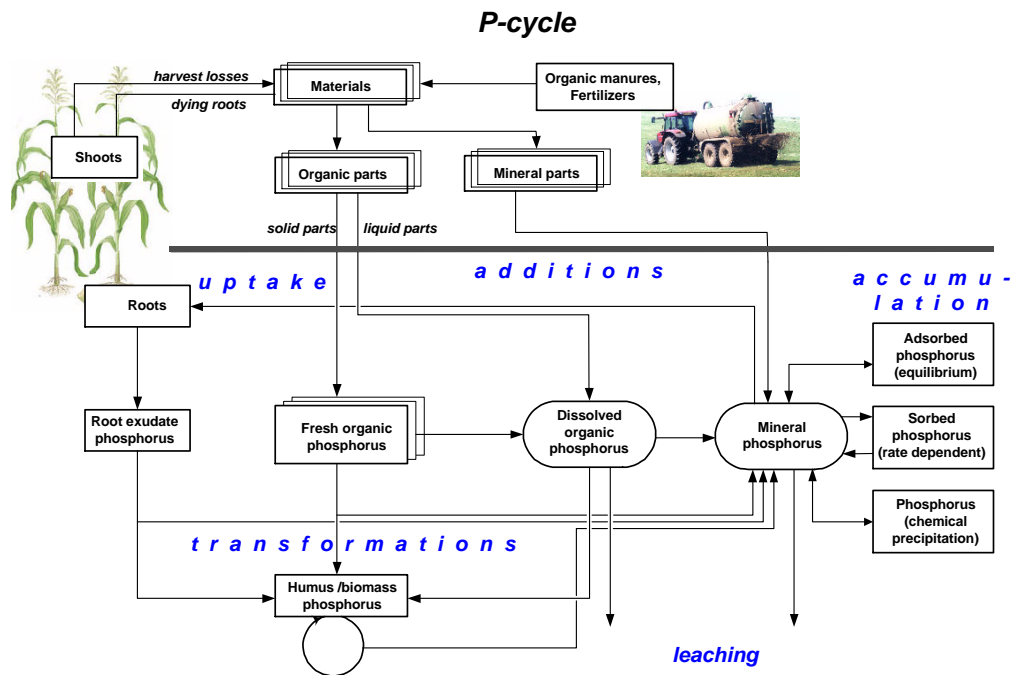


Figure 8.1: Phosphorus transformation-, accumulation- and transport processes considered in the ANIMO model

Depending on the assimilation ratio and the ratio between phosphorus content in parent fresh organic material and the phosphorus weight fraction of the humus/biomass pool, mineral P will be released or incorporated. The net mineralization has been formulated as a zero-order term in the *conservation and transport*

equation of mineral phosphate, defined by:

$$\begin{aligned}
R_{p,PO_4} &= \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left(\sum_{fn=1}^{nf} (f_P^{fn} - a_{fn} f_P^{hu}) f_{hu} k_{fn} OM_{fn}(t) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left(k_{dom} \theta (c_{doP}(t) - a_{dom} f_P^{hu} c_{dom}(t)) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \left((f_P^{ex} - a_{ex} f_P^{hu}) k_{ex} EX(t) \right) dt \\
&+ \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} f_P^{hu} k_{hu} HU(t) dt
\end{aligned} \tag{8.1}$$

where f_P^{hu} is the phosphorus weight fraction of humus/biomass (–). When the right hand side of the equation takes a negative value, phosphate is immobilized. In case the initial quantity of readily available phosphate at the beginning of the time step is not sufficient to cover the total immobilization requirement, the assimilation ratio is decreased and less humus/biomass will be formed.

8.2 Sorption and diffusion–precipitation

Phosphate sorption is modeled by assuming a reversible adsorption reaction and an irreversible diffusion (fixation) process. The *Langmuir* isotherm is derived from the assumption of a homogeneous monolayer of adsorbate on the adsorbent. The Langmuir equation is used to describe instantaneous sorption of phosphates to soil constituents (Enfield *et al.*, 1981; van Noordwijk *et al.*, 1990; Schoumans *et al.*, 1997; Schoumans and Groenendijk, 2000):

$$X_{e,P} = \frac{K_L c_P}{1 + K_L c_P} X_{max,P} \tag{8.2}$$

where $X_{e,P}$ is the content of reversibly adsorbed P ($kg\ kg^{-1}$), $X_{max,P}$ is the maximum content of adsorbed P ($kg\ kg^{-1}$) and K_L is the adsorption constant ($m^3\ kg^{-1}$). The quantity adsorbed to the soil matrix never exceeds the maximum sorption capacity $X_{max,P}$. The formulations given above can be incorporated into the *conservation and transport equation* by elaborating the differential quotient $\frac{\partial X_e}{\partial t}$:

$$\rho_d \frac{\partial X_{e,P}}{\partial t} = \rho_d \left(\frac{dX_{e,P}}{dc_P} \right) \frac{\partial c_P}{\partial t} = \rho_d K_a(c_P) \frac{\partial c_P}{\partial t} \tag{8.3}$$

where $K_a(c_P)$ is the differential sorption coefficient which is approximated by the average value $\bar{K}_a(c_P)$. This value is assessed by calculating the slope of the chord of the adsorption isotherm:

$$\bar{K}_a(c_P) = \frac{1}{c_P(t) - c_P(t_0)} \int_{t_0}^t \left(\frac{dX_{e,P}}{dc_P} \right) dc_P = \frac{X_{e,P}(t) - X_{e,P}(t_0)}{c_P(t) - c_P(t_0)} \tag{8.4}$$

Although $\bar{K}_a(c_P)$ is a function of the concentration, its average value is considered to be constant during the time step. Schoumans (1995) established parameters of the Langmuir-isotherm describing the reversible phosphate sorption for a wide range of sandy soils:

$$\begin{aligned} K_L &= 1129 \\ X_{max} &= 5.167 \cdot 10^{-6} \cdot \rho_d \cdot [Al + Fe] \end{aligned} \quad (8.5)$$

where K_L is expressed in ($m_w^3 kg^{-1} P$) and $[Al + Fe]$ is the aluminium + iron content of the soil ($mmol kg^{-1}$). Descriptive formulations have been chosen which have also been utilized to address time dependent sorption behavior of pesticides (Boesten, 1986). The diffusive transition zone is described by one lumped first order rate equation and the chemical fixation by a Freundlich sorption isotherm. The Freundlich equation represents a composition of Langmuir-curves. An individual Langmuir-curve describes the fixation of a chemical substance to a sorptive medium of limited capacity. Therefore, the Freundlich relation appears more suitable for a heterogeneous soil medium, composed of a finite number of homogeneous soil aggregates. The general formulation of a first order rate sorption (chemical non-equilibrium) model is:

$$\begin{aligned} f_s(c_P) > X_{n,P} \quad \rho_d \frac{\partial X_{n,P}}{\partial t} &= \rho_d k_{ads} (f_s(c_P) - X_{n,P}) \\ f_s(c_P) < X_{n,P} \quad \rho_d \frac{\partial X_{n,P}}{\partial t} &= \rho_d k_{des} (f_s(c_P) - X_{n,P}) \end{aligned} \quad (8.6)$$

where k_{ads} and k_{des} (d^{-1}) are rate constants and $f_s(c_P)$ is the non-equilibrium sorption pool content in the equilibrium state as a function of the concentration ($kg kg^{-1}$). The difference between the equilibrium concentration which is reached in the steady state situation and the actual solid phase concentration is considered as the driving force for mass transfer. The validity of either the adsorption relation or the desorption relation depends on $X_{n,P}$ relative to $f_s(c_P)$. In the further text the choice for one of the relations is indicated by the use of $k_{ads,des}$. In the case of kinetic phosphate sorption, the rate equation is defined as follows:

$$\rho_d \frac{\partial X_n}{\partial t} = \rho_d k_{ads,des} (K_F c_P^N - X_n) \quad (8.7)$$

When appropriate parameters are chosen, the formulations given in the preceding section can be used to simulate the phosphate diffusion/precipitation model presented by van der Zee and Bolt (1991); van der Zee and van Riemsdijk (1991). Mansell *et al.* (1977) applied a rate dependent model to describe non-equilibrium behavior of phosphate sorption in sandy soils.

The ANIMO model describes the rate dependent phosphate sorption to soil constituents by considering three separate sorption sites:

$$\rho_d \frac{\partial X_n}{\partial t} = \rho_d \sum_{i=1}^3 \frac{\partial X_{n,i}}{\partial t} = \rho_d \sum_{i=1}^3 k_{ads,des,i} (K_{F,i} c_P^{N_i} - X_{n,i}) \quad (8.8)$$

Schoumans (1995) assessed the sorption parameters in a validation study for a wide range of Dutch sandy soils (Table 8.1).

Data on the first order rate coefficient of the desorption relation $k_{des,i}$ are still missing.

Table 8.1: Parameters describing the rate dependent phosphate sorption for a wide range of Dutch sandy soils (after *Schoumans (1995)*). ρ_d is the dry bulk density (kg m^{-3}) and $[Al + Fe]$ is the aluminium+iron content (mmol kg^{-1}).

Sorption class	k_{ads} (d^{-1})	K_F (kg m_s^{-3}) (kg m_w^{-3}) $^{-N}$	N (-)
1	1.1755	$11.87 \cdot 10^{-6} \rho_d [Al + Fe]$	0.5357
2	0.0334	$4.667 \cdot 10^{-6} \rho_d [Al + Fe]$	0.1995
3	0.0014382	$9.711 \cdot 10^{-6} \rho_d [Al + Fe]$	0.2604

Numerical elaboration of the rate dependent sorption equation requires an expression for the differential quotient. This expression can be obtained by taking the value of the time averaged concentration instead of the concentration $c_P(t)$ at time $t = t$. Integration of the differential equation between limits t_0 and $t_0 + \Delta t$ and dividing by the time increment Δt yields:

$$\frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} \frac{dX_n}{dt} dt = \frac{X_n(t_0 + \Delta t) - X_n(t_0)}{\Delta t} \quad (8.9)$$

where $X_n(t_0)$ is the amount of chemical bounded to non-equilibrium sorption sites at the beginning of the time interval. In order to calculate the phosphate amount $X_{n,P}$ at the end of the time interval, the function which describes the exchange between solution and time dependent sorption phase $f_s(c)$ is linearized. The function $f_s(c)$ is approximated by $f_s(\bar{c}_P)$ where \bar{c}_P is the average concentration during the time-interval.

$$\frac{\partial X_n}{\partial t} = k_{ads,des} (f_s(\bar{c}_P) - X_n) \quad (8.10)$$

Although the average concentration is unknown at the start of the computations, \bar{c}_P can be considered as a constant. The following solution can be derived subject to the condition $X_{n,P} = X_{n,P}(t_0)$ at the beginning of the time interval.

$$X_n(t_0 + \Delta t) = f_s(\bar{c}_P) + (X_n(t_0) - f_s(\bar{c}_P))e^{-k_{ads,des}\Delta t} \quad (8.11)$$

In order to obtain an expression for Eq. 8.9, Eq. 8.11 can be rewritten as:

$$\frac{X_n(t_0 + \Delta t) - X_n(t_0)}{\Delta t} = (f_s(\bar{c}_P) - X_n(t_0)) \frac{(1 - e^{-k_{ads,des}\Delta t})}{\Delta t} \quad (8.12)$$

For concentration ranges below the equilibrium level of phosphate precipitation processes, the following *conservation transport equation* holds for soil compartment i :

$$\begin{aligned} \frac{d\theta(t)c_{P,i}(t)}{dt} + \rho_d \bar{K}_a(c_{P,i}) \frac{dc_{P,i}(t)}{dt} &= \frac{q_{i-\frac{1}{2}}c_{i-1}}{\Delta z} - \frac{q_{i+\frac{1}{2}}c_{P,i}(t)}{\Delta z} - \frac{\sigma_P q_{ep}}{\Delta z} - k_1 \theta(t) c_{P,i}(t) \\ &+ R_{p,i} + \rho_d \sum_{i=1}^3 \left(X_{n,i}(t_0) - K_{F,i} \bar{c}_{P,i}^{N_i} \right) \frac{(1 - e^{-k_{ads,des}\Delta t})}{\Delta t} \end{aligned} \quad (8.13)$$

8.3 Chemical precipitation

Phosphate precipitation is modeled as an instantaneous reaction. The reaction occurs immediately and complete when the solute concentration exceeds the equilibrium concentration c_{eq} . The precipitated minerals dissolve immediately when the

concentration of the water phase drops below the buffer concentration. For most of the Dutch sandy soils, the parametrization of the model has been restricted to the instantaneous precipitation formulation. For establishing the equilibrium concentration it is assumed that c_{eq} is a function of pH .

For establishing the equilibrium concentration, the following relation between pH and c_{eq} has been formulated:

$$c_{eq} = 0.135 \cdot 3^{5-pH} \approx 10^{-0.447pH+1.516} \quad (8.14)$$

It should be noted that the parameters describing the diffusion/precipitation reaction ($k_{ads,i}$, $K_{F,i}$ and N_i) are also dependent on pH . The parameter assessment was done by statistical interpretation of laboratory experiments where a certain pH was maintained. Processing the laboratory results performed at other sub-optimal pH -levels should have resulted to slightly other $k_{ads,i}$, $K_{F,i}$ and N_i -values. For this reason, the pH -dependency of c_{eq} has been disabled in recent studies using ANIMO in the STONE framework (Schoumans *et al.*, 2002, 2004a) for national studies. The c_{eq} variable was fixed at a level that corresponds to the pH maintained in the laboratory experiments for phosphate diffusion/precipitation parameter assessment.

While applying the model in combination with the instantaneous precipitation reaction, four situations with respect to the concentration course with time within a time increment are relevant to consider:

1	$t_0 \leq \text{time} \leq t_0 + \Delta t$	$c_P < c_{eq}$	$X_{p,P} = 0$	$\frac{\partial X_{p,P}}{\partial t} = 0$
2	$t_0 \leq \text{time} \leq \tau$	$c_P < c_{eq}$	$X_{p,P} = 0$	$\frac{\partial X_{p,P}}{\partial t} = 0$
	$\tau \leq \text{time} \leq t_0 + \Delta t$	$c_P = c_{eq}$	$X_{p,P} \geq 0$	$\frac{\partial c_P}{\partial t} = 0$
3	$t_0 \leq \text{time} \leq \tau$	$c_P = c_{eq}$	$X_{p,P} > 0$	$\frac{\partial c_P}{\partial t} = 0$
	$\tau \leq \text{time} \leq t_0 + \Delta t$	$c_P \leq c_{eq}$	$X_{p,P} \geq 0$	$\frac{\partial X_{p,P}}{\partial t} = 0$
4	$t_0 \leq \text{time} \leq t_0 + \Delta t$	$c_P = c_{eq}$	$X_{p,P} > 0$	$\frac{\partial c_P}{\partial t} = 0$

The four possibilities to consider are explained in Fig. 8.2. In the 2th and 3th situation the time interval has to be split up into two parts. The length of the first part τ is calculated from its specific conditions combined with the conservation equation.

Under the presence of precipitated phosphate, the concentration $c_P(t)$ as well as the average concentration \bar{c}_P equals the equilibrium concentration c_{eq} ($\frac{\partial c_P}{\partial t} = 0$). Then, the *conservation and transport equation* for soil compartment i reads as follows:

$$\begin{aligned} \rho_d \frac{dX_p}{dt} &= \frac{q_{i-\frac{1}{2}} c_{i-1}}{\Delta z} - \frac{q_{i+\frac{1}{2}}}{\Delta z} c_{P,i}(t) - \frac{\sigma_P q_{ep}}{\Delta z} - k_1 \theta(t) c_{P,i}(t) \\ &+ R_{p,i} + \rho_d \sum_{i=1}^3 \left(X_{n,i}(t_0) - K_{F,i} \bar{c}_{P,i} \right) \frac{(1 - e^{-k_{ads,des} \Delta t})}{\Delta t} \end{aligned} \quad (8.15)$$

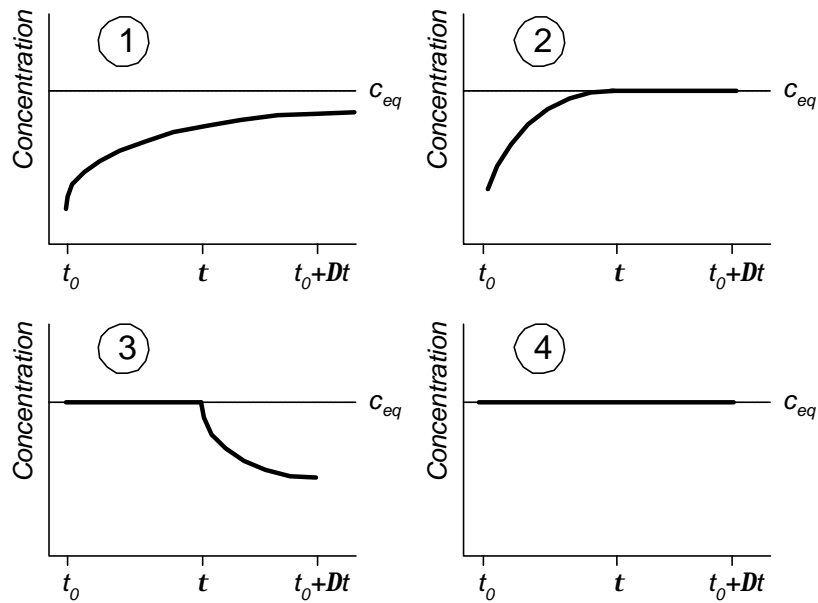


Figure 8.2: Four possibilities of the concentration course with time within a timestep Δt establishing an eventual exceeding of the equilibrium concentration c_{eq}

8.4 Soil P status

To compare the simulated adsorbed P contents with readily available agronomic soil test, Pw values ($\text{mg } P_2O_5 l^{-1}$) can be calculated using the following expression (Schoumans *et al.*, 1997; Schoumans and Groenendijk, 2000):

$$Pw = 2.4163 \cdot 10^3 \cdot \left(\frac{y\sqrt{D} pe^{yt\sqrt{D}} + 1}{2k_a pe^{yt\sqrt{D}} - 1} - \frac{y}{2} (Q_m - Q_0) - \frac{k_d}{2k_a} \right) \quad (8.16)$$

where:

2.4163	: stoichiometric conversion factor between P_2O_5 and P	(mmol mmol^{-1})
10^3	: unit conversion	(mmol mol^{-1})
y	: $\frac{\rho_d V_{soil}}{10^3 V_{H_2O}}$	
V_{soil}	: incubated volume of the soil sample	(m^3)
V_{H_2O}	: volume of the extractant	(m^3)
ρ_d	: dry bulk density	(kg m^{-3})
Q_0	: initial adsorbed content	(mmol kg^{-1})
k_a	: adsorption rate constant	$(\text{l mmol}^{-1} \text{d}^{-1})$
k_d	: first order desorption rate constant	(d^{-1})

The constants p and \sqrt{D} are calculated as follows:

$$p = \frac{y k_a (Q_m - Q_0)^2 + (k_d + y\sqrt{D}) (Q_m - Q_0) + 2k_d \frac{Q_T}{36}}{y k_a (Q_m - Q_0)^2 + (k_d - y\sqrt{D}) (Q_m - Q_0) + 2k_d \frac{Q_T}{36}}$$

$$\sqrt{D} = \sqrt{k_a^2 (Q_m - Q_0)^2 + 2k_a \frac{k_d}{y} (Q_m + Q_0) + \left(\frac{k_d}{y}\right)^2} \quad (8.17)$$

where Q_T is the sum of phosphate quantities present in the liquid and the adsorbed phase.

To validate the Pw -relation as function of sorption parameters, Pw -values were predicted as a function of measured adsorbed $P(Q)$ using the data set of [Schoumans et al. \(1991\)](#). The predicted and measured values are in close agreement (Fig. 8.3).

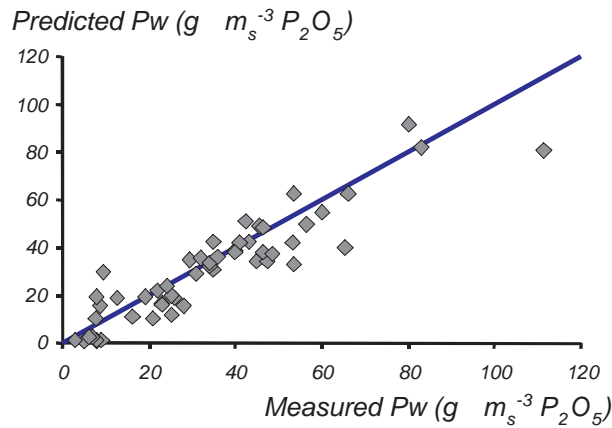


Figure 8.3: Validation of the Pw -relation on a data set of [Schoumans et al. \(1991\)](#)

As a result of this good relationship the water soluble soil P -test is a powerful tool from an environmental point of view, because the soil fertility level can be directly translated to an equilibrium soil P concentration (ortho P) in the tillage layer. Furthermore, the effect of P surplus/deficiency on changes in soil P test values, P concentrations (ortho P) and P content can be predicted for the non calcareous sandy soils which were used in the assessment of model parameters.

9 Rate response functions

Transformation rate coefficients concerning transformation of fresh organic materials, dissolved organic matter, exudates and humus biomass and the nitrification rate coefficient are defined by a reference value k_{ref} . Environmental influences are taken into account by response factors for reduced aeration at wet conditions, drought stress at dry conditions, temperature and pH . Although some other models select the minimum value of the different factors as the final reduction factor [e.g. [Huwe \(1992\)](#)], the ANIMO model applies a multiplication of all the factors to obtain the final reduction. The parameter assessment procedure of decomposition rate constants should take into account for the reduction due to sub-optimal conditions. For transformation processes concerning the decomposition of *Fresh Organic Matter* the actual decomposition rate constant is calculated as:

$$k = f_{ae,OM} f_T f_{\theta} f_{pH} k_{ref} \quad (9.1)$$

for the decomposition of the humus/biomass pool the multiplicative expressions reads:

$$k = f_{ae,OM} f_T f_{\theta} f_{pH} f_Z k_{ref} \quad (9.2)$$

for the nitrification process:

$$k = f_{ae,nit} f_T f_{\theta} f_{pH} k_{ref} \quad (9.3)$$

where:

$f_{ae,OM}$: aeration response factor for organic matter transformations	(-)
$f_{ae,nit}$: aeration response factor for nitrification	(-)
f_T	: temperature response factor	(-)
f_{θ}	: drought stress response factor	(-)
f_{pH}	: acidity response factor	(-)
f_Z	: depth response factor	(-)
k_{ref}	: first order rate constant at a given reference temperature T_{eref}	(d^{-1})

The denitrification the rate constant equals to k_{ref} for cases where the denitrification rate is limited by the nitrate concentration.

9.1 Soil temperature

The temperature response factor (f_T) is described by the Arrhenius equation:

$$f_T = \exp \left[-\frac{\mu}{R_{gas}} \left(\frac{1}{Te + 273} - \frac{1}{T_{eref} + 273} \right) \right] \quad (9.4)$$

where:

μ	: molar activation energy	($J mol^{-1}$)
R_{gas}	: gas constant	($J mol^{-1} K^{-1}$)
T_{eref}	: reference temperature	($^{\circ}C$)
Te	: actual soil temperature at a certain depth	($^{\circ}C$)

The gas constant R_{gas} equals 8.314 ($J mol^{-1}$). In most of the model applications up to the current version 4.0, the molar activation energy was taken 74826 ($J mol^{-1}$) for

all biologically controlled transformations of the organic pools. However the process of *dissolving* solid fresh organic fractions as described in the ANIMO model and the decay of the dissolved organic matter pool could be regarded as a chemically and physically controlled process instead of a biologically controlled transformation. A lower value of the molar activation energy yields a reduced response to soil temperature and is assumed to approach the temperature response of chemically and physically controlled processes (Fig. 9.1). The ANIMO model has the ability to read

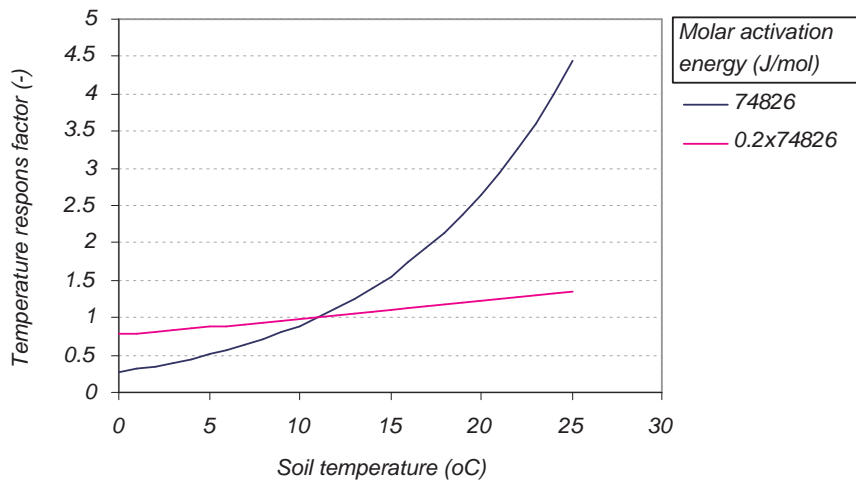


Figure 9.1: Response to soil temperature at $\mu=74826$ and $\mu=0.2 \times 74826$ ($J mol^{-1}$)

soil temperatures per soil compartment and per time step from an input file generated by a supporting hydrological model [e.g. SWAP, (Kroes and van Dam, 2003)]. If no soil temperatures are specified in the input, the model simulate values using a sinus wave sub-model:

$$Te = Te_{av} + Te_{am} \exp\left(-\frac{z}{\sqrt{\frac{2\lambda_h}{\omega C_h}}}\right) \cos\left(\omega t + \phi - \frac{z}{\sqrt{\frac{2\lambda_h}{\omega C_h}}}\right) \quad (9.5)$$

where:

Te_{av}	: average annual temperature at soil surface	(°C)
Te_{am}	: amplitude of the temperature wave	(°C)
ω	: frequency of the temperature wave	($rad d^{-1}$)
ϕ	: phase shift	(-)
λ_h	: heat conductivity	($J m^{-1} d^{-1} °C^{-1}$)
C_h	: differential heat capacity	($J m^{-3} °C^{-1}$)

9.2 Soil moisture

9.2.1 ANIMO3.5 drought stress concept

Drought stress of micro-organisms has been described by the drought response factor f_{θ} . The pF -value has been used to describe the drought response of micro-organisms, based on the analogy of the root activity response to dry conditions. Below wilting point, micro-organisms are assumed to function at a minimum level. Based on experimental data from Ruurlo (Fonck, 1982b,a) and model calibration it has been assumed that within the root zone between the values pF 3.2 and pF 4.2 the response factor f_{θ} decreases linearly from 1.0 to 0.2. The influence of the moisture content is described by:

$$\begin{aligned} pF \leq 3.2 \quad f_{\theta} &= 1 \\ 3.2 < pF < 4.2 \quad f_{\theta} &= 1 - 0.8(pF - 3.2) \\ pF \geq 4.2 \quad f_{\theta} &= 0.2 \end{aligned} \quad (9.6)$$

Below the root zone, no adaptation for dry conditions is considered.

9.2.2 ANIMO3.5 limited aeration concept

Since one of the model aims is to evaluate the environmental impacts of water management for a wide range of soil types and a wide range of hydrological conditions, a detailed sub-model describing oxygen diffusion in the soil gas phase and in soil aggregates has been implemented. In this sub-model the aerated fraction per soil compartment depends on:

- oxygen demand, as a result of organic transformations and nitrification. Oxidation of other reduced components (e.g. sulphur) has been ignored.
- soil physics.
- hydrological conditions (partitioning between soil moisture and soil air).

The aeration factor f_{ae} has been formulated as an multiplicative factor where $f_{ae} = 1$ at optimal conditions. For sub-optimal conditions ($f_{ae} < 1$), the diffusive capacity of the unsaturated zone is insufficient to fulfill the oxygen requirement. In situations where partial anaerobiosis occurs, the oxygen demand for the organic transformations is met by atmospheric oxygen as well as by nitrate-oxygen (Fig. 9.2). The nitrification rate will be sub-optimal. Under these conditions, the available nitrate will be reduced partial or complete (denitrification). Under unfavorable wet conditions the upper compartments consume all oxygen which can enter the soil profile by diffusion and no atmospheric oxygen will penetrate into the lower part of the unsaturated zone. The partitioning between the aerobic soil fraction and the anaerobic soil fraction is determined by the equilibrium between oxygen demand for organic conversion processes plus nitrification and the oxygen supply capacity of the soil air and soil water system. Both the vertical diffusion in air filled pores and the lateral oxygen diffusion in the soil moisture phase have been taken into account. Fig. 9.3 shows the two diffusive transport mechanisms schematically.

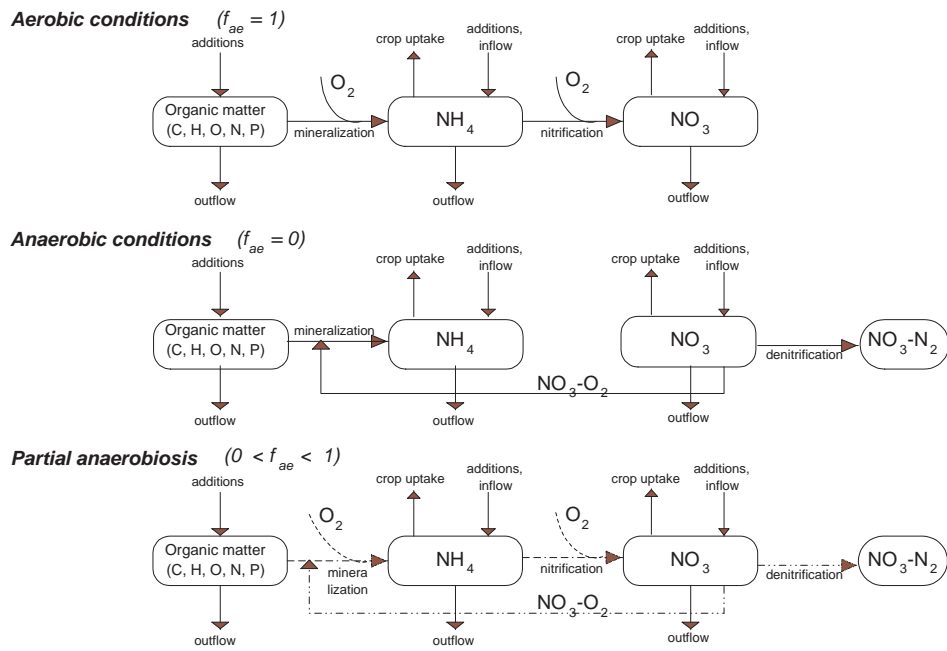


Figure 9.2: Atmospheric oxygen and nitrate oxygen related processes in the ANIMO model

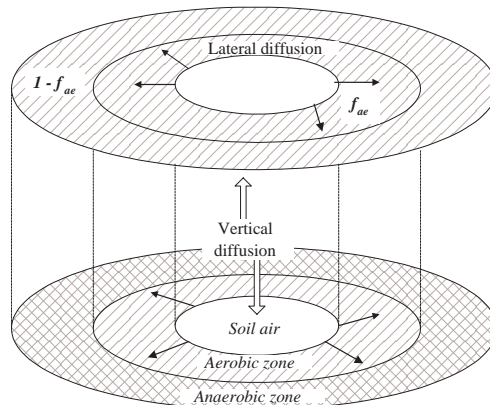


Figure 9.3: Schematic representation of oxygen diffusion transport in the aeration module

Diffusion in soil gas phase

The vertical diffuse transport of oxygen in the air-filled pores in the soil system is described by:

$$\frac{\partial \theta_g c_g}{\partial t} = \frac{\partial}{\partial z} \left(D_g \frac{\partial c_g}{\partial z} \right) - f_{ae} 2.564 \cdot 10^{-3} (T_e + 273) \Omega_{ox} \quad (9.7)$$

where:

c_g	:	oxygen concentration of soil air	$(m^3 O_2 m^3 \text{soilair})$
θ_g	:	soil air fraction	$(-)$
D_g	:	gas diffusion coefficient	$(m^2 d^{-1})$
Ω_{ox}	:	demand for atmospheric oxygen	$(kg m^{-3} d^{-1})$
$2.564 \cdot 10^{-3}(Te + 273)$:	conversion based on the Boyle Gay-Lussac law	$(J m^{-3} ^\circ C^{-1})$

The actual diffusion coefficient D_g is described as a function of soil air fraction and the diffusion coefficient in free air (D_0):

$$\frac{D_g}{D_0} = p_1(\theta_{sat} - \theta)^{p_2} \quad (9.8)$$

In literature different relations between the diffusion coefficient and the volumetric gas content can be found, but the formulation implemented in the ANIMO model has been chosen for reasons of data availability. Bakker *et al.* (1987) provide a review on different formulations and experimental data. Parameters (Bakker *et al.*, 1987) assessed for different soil types are given in Table 9.1. In most regional model appli-

Table 9.1: *Parametrization of the oxygen diffusion coefficient as a function of the volumetric gas content*

Soil type	p_1	p_2
Poor loamy and humusless sands	1.5	3.0
Structureless loamy sands	7.5	4.0
Weakly aggregated topsoils of loamy sands, light clays and humus sands, subsoils of light clays	2.5	3.0
Aggregated light clays	2.0	2.5
Dense clay soils	0.3	1.5

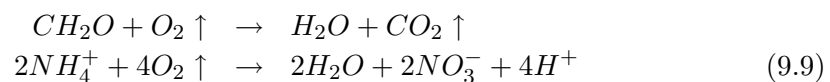
cations, the diffusive properties of soils have been schematized to three classes: good, moderate and bad capabilities for oxygen diffusion (see Table 9.2). Decomposition

Table 9.2: *Parameters p_1 and p_2 for different soil types to be used in regional studies*

Diffusive property	p_1	p_2	Soil unit according to the Staring series [†]
Good	0.3	1.5	B07, B09, B10, B11, B12, B16, B18
Moderate	2.0	2.5	B03, B04, B08, B13, B14, B15, B17
Bad	2.5	3.0	B01, B02, B05, B06

[†] The Staring series comprise the soil physical relations for a selected number of representative Dutch soils. "B" refers to topsoils.

of organic pools as well as nitrification requires oxygen. Stoichiometric factors are based on the assumption that these transformations are governed by:



The oxygen demand which results from nitrification and aerobic decomposition of

organic materials is expressed by Ω_{ox} :

$$\begin{aligned}\Omega_{ox} &= \frac{32}{12}0.58 \sum_{fn=1}^{nf} (1 - a_{fn})f_{hu}k_{fn}OM_{fn}(t) + \frac{32}{12}0.58 (1 - a_{ex})k_{ex}EX(t) \\ &+ \frac{32}{12}0.58 (1 - a_{dom})k_{dom}\theta c_{dom}(t) + \frac{32}{12}0.58 k_{hu}HU(t) \\ &+ \frac{128}{28}k_{nit}\theta c_{NH_4}(t)\end{aligned}\quad (9.10)$$

where:

$OM_{fn}(t)$: fresh organic matter content attributed to fraction fn	$(kg\ m^{-3})$
$EX(t)$: root exudate content	$(kg\ m^{-3})$
$c_{dom}(t)$: concentration dissolved organic matter	$(kg\ m^{-3})$
$HU(t)$: humus/biomass content	$(kg\ m^{-3})$
k_{fn}	: fresh organic matter transformation rate constant	(d^{-1})
k_{ex}	: root exudate transformation rate constant	(d^{-1})
k_{dom}	: dissolved organic matter transformation rate constant	(d^{-1})
k_{hu}	: humus/biomass transformation rate constant	(d^{-1})
k_{nit}	: nitrification rate constant	(d^{-1})
a_{fn}	: assimilation ratio of a specific fresh organic matter pool	(-)
a_{ex}	: assimilation ratio of the root exudates pool	(-)
a_{dom}	: assimilation ratio of the dissolved organic matter pool	(-)
f_{hu}	: partitioning factor of decomposing fresh organic matter	(-)

The oxygen requirement of respiratory processes of living roots has been disregarded. When the defined oxygen requirement can be fully satisfied by supply from the atmosphere, the factor f_{ae} takes the value one. However, when the diffusive process in the partial water filled aggregate pores is not fast enough to create complete aerobic circumstances, part of the soil compartment will be anaerobic. The oxygen consumption of such a compartment will be smaller than Ω_{ox} . Under these circumstances no nitrification will occur. It has been assumed that organic matter transformations proceed slower when only nitrate oxygen is available. Therefore, a factor f_{hetero} has been introduced to account for the reduced process rates.

$$\begin{aligned}\Omega_{ox} &= \frac{32}{12}0.58f_{hetero} \sum_{fn=1}^{nf} (1 - a_{fn})f_{hu}k_{fn}OM_{fn}(t) + \frac{32}{12}0.58f_{hetero} (1 - a_{ex})k_{ex}EX(t) \\ &+ \frac{32}{12}0.58f_{hetero} (1 - a_{dom})k_{dom}\theta c_{dom}(t) + \frac{32}{12}0.58f_{hetero} k_{hu}HU(t)\end{aligned}\quad (9.11)$$

The introduction of the reduction factor f_{ae} enables the calculation of an oxygen profile on the basis of actual oxygen consumption rates. Under field conditions, the oxygen transport in the soil gas phase will be in equilibrium within a few hours. The diffusion coefficient of oxygen in air will take the value $1.64\ (m^2\ d^{-1})$ at $10\ ^\circ C$. Taking p_1 and p_2 as 2.0 and 2.5 and assuming a volumetric gas content of 0.1 (-) yields $0.01\ (m^2\ d^{-1})$ as the value of D_g . When the compartment thickness equals $0.1\ (m)$, the factor $\frac{D_g}{(\Delta z)^2}$ will amount $1\ (d^{-1})$. For longer time increments (e.g. 10 days), equilibrium will be achieved within a fraction of the time step and the diffusion process can be approximated by steady-state diffusion profiles. Such a diffusion equation reads:

$$\frac{d}{dz} \left(D_g \frac{dc_g}{dz} \right) = f_{ae} 2.564 \cdot 10^{-3} (Te + 273) \Omega_{ox}\quad (9.12)$$

The factor f_{ae} is a function of the oxygen concentration in the gas phase, the potential oxygen consumption rate and soil moisture conditions related to the soil type.

The soil system is divided into a number of compartments, each with its own thickness. The diffusion coefficient D_g and the oxygen consumption rates are considered to be constant per time step. Since the factor f_{ae} is dependent on the oxygen concentration, an iterative computation scheme is required to determine its value. In the first iteration round, the factor is set to 1 and oxygen concentrations are calculated using the vertical diffusion model. Then new values of f_{ae} are calculated per compartment using the radial diffusion model. This model uses the calculated oxygen concentrations and the potential oxygen consumption rate as input. After determining f_{ae} -values, a new computation round starts. The iteration procedure will be terminated when the difference between old and new values is less than a certain criterium.

When solving the differential equation for vertical diffusive transport, two boundary conditions can be identified. At the ground surface, the soil air concentration equals the concentration in the free atmosphere. At the groundwater level, a zero-diffusion flux is assumed. If the diffusive capacity is not sufficient to satisfy the oxygen demand, anaerobic conditions in the unsaturated compartments above the groundwater table can occur. In this case, the effective diffusion depth can be calculated from the condition that the concentration and consequently the diffusive flux will take the value zero.

Partial anaerobiosis fraction

The aerated soil fraction f_{ae} is related with the partial anaerobiosis fraction. This fraction is calculated utilizing a sub-model which describes the radial diffusion in soil water around a pore. The general equation for radial diffusion:

$$\frac{\partial \theta_{sat} c_w}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\theta_{sat} D_w}{\lambda_r} \frac{\partial c_w}{\partial r} \right) - \Omega_{ox} \quad (9.13)$$

where:

c_w	: aqueous oxygen concentration	$(kg \ m_w^{-3})$
θ_{sat}	: moisture fraction at saturation	$(m_w^3 \ m_s^{-3})$
D_w	: oxygen diffusion coefficient in water	$(m^2 \ d^{-1})$
λ_r	: tortuosity factor	$(m_w \ m_s^{-1})$
r	: distance from the center of air-filled pores	(m)

A default value 0.3 has been assumed for the tortuosity factor λ_r . Under normal field conditions, $\frac{\theta_{sat} D_w}{\lambda_r}$ takes the value $7.5 \cdot 10^{-6} - 8.0 \cdot 10^{-6} \ (m^2 d^{-1})$. The average radius of an aerated zone around an air-filled pore amounts less than $10^{-4} \ m$, so the factor $\frac{\theta_{sat} D_w}{r^2 \lambda_r}$ will be greater than 10. The oxygen profile around an air filled pore will be at equilibrium within one hour. This allows a steady state approximation of Eq. 9.13:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\theta_{sat} D_w}{\lambda_r} \frac{\partial c_w}{\partial r} \right) = \Omega_{ox} \quad (9.14)$$

This equation is subject to the following boundary conditions (Fig. 9.4):

- The aqueous concentration is in equilibrium with the concentration in air filled pores at the air-water interface ($r = r_{por} \rightarrow c_w = c_{we}$).

- At the outer-side of the aerobic zone, the flux and the concentration equal zero ($r = r_{aer} \rightarrow \frac{\partial c_w}{\partial r} = 0$).

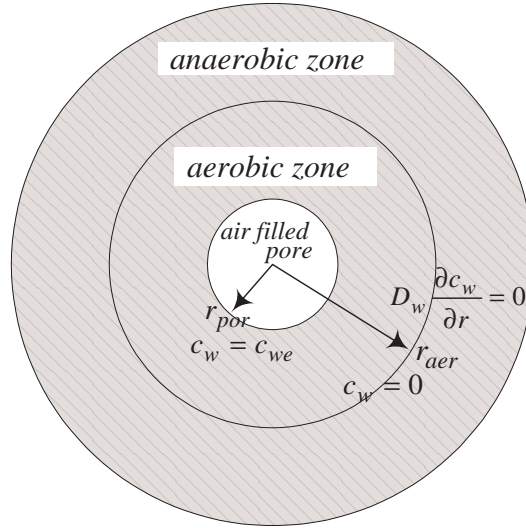


Figure 9.4: Schematization of an aerobic and an anaerobic zone around an air filled pore

The solution to the radial diffusion equation which satisfies the zero flux condition at $r = r_{aer}$ and the concentration condition at $r = r_{por}$, combined with the zero concentration condition at $r = r_{aer}$ yields an expression from which the variable r_{aer} can be derived iteratively:

$$4 \frac{\theta_{sat} D_w}{\lambda_r} \frac{c_{we}}{\Omega_{ox} r_{por}^2} = \left(\frac{r_{aer}}{r_{por}} \right)^2 \ln \left(\frac{r_{aer}}{r_{por}} \right)^2 - \left(\frac{r_{aer}}{r_{por}} \right)^2 + 1 \quad (9.15)$$

Rijtema *et al.* (1999) found an explicit expression for $\frac{r_{aer}}{r_{por}}$ which approaches the relation with high accuracy:

$$\frac{r_{aer}}{r_{por}} = \left(1 - 4 \frac{D_w c_{we}}{\Omega_{ox} r_{por}^2} \right)^{0.391} \quad (9.16)$$

The equilibrium concentration at the air-water interface can be calculated from the oxygen concentration in gas:

$$r = r_{por} \rightarrow c_{we} = \frac{\alpha_B}{2.564 \cdot 10^{-3} (T_e + 273)} c_g \quad (9.17)$$

where α_B is Bunsen's coefficient of solubility ($m^3 m^{-3}$) and the denominator is a factor to convert from volume concentration to mass concentration, as can be derived from Boyle Gay-Lussac's law. Both the diffusion coefficient of oxygen in water and the Bunsen's coefficient depend on temperature. Table 9.3 represents data reported by Gliński and Stepniewski (1985).

Table 9.3: Diffusion coefficient in water and Bunsen's coefficient of oxygen (Gliński and Stepniewski, 1985)

Temperature (°C)	Diffusion coefficient ($m^2 d^{-1}$)	Bunsen's coefficient ($m^3 m^{-3}$)
0	$8.554 \cdot 10^{-5}$	0.0489
5	$1.097 \cdot 10^{-4}$	0.0436
10	$1.331 \cdot 10^{-4}$	0.0394
15	$1.572 \cdot 10^{-4}$	0.0360
20	$1.814 \cdot 10^{-4}$	0.0333
25	$2.056 \cdot 10^{-4}$	0.0309
30	$2.307 \cdot 10^{-4}$	0.0290

The average radius of air filled pores r_{por} follows from the relation between suction and height of capillary rise in thin tubes at static equilibrium. In general:

$$r = \frac{2\eta}{\Delta p} \quad (9.18)$$

where:

$$\begin{aligned} \eta & : \text{ surface tension of water} && (Nm^{-1}) \\ \Delta p & : \text{ pressure difference between soil air and soil water} && (Pa) \end{aligned}$$

If ψ is the suction in cm's water pressure in the soil compartment, the corresponding smallest air-filled pore radius r (m) can be calculated as:

$$r = \frac{0.0015}{\psi} \quad (9.19)$$

When the air entry point of the soil is at suction ψ_a (cm), the corresponding radius of the biggest pore equals r_a (m). The average radius r_{por} of the air-filled pores is assumed to equal the geometrical mean of r_a and r_ψ :

$$r_{por} = \frac{0.0015}{\sqrt{\psi_a \psi}} \quad (9.20)$$

From Eq. 9.16 the aerated radius r_{aer} can be solved. For a soil system containing one pore, the aerated area around the pore A_{ae} per surface unit can be calculated as follows:

$$A_{ae} = \pi (r_{aer}^2 - r_{por}^2) \quad (9.21)$$

If the volume per unit depth of a pore in soil compartment is estimated as $\lambda_v \cdot \pi \cdot r_{por}^2$ and the soil moisture difference between the suctions ψ_a and ψ is $\Delta\theta$, the number of air-filled pores can be approximated as:

$$N_{por} = \frac{\Delta\theta}{\lambda_v \pi r_{por}^2} \quad (9.22)$$

where λ_v is a factor accounting for the tortuosity of the air-filled pores. If all air-filled pores would be regularly distributed, without any interference, the aerated soil fraction would read:

$$f_{ae} = N_{por} A_{ae} = \frac{\Delta\theta}{\lambda_v} \frac{r_{aer}^2 - r_{por}^2}{r_{por}^2} \quad (9.23)$$

In practise, the distribution of the pores is a random one, so that the aerated soil volume will not increase linearly with the number of air-filled pores. Assuming a geometric distribution of air-filled pores, the aerated soil surface per square unit can be expressed as the sum of a geometric sequence with first term A_{ae} and ratio $(1 - A_{ae})$. In other words, when the chance that a new air-filled pore interferes with an already aerated soil part is defined as being proportional to the aerated part, the total aerated soil fraction will be:

$$f_{ae} = A_{ae} + (1 - A_{ae})A_{ae} + (1 - A_{ae})^2 A_{ae} + \dots + (1 - A_{ae})^{N_{por}} A_{ae} = 1 - (1 - A_{ae})^{N_{por}} \quad (9.24)$$

Even at small moisture suctions the number of air filled pores per unit of soil surface will be very large, so the limit rule for large numbers can be applied:

$$f_{ae} = 1 - \lim_{N_{por} \rightarrow \infty} (1 - A_{ae})^{N_{por}} \approx 1 - e^{-A_{ae}N_{por}} \quad (9.25)$$

In anaerobic part of the soil, the oxygen demand for organic matter transformations is met by the utilization of nitrate oxygen (Fig. 9.2). When only nitrate oxygen is available for oxidation of reduced compounds, it has been assumed that the process rate proceeds sub-optimal. To account for the reduced process rates, a factor f_{hetero} has been introduced (see Eq. 9.11). The multiplication factor for the combined availability of atmospheric oxygen and nitrate oxygen on respiratory activities has been formulated as:

$$f_{ae,OM} = f_{ae} + (1 - f_{ae}) \min \left(1, \frac{-\frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} R_{d,den} dt}{R_{p,den}} \right) \quad (9.26)$$

The minimum function at the right hand side of the equation expresses the selection

of the rate limiting process. When $\frac{-\frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} R_{d,den} dt}{R_{p,den}}$ takes a value less than one, the nitrate availability seems to be rate limiting.

9.2.3 SONICG concept

A second more commonly used approach to account for the impact of soil moisture has been implemented in version 4.0 of the ANIMO model. Water Filled Pore Space (*WFPS*) is defined as the ratio between the actual soil moisture content and the content at saturation. The *WFPS*-variable affects all the biological transformation processes:

- Mineralization
- Nitrification
- Denitrification

In the SONICG-model (Bril *et al.*, 1994) only the *Water Filled Pore Space*-variable has been used to describe the moisture response to biological transformation processes. The module NITDEN was developed to simulate the dynamics in conversion and

production rates of ammonium and nitrate in the soil and the gaseous losses of N_2 and N_2O due to denitrification from grassland. The NITDEN-model has been primarily based on the SONICG-model, but some adaptations and refinements were implemented by Conijn (2002). The NITDEN module has been adopted by Heinen and de Willigen (1998, 2001) in the FUSSIM2-model. The moisture response functions in version 4.0 of the ANIMO-option were based on the original SONICG concept

Organic matter transformation

The organic matter module of the SONICG model distinguishes a number of pools. Transformations between pools has been described by first process rate equations where the rate constant is adjusted for temperature and water content. A response function for the influence of soil moisture was derived by Bril *et al.* (1994) from some literature sources.

$$f_{ae,OM} = \frac{6 \left(\frac{\theta}{\theta_{sat}} \right)^2}{1 + 9 \left(\frac{\theta}{\theta_{sat}} \right)^4} \quad (9.27)$$

The drought stress part of the relations between $WFPS=0$ and $WFPS=\frac{1}{\sqrt{3}}$ expresses the increasing biological activity with respect to biodegradation of organic matter with increasing soil moisture content. From $WFPS=\frac{1}{\sqrt{3}}$ onwards the biodegradation is reduced by limited oxygen availability.

Differences in soil air volumes at equal $WFPS$ -values between soil types were not taken into account. The SONICG-concept assumes a $WFPS$ value $\frac{1}{\sqrt{3}}$ for optimal mineralization conditions. At lower values the organic transformations will be reduced due to drought stress. Higher $WFPS$ values imply a reduced aeration and therefore the transformation processes will be limited by unfavorable oxygen supply. The original SONICG relation assumes a relative organic matter decomposition rate of $f_{ae,OM} = \frac{6}{1+9} = 0.6$ at complete saturation ($\frac{\theta}{\theta_{sat}} = 1$). The ANIMO model is used to simulate nitrogen and phosphorus leaching for different types of top soils and sub-soils. Mineralization in saturated peat sub-soils will be obviously less than 60% of the process rate at optimal moisture conditions. The SONICG relation (Bril *et al.*, 1994) has been based on scarce literature data for top soils and does not take account for anaerobic processes in soils at greater depth. An additional relation for the response of organic matter decomposition to moisture contents at near saturation has been implemented to avoid the simulation of unrealistic high mineralization rates. When $\frac{\theta}{\theta_{sat}}$ exceeds a critical value ($WFPS_{crit}$) value, $f_{ae,OM}$ is calculated according to:

$$f_{ae,OM} = \varrho_0 + \varrho_1 WFPS + \varrho_2 WFPS^2 \quad (9.28)$$

The parameters ϱ_0 , ϱ_1 and ϱ_2 are estimated by assuming a smooth function at $WFPS = WFPS_{crit}$ and defining an organic matter decomposition at complete saturation (f_{anae}). The parameters are then found by solving a linear set of three

equations:

$$\begin{aligned}
\frac{\theta}{\theta_{sat}} &= 1 & : \quad \varrho_0 + \varrho_1 + \varrho_2 &= f_{anae} \\
\frac{\theta}{\theta_{sat}} &= WFPS_{crit} & : \quad \varrho_0 + \varrho_1 WFPS_{crit} + \varrho_2 WFPS_{crit}^2 &= \frac{6 WFPS_{crit}^2}{1 + 9 WFPS_{crit}^4} \\
\frac{\theta}{\theta_{sat}} &= WFPS_{crit} & : \quad \varrho_1 + 2\varrho_2 WFPS_{crit} &= \frac{12 WFPS_{crit} (1 - 9 WFPS_{crit}^4)}{(1 + 9 WFPS_{crit}^4)^2} \quad (9.29)
\end{aligned}$$

Nitrification

Nitrification in the NITDEN module is described as a function of soil temperature, pH , the fraction water-filled pore space and the ammonium content of the soil according to:

$$-\frac{d c_{NH_4}}{d t} = f_{ae,nit} f_T f_{pH} f_{CEC} \frac{c_{NH_4}}{k_{nit} + 10^3 \frac{c_{NH_4}^2}{14 \rho_w}} \quad (9.30)$$

where:

c_{NH_4}	: ammonium concentration	$(kg m^{-3})$
f_{CEC}	: CEC dependent parameter	$(-)$
ρ_w	: mass of wet soil	$(kg m^{-3})$
k_{nit}	: value of $\frac{10^3}{14 \rho_w} c_{NH_4}^2$ where the function reaches its maximum	$(kg m^{-3})$

The non-linear dependency of nitrification on the ammonium concentration has not been adopted by the ANIMO model since it requires more parameters and the experimental evidence of the SONICG relation is rather poor. In the SONICG model the dependence on $WFPS$ has the same optimum as organic matter transformation but the rate proceeds to zero at complete saturation:

$$f_{ae,nit} = \max \left[0, \sin \left(\pi \left(\frac{\theta}{\theta_{sat}} \right)^{1.2} \right)^{1.75} \right] \quad (9.31)$$

Regional and national applications of the ANIMO model utilizing this concept resulted to underestimation of nitrification rates and overestimation of ammonium/nitrate ratios in moderately wet and wet soils (de Willigen *et al.*, 2003). It was found that this concept yielded unrealistic low nitrification rates in clay soils and peat soils. The original SONICG concept assumes optimal nitrification rates at 10% soil air fractions or more. For soil air fractions lower than 5% the nitrification rate will be reduced considerably. For identical soil air fractions, different soil types with different soil moisture suction relations have different reduction values (Fig. 9.5).

The SONICG concept has been replaced by a simple functional expression which assumes nitrification rate to be related to the soil air fraction instead of the $WFPS$ (Fig. 9.6). It is assumed that nitrification will not be affected by soil moisture conditions when the soil air fraction exceeds 0.08.

$$f_{ae,nit} = 1 - e^{-100(\theta_{sat}-\theta)} \quad (9.32)$$

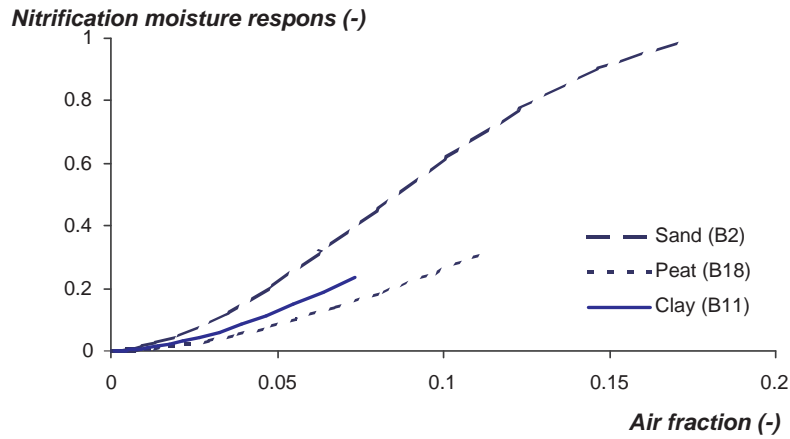


Figure 9.5: Moisture response to nitrification rate (Bril et al., 1994)

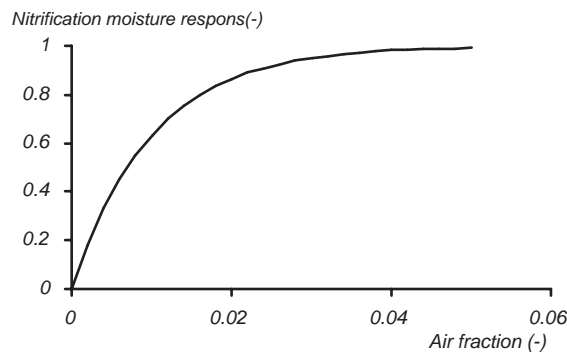


Figure 9.6: New relation for the moisture dependency of the nitrification rate

Denitrification

In the SONICG model it was assumed that the nitrate disappearance rate can be described as a fraction of the organic matter degradation rate:

$$-5 \frac{dc_{NO_3}}{dt} = f_{ae,den} \frac{c_{NO_3}}{k_{den} + c_{NO_3}} 4 \frac{dC}{dt} \quad (9.33)$$

where:

c_{NO_3}	: nitrate concentration	$(kg\ m^{-3})$
$\frac{dC}{dt}$: organic matter conversion rate	$(kg\ m^{-3})$
$f_{ae,den}$: functional relation for the influence of moisture content on the denitrification rate	(-)
k_{den}	: nitrate concentration where the Monod equation results to $\frac{1}{2}$	$(kg\ m^{-3})$

The value of $\frac{dC}{dt}$ is derived from results of ANIMO organic matter simulations. The functional relation for the influence of moisture content on the denitrification rate is related to the decrease of the oxygen supply by gas diffusion and has been formulated as the scaled complementary function relative to the response on organic matter transformations. For $WFPS > \frac{1}{\sqrt{3}}$:

$$f_{ae,den} = \frac{10}{4} \frac{\left(1 - 3 \left(\frac{\theta}{\theta_{sat}}\right)^2\right)^2}{1 + 9 \left(\frac{\theta}{\theta_{sat}}\right)^4} \quad (9.34)$$

Heinen (2003) found a wide range of relations in his investigation of series of models describing the impact of moisture content on denitrification rates. Most of the experimental data hold for the root zone. The original SONICG formulation was only based on a few literature sources and further analysis of simulation results indicated an underestimation of denitrification for dry sandy soils. It was concluded that the $f_{ae,den}$ -curve should start at lower $WFPS$ -values (Fig.9.7).

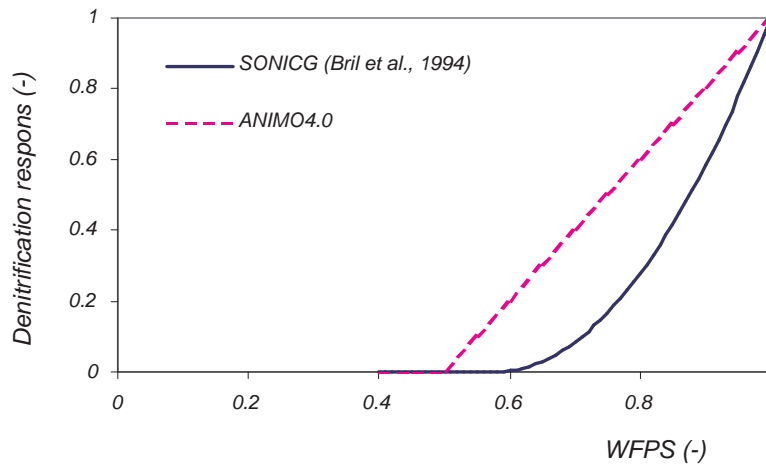


Figure 9.7: Moisture response to denitrification rate

The lower starting point agrees with findings of Conijn (2002) who assumes a small denitrification activity between $0.5 < WFPS < 0.6$. For sandy soils a linear relation is assumed for $f_{ae,den}$ which start at $WFPS=0.5$. The relation assumes higher denitrification rates than Conijn (2002) but is still in the range of parameters given by Heinen and de Willigen (2001).

9.3 Acidity

For the influence of pH on reaction rates only one function for the organic transformation processes and the nitrification process has been implemented. The response factor f_{pH} for acidity is given as:

$$f_{pH} = \frac{1}{1 + e^{-2.5(pH-5)}} \quad (9.35)$$

Time independent pH -values are specified by the user for each soil horizon. It has been assumed that under optimal agricultural practises, the pH -value will not change and the seasonal fluctuation has been ignored.

The relation is based on soil water quality data, so pH -values have to be considered as $pH-H_2O$ values. In most model applications, only $pH-KCl$ values are available from soil information systems. A linear relation has been fitted between $pH-KCl$ and $pH-H_2O$ values which yielded a set of regression coefficients (Table 9.3).

Table 9.4: Transfer functions for assessment of $pH-H_2O$ -values from soil chemical properties

Soil type	Relation	Soil units according to Staring series
Sand	$pH-H_2O=0.7262pH-KCl+2.1160$	B7, B8, B9, B10, B11, B12, B13, B14
Peat	$pH-H_2O=0.8510pH-KCl+1.3842$	B1, B2, B3, B4, B5, B6
Sandy loam	$pH-H_2O=0.7819pH-KCl+1.9772$	B15, B16
Dense clay	$pH-H_2O=0.7623pH-KCl+2.2517$	B17, B18, B19, B20, B21

9.4 Soil depth

In the original ANIMO3.5 model the decomposition rate of humus biomass in the subsoil below the the rootzone, was reduced to a user supplied percentage of the value specified for the rootzone. The corresponding N-fraction was reduced to 20% of the specified N-fraction of humus/biomass. These rules were implemented on the basis of field investigations and calibration with the first version of the ANIMO model (Berghuijs-van Dijk *et al.*, 1985). The reduction caused an acute change of humus/biomass characteristics at the rootzone – subsoil interface. In order to take account for the variability of subsoil characteristics in regional applications the ANIMO4.0 model has been extended by the possibility to impose a $\frac{C}{N}$ -ratio for each soil horizon. The N-weight content is calculated as $f_N^{hu} = \frac{0.58}{\frac{C}{N}-ratio}$. The P-weight content is calculated according to:

$$f_P^{hu} = \left(f_P^{hu}\right)_{rootzone} \frac{f_N^{hu}}{\left(f_N^{hu}\right)_{rootzone}} \quad (9.36)$$

The imposed $\frac{C}{N}$ -ratio does not affect the composition of peat soils, since the peat material is considered as a special organic material (see Par. 10.1). It has been assumed that the decomposition rate of the humus/biomass pool decreases as a function of depth. The user specified value is maintained for the rootzone. For

the compartments deeper than the rootzone the response factor for soil depth is calculated according to:

$$z > Z_r \rightarrow f_z = (1 - f_z^*)e^{-3(z-Z_r)} + f_z^* \quad (9.37)$$

z : soil depth (m)
 Z_r : depth of rootzone (m)
 f_z^* : parameter expressing the dependency of soil depth (-)

Setting the parameter f_z^* to 1 yields the original value and setting f_z^* to 0 results to an infinite small value of f_z at greater depth. In the recent regional applications of the ANIMO model (Schoumans *et al.*, 2002, 2004a) f_z^* was set to 0.5

10 Initial values of state variables

The attribution of initial values to the organic matter pools and the assessment of the initial phosphate content of the soil has a major influence on the final simulation results. Also the ammonium content in the subsoil of soil profiles exposed to upward seepage flow may have an influence on the final calculated load on surface waters. Even the results of long-term scenario studies may be affected by the initial estimates of the organic matter pools and the phosphate state variables. This aspect has long been recognized and therefore a so-called initialization protocol has been designed to overcome some of the difficulties of applying a detailed mechanistic ANIMO model at the regional scale. In most of the national model applications (Kroes *et al.*, 1990; Boers *et al.*, 1997; Overbeek *et al.*, 2001a; Milieu- en Natuurplanbureau, 2002, 2004) a pre-run has been conducted with assumed land use and fertilizations rates between 1941 and 1985 or between 1941 and 2000. The resulting contents of the organic matter pools and phosphate pools is used as an input for further model analysis for the period thereafter. It is assumed that the total contents and subdivision can be approached as a function of historical land use. The results of these historical simulation runs allow verification to measured field data and provide insight in the overall model performance.

10.1 Organic matter pools

10.1.1 Field study

The model requires initial values of soil organic matter contents for each distinguished class of fresh material, the humus/biomass pool, the exudate pool and the dissolved organic matter pool. In general, the exudate and the dissolved organic matter pool are defined as rapidly decomposing substances. Input errors with respect to the initial contents of these pools will not affect the final results of the model simulation to a large extent. The initial estimates of fresh materials and the humus/biomass pool however, can have a great influence on the mineralization.

In most validation studies, the sub-division of initially present fresh organic matter and humus biomass has been based on a rule of thumb resulting from the model calibrations of Berghuijs-van Dijk *et al.* (1985). They derived a fractional division of 90% assigned to humus/biomass and 10% attributed to fresh organic matter within the root zone. In most of the simulations the assignments of organic fractions in the subsoil was based on the assumption of an increasing stability with depth. The upper soil compartment contains more readily decomposable material and the deeper soil compartment shows a decreased average decomposition rate.

10.1.2 Regional application

In regional applications of the model, (e.g. in the context of STONE-applications, (Wolf *et al.*, 2003)) the so-called initialization pre-run has been conducted to describe the initial values of state variables as a function of historical land use and model parameters. Before the start of the pre-run (e.g. 1941), the organic matter content

of each pool is specified for each simulation plot. The total organic matter content in each soil compartment is sub-divided into humus/biomass and a number of fresh organic matter classes. This distribution depends on land use, soil type, depth (root zone or sub-soil). The attribution of relative organic matter contents to the different pools is given in Table 10.1.2 and 10.1.2. For peat soils two types of subsoils (*Eutrophic* and *Mesotrophic*) have been distinguished on the basis of literature data reported by Hendriks (1993). The regional soil schematization of the STONE-model does not comprise *Oligotrophic* peat soils.

Table 10.1: Attribution of total organic matter to different pools for the root zone or 'B'-horizons of peat soils

Land use	Humus / biomass	Fresh Org.Mat. fractions			
		4	5	9	10
Rate constant (a^{-1})	0.008	2.0	0.22	2.0	0.22
N-fraction (-)	var. [†]	0.008	0.008	0.016	0.016
P-fraction (-)	var. [‡]	0.00219	0.00219	0.00198	0.00198
Grassland	90%			5%	5%
Arable land	90%	5%	5%		
Nature	90%				10%

[†]) $\frac{C}{N}$ -ratio specified in from input file. $N\text{-fraction} = \frac{0.58}{\frac{C}{N}\text{-ratio}}$

[‡]) calculated as $P\text{-fraction} = \frac{0.006}{0.048} N\text{-fraction}$

For the subsoils covered by a peat topsoil a criterion is formulated to decide whether the compartment can be characterized as a peaty compartment or not. The compartment will be considered as peaty if one of the following conditions holds:

- Organic matter weight content > 70%
- Organic matter weight content > 35% and lutum weight content < ($\frac{1}{1.167}$ organic matter weight content - 30)%
- Horizon has been characterized as 'O17'

Initially some part of the organic matter in the grassland root zone is attributed to fraction 9 and 10. It should be noted that crop residues as calculated by the QUADMOD model during an initialization pre-run and a scenario-run of the STONE model are assigned to other fractions with higher transformation rate constants

10.2 Phosphate pools

10.2.1 Field study

The model user should use one of three options for the attribution of the initial mineral phosphorus contents. Options:

1. should be selected if the contents of all individual phosphorus pools (liquid concentration, fast sorption, rate dependent sorption) are known from lab-experiments or previous model simulations.

2. should be chosen if total P-contents P_{tot} ($kg\ kg^{-1}$) and the liquid concentrations ($c_P(t_0)$) are known. The content of the equilibrium sorption pool can be estimated from the liquid concentration: ($X_e(t_0) = X_{max} \frac{K_{LCP}(t_0)}{1+K_{LCP}(t_0)}$) and the sum of the slow sorption fractions is the remaining part. These quantities are calculated assuming a hypothetical equilibrium concentration c_{eq}^* . This equilibrium concentration can be calculated by solving the equality:

$$\rho_d \sum_{i=1}^3 K_{F,i}(c_{eq}^*)^{N_i} = \rho_d P_{tot} - \theta_{cP}(t_0) - \rho_d \frac{K_{LCP}(t_0)}{1 + K_{LCP}(t_0)} X_{max} \quad (10.1)$$

The resulting value of c_{eq}^* is used to calculate the initial quantities $X_{n,i}(t_0)$ of the rate dependent sorption pool according to $X_{n,i}(t_0) = K_{F,i}(c_{eq}^*)^{N_i}$

3. should be used when only total P-contents are known. The diffusion-precipitation pool is assumed to be at equilibrium. Both sorption pools can be written as a function of the liquid concentration. For the sum of all pools (P_{tot}) holds:

$$\theta_{cP}(t_0) + \rho_d \frac{K_{LCP}(t_0)}{1 + c_P(t_0)} X_{max} + \rho_d \sum_{i=1}^3 K_{F,i} c_P(t_0)^{N_i} = \rho_d P_{tot} \quad (10.2)$$

The value of $c_P(t_0)$ is obtained iteratively by a Newton-Raphson procedure and then the quantities of the equilibrium pool and the rate dependent sorption pool are calculated straight forward.

10.2.2 Regional application

For model applications within the STONE framework (Wolf *et al.*, 2003) the initial phosphorus contents in 1941 serve as model input to the initialization pre-run. Estimations of soil P-contents are made based on soil map information concerning the aluminium+iron content, the ratio between oxalate extractable phosphorus and the aluminium+iron content and assumed ortho-P concentrations in soil moisture. The total P-content ($kg\ m^{-3}$) is approximated as:

$$P_{tot} = 31 \cdot 10^{-6} \frac{P_{ox}}{[Al] + [Fe]} ([Al] + [Fe]) \rho_d 10^3 \quad (10.3)$$

where 31 is the atomic weight of P ($g\ mol^{-1}$), 10^{-6} is a unit conversion from (mg) to (kg), $\frac{P_{ox}}{[Al]+[Fe]}$ is the ratio between oxalate extractable phosphorus and aluminium and iron, ($[Al] + [Fe]$) is the aluminium and iron content ($mmol\ kg^{-1}$) as can be derived from the Dutch soil information system, ρ_d is the dry bulk density ($kg\ l^{-1}$) and 10^3 converts from (m^3) to (l). The initial $\frac{P_{ox}}{[Al]+[Fe]}$ -ratios for 1941 have been estimated by (Schoumans, pers. comm.) assuming that with respect to the mineral P contents of soils in nature areas no major change took place during the last 50 years.

Table 10.3: Initial values of $\frac{P_{ox}}{[Al]+[Fe]}$ for the initialization pre-run of STONE model applications, (Schoumans, pers. comm.)

Depth	Sand	Clay	Peat	Löss
0–10 cm	0.021	0.05	0.04	0.06
10–30 cm	0.021	0.04	0.02	0.04
30–60 cm	0.02	0.02	0.02	0.03
60–100 cm	0.016	0.03	0.02	0.03
> 100 cm	0.016	0.03	0.02	0.03

Three zones are distinguished to determine the initial distribution of the phosphate pools:

1. For the root zone of soils used for agricultural crop production it is assumed that the adsorption pool and the diffusion/precipitation are in equilibrium with a liquid concentration required for unconstrained production ($0.2\text{--}0.4\text{ mg l}^{-1}$). The user should specify this concentration in the model input. For the root zone of nature areas it is assumed that P_{tot} results from Eq. 10.3 and Table 10.2.2 and that the sub-division is determined by Eq. 10.2. When the resulting ortho-P concentration is lower than a defined minimum level, the ortho-P concentration is set to this minimum value (c_P^{min}) and the contents of the adsorption pool and the diffusion/precipitation are recalculated.
2. The compartments between the root zone and the *seepage surface* (see Par.3.4 and Fig.3.7) are treated analogously to the root zone of nature areas.
3. For the compartments deeper than the *seepage surface* it is assumed that the adsorption pool and the diffusion/precipitation are in equilibrium with the seepage concentration as defined in the model input (Par. 3.4). If the depth of the *seepage surface* is less than 1.0 m, option 3 is omitted and if the depth is even less than the thickness of the root zone option 2 is omitted also.

For recent applications of the STONE model (Overbeek *et al.*, 2001a; Schoumans *et al.*, 2002; Milieu- en Natuurplanbureau, 2002) c_P^{min} was set to 0.05 mg l^{-1} for nearly all soil types. Only for marine clay soil a higher value was specified: 0.15 mg l^{-1} . In the newest version of the STONE-model the model was adapted slightly. The user can specify a c_P^{min} -value for each plot. For the model applications reported by Schoumans *et al.* (2004a); Milieu- en Natuurplanbureau (2004) the subsoil of the Netherlands with respect to c_P^{min} has been schematized to three classes:

1. Southern and western coastal areas with marine sediments: $c_P^{min}=0.3\text{ mg l}^{-1}$.
2. Other areas with marine sediments, eutrophic peat areas or areas with eutrophic peaty subsoil: $c_P^{min}=0.2\text{ mg l}^{-1}$.
3. All other areas $c_P^{min}=0.05\text{ mg l}^{-1}$.

The initial c_P estimate determines the simulation results for long periods, since the quantity in the adsorption pool and the diffusion/precipitation pool are most of the time more than 1000 larger than the quantity in the aqueous phase and leaching by

groundwater displacement reduces the total phosphate quantity slowly. Better c_P^{min} and c_P^{max} estimates based on field investigations can improve the model performance with respect to the prediction of the P-load on surface waters.

Table 10.2: Attribution of total organic matter to different pools for compartments deeper than the root zone or 'O'-horizons of peat soils

Type of subsoil	Humus / biomass	Fresh Org.Mat. fractions
	11	12 13 14
	Rate constant (a^{-1})	0.001 0.0383 0.001 0.024
	N-fraction (-)	var. 0.043 0.028 0.020 0.019
	P-fraction (-)	var. 0.0001 0.0006 0.0001 0.0006
Non peat topsoil	Org.Mat.<5%	100%
	5%<Org.Mat.<25%	$(1-\beta^\ddagger) \cdot 100\%$ $\beta \cdot 33\%$ $\beta \cdot 67\%$
	Org.Mat.>25%	33% 67%
'O'-horizons of peat topsoils + peaty subsoil	Eutrophic	33% 67%
	Mesotrophic	33% 67%
'O'-horizons of peat topsoils + non-peaty subsoil		100%

†) at bottom of root zone, decreases with depth

‡) where $\beta = \frac{Org.Mat.\% - 5}{25 - 5}$

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List of symbols

$a_1 \cdots a_{nf}$: assimilation ratio of an organic class	(-)
a_{dom}	: assimilation ratio of the dissolved organic matter pool	(-)
a_{ex}	: assimilation ratio of the root exudates pool	(-)
A	: area of a discharging catchment	(m^2)
A_N	: total applied nitrogen dose (QUADMOD)	($kg\ ha^{-1}$)
c	: mass concentration in the liquid phase	($kg\ m_w^{-3}$)
c_1	: time averaged solute concentration in soil compartment 1	($kg\ m^{-3}$)
c^*	: mass concentration	($kg\ m_s^{-3}$)
$c_{dom}(t)$: concentration dissolved organic matter	($kg\ m^{-3}$)
$c_{dom}(t + \tau)$: concentration dissolved organic matter after addition	($kg\ m^{-3}$)
$c_{dom}(t)$: concentration dissolved organic matter before fertilization	($kg\ m^{-3}$)
$c_{doN}(t)$: concentration dissolved organic nitrogen	($kg\ m^{-3}$)
$c_{doP}(t)$: concentration dissolved organic phosphorus	($kg\ m^{-3}$)
c_{eq}	: equilibrium concentration for chemical P precipitation	($kg\ m^{-3}$)
c_g	: oxygen concentration of soil air	($m^3 O_2\ m^3\ soil\ air$)
c_{i-1}	: concentration in an adjacent upstream soil compartment	($kg\ m^{-3}$)
$c_{opt,1}; c_{opt,2}$: optimal N or P concentrations in plant evaporation flow during resp. 1 st and 2 nd growing stage	($kg\ m^{-3}$)
c_{pl}	: nitrate concentration in grass shoot liquids	($kg\ m^{-3}$)
c_{po}	: time averaged concentration of ponded water	($kg\ m^{-3}$)
c_{pr}	: weighted concentration of hydrological entry routes	($kg\ m^{-3}$)
c_w	: aqueous oxygen concentration	($kg\ m_w^{-3}$)
c_{NH_4}	: ammonium concentration	($kg\ m^{-3}$)
c_{NO_3}	: nitrate concentration	($kg\ m^{-3}$)
c_P^{min}	: minimum value of P-concentration in subsoil initialization	($kg\ m^{-3}$)
$\bar{c}_{NH_4,i}$: time averaged ammonium concentration in compartment i	($kg\ m^{-3}$)
$\bar{c}_{NO_3,i}$: time averaged nitrate concentration in compartment i	($kg\ m^{-3}$)
C_h	: differential heat capacity	($J\ m^{-3}\ ^\circ C^{-1}$)
CEC	: Cation Exchange Capacity	($meq\ (100gr)^{-1}$)
D_g	: gas diffusion coefficient	($m^2\ d^{-1}$)
D_n	: mathematical dispersion coefficient	($m^2\ d^{-1}$)
D_w	: oxygen diffusion coefficient in water	($m^2\ d^{-1}$)
$EX(t)$: root exudate content	($kg\ m^{-3}$)

f_1	: fraction of surface runoff to which the concentration of soil compartment 1 is assigned	(-)
$f_1^N \dots f_{nf}^N$: nitrogen weight fraction of an organic class	($kg\ kg^{-1}$)
$f_1^P \dots f_{nf}^P$: phosphorus weight fraction of an organic class	($kg\ kg^{-1}$)
$f_{ae,den}$: factor for moisture response on the denitrification rate	(-)
$f_{ae,OM}$: aeration response factor for organic matter transformations	(-)
$f_{ae,nit}$: factor for moisture response on the nitrification rate	(-)
f_{cl}	: cloudiness factor	(-)
f_{CEC}	: CEC response factor in the SONICG model	(-)
f_{ds}	: dry matter fraction of fresh biomass	(-)
f_{def}	: recoverable uptake deficit factor	(-)
$f_{gr,loss}$: fraction of grass shoots lost by grazing	(-)
$f_{ha,loss}$: fraction of grass shoots lost by harvesting	(-)
f_{hu}	: partitioning factor of decomposing fresh organic matter	(-)
$f_{i,fn}$: fraction of the fn^{th} class as a part of material applied	(-)
$f_{i,fn}$: fraction of the fn^{th} class as a part of the i^{th} material	(-)
$f_{i,fn}^L$: liquid fraction of the fn^{th} class as a part of material applied	(-)
f_i^O	: organic fraction of the applied material	(-)
f_{Ne}	: factor expressing the contribution of N_e to N_{dose}	(-)
f^{NH_4N}	: ammonium-N content of a material	($kg\ kg^{-1}$)
f^{NO_3N}	: nitrate-N content of a material	($kg\ kg^{-1}$)
f_{NP}	: reduction factor for nutrient limitation	(-)
f_{N}^{flux}	: factor used to express the potential for luxurious N uptake	(-)
f^{PO_4P}	: phosphate-P content of a material	($kg\ kg^{-1}$)
f_P^{flux}	: factor used to express the potential for luxurious P uptake	(-)
f_{po}	: fraction of surface runoff to which the concentration in the ponding layer is assigned	(-)
f_{sh}	: shoot fraction	(-)
f_N^{ex}	: nitrogen weight fraction of exudates	(-)
f_N^{hu}	: nitrogen weight fraction of humus/biomass	(-)
$f_{N,r}$: nitrogen weight content of grass root dry matter	(-)
$f_{N,r}^{min}$: minimum nitrogen weight fraction in grass roots	(-)
$f_{N,r}^{max}$: maximum nitrogen weight fraction in grass roots	(-)
$f_{N,s}$: nitrogen weight content of grass shoot dry matter	(-)
$f_{N,s}^{min}$: minimum nitrogen weight fraction in grass shoots	(-)
$f_{N,s}^{max}$: maximum nitrogen weight fraction in grass shoots	(-)
f_{NP}	: nutrient limited reduction factor for grass biomass production	(-)
f_P^{ex}	: phosphorus weight fraction of exudates	(-)
f_P^{hu}	: phosphorus weight fraction of humus/biomass	(-)
$f_{P,r}^{min}$: minimum phosphorus weight fraction in grass roots	(-)
$f_{P,s}^{min}$: minimum phosphorus weight fraction in grass shoots	(-)
$f_{P,r}^{max}$: maximum phosphorus weight fraction in grass roots	(-)
$f_{P,s}^{max}$: maximum phosphorus weight fraction in grass shoots	(-)
$f_{pl,N_{tot}}$: total nitrogen fraction of shoots	(-)
f_{pl,NO_3}	: nitrate-nitrogen fraction of shoots	(-)
$f_s(cP)$: non-equilibrium sorption pool content in the equilibrium state as a function of the concentration	($kg\ kg^{-1}$)
f_z	: factor for humus/biomass decomposition response to depth	(-)
f_z^*	: parameter expressing the dependency of soil depth	(-)
f_{rN}	: nitrogen fraction of arable crop dry matter biomass	(-)
f_{rP}	: phosphorus fraction of arable crop dry matter biomass	(-)
h_{pond}	: ponding height	(m)
H	: aquifer thickness	(m)
H_i	: thickness of discharge layer i	(m)
$HU(t)$: humus/biomass content	($kg\ m^{-3}$)
J_s	: vertical solute flux	($kg\ m^{-2}\ d^{-1}$)
$J_{s,r}$: surface runoff transport to surface waters	($kg\ m^{-2}\ d^{-1}$)

$k_1 \cdots k_{n,f}$: first order decomposition rate constant of an organic class	(a^{-1})
k_{ads}	: phosphate adsorption rate constant	(d^{-1})
k_{des}	: phosphate desorption rate constant	(d^{-1})
$k_{ads,des}$: adsorption or desorption rate constant; the value depends on	
	: ratio between $f_s(c_P)$ and $X_{n,P}$	(d^{-1})
k_a	: adsorption rate constant (<i>Pw-relation</i>)	$(l\ mmol^{-1}\ d^{-1})$
k_d	: desorption rate constant (<i>Pw-relation</i>)	(d^{-1})
k_{ref}	: optimal value of first order rate constant	(d^{-1})
k_{ex}	: root exudate transformation rate constant	(d^{-1})
k_{dom}	: dissolved organic matter transformation rate constant	(d^{-1})
k_{hu}	: humus/biomass transformation rate constant	(d^{-1})
k_{nit}	: nitrification rate constant	(d^{-1})
k_{nit}^*	: value of $\frac{10^3}{14 \rho_w} c_{NH_4}^2$ where	
	the function reaches its maximum	$(kg\ m^{-3})$
k_{den}	: nitrate concentration where the <i>Monod</i> equation	
	results to $\frac{1}{2}$	$(kg\ m^{-3})$
$k_{gr,decease}$: first order rate constant for living grass root turn-over	(a^{-1})
$k_{gr,dif}$: rate constant for diffusive nitrate transport to grass roots	(d^{-1})
$k_{0,NO_3,i}$: zero-order production of nitrate in soil compartment i	$(kg\ m^{-3}\ d^{-1})$
$k_{0,NO_3,i}^*$: zero-order production of nitrate in soil compartment i	
	including a term for backward diffusive nitrate uptake	$(kg\ m^{-3}\ d^{-1})$
K_F	: Freundlich adsorption constant	$(kg\ m_s^{-3}) (kg\ m_w^{-3})^{-N}$
$K_d(c)$: differential sorption coefficient	$(m^3\ kg^{-1})$
K_{e,NH_4}	: linear adsorption coefficient of ammonium	$(m^3\ kg^{-1})$
K_e^{app}	: phosphate apparent linear sorption coefficient	$(m^3\ kg^{-1})$
K_L	: adsorption constant	$(m^3\ kg^{-1})$
$K_a(c_P)$: differential sorption coefficient	$(m^3\ kg^{-1})$
$\overline{K}_a(c_P)$: concentration averaged sorption coefficient	$(m^3\ kg^{-1})$
L	: distance between drains	(m)
M_r	: fertilizer released from surface reservoir	$(kg\ m^{-2})$
M	: fertilizer added to surface reservoir	$(kg\ m^{-2})$
M_i	: areic mass of applied material	$(kg\ m^{-2})$
n_{dr}	: number of drainage systems considered	$(-)$
N_e	: readily available organic N in manure and slurry	$(kg\ ha^{-1})$
$N_{fertilizer}$: annual fertilizer N dose	$(kg\ ha^{-1})$
N_F	: Freundlich adsorption exponent	$(-)$
N_{isu}	: number of grazing live stock units areal unit	$(-)$
N_{min}^{om}	: annual N dose by manure and slurry	$(kg\ ha^{-1})$
N_{org}	: annual addition of manure organic nitrogen	$(kg\ ha^{-1})$
N_r	: number of soil compartments with water extraction for	
	plant evaporation	$(-)$
$NH_3 \uparrow$: ammonia volatilization	$(kg\ ha^{-1})$
n_f	: number of organic matter classes	$(-)$
nm	: number of materials	$(-)$
$Nwdose$: effective nitrogen dosage	$(kg\ ha^{-1})$
$NetNSoil$: soil nitrogen supply	$(kg\ ha^{-1})$
$OM(t)$: total quantity organic material present at time t	$(kg\ m^{-3})$
$OM(t_0)$: total quantity organic material present at time t_0	$(kg\ m^{-3})$
$OM_{fn}(t)$: quantity organic material attributed to the fn^{th} class	$(kg\ m^{-3})$
$OM_{fn}(t + \tau)$: volumic mass of organic matter class fn after addition	$(kg\ m^{-3})$
$OM_{fn}(t)$: volumic mass of organic matter class fn before addition	$(kg\ m^{-3})$
$OM_{fn}(t)$: fresh organic matter content attributed to fraction fn	$(kg\ m^{-3})$
$P_{st}(t)$: gross photosynthesis under standard conditions	$(kg\ m^{-2})$
P_w	: water extractable phosphorus content	$(mg\ l^{-1}\ P_2O_5)$

$q_{d,i}$: flux density of water flowing to drainage system i	$(m d^{-1})$
$q_{d,i,k}$: flux density at node k of water flowing to drainage system i	$(m d^{-1})$
q_{eow}	: evaporation from ponded water layer	$(m d^{-1})$
q_{ep}	: plant evaporation	$(m d^{-1})$
$q_{ep,i}$: plant evaporation flux of compartment i	$(m d^{-1})$
q_{ep}^{pot}	: potential plant evaporation	$(m d^{-1})$
q_{es}	: soil evaporation	$(m d^{-1})$
q_{inu}	: inundation from adjacent watercourses	$(m d^{-1})$
q_{irr}	: irrigation	$(m d^{-1})$
q_{me}	: snow melt	$(m d^{-1})$
q_{per}	: percolation at lower boundary	$(m d^{-1})$
q_p^n	: net precipitation	$(m d^{-1})$
q_{ro}	: run-on from adjacent fields	$(m d^{-1})$
q_{ru}	: areal surface runoff water flux	$(m d^{-1})$
q_s	: upward seepage at lower boundary	$(m d^{-1})$
q_y	: vertical flux at a point of a two-dimensional cross-section	$(m d^{-1})$
$\bar{q}_y(y)$: vertical flux averaged over the span of a cross-section	$(m d^{-1})$
$q_{i-\frac{1}{2}}$: water flux entering in compartment i from an adjacent upstream compartment	$(m d^{-1})$
$q_{i+\frac{1}{2}}$: water flux leaving from compartment i to an adjacent downstream compartment	$(m d^{-1})$
Q_d	: total discharge of a cross section between $x = 0$ and $x = \frac{L}{2}$	$(m^2 d^{-1})$
$Q_{d,i}$: discharge rate of water flowing to drainage system i	$(m^2 d^{-1})$
Q_0	: initial adsorbed content (<i>Pw-relation</i>)	$(mmol kg^{-1})$
$Q_s(t)$: shoot dry matter amount as a function of time	$(kg m^{-2})$
$Q_s(t)$: biomass present in grass shoot system	$(kg m^{-2})$
$Q_{s,ref}$: reference value Q_s related to κ	$(kg m^{-2})$
Q_T	: total phosphate quantity present in aqueous and solid phase (<i>Pw-relation</i>)	$(mmol kg^{-1})$
r	: distance from the center of air-filled pores	(m)
R	: recharge of an aquifer	$(m d^{-1})$
R_d	: decomposition sink term	$(kg m^{-3} d^{-1})$
$R_{d,den}$: denitrification rate calculated as a first order rate process	$(kg m^{-3} d^{-1})$
$R_{d,DOM}$: decomposition rate of the dissolved organic matter pool	$(kg m^{-3} d^{-1})$
$R_{d,EX}$: decomposition rate of the root exudate pool	$(kg m^{-3} d^{-1})$
$R_{d,HU}$: decomposition rate of humus/biomass	$(kg m^{-3} d^{-1})$
R_{d,NH_4}	: transformation rate of ammonium (nitrification)	$(kg m^{-3} d^{-1})$
$R_{d,OM \rightarrow HU}$: transformation rate of fresh organic matter to the humus/biomass pool	$(kg m^{-3} d^{-1})$
$R_{d,OM \rightarrow DOM}$: transformation rate of fresh organic matter to the dissolved organic matter pool	$(kg m^{-3} d^{-1})$
R_{dr}	: drainage sink term	(d^{-1})
R_{gas}	: gas constant	$(J mol^{-1} K^{-1})$
R_p	: production source term	$(kg m^{-3} d^{-1})$
$R_{p,den}$: denitrification rate calculated as a zero-order sink-term	$(kg m^{-3} d^{-1})$
$R_{p,DOM}$: production rate of the dissolved organic matter pool	$(kg m^{-3} d^{-1})$
$R_{p,EX}$: production rate of the root exudate pool	$(kg m^{-3} d^{-1})$
$R_{p,OM \rightarrow HU}$: formation rate of humus/biomass from fresh organic matter	$(kg m^{-3} d^{-1})$
$R_{p,DOM \rightarrow HU}$: formation rate of humus/biomass from dissolved organic matter	$(kg m^{-3} d^{-1})$
$R_{p,EX \rightarrow HU}$: formation rate of humus/biomass from exudates	$(kg m^{-3} d^{-1})$
R_{p,NH_4}	: production rate of ammonium (mineralization)	$(kg m^{-3} d^{-1})$
R_{p,NO_3}	: production rate of nitrate (nitrification)	$(kg m^{-3} d^{-1})$
R_{p,PO_4}	: P-mineralization rate	$(kg m^{-3} d^{-1})$
R_u	: plant uptake sink term	$(kg m^{-3} d^{-1})$
$R_{u,c}$: nitrate uptake rate by convective transport	$(kg m^{-3} d^{-1})$
$R_{u,d}$: nitrate uptake rate by diffusive transport	$(kg m^{-3} d^{-1})$
R_{u,NO_3}	: nitrate uptake rate by grass roots	$(kg m^{-3} d^{-1})$
R_{u,NH_4}	: ammonium uptake rate by grass roots	$(kg m^{-3} d^{-1})$

$R_{t_0+\Delta t}$: arable crop root biomass quantity at end of time step	$(kg\ m^{-2})$
R_{t_0}	: arable crop root biomass quantity at start of time step	$(kg\ m^{-2})$
R_x	: drainage sink term in <i>conservation and transport equation</i>	$(kg\ m^{-3}\ d^{-1})$
S	: N uptake derived from indigenous soil N (QUADM0D)	$(kg\ ha^{-1})$
t_{res}	: residence time of soil moisture	(d)
t_p	: planting date	$(-)$
t_c	: date of transition between 1 st and 2 nd growing period	$(-)$
t_h	: harvesting date	$(-)$
T	: transmissivity	$(m^2\ d^{-1})$
Te	: actual soil temperature	$(^{\circ}C)$
Te_{ref}	: reference temperature	$(^{\circ}C)$
Te_{av}	: average annual temperature at soil surface	$(^{\circ}C)$
Te_{am}	: amplitude of annual temperature wave	$(^{\circ}C)$
$U(t)$: amount of nitrogen present in grass shoot system	$(kg\ m^{-2})$
$U_1^*; U_2^*$: long term averaged cumulative uptake during resp. 1 st and 2 nd growing stage	$(kg\ m^{-2})$
U_N	: total seasonal nitrogen yield (QUADM0D)	$(kg\ ha^{-1})$
V_i	: groundwater volume occupied by discharge to system i	(m^2)
V_{soil}	: incubated volume of the soil sample	(m^3)
V_{H_2O}	: volume of the extractant	(m^3)
W	: grass intake rate by grazing cattle	$(kg\ m^{-2}\ d^{-1})$
X_e	: content adsorbed to the solid phase in equilibrium with c	$(kg\ kg^{-1})$
$X_{e,P}$: content reversibly adsorbed P	$(kg\ kg^{-1})$
X_{e,NH_4}	: adsorbed ammonium content	$(kg\ kg^{-1})$
$X_{max,P}$: maximum content reversibly adsorbed P	$(kg\ kg^{-1})$
X_n	: content of non-equilibrium sorption phase	$(kg\ kg^{-1})$
$X_{n,P}$: phosphate non-equilibrium sorption pool content	$(kg\ kg^{-1})$
X_p	: content of the substance involved in precipitation reaction	$(kg\ kg^{-1})$
$X_P^{eq.s}$: adsorbed phosphorus content of the equilibrium sorption pool	$(kg\ kg^{-1})$
X_P^{prec}	: adsorbed phosphorus content of the precipitated pool	$(kg\ kg^{-1})$
Y	: crop yield (QUADM0D)	$(kg\ ha^{-1})$
Y_{max}	: maximum crop yield as limited by environmental conditions but under abundant N-availability (QUADM0D)	$(kg\ ha^{-1})$
z	: soil depth	(m)
Z_r	: height of rootzone	(m)
Z_{surf}	: user specified thickness of surface reservoir	(m)
$\frac{dC}{dt}$: organic matter conversion rate	$(kg\ m^{-3})$
$\frac{\Delta V}{\Delta t}$: change of areal water volume per time step	$(m\ d^{-1})$
(x_d, y_d)	: coordinates of the deepest point of a streamline	(m, m)

α_{min}	:	minimum N concentration in crop biomass (QUADMOD)	$(kg\ kg^{-1})$
α_{crit}	:	N concentration in crop biomass at critical point (QUADMOD)	$(kg\ kg^{-1})$
α_{max}	:	maximum N concentration in crop biomass (QUADMOD)	$(kg\ kg^{-1})$
β	:	factor to partition organic matter initially present to humus/biomass and fresh organic matter	$(-)$
γ	:	crop yield at critical point, expressed as a fraction of Y_{max}	$(-)$
η	:	surface tension of water	$(N\ m^{-1})$
$\eta_1 \cdots \eta_3$:	transformed organic matter decomposition parameters	$(-)$
θ	:	volume moisture fraction	$(m^3\ m^{-3})$
θ_g	:	soil air fraction	$(m_w^3\ m_s^{-3})$
θ_{sat}	:	moisture fraction at saturation	$(m_w^3\ m_s^{-3})$
κ	:	coefficient related to light absorption by shoot biomass	$(-)$
λ_h	:	heat conductivity	$(J\ m^{-1}\ d^{-1}\ ^\circ C^{-1})$
λ_r	:	tortuosity factor	$(m_w\ m_s^{-1})$
μ	:	molar activation energy	$(J\ mol^{-1})$
$\mu(h_{pond})$:	ponding storage coefficient as a function of ponding height	$(m\ m^{-1})$
ρ_d	:	dry bulk density	$(kg\ m^{-3})$
ρ_w	:	mass of wet soil	$(kg\ m^{-3})$
ρ_{ini}	:	initial apparent N recovery (QUADMOD)	$(-)$
$\varrho_0 \cdots \varrho_2$:	coefficients of $f_{ae,OM}$ -relation at near saturation	(\cdots)
σ_{NO_3}	:	nitrate transpiration concentration stream factor	$(-)$
σ_{NH_4}	:	ammonium transpiration concentration stream factor	$(-)$
σ_{PO_4}	:	phosphate transpiration concentration stream factor	$(-)$
σ_N^{max}	:	maximum value of nitrogen transp. concentration stream factor	$(-)$
τ	:	infinite small time increment	(d)
τ_a	:	apparent age of the organic material	(a)
ϕ	:	phase shift	$(-)$
χ_o	:	grass biomass growth efficiency factor (optimal conditions)	$(-)$
χ_p	:	grass biomass growth efficiency under practical farm conditions relative to optimal conditions	$(-)$
ω	:	frequency of the temperature wave	$(rad\ d^{-1})$
Δp	:	pressure difference between soil air and soil water	(Pa)
Δz_i	:	thickness of soil compartment i	(m)
Δz	:	thickness of a soil compartment	(m)
Φ_{NH_4}	:	ammonium in soil available for uptake	$(kg\ m^{-2})$
Φ_{NO_3}	:	nitrate in soil available for uptake	$(kg\ m^{-2})$
$\Psi(x, y)$:	streamfunction	$(m^2\ d^{-1})$
Ψ_0	:	streamfunction value for which a streamline is constructed	$(m^2\ d^{-1})$
Ω_N^{def}	:	nitrogen uptake deficit of previous time steps	$(kg\ m^{-2})$
Ω_N^{gr}	:	demand for nitrogen due to biomass growth in current time step	$(kg\ m^{-2})$
Ω_N^{lux}	:	luxurious nitrogen uptake in case of excessive supply conditions	$(kg\ m^{-2})$
Ω_P^{def}	:	phosphorus uptake deficit of previous time steps	$(kg\ m^{-2})$
Ω_P^{gr}	:	demand for phosphorus due to biomass growth in current time step	$(kg\ m^{-2})$
Ω_P^{lux}	:	luxurious phosphorus uptake in case of excessive supply conditions	$(kg\ m^{-2})$
Ω_N^{max}	:	maximum nitrogen uptake requirement of grass	$(kg\ m^{-2})$
Ω_N^{mean}	:	mean nitrogen uptake requirement of grass	$(kg\ m^{-2})$
Ω_{ox}	:	demand for atmospheric oxygen	$(kg\ m^{-3}\ d^{-1})$
$\sum l_i$:	total length of watercourses attributed to drainage system i	(m)
$\sum_{i=1}^{N_r} q_{eq,i}$:	actual plant evaporation in a time step, summed over the soil compartments of the root zone	$(m\ d^{-1})$
$\sum_{k=1}^{n_{dr}} q_{dr,k}$:	flux intensity of water flowing to drainage systems, summed over the number of drainage systems	$(m\ d^{-1})$
$\sum q_p \Delta t$:	cumulative precipitation since an addition event	(m)
$\sum_{t_p}^{t_c} q_{ep}$:	long term averaged plant evaporation during 1 st growing stage	(m)
$\sum_{t_c}^{t_h} q_{ep}$:	long term averaged plant evaporation during 2 nd growing stage	(m)

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