Simulation of nitrogen-limited crop growth with SWAP/WOFOST

Process descriptions and user manual

Piet Groenendijk, Hendrik Boogaard, Marius Heinen, Joop Kroes, Iwan Supit, Allard de Wit

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Wageningen Environmental Research
Wageningen, December 2016

Report 2721
ISSN 1566-7197

Piet Groenendijk, Hendrik Boogaard, Marius Heinen, Joop Kroes, Iwan Supit, Allard de Wit, 2016. *Simulation of nitrogen-limited crop growth with SWAP/WOFOST; Process descriptions and user manual.* Wageningen, Wageningen Environmental Research, Report 2721. 60 pp.; 25 fig.; 8 tab.; 72 ref.

This report describes a soil nitrogen module (Soil-N), which is combined with the agro-hydrological model, SWAP, and the crop growth model, WOFOST. The core of the Soil-N module is a description of the nitrogen cycle, which is coupled to the organic matter cycle based upon the RothC-26.3 model. Nitrogen can be supplied to the soil as different types of fertilizer applications and through mineralisation of organic nitrogen. Ammonium and nitrate balances are calculated including uptake by plant roots, de-nitrification and leaching of nitrate.
Data exchange is on a daily base. The partitioning of nitrogen within crops and the nitrogen contents of crop residues are calculated by WOFOST and passed to the Soil-N module. SWAP generates the data for establishing the water balance of the soil compartment for which the Soil-N perform the simulations. Nitrogen uptake by the crop is calculated as the minimum of the demand by the crop and the availability of nitrogen in the soil. The crop production rate is reduced when the mineral nitrogen stock is limited. Nitrogen-fixation is based on a simple approach. An improved sub-model for phenological stages of soybean was implemented. Increasing atmospheric CO_2 concentrations can be accounted for. The innovated integrated model was tested using data sets from The Netherlands, China and Argentina, for which examples are given. This new model can be used as a tool in studies, in which both water and nitrogen can be limited for crop growth.

Keywords: crop growth, crop uptake, soil nitrogen dynamics, organic matter, mineralisation, leaching, simulation model, SWAP, WOFOST, nitrate.

Wageningen Environmental Research Report 2721 | ISSN 1566-7197

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Preface

This research was (partly) funded by the European Commission’s Research Framework Programme (FP7), within the SIGMA-project (Stimulating Innovation for Global Monitoring of Agriculture), under grant agreement No. 603719. The aim of this project is to develop innovative methods and indicators to monitor and assess progress towards ‘sustainable agriculture’, focused on the global monitoring of agricultural production and the assessment of longer term impact of agricultural production on the environment and *vice versa*.

The SIGMA project also initiated the Environmental Impact Assessments for the so-called ‘JECAM sites’ (www.jecam.org). To enable these assessments, we developed and integrated a soil hydrological module and a soil nitrogen module within a crop growth model. This integrated instrument is an innovation that allows improved crop yield forecasts and increases transparency on agricultural production through the creation of an operational global agricultural monitoring system based on crop growth models, earth observation and *in situ* data.

Summary

A newly developed soil nitrogen (N) module enables the simulation of nutrient limited crop growth and the elucidation of the causes of yield gaps by either water scarcity, nutrient deficiency or a combination of both. The module interacts by exchanging information with the soil water model SWAP and the crop growth model Wofost on a daily basis (Figure 1).

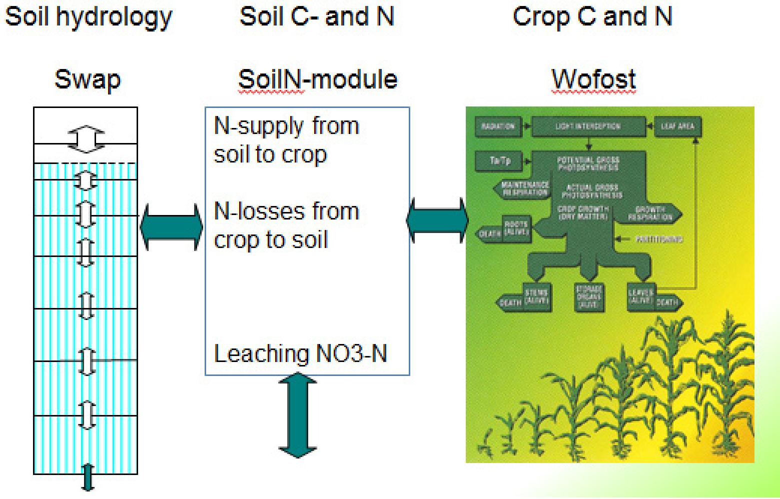


Figure 1 *Schematic representation of the exchange of information between the Soil-N module interacting between the models SWAP for soil hydrology and WOFOST for crop growth*

The RothC-26.3 model (Coleman et al., 1997) was taken as the starting point for the development of an organic matter module. Attention was given to allow for a low parameter demanding, but flexible formulation of the model, by defining a number of characteristic parameters as a function of the ‘initial age’. The ‘initial age’ concept was initially developed by Janssen (1984) to predict the organic matter decay using a one parameter model.

The nitrogen (N) balance of the soil is implemented parallel to the organic matter balance. Nitrogen supplied to the soil through fertilizer applications and organic matter decay is stored in the soil. Mineralisation rates of ammonia (NH_4) and nitrous oxide (NO_3) control nitrogen mineralisation and immobilisation in relation to the processes in the organic matter cycle.

Ammonium and nitrate balances are calculated as a result of mineralisation, nitrification, de-nitrification, plant uptake and nitrate leaching rates. Both the amounts of organic matter and the associated N-contents of crop residues are calculated by the WOFOST model and passed to the Soil-N module. The SWAP module provides information on daily water balances of the single compartment Soil-N module. The Soil-N module provides information on the resulting daily plant uptake rates, which are the minimum of the uptake demand and the mineral nitrogen availability in the soil.

The nitrogen distribution within a crop is, implemented in WOFOST based on Shibu et al. (2010). Nitrogen fixation is based on a user defined fraction that indicates the amount of nitrogen demand which is met by N-fixation from air and soil. For soybean an improved sub model to establish phenological stages was implemented in WOFOST based on Setiyono et al. (2007).

The increasing atmospheric CO_2 concentrations can be accounted for using the same method as Supit et al. (2012).

The innovated SWAP/WOFOST model, extended by the Soil-N module and descriptions for soybean development, enables the evaluation of the impacts of changes of land use and management on environmental factors. The model enables also the unravelling of interactions between water stress and limited nitrogen availability and in this way facilitates the analysis of yield gaps. A number of management actions, such as: i) addition of organic manure, ii) addition of inorganic fertilizer, iii) crop rotations, iv) irrigation, and v) drainage, can be imposed by specification of parameters in the model's input files.

The innovated model was tested using datasets from Argentina, China and the Netherlands, for which examples are given.

1 Introduction

Water and nitrogen are the two most limiting factors of crop growth that can be controlled. With increasing competition for water and concern for the nitrate pollution of our environment, agriculture must optimise growth factors that can be controlled. The cycling of nitrogen (N) in the soil/plant system is complex and involves many pathways, states and regulatory processes. All of these flows and transformations are influenced by water availability and moisture conditions. Since irrigation water may leach nitrate out of the root zone, the system cannot be optimised by considering the variables separately. A mathematical model is essential to evaluate the numerous combinations of time and amount of both water- and fertilizer applications.

A second objective of developing a model is to provide a research tool for assessing our understanding of the behaviour of water and nitrogen in the soil—plant system. A good predictive model can be developed for a given crop and area with empirical relations, but the empirical relations must be replaced by sound scientific principles for a universal model.

In the past 40 years, a series of simulation models was developed and applied for simulation of crop growth dependent on water and nutrient availability. Most models are suitable for the climatic zone and soil conditions, for which the data that are used for parameter population and validation have been collected. The model structure is usually tailored to the specific area of interest of the developers. Model developers with botanical and agronomic background describe the crop development usually in detail and approach soil water flow with less detail. On the other hand, modellers with a soil science background treat the crop development in a simple way and pay more attention to the description of the organic matter cycle and mineralisation processes. We believe that a detailed description of the soil water flow and crop development is a prerequisite for the description of water- and nitrogen limitation of crop growth, and the nitrogen availability in the soil should be addressed by taking account of to the organic matter cycle and the dynamics of nitrogen mineralisation.

The SWAP / WOFOST model was already equipped to dynamically simulate the impact of soil moisture on crop production. The development of a soil nitrogen module, incorporated in the SWAP / WOFOST model, the interdependencies between crop growth, moisture and nitrogen processes can be unravelled. The new model was calibrated and tested for field data of fertilizer application trials in Maarheze in the Southern sand district of the Netherlands (Schröder et a;,1985a).

Major parts of the development, testing and application were made possible by support from the SIGMA project (www.geoglam-sigma.info). Within this project, Environmental impacts of land use changes on groundwater and soil nitrogen were analysed for several sites from the global Joint Experiment for Crop Assessment and Monitoring (JECAM) network (www.jecam.org). Selected JECAM sites in Argentina and China were used to test the implementation. Some preliminary results are given.

2 General set-up of the model

2.1 Connection between modules

The newly developed soil nitrogen module interacts by exchanging information with the soil water model, SWAP (Van Dam et al., 2008; Kroes et al., 2009; Kroes et al., in prep), and the crop growth model WOFOST (Van Diepen et al., 1989; Supit et al., 1994; Boogaard et al., 2014, Boogaard et al., 2013), on a daily basis. The interdependencies between the module Soil N and the models SWAP and WOFOST is illustrated in Figure 2.

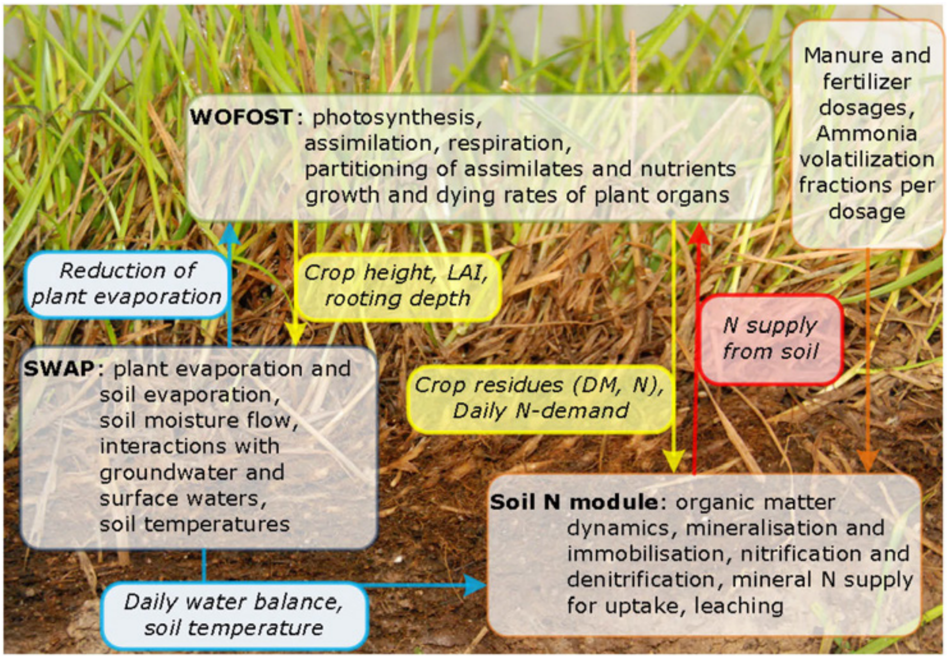


Figure 2 *Interdependencies between the SWAP, WOFOST and Soil N modules in the SWAP/WOFOST model*

The computation sequence and information exchange between modules implemented in the innovated model is depicted in Figure 2 and described, as follows:

1. Water balance is calculated by the SWAP Model, based on the initial moisture profile at the start of the day, daily precipitation and potential evaporation rates. Water extraction by plant roots is accounted for on the basis of the pressure head distribution in the root zone, which results in the extent to which the evaporative demand can be met by the soil moisture conditions. The ratio between the actual and potential plant evaporation is calculated and passed to the WOFOST Model.
2. WOFOST calculates the potential rates of gross assimilation, growth and maintenance respiration and dry matter production in the different parts of the plant. The new values of the state variables at the end of the day are calculated ignoring possible restriction by moisture deficit or nitrogen insufficiency. Then the growth rates of the plant organs are adjusted for the ratio between actual and potential plant evaporation and the nutritional demand is calculated on the basis of these adjusted growth rates. The portion of this demand provided by biological nitrogen fixation is subtracted from the total demand. The resulting demand is passed to the Soil-N module.

3. The Soil-N module calculates new values for the stocks of organic matter and nitrogen in the various soil pools at the beginning of the day, on the basis of the stocks at the end of the previous day, the application of fertilizers (organic + mineral) during the current day and crop residues from the previous day. Ammonia volatilisation is accounted for by a user-defined factor per application event. Following this, the decomposition and transformation of organic matter is calculated. The amount of mineralised and immobilised nitrogen results from this calculation. After that, the soil balance for ammonium is drawn up, taking into account adsorption on soil particles, nitrification, crop demand and leaching. The ammonium balance yields a value of the nitrified quantity of ammonium. The nitrification rate is imposed as a production term in the establishment of the nitrate balance. This balance counts for the remaining demand of the crop, de-nitrification and leaching. The terms for plant uptake of the ammonium and nitrate balance yield the amount of mineral N that can be delivered by the soil.
4. The N-delivery from soil is used by the WOFOST model to adjust the resultant growth rates from Section 2. Then, WOFOST calculates the final values of the state variables at the end of the day and establishes values for crop height, leaf area index, rooting depth, dry matter quantities of starved off leaves, stems and roots and the corresponding nitrogen quantities in these crop residues.

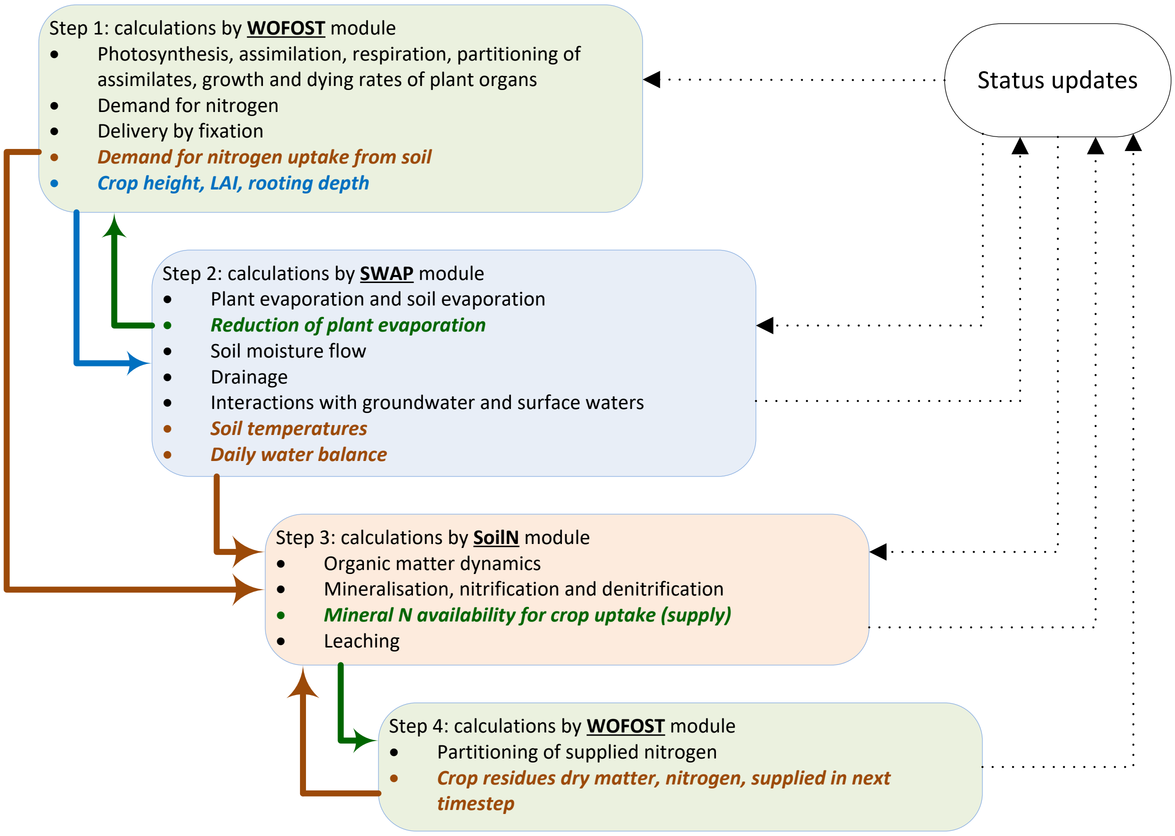


Figure 3 *Computational sequence and information exchange between modules implemented in the innovated model.*

2.2 Geometry and spatial discretization

The newly developed module is controlled from the main program, which also controls the Soil Water and WOFOST routine. SWAP uses for the simulation of soil water flow a detailed spatial discretization of the topsoil. The spatial discretization is usually coarser at greater depth. In the original WOFOST model, the soil is represented by a single layer (root zone), for which some water balance terms were calculated. For compatibility reasons, it was decided that the Soil-N module also represents the root zone by a single layer.

Advantages:

- It is consistent with the WOFOST concept, in which the plant is considered as one system. Different organs are distinguished, but no spatial discretization is applied.
- It is not necessary to formulate processes, in which the reaction of the plant to local surpluses and deficiencies in the root zone are described. Such descriptions are complex and difficult to parameterise.
- The simplicity of the Soil-N module and a small number of parameters

Disadvantages:

- In the SWAP model, the rooting depth is described as a function of time. At the beginning of the growing season, the crop is not able to utilise the whole depth for the extraction of nutrients. The single layer concept could possibly lead to an overestimation of the N-availability.
- In the SWAP model, the water balance is calculated for the fine computational grid of the root zone. The results of the SWAP model are aggregated for use in the Soil-N module. This concerns both the water balance and the calculation of soil temperature.
- The effects of any gradients of ammonium and nitrate concentrations with depth within the root zone are not reflected in leaching to groundwater and surface water.

3 Soil organic matter cycle

3.1 Background

Organic compounds are generally decomposed relatively quickly, as long as enough molecular oxygen is available. If this is not the case, degradation in top soils takes place under anaerobic circumstances with nitrates and sulphates as oxygen donors. At sufficient oxygen supply, these reactions terminate in the production of carbon dioxide (CO_2) and water (H_2O). The decomposition of organic matter is mostly a process of oxidation. The microorganisms involved in the decomposition process are mostly aerobic or facultative aerobic, which means that they can live under both aerobic and anaerobic conditions. The anaerobic decomposition process is 100 to 1,000 times smaller than the process under aerobic conditions (Hämäläinen, 1991).

Dead plant parts and all other organic materials added to the soil can be considered as additions of fresh organic materials. Living plant roots excrete soluble organic materials into the soil solution, but also dead root-cells during growth. These products become available for decomposition and partake in the carbon- and nutrient cycles too. When this material starts to decompose, it is partially oxidised to CO_2 and H_2O and partially transformed into biomass. The ratio between formed soil biomass and total amount of material transformed is given as the assimilation efficiency. Some of these transformations take place via the stage of dissolved organic material. The first step in the decomposition process, in which big molecules, such as cellulose, hemicellulose, pectin and lignin, are involved is the splitting of these molecules into smaller parts. Microorganisms use exo-enzymes that operate outside the biomass cells, to perform this task. Generally, the smaller the compounds formed, the higher their solubility is. These smaller molecules are absorbed by the micro-organism cell for further transformation.

Two main approaches are followed in modelling the mineralisation of organic materials, both based on the principle of first order kinetics. One approach is to partition substrates into various components each with its own characteristic constant decomposition rate. Another approach is to treat organic materials with a characteristic mineralisation rate, which is described either as a concentration-dependent function or as a time-dependent function. Natural organic materials show a reduction in the decomposition rate with time caused by the heterogenetic composition of the organic material considered. Materials that decompose easily, such as carbohydrates and proteins, will be used first, resulting in a relative increase of more resistant compounds of the residual material.

Jenkinson and Rayner (1977) considered five different fractions of organic compounds in their model. Two of them are connected to fresh organic material, i.e. a rapid decomposable plant material (DPM) and a resistant plant material (RPM). The soil organic material is divided into three different fractions. The first fraction is considered as biomass, with a low C/N ratio and a relatively high decomposition rate. The second fraction is the active humus compound of physically stabilised organic material with a medium C/N ratio. The third fraction is chemically stabilised organic material with a high value of the C/N ratio and a very low decomposition rate. Part of each fraction of the soil organic material in the Jenkinson and Rayner model returns during decomposition, as a result of assimilation into the three soil organic compounds.

Within the SIGMA-project, the structure of the RothC-26.3 model (Coleman et al., 1997) was taken as the starting point for the development of an organic matter module within WOFOST. The RothC-26.3 is widely used for research of the development of organic matter stocks in relation to the sustainability of agricultural systems. RothC-26.3 is relatively simple, but has the flexibility to address different types of soils and crops. Contrary to the original model of Jenkinson and Rayner (1977), the RothC-26.3 model describes the organic matter cycle through four biological transformable pools and an inert organic matter pool (Figure 4).

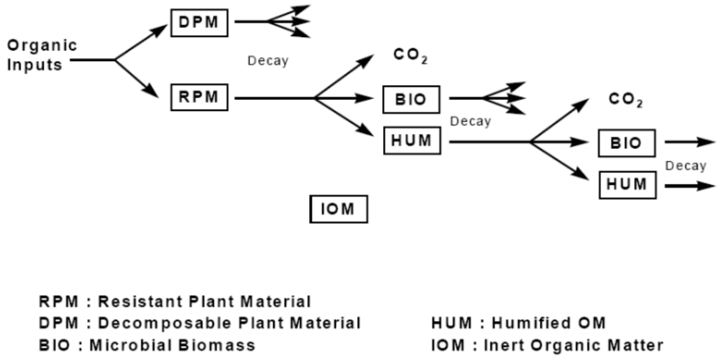


Figure 4 *Organic carbon pool structure of the RothC26.3 model*

The DPM- and RPM-pools are transformed into the BIO- and the HUM-pool (assimilated) and this transformation is accompanied by the degradation of organic molecules to carbon dioxide. The BIO and the HUM-pool are also transformed to a next stage. The RothC-26.3 model approximates this transformation by returning a return portion in the parent pool and transforming a portion to the other pool. This conversion is also accompanied by the degradation of organic molecules to carbon dioxide. The rapid decomposable plant material (DPM) and a slowly decomposing material (RPM) pools are amended to the soil by:

- application of farmyard manure and cattle slurry.
- crop residues (during the growing season died off leaves, stems and roots, after harvest residues).
- application of other organic materials (compost, straw for frost protection, tree shred, etc.).

As mentioned, the structure of the RothC-26.3 model was adopted within the WOFOST Soil-N module, but additional features were added to enable the parameterisation of the model for a wide variety of different organic materials. For this purpose, the one-parameter model of Janssen (1984) was utilized to construct relations with time of the residue of an organic material in an incubation experiment. Janssen (1984) derived a time dependent decomposition rate of peat and other organic materials using the data published by Kolenbrander (1969, 1974). The model of Janssen 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 structure.

3.2 Mathematical description

The IOM pool is considered as a fraction that is found in measurements, but does not participate in the transformations, and is not affected by the amendments. This pool has no further effect on nitrogen mineralisation. When parameterisation of the model is based on measured organic matter contents, one should take this pool into account. The four biological active pools are schematically represented in Figure 5.

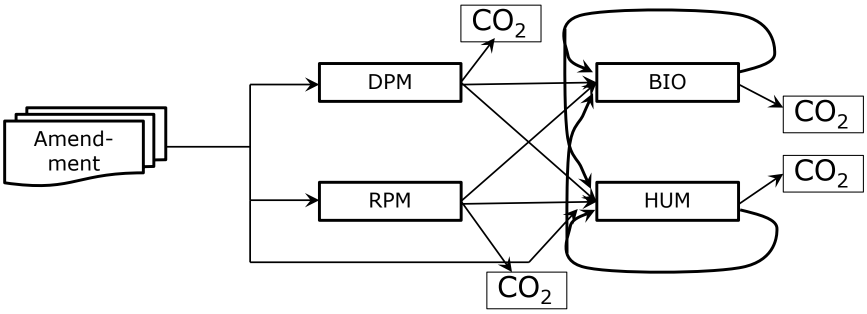


Figure 5 *Schematic representation of organic matter stocks and transformation in the RothC-26.3 model*

The transformations are described as first order rate processes where the rates are dependent on the amounts of organic matter in the pools. The interdependence of the BIO-pool and the HUM-pool can be expressed mathematically by describing the processes as a set of linear differential equations (see also Groenendijk et al., 2005; Heinen & De Willigen, 2005; De Willigen et al., 2008):

$$\begin{pmatrix} \frac{d\,DPM}{dt} \\ \frac{d\,RPM}{dt} \\ \frac{d\,BIO}{dt} \\ \frac{d\,HUM}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & 0 & 0 & 0 \\ 0 & -k_2 & 0 & 0 \\ f\,\varepsilon\,k_1 & f\varepsilon\,k_2 & -(1-f\varepsilon)k_3 & f\varepsilon\,k_4 \\ (1-f)\,\varepsilon\,k_1 & (1-f)\,\varepsilon\,k_2 & (1-f)\,\varepsilon\,k_3 & -(1-(1-f)\,\varepsilon)k_4 \end{pmatrix} \begin{pmatrix} DPM \\ RPM \\ BIO \\ HUM \end{pmatrix} \tag{1}$$

Where k_1 .. k_4 are transformation rate constants, ε is the assimilation fraction (fraction of total decayed C that is newly incorporated in the BIO and HUM pool) and f is the fraction of assimilated carbon that is incorporated in the BIO pool). Inputs are imposed by an instantaneous increase of the DPM and RPM pools at the beginning of the time step. The state variables DPM and RPM are recalculated according to:

$$\begin{aligned} DPM(t+\delta t) &= DPM(t) + p\,Q \\ RPM(t+\delta t) &= RPM(t) + (1-p)\,Q \end{aligned} \tag{2}$$

where Q is the quantity of added organic matter and p is a parameter to fractionate the amendment to either the DPM and the RPM pool.

The mathematical set of linear differential equations is solved analytically by:
- deriving the solutions for the DPM(t) and RPM(t) values at the end of the time step;
- calculating the Eigenvalues for the BIO and HUM subsystem;
- deriving the solutions for the BIO(t) and HUM(t) values at the end of the time step, taking into account the quantities assimilated from the DPM and RPM-pool and the internal assimilation and dissimilation rates of this subsystem;
- deducing the dissociation, assimilation and dissimilation rates from the quantities of DPM, RPM, BIO and HUM at the start and the end of the time step;
- calculating the quantities on nitrogen mineralised and carbon dioxide produced by multiplying the different process rates by a nitrogen fraction and carbon fraction, respectively, and setting up balances according to the transformation scheme.

The transformation rate constants k_1 .. k_4 (summarised as k_R^*) are calculated from a default value k_R expressing optimal conditions and a number of rate-modifying factors:

$$k_R^* = m_W \times m_t \times m_C \times m_{pH} \times k_R \tag{3}$$

The transformation rates at optimal conditions taken from the literature (Jenkinson et al., 1990; Coleman et al., 1997) are denoted in Table 1.

Table 1 *Rate constant values applied in the Soil-N module.*

Rate constant	Year
k_1	3.0
k_2	0.3
k_3	0.66
k_4	0.02

Originally the transformation rate k_1 was taken 10 years, but in later reports k_1 values of three years can be found. The assimilation products of the transformations are attributed for 46% to the BIO-pool and 54% to the HUM-pool. The total assimilation fraction ε and the partitioning (*p*) of organic material amendments into fractions attributed to DPM, RPM and eventually HUM differs from the standard model and is explained in the next section.

3.3 Deduction of partitioning fractions from the Janssen model

The model of Janssen (1984) is a single parameter model that describes the course of time of residue of a unit incubated organic matter:

$$\frac{OM(t)}{OM(t_0)} = \frac{exp\left(4.7(t+a)^{-0.6}\right)}{exp\left(4.7(a)^{-0.6}\right)} \tag{4}$$

where OM(t) is the organic matter weight after a certain time span, OM(t_0) is the initial weight and *a* is the apparent age. This parameter characterises the degradability of the organic material considered. The model is widely used for advising farmers in Europe and developing countries, with respect to cropping systems with a view to optimal production conditions and sustainable management of the soil. The apparent age parameter has been listed in different reports for a number of materials. A number of them have been defined in the Soil-N module (Table 2).

Table 2 *Characterisation of organic materials by the Janssen model's parameter a.*

Material	*a*-value (year)
Cattle manure and slurry	3.16
Pig manure and slurry	1.36
Poultry manure and slurry	1.36
Compost	1.96
Champost	1.36
Green leaves of e.g. Vegetables	0.92
Over ground crop residues	0.99
Root and stubble residues	1.57
Grass shoots	0.92
Grass roots	1.20
Tree leaves	2.25
Spruce needles	3.34

The rapidly decomposing materials with low *a* values degrade for the most part within a few years, leaving only a small portion of the initial amount. The assimilation fraction ε is defined in the RothC-26.3 model as a function of the clay percentage (*pClay*) in mineral soils (Jenkinson et al, 1990).

$$\boldsymbol{\varepsilon} = \frac{\mathbf{1}}{\mathbf{1+1.67(1.85+1.60exp(-0.0786}\,\boldsymbol{pClay}\mathbf{))}} \qquad (5)$$

Consequently, for low clay contents the ε parameter amounts to 0.15 and for high clay contents ε is ca. 0.22. Keeping in mind the low value of the transformation rate k_4, the RothC-26.3 model is not able to simulate the degradation of organic materials for more than 90% within a few years as it is described by the Janssen model for materials with *a*-values less than 1.20. For this reason, an alternative approach to calculate the ε-parameter was adopted. The assimilation fraction ε for products that result from the conversion of the BIO- and the HUM-pool was set to 0.2 and material dependent values were established for the products that result from the conversion of the DPM and the RPM-pool.

Another adaptation with respect to the RothC-26.3 model concerns the partitioning of soil amendments into the DPM-pool and the RPM-pool. The RothC-26.3 model sets the *p*-value to 0.59. This value results to a degradation curve with time of crop residues (stubbles and roots). By setting *p* to a fixed value, the model would only be able a limited number of organic materials.

To formulate an organic model for a wider range of applications, relationships were derived for the assimilation fraction as a function of the apparent age in the Janssen model. Relationships for the partitioning factor *p* were also derived. It was concluded that for stable materials, such as peat materials and native soil organic matter, the attribution to DPM and RPM would over-estimate the degradation rates, irrespective of the assimilation factor. Therefore, for materials characterised by an apparent age higher than 2.5 years, a part of the amendment can also be attributed to the HUM-pool.

For 10 values of the apparent age, a degradation curve with time of a certain unit of organic material was constructed according to the Janssen model. For each of the apparent age values, three parameters of the RothC-26.3 model were fitted by an optimisation algorithm that minimises the sum of squared differences between curves generated by the Janssen model and by the RothC-26.3 model. The 10 sets of parameters were plotted as a function of the apparent age and continuous functions were formulated to enable interpolation between the values. The resulting relations are depicted in Figures 6 and 7.

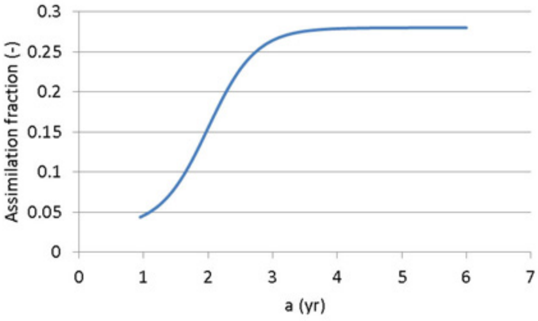


Figure 6 *Assimilation fraction for the products that result from the conversion of the DPM and the RPM-pool in the adjusted RothC-model to enable the simulation of a wide variety of organic materials*

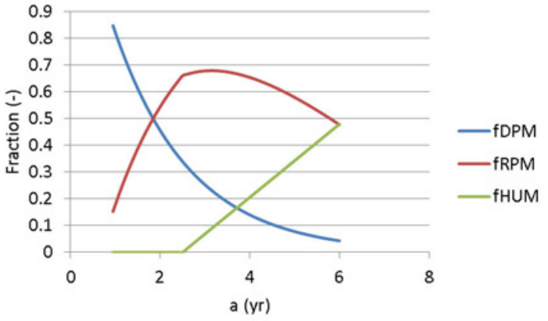


Figure 7 *Attribution fractions of organic soil amendments in the adjusted RothC-model to enable the simulation of a wide variety of organic materials*

For rapidly degradable materials, the values are much lower than in the original RothC-26.3 model and the values are actually higher stable materials. Materials with an apparent age ranging from two to three years have similar values as in the RothC-26.3 model. The attribution fractions of organic soil amendments were fitted subject to the condition that the sum should be equal to one (Figure 6).

Only for materials with *a* greater than 2.5 years, a part is attributed to the HUM-pool. Rapid degradable materials are attributed for a large proportion to the DPM-pool, but slow degradable materials are only allocated for a small part to this pool.

The model was verified by comparing the results of the Janssen model and the RothC-model for a number of materials.

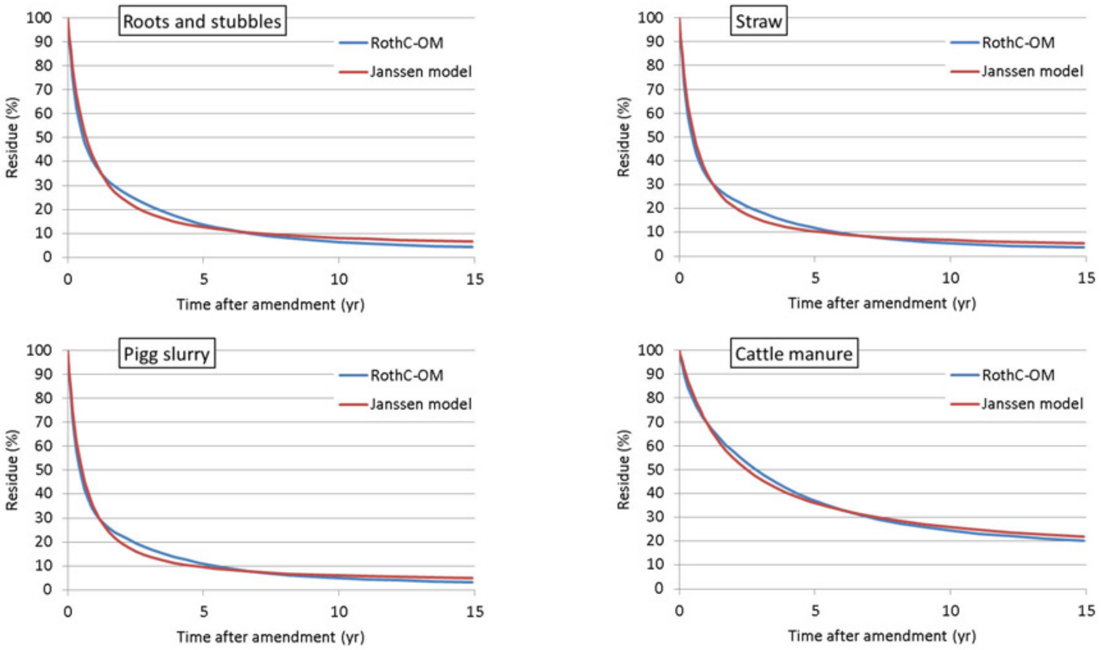


Figure 8 *Verification of the relations introduced in the RothC-model to enable the simulation of a wide variety of organic materials*

It is assumed that in practice, farmyard fertilizers are defined by wet weight. To this end, the module comprises a list of material definitions with the organic weight fractions of the materials (Table 3). For the crop residues that amended to the soil during or at the end of the growing season, it is assumed that they are calculated by WOFOST and that their weight fractions are equal to one.

Table 3 *Organic weight fractions of organic materials*

Material	Organic matter weight fraction of wet (total) weight
Cattle manure	0.150
Pig manure	0.161
Poultry manure	0.376
Cattle slurry	0.064
Pig slurry	0.060
Poultry slurry	0.093
Compost	0.190
Champost	0.460

4 Soil nitrogen balance

The logic used in developing the nitrogen (N) balance is somewhat parallel of the organic matter balance. Nitrogen supplied to soil through fertilizer applications and organic matter decay is stored in the soil (Figure 9). The processes that control the nitrogen mineralisation and immobilisation in relation to the processes in the organic matter cycle are:

- The net total mineralisation rate of NH_4 follows from the formation/decomposition balance of the different organic materials, taking into account their diverse N contents.
- The decomposition rate of NO_3 is determined by the part of the total decomposition of organic material that takes place under anaerobic conditions. The decomposition rates under strict anaerobic conditions are much lower and in top soils complete anaerobic decomposition can mostly be neglected.

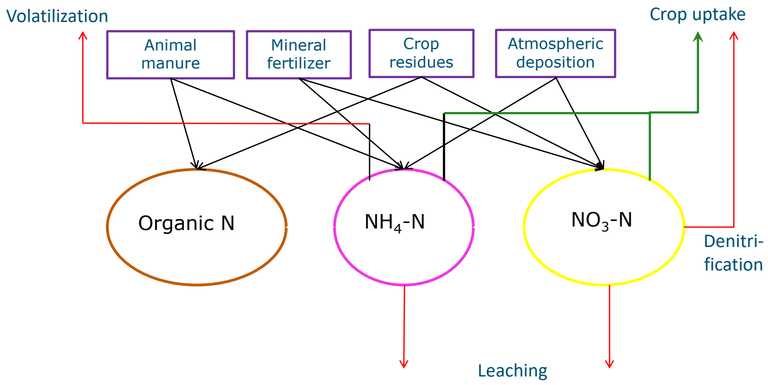


Figure 9 *Schematic representation of the nitrogen pools, transformations and transport described in the Soil-N module*

Other processes in the nutrient cycles that are not directly parallel with those in the carbon cycle are:

- The oxidation of ammonium to nitrate is called nitrification. The process takes place in two steps, performed by different groups of micro-organisms:
- Under normal circumstances the second step is much faster than the first, so no accumulation of nitrite (NO_2^-) will occur.
- Volatilisation is the process of gaseous losses of nitrogen from the top soil to the free atmosphere after the formation of ammonia gas (NH_3) from NH_4.
- In addition to animal slurry and inorganic nitrogen fertilizers, another source of nitrogen is available for crops as a result of nitrogen fixation by free-living soil bacteria and symbiosis with leguminous plants.

4.1 Mineralisation

The organic materials considered all have a different N-content. Table 4 shows values for the nitrogen weight fraction of the organic matter, as these are commonly used for the Dutch situation. In addition, the weights of mineral N in ammonium and nitrate are shown as a fraction of the wet weight. The N-contents of crop residues are calculated by the WOFOST model and are passed to the Soil-N module.

Table 4 *Nitrogen fractions of animal manure, recycling products and synthetic fertilizers*

Material	**Nitrogen weight as a fraction of organic matter added**	**NH_4-N weight as a fraction of amendment wet weight**	**NO_3-N weight as a fraction of amendment wet weight**
Cattle manure	0.035	0.0012	0
Pig manure	0.037	0.0015	0
Poultry manure	0.058	0.0024	0
Cattle slurry	0.034	0.0022	0
Pig slurry	0.050	0.0042	0
Poultry slurry	0.047	0.0058	0
Compost	0.041	0.0008	0
Champost	0.025	0.0003	0
Urea		0.46	0
Synthetic fertilizer		0.50	0.50

In order to describe the wide variation in the N content of different materials, the DPM-pool and the RPM-pool are each split into two sub-pools. Only the N-contents are different, but the degradation rates are equal. Sub-pool 1 has a low N-content (fN_{min}), which can be regarded as a minimum value, and the N-content of sub-pool 2 is considered as a maximum value (fN_{max}). Amendments are assigned to the sub-pools on the basis of their N-content ($fN_{material}$). The part assigned to the sub-pool with the low N-content (Fr_1) and the high N-content (Fr_2) is calculated as:

$$Fr_1 = \frac{fN_{max} - fN_{material}}{fN_{max} - fN_{min}}; \qquad Fr_2 = \frac{fN_{material} - fN_{min}}{fN_{max} - fN_{min}} \tag{6}$$

The mineralisation rate R_{Nmin} (kg m^{-3} d^{-1}) follows from the results of the organic matter transformations:

$$R_{Nmin} = \Big(fN_{min}\big(DPM_1(t_0) - DPM_1(t)\big) + fN_{max}\big(DPM_2(t_0) - DPM_2(t)\big) + fN_{min}\big(RPM_1(t_0) - RPM_1(t)\big) + fN_{max}\big(RPM_2(t_0) - RPM_2(t)\big) + fN_{BIO}\big(BIO(t_0) - BIO(t)\big) + fN_{HUM}\big(HUM(t_0) - HUM(t)\big)\Big)\frac{1}{\Delta t} \tag{7}$$

4.2 Ammonium balance

The ammonium balance is defined by a number of inputs and outputs and the change of stocks. Most of the processes are defined as time-dependent functions, but some are formulated as event-based functions:

- Fertilizer additions.
- Volatilisation.

The only form of volatilisation we considered is the gaseous emission of NH_3 at the time of the fertilizer dosage. The fraction of ammonium dosage that is lost should be specified in the model input file for each fertilization event. For the time-dependent functions, we take the mass conservation equation as a starting point in the Soil-N-module:

$$K_{sorp}\rho_d \frac{dc_{NH4}}{dt} + \frac{d\theta c_{NH4}}{dt} = q_{in}c_{NH4,in} - q_{out}c_{NH4} + R_{Nmin} - R_{NH4,upt} - R_{nitr} \tag{8}$$

where:

c_{NH4}	ammonium concentration of soil water	(kg m^{-3})
$c_{NH4,in}$	ammonium concentration of in-flowing water	(kg m^{-3})
q_{in}	In-flowing water flux	(m d^{-1})
q_{out}	Out-flowing water flux	(m d^{-1})
θ	moisture volume fraction	(m^3 m^{-3})
K_{sorp}	linear sorption constant	(m^3 kg^{-1})
ρ_d	dry bulk density	(kg m^{-3})
R_{Nmin}	mineralisation rate	(kg m^{-3} d^{-1})
$R_{NH4,upt}$	ammonium-N uptake rate	(kg m^{-3} d^{-1})
R_{nitr}	nitrification rate	(kg m^{-3} d^{-1})

The linear sorption coefficient and the dry bulk density should be specified in the model input file. The water and the information about soil water contents are derived from the SWAP simulation results. Inflow of ammonium from deeper soil layers can occur in periods when the evaporative demand is met by capillary rise. Therefore, the ammonium concentration at the lower boundary should be specified. In the ammonium balance, the mineralisation rate is treated as a zero order production. Nitrification is formulated as a first order rate process, according to:

$$R_{nitr} = k_{nitr}(\theta\, c_{NH4}) \tag{9}$$

The value of the first order rate constant k_{nitr} depends on soil temperature, soil pH and the relative water saturation degree. The calculation of the modification factors will be explained in a subsequent section.

For establishing the ammonium uptake by plant roots ($R_{NH4,upt}$) of a half fully grown to a full-grown crop, two calculations of the mass conservation equation are performed.

1. Firstly, the uptake is set equal to the demand of the crop as it is calculated by the WOFOST model.
2. Secondly, $R_{NH4,upt}$ is formulated as a first order term and it is assumed that the uptake is limited by the ammonium amount in soil. In this case, $R_{NH4,upt}$ is defined as:

$$R_{NH4,upt} = \delta_{NH4} \frac{q_{evtr}}{\Delta z} c_{NH4} \tag{10}$$

where q_{evtr} is the transpiration flux (m d^{-1}), Δz is the depth of the root zone (m) and δ_{NH4} is a so-called ‘transpiration–concentration stream factor’. If the demand of the plant is large, but the concentration in the soil moisture is low, the $R_{NH4,upt}$ value will be relatively high in the first calculation of the mass conservation equation, and in the second calculation it will be relatively low. In the end, the first or the second is chosen for on the basis of the highest value of c_{NH4}. From the resulting ammonium concentration values, the time averaged nitrification rate is calculated and its value is passed to the nitrate balance.

For recently emerged crops, the uptake rate limitation due to ammonium availability appears to be sensitive for the accuracy of plant transpiration simulations. The parameter sets of the WOFOST model and the SWAP model need to be tuned to each other for 100%. In practice, this is difficult to achieve. WOFOST can calculate a nitrogen demand, whilst there is still no root development, and, thus, no transpiration flux calculated. In addition, the plant evaporation of an early crop calculated by SWAP appears to be uncertain. Therefore, an alternative approach is applied to calculate the nitrogen uptake by a recently emerged crop. If the development stage is less than one and the LAI of the crop is less than a user defined critical value $\mathrm{LAI}_{\mathrm{CNU}}$, a factor F_{CNU} is calculated according to:

$$F_{CNU} = \frac{LAI_{CNU} - LAI}{LAI_{CNU}} \tag{11}$$

The uptake rate is then calculated as the sum of the demand multiplied by the factor F_{CNU} and the uptake rate based on the ammonium availability, which is calculated as:

$$R_{NH4,upt} = (1 - F_{CNU})\, \delta_{NH4} \frac{q_{evtr}}{\Delta z} c_{NH4} \tag{12}$$

4.3 Nitrate balance

Similar to the ammonium balance, the nitrate balance is defined by a number of inputs and outputs and the change of stocks. Only the process of *fertilizer addition* is defined as an event-based function, all other processes are computed as time-dependent functions. The mass conservation equation that is taken as a starting point in the Soil-N module:

$$\frac{d\theta c_{NO3}}{dt} = q_{in}c_{NO3,in} - q_{out}c_{NO3} + R_{nitr} - R_{NO3,upt} - R_{denitr} \tag{13}$$

where:

c_{NO3}	ammonium concentration of soil water	(kg m^{-3})
$c_{NO3,in}$	ammonium concentration of inflowing water	(kg m^{-3})
$R_{NO3,upt}$	ammonium-N uptake rate	(kg m^{-3} d^{-1})
R_{denitr}	nitrification rate	(kg m^{-3} d^{-1})

In the nitrate balance the nitrification rate is treated as a zero-order production. From the resulting ammonium concentration values, the time averaged nitrification rate is calculated and its value is passed to the nitrate balance. De-nitrification is also formulated as a first order rate process:

$$R_{denitr} = k_{denitr}(\theta\ c_{NO3}) \tag{14}$$

where the value of the first order rate constant k_{denitr} depends on soil temperature, soil pH and the relative water saturation degree. Many soil nitrogen models describe de-nitrification with a nitrate concentration based Michealis-Menten kinetics. In our model, de-nitrification is defined as a first order rate process, but the rate constant depends on the organic matter dissimilation rate which is described by a Michealis-Menten equation.
Apart from that, depending on the half-value of the MM relationship, there would be little difference with a first order approximation for not too high concentrations (Heinen, 2006).

De-nitrification occurs only in wet conditions. The model is not able to describe the process of de-nitrification in detail, because of the chosen spatial discretization and the temporal discretization (1 day). At the selected computation time, step and thickness of the soil layer, it is anticipated that de-nitrification is under-estimated. On the other hand, by omitting the influence of the nitrate concentration on the process rate constant, de-nitrification reaction may be over-estimated. We assume that both effects usually balance out.

For establishing the nitrate uptake by plant roots ($R_{NO3,upt}$), two calculations of the mass conservation equation are performed. In the first calculation, the uptake is set equal to the demand of the crop, as calculated by the WOFOST model. In the second calculation, $R_{NO3,upt}$ is formulated as a first order term and it is assumed that the uptake is limited by the nitrate amount in soil. In this case, $R_{NO3,upt}$ is defined as:

$$R_{NO3,upt} = \delta_{NO3}\frac{q_{evtr}}{\Delta z}c_{NO3} \tag{15}$$

where δ_{NO3} is a so-called transpiration – concentration stream factor for nitrate uptake. If the demand of the plant is large, but the concentration in the soil moisture is low, the $R_{NO3,upt}$ value will be relatively high in the first calculation of the mass conservation equation, and in the second calculation it will be relatively low. In the end, the first or the second is chosen for on the basis of the highest value of c_{NO3}. If both ammonium and nitrate concentrations in the soil are too low, the crop demand cannot be fulfilled and the WOFOST model should adjust its growth rates to the soil conditions.
For recently emerged crops, the LAI based procedure for calculating the uptake as the sum of the demand driven uptake, multiplied by the factor F_{CNU}, and the availability driven uptake, multiplied by (1 - F_{CNU}), is maintained.

4.4 Crop uptake

The calculation sequence of the coupled models, the WOFOST model defines an optimal demand for mineral nitrogen for the current time step. The proportion that can be delivered by biological nitrogen fixation is subtracted from this demand and the remaining quantity (N_{demand}) is passed to the Soil-N module. The final amount of mineral nitrogen that can be delivered by the soil is given by:

$$N_{supply} = \min(\delta_{NO3} q_{evtr} \overline{c}_{NO3}, N_{demand} - \min(\delta_{NH4} q_{evtr} \overline{c}_{NH4}, N_{demand})) + \min(\delta_{NH4} q_{evtr} \overline{c}_{NH4}, N_{demand}) \tag{16}$$

Where $\overline{c}_{NO3}$ and $\overline{c}_{NH4}$ are the time averaged nitrate and ammonium concentration for the current time step. The calculation scheme implies a preference for the uptake of ammonium, and if there is too little ammonium present, the remaining demand is being met by the uptake of nitrate.

4.5 Rate modification factors

Rate constant values are defined in the model inputs, but are adjusted for environmental influences, with respect to soil temperature and moisture content. It is assumed that influences of the soil clay content and the soil pH were accounted for in the definition of the rate constant, as they are specified in the model input files.

All rate constants used in the simulation of the organic matter cycle (k_1, k_2, k_3, k_4), the nitrification rate constant k_{nitr} and the de-nitrification rate constant k_{denitr} are adjusted for the influence of temperature T (range 0 – 42°C), according to a function given by Rijtema et al. (1999):

$$\boldsymbol{m_T = \frac{1}{1+\exp(-0.26\times(T-17))} - \frac{1}{1+\exp(-0.77\times(T-41.9))}} \tag{17}$$

This function reaches its maximum level at temperature values ranging from 30–37°C, but disregards the temperature of the field of laboratory circumstances, for which experimental values of rate constants have been assessed. Therefore the equation is normalised and adjusted to:

$$\boldsymbol{m_T = \frac{\frac{1}{1+\exp(-0.26\times(T-17))} - \frac{1}{1+\exp(-0.77\times(T-41.9))}}{\frac{1}{1+\exp\left(-0.26\times\left(T_{ref}-17\right)\right)} - \frac{1}{1+\exp\left(-0.77\times\left(T_{ref}-41.9\right)\right)}}} \tag{18}$$

where T_{ref} is the reference temperature for the rate constants specified. The m_T value according to Eq. (16) takes the value of one at the reference temperature T_{ref}. It should be denoted that for T_{ref} values smaller than 12°C, Eq. (16) results in higher m_T values for the range $T_{ref} < T < T_{ref}+20$ than the Arrhenius equation used for the temperature response in the ANIMO model (Groenendijk et al, 2005). Therefore, the T_{ref} is not considered as an empirical constant and its value should be established by optimisation procedures.

The influence of the moisture content is accounted for in different ways.

1. For the transformation of the organic matter pools, we follow the rules as they are implemented in the ANIMO model (Groenendijk et al, 2005). The modification factor is calculated as a function of the water-filled pore space (water saturation degree):

   $$m_W = \frac{6WFPS^2}{1+9WFPS^4} \qquad 0 < WFPS < WFPS_{crit}$$

   $$\boldsymbol{m_W = a_2\, WFPS^2 + a_1\, WFPS + a_0 \qquad WFPS_{crit} < WFPS < 1} \tag{19}$$

   The coefficients a_0, a_1, and a_2 are obtained by requiring continuity of both the function and the derivative of the function for the range 0 < $WFPS$ < $WFPS_{crit}$. At complete saturation m_w is set to 0.01.

2. For the nitrification reaction, the rate modification is described by:

$$\boldsymbol{m_W} = \frac{\mathbf{0.9}}{\mathbf{1+exp\left(-15\times(\boldsymbol{WFPS}-0.45)\right)}} + \mathbf{0.1} - \frac{\mathbf{1}}{\mathbf{1+exp(-50\times(\boldsymbol{WFPS}-0.95))}} \tag{20}$$

This equation is graphically represented in *Figure 10*.

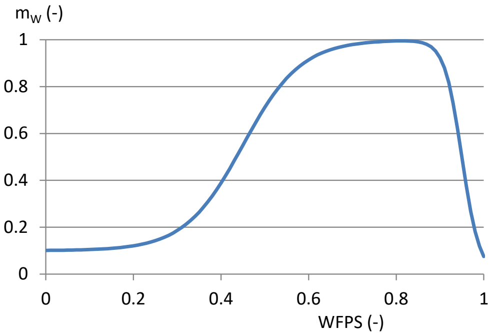


Figure 10 *Rate modification factor of nitrification for water saturation degree*

In very dry conditions, the nitrification rate is inhibited by drought stress and m_W takes a value of 0.1. Optimum values of nearly one are reached at WFPS-values ranging from 0.6 – 0.9. At WFPS = 1 (complete saturation), again m_W takes a small value.

For the de-nitrification reaction, the rate modification is formulated as:

$$\begin{array}{ll} 0 < WFPS < WFPS_{critden} & m_W = 0 \\ \boldsymbol{WFPS > WFPS_{critden}} & \boldsymbol{m_W} = \left(\frac{\boldsymbol{WFPS-WFPS_{critden}}}{\boldsymbol{1-WFPS_{critden}}}\right)^{\mathbf{2}} \end{array} \tag{21}$$

De-nitrification occurs under very wet conditions. The parameter $WFPS_{critden}$ is supplied by the user in the model input and can ranges from 0.7 – 0.9, depending upon the soil type and the agricultural use of the soil.

A third modification factor is implemented in the Soil-N module for de-nitrification only. The de-nitrification rate is also adjusted for soil respiration circumstances. When the demand for oxygen, either donated from atmospheric oxygen of from nitrate, is low, the potential de-nitrification rate will also be low. The dissimilation rate is derived from the organic matter transformations and the modification factor m_C reads as follows:

$$\boldsymbol{m_C} = \frac{\boldsymbol{C_{dis}}}{\boldsymbol{c_{½}+C_{dis}}} \tag{22}$$

Where C_{dis} is the dissimilation rate obtained from the organic matter balance and $c_{½}$ is a user supplied parameter such that $m_c = 0.5$ at $c_{dis} = c_{1/2}$.

5 Crop dry matter and nitrogen balances

5.1 Dry matter balance

The crop growth simulation model WOFOST (Van Diepen et al.,1989; Supit et al., 1994; Boogaard et al., 1998, Boogaard et al., 2013) is applied to simulate crop growth. It is implemented as a separate module and computes daily biomass accumulation and its distribution over crop organs during the growth period using a photosynthesis approach. Crop growth is simulated and expressed as dry weight (0% moisture). Dry weight or dry matter of plants generally can be expressed as carbon balance, assuming a nearly fixed carbon content, which according to Schlesinger (1991) is almost always found to be between 45 and 50% (by oven-dry mass).
In this model, we simulate dry matter and control and export the dry matter balance of plant parts in two ways:

1. Dry matter Balance 1: from air to partitioning (kg/ha DM CH2O)

   ```
   check on carbon balance:
   ccheck = (gasspot-mrespot-(fr+(fl+fs+fo)*(1.0d0-fr))*dmipot/cvf) /
             max(0.0001d0,gasspot)
   ```

   A check is carried out on the closure of the dry matter balance and the simulation is interrupted when |ccheck| > 0.0001 kg/ha DM CH2O

2. Dry matter Balance 2: storage difference(kg/ha DM CH2O):

   ```
   storagediff = ((wlv+wst+wso+wrt) - (wlvt0+wstt0+wsot0+wrtt0))
   ombalan = storagediff - ((gwst+gwrt+gwso) + (grlv-drleaf))*delt
   ```

   A check is carried out on the closure of the dry matter balance and the simulation is interrupted when ombalan > 1 kg/ha DM CH2O

Both balances are exported to output files.

5.2 CO_2 changes

CO_2 changes can be simulated using explicit input of the CO_2 concentration and three tables defining the relation between CO_2 and Amax, Eff and Tra, respectively. These relations vary per crop and also allow distinction between C3 and C4 crops.
The increasing atmospheric CO_2 concentrations can be accounted for using the same method as Supit et al. (2012). For maize (C4-crop), literature reviews by Cure (1985) and Cure and Acock (1986) indicate a stomatal conductance reduction of 40% and a transpiration decrease of 28% for maize at doubled atmospheric CO_2 and high light conditions. For grassland and potatoes (C3-crops), effects of increasing atmospheric CO_2 concentration on the CO_2 assimilation and growth are incorporated via the maximum and initial angle of the CO_2 assimilation–light response and a small decrease in transpiration rate. Note that yield increases in free air CO_2 enrichment (FACE) studies are lower than for enclosure studies (Long et al., 2006) due to more plant interaction (e.g. shadowing in canopy). Yield increases of 25–40% for doubled CO_2 (De Temmerman et al., 2002; Wolf and van Oijen, 2002, 2003; Wolf et al., 2002) were found in such circumstances.

5.3 Nitrogen balance

The nitrogen routines, implemented in SWAP-WOFOST are based on Shibu et al. (2010). Large parts of their manuscript are used in the text below to describe the implemented nitrogen model. Total crop nitrogen demand equals the sum of the nitrogen demands of its individual organs (excluding storage organs, for which nitrogen demand is met by translocation from the other organs, i.e. roots, stems and leaves). Nitrogen demand of the individual organs is calculated as the difference between maximum and actual organ nitrogen contents. The maximum nitrogen content is defined as a function of canopy development stage (Drenth et al., 1994). Total N demand (TN_{dem}: kg ha^{-1} d^{-1} N) of the crop is:

$$\boldsymbol{TN_{dem} = \sum_{i=1}^{n} \frac{W_i N_{\max,i} - AN_i}{\Delta t}} \tag{23}$$

where $N_{\max,i}$ is the maximum nitrogen concentration of organ i (kg N kg^{-1} biomass), with i referring to leaves, stems and roots), W_i is the weight of organ i (kg biomass ha^{-1}), and AN_i is the actual nitrogen content of organ i (kg N ha^{-1}).

Nitrogen uptake is determined by crop demand, indigenous soil nitrogen supply and fertilizer application. Nitrogen uptake processes like mass flow and diffusion are not explicitly simulated in the model. Crop N uptake is estimated via a simple book-keeping approach. Nitrogen from indigenous sources is assumed to have a higher (nearly 100%) recovery compared to applied fertilizers, as it is the amount of N actually taken up by a crop under zero nitrogen fertilizers. Therefore, in the model, it is assumed that the crop first takes up nitrogen mineralized from indigenous organic matter, and then from fertilizer. Total nitrogen taken up by the crop (dNU/dt) is partitioned among leaves, stems, roots and storage organs in proportion to their demands:

$$\boldsymbol{\left(\frac{dNU}{dt}\right)_i = \left(\frac{N_{dem,i}}{TN_{dem}}\right)\left(\frac{dNU}{dt}\right)} \tag{24}$$

where $(dNU/dt)_i$, and $N_{dem,\,i}$ are the rate of nitrogen uptake (g m^{-2} d^{-1}) and nitrogen demand (g m^{-2} d^{-1}) of organ i (i refers to leaves, stems, roots and storage organs), respectively.

In SWAP-WOFOST the nitrogen uptake is assumed to stop at a predefined development stage (after anthesis), as nitrogen content in the vegetative parts hardly increases (Groot, 1987; Sinclair and Amir, 1992). Nitrogen demand of the storage organs is also assumed to be met exclusively by translocation from leaves, stems, and roots as soon as grain formation starts. Hence, the rate of nitrogen accumulation in the storage organs is determined by their nitrogen demand calculated by the maximum N content and the actual N content and by the total amount of translocatable nitrogen in the other crop organs. Total translocatable nitrogen in the crop equals total nitrogen content of the organs, minus their residual non-transferable nitrogen content, which is the nitrogen incorporated in structural crop components. The net rate of change of nitrogen $(dN/dt)_i$ in each of the organs AN_i, where i refers to leaves, stem and roots, is:

$$\boldsymbol{\left(\frac{dN}{dt}\right)_i = \left(\frac{dNU}{dt}\right)_i - \left(\frac{dNT}{dt}\right)_i - \left(\frac{dND}{dt}\right)_i} \tag{25}$$

where $(dNU/dt)_i$, $(dNT/dt)_i$ and $(dND/dt)_i$ are the contributions of nitrogen uptake to the organ, translocation from the organ and loss of nitrogen due to the death of the organ, respectively. It is assumed that the stem does not die and therefore $(dND/dt)_{stem}$, equals zero and the outflow rate is not included.

A crop is assumed to experience N stress at N concentrations below a critical value for unrestricted growth. To quantify crop response to nitrogen shortage, a Nitrogen Nutrition Index (NNI) is defined, ranging from 0 (maximum N shortage) to 1 (no shortage) (Lemaire et al., 1989; Van Delden, 2001):

$$\boldsymbol{NNI = \frac{actual\ crop[N] - residual[N]}{critical[N] - residual\ [N]}} \tag{26}$$

The critical crop nitrogen concentration is defined as the lower limit of canopy nitrogen concentration in leaves and stems required for unrestricted growth. It is assumed to be half of the maximum nitrogen concentration (Porter, 1993; Jamieson et al., 1998).

The nitrogen balance of the crop is controlled:

```
Check on N balance:
NBALAN = ABS(NUPTT+NFIXTT+(ANLVI+ANSTI+ANRTI+ANSOI)-(ANLV
           +ANST+ANRT+ANSO+NLOSSL+NLOSSR+NLOSSS))
```

A check is carried out on the closure of the N balance and the simulation is interrupted when NBALAN > 0.001 kg ha^{-1} N.
The N balances is exported to an output file with the extension `.nba`

5.4 Nitrogen-fixation

Nitrogen-fixation (N-fixation) was based on a simple approach, assuming that nitrogen-fixation from the air is potentially unlimited. The crop defines the demand for nitrogen and a simple user defined fraction indicates the amount of nitrogen-demand (N-demand) which met by N-fixation from air and soil.

Crop growth and the corresponding N-demand are already limited by drought, which is simulated using the detailed hydrology from the SWAP-model.

If we assume that other factors, especially phosphorus, are not limiting this approach may be valid. It seems in agreement with Giller (2001) who states that "*The main environmental factors that constrain N2-fixation in the tropics include limitations of water, nutrients (particularly phosphorus) and toxicities*".

A future improvement may be achieved when the dynamics and quantities of Rhizobial populations are described by a separate pool.

6 Soybean simulation

6.1 Water

Water is an extremely important factor in crop growth situations. Due to an atmospheric demand, crops transpire water after that has been taken up from the root zone. Other than for nutrients, almost all water taken up by the root system leaves the plant through transpiration via the stomata in the leaves. Shortage of water in the root zone causes a decrease in root water uptake, and, thus, a decrease in crop transpiration. Once this occurs, the plant will partly close its stomata. This then causes a problem in gas exchange (CO_2 assimilation) between the leaves and the atmosphere. Consequently, the crop respiration cannot occur at optimal rate, causing a decrease in crop growth. Even in situations where ample nutrients are available in the root zone, crop growth may not be optimal when water shortage occurs during the growing season.

Soil compaction may, dependent on prevailing weather conditions, cause decreased pressure heads in the top soil (say 0-15 cm) and thus in a decrease in soil water availability. This can be partly diminished by using mulching (Siczek et al., 2015).

Based on a modelling study Videla Mensegue et al. (2015) concluded that the water contribution from a water table located approximately 1.5 to 2m deep can contribute up to 30% of the total water requirement of soybeans in the Argentinian pampas region, thus, stabilising the inter-annual variability of grain yield.

6.2 Soil

Soils may be characterised by their natural (indigenous) soil fertility. That is, nutrients may be released from the soil and become available for uptake by the plant roots. Nitrogen (N) availability is determined by the mineralisation of the organic matter (often plant residues and added manure or compost) present in the soil. To a lesser extent this is also the case for other nutrients, such as phosphorus (P) and potassium (K). Phosphorus can be released from the P-adsorption sites, whereas K can be released from the cation-exchange sites. Often the indigenous soil supply of nutrients is not enough for optimal crop production. Therefore, nutrients are added via inorganic and organic (compost, manure) fertilizers. Relatively young soils, e.g., un-weathered volcanic deposits or alluvial material, are the most fertile. Highly weathered and leached soils show nutrient deficiencies.

6.3 Biological nitrogen-fixation

Soybeans (*Glycine max*) belong to the family of *Leguminosae* or *Fabaceae*, sub-family *Papilionoideae*, tribe *Phaseoleae*. Leguminous crops live in symbiosis with nitrogen-binding bacteria. Often these are *Rhizobium* bacteria. For soybeans these are bacteria of the genus *Bradyrhizobium* (dominant), *Mesorhizobium* and *Sinorhizobium* (Giller, 2001). These bacteria are able to transform the gaseous (atmospheric) N_2 into N-ammonia, a form that can be used by the hosting crop. In formula, N-fixation is given by (Giller, 2001)

$$\mathrm{N_2 + 8H^+ + 8e^- + 16ATP \rightarrow 2NH_3 + H_2 + 16ADP + 16P_i} \tag{27}$$

The reaction is carried out by an enzyme known as nitrogenase. Some proteins serve as electron donors. N-ammonia will be further protonated to form N-NH_4^+ which can be assimilated by the host plant. N-fixation is energetically inefficient (it requires 16 ATP molecules), since the triple bond between the two nitrogen atoms needs to be broken[1]. Nitrogenase is a highly O_2-sensitive enzyme and the process may become irreversibly inactivated on exposure to atmospheric levels of O_2. The presence of other nitrogen sources will hinder the process of N-fixation: nodulation may be suppressed completely; the total nodule mass may be reduced; or the nitrogenase activity of mature nodules may be inhibited (Giller, 2001).

Often the nodulation occurs below-ground at the root hairs or roots. This means that in the surroundings of the roots there must be N_2-gas present. This gas comes from the atmosphere. Thus, there is a need for gas exchanges from the atmosphere to the rooted zone. Gas exchange occurs via the air-filled pore system. Therefore, too wet conditions need to be prevented, as well as the formation of crusts at the soil surface and dense layers inside the root zone.

The proportion of soybean N derived from N_2-fixation varies between the different studies (with low mineral N supply and ample P supply) and ranges from 12 to 100% (Giller, 2001), but in many studies this was >70%. This indicates that N_2-fixation can contribute significantly in the N supply for the plant. Peoples et al. (1995) reported percentages of N-fixation in the range 0 - 95%, which is equal to 0 - 450 kg N ha^{-1}. With protein levels of 20 - 40%, legume seeds have a high demand for N and up to 60 kg N ha^{-1} can be removed with every tonne of seed harvested (Peoples et al., 1995). For example, for a yield of two tonnes ha^{-1} this means at least 120 kg N ha^{-1} should come from N-fixation so that we can speak of any net benefit of biological N-fixation. For soybean final N-balances (N-fixation compared to N harvested) ranged from -132 to + 80 kg N ha^{-1} (Peoples et al., 1995).

From a literature review (covering the period 1966-2006) Salvagiotti et al. (2008) made the following observations:

- On average, 50–60% of soybean N demand was met by biological N-fixation. On average this corresponds to 111-125 kg N ha^{-1} (N-content in the grains ranges from 4 – 8%).
- N-fixation was not always enough to replace all N exported in the soybeans seeds. A negative partial N balance (fixed N in above-ground biomass minus N in seeds) was observed in 80% of the studies (mean: -40 kg N ha^{-1}). However, after applying a correction for N contribution from below-ground biomass the partial N balance was close to zero but still slightly negative (on average -4 kg N ha^{-1}). This gap tended to increase with increasing seed yields.
- Soybeans responded more to N-fertilization in situations with high yields (>4.5 ton ha^{-1}).
- The amount of N fixed decreased exponentially with increasing fertilizer N application, when the latter was applied at the soil surface or at shallow depths. When applied at greater depths, at later times, or by using slow-release fertilizers, N-fixation was much less hindered (see also Yinbo et al., 1997).
- There remains a need for studies looking at the interaction between N-fixation, N-fertilization and other management factors.

For the Argentinian Pampas region, Di Ciocco et al. (2011) reported from several studies that the N-fixation accounted for 20 to 55% of the plant N. Collino et al. (2015) determined N-fixation in the northern half of Argentina. The percentage of N by N-fixation in the above-ground part of soybean was on average 60% (interquartile range 46-71%). At high yields (>3.7 ton ha^{-1}) this fraction was correlated with effective rainfall during the fallow period and with the mean temperature during the seed-filling period. At lower yields it was correlated with the soil P-content, soil pH, and the effective rainfall during the vegetative period.

Nitrogen-fixation can be enhanced by adding (inoculating) *Rhizobium* bacteria to the soil.

In many studies with leguminous crops (including soybeans), it is observed that during and after the growth period the mineral N ($N-NO_3$) content increases. This attributed to a reduced use of soil nitrate ('nitrate-sparing'), the possible release of products of N- fixation from nodulated-roots, or from N mineralised from fallen leaves or roots and nodules lost during growth and development (Peoples et al., 1995).

---

[1] Producing nitrogen fertilizers also costs a lot of energy!

6.4 Phenological development for soybean

Simulation of phenological development in WOFOST 7.1 is based upon the phenological development pattern of a typical cereal plant. It is defined by a dimensionless variable called the Development Stage (DVS) where DVS equals zero at crop emergence, DVS equals one at anthesis (flowering) and DVS equals two at maturity. The development rate from one stage to the next is calculated from the daily average temperature adjusted for a base temperature and divided by the temperature sum needed to reach the next development stage: TSUM1 for the stage from emergence to anthesis and TSUM2 for the stage from anthesis to maturity. For long-day plants, such as cereals, WOFOST allows the impact of day-length on phenological development to be taken into account; limiting the development rate under conditions of too short day-length.

An important characteristic of the phenological development scheme used in WOFOST is that phenological development is essentially sequential. The plant undergoes a defined set of sequences, which do not overlap. This type of phenological development is typical for cereals and it is appropriate for tuber crops (potato, sugar beet), as well given that those crops have a very simple phenological development pattern. For tuber crops, the anthesis date does not correspond to flowering, but to the start of tuber development.

However, in the case of soybean the sequential phenological development scheme used by WOFOST 7.1 does not describe the growth stages of soybean very well, for several reasons:

- The phenological development of soybean is to a large extent parallel. Following the definition of soybean phenology by Fehr and Caviness (1977), the vegetative development of stems and leaves (the ‘V’ stages) runs parallel to the reproductive development of pods and seeds (The ‘R’ stages) for a considerable part of the growth cycle.
- The influence of temperature on the development rate of soybean is more complicated and cannot be simulated by accumulating the daily average temperature above a base temperature.
- In contrast to cereals, soybean is a short-day plant meaning that the phenological development rate of soybean accelerates under shorter day length. The short-day dependence of soybean cultivars is formalised in so-called ‘maturity groups’, which indicate the critical and optimal day-length for a given cultivar.

Therefore, an improved sub-model for phenological development in soybean in WOFOST was required. However, the principle of the development stage (DVS) cannot be eliminated from the WOFOST model completely, given that many internal variables and parameters rely on the DVS to receive an appropriate value. Thus, we developed a hybrid phenological development model that uses elements from established models for soybean phenology (SoyDev – Setiyono et al. 2007), but still applies the sequential DVS logic that is needed for WOFOST.

The new phenological development model contains the following elements:

1. It is defined as in Table 5, where DVS=0 means emergence, DVS=1.0 is equivalent to the R1-stage (*beginning of flowering*) and DVS=2.0 is equivalent to the R8 stage (*fully ripe*). There is an inconsistency with the definition of the partitioning scheme for WOFOST as defined by Van Heemst (1988). According to this source, it would be more logical set DVS=1 at the R3 stage (beginning of pod development). However, simulations demonstrated that this leads to a very low yield, which is lower than the observed values. Moreover, there are very few observations of R3 available. Therefore, we decided to match DVS=1 with the R1 stage (beginning of flowering).

2. The vegetative part from DVS=0 to 1 is driven by temperature and day length. It is simulated by a maximum development rate multiplied by a temperature reduction function, which is modelled as a beta function defined by an optimal temperature, *Topt,* where phenological development rate is maximal and the cardinal temperatures, *Tmin* and *Tmax,* below or above phenological development is halted (Figure 11 left, similar to Figure 3b Setiyono et al., 2007). The day-length effect is simulated as in Setiyono et al. 2007. This includes the empirical relation for dependency of the critical and optimal day-length on maturity group number (Figure 11 right, similar to Figure 4 in Setiyono et al. 2007).
3. The reproductive part from DVS=1 to 2 is simulated in the same way as the vegetative part except that another maximum development rate is used.

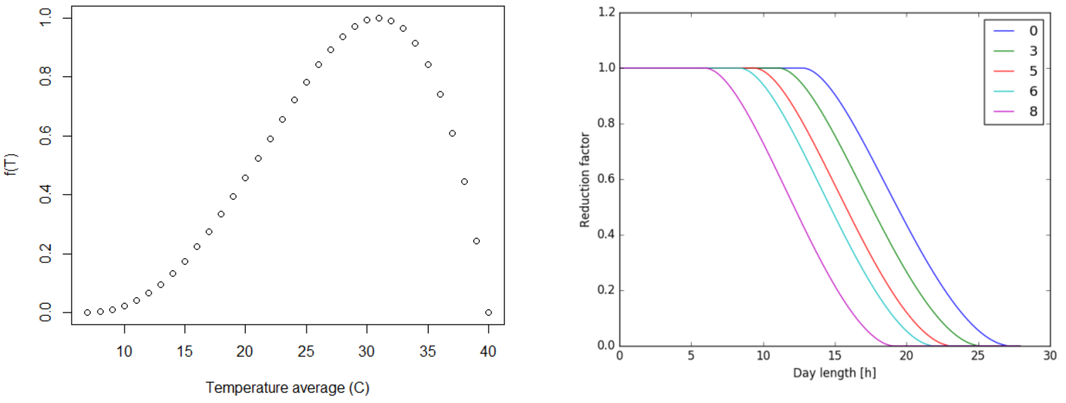


Figure 11 *Reduction factor as a function of the actual daily average Temperature according to Setiyono (2007) with Tmin=7, Tmax=40, Topt=31 gr C (left). Reduction factor as a function of day-length for several maturity groups (right)*

Calibration of the new WOFOST hybrid phenology is carried out using observed phenological stages for soybean, as provided by INTA. Application of WOFOST-soybean requires two parameters for calibration, these are the maximum development rate for the vegetative and reproductive stages (DVRMAX1 and DVRMAX2), which can be accomplished by minimising the differences between the observed and simulated R-stages (Table 5).

Table 5 *Relation between R-stages that are common to soybean phenology data and the WOFOST DVS-phenology*

Stage	WOFOST DVS	description
RA	N/A	Sowing
EMG	DVS = 0	Emergence
R0	N/A	Floral induction: not observable and no BBCH equivalent
R1	DVS = 1.0	Beginning of flowering, equivalent to DVS=1.0
R3	N/A	Beginning of pod development, no WOFOST equivalent
R5	DVS = 1.15	Beginning of seed development
R7	N/A	10% pods ripe, no WOFOST equivalent
R8	DVS = 2.0	Fully ripe.

7 Land management

The SWAP/WOFOST model, extended by the Soil-N module and descriptions for soybean development, enables the evaluation of the impacts of land-use and land-management on environmental factors. A number of management actions can be imposed by specification of parameters in the model's input files:

- Addition of organic manure (see par.7.4).
- Addition of inorganic fertilizers (see par.7.4).
- Crop rotations.
- Irrigation.
- Drainage.

A detailed discussion about management options for crop rotations, irrigation and drainage is given in the SWAP-manual (Kroes et al., 2009; Kroes et al, in prep).

Management of soybean

Soybean is produced in different (sub)tropical cropping systems, e.g. shifting cultivation, fallow system and permanent farming system. Soybean production is managed by (e.g. Woomer et al., 2014):

- Choosing the best variety. For example, Rotundu et al. (2014) analysed cultivars used in Argentina and USA for highest yield and highest N-uptake.
- Inoculating *Rhizobium* bacteria, in case not abundantly present in the soil.
- Other nutrients (e.g., P, micronutrients) and water must be present.
- Prevent build-up of soil nitrate: potentially lost via leaching; resulting in acidification (Peoples et al., 1995; p. 16-17).
- Integrated pest and disease management; but this should be done with care, e.g. not abundantly use high amounts of fungicides, herbicides (f.i. glyphosate) or pesticides.
- Planting density, intercropping, crop rotation.

Soil mulching may increase soil water availability and causes a decrease in soil temperature during the growing seasons (Siczek et al., 2015). Depending upon the actual weather conditions during the growing season, the yields of seeds, straw, protein and oil, as well as water productivity of soybean seed and biomass, were improved by mulching (Siczek et al., 2015). From other studies, it is generally observed that soil compaction has a negative effect on crop yields (e.g., Alakukku and Elonen, 1995; 1996).

The effect of climate change, typically the increase in temperature, may result in using a different type of soybean cultivar, e.g. a late-maturing cultivar (Kumagai and Sameshima, 2014). Hao et al. (2016) experimentally determined the effect of free-air CO_2-enrichment on N, P and K uptake of soybean in northern China. They concluded that at harvest, elevated CO_2 significantly increased N, P and K uptake in soybean seed and that more N, P and K input may be required to maintain the availability of these elements in the soil for soybean under future elevated CO_2 environments.

8 User’s manual

8.1 Model inputs

Model inputs for the simulation of nitrogen-limited crop growth are given in six files:

- A nitrogen section in the crop file (also input to the SWAP model) with extension .crp.
- A CO_2 section in the crop file (also input to the SWAP model) with extension .crp.
- Atmospheric concentrations of CO_2 in a separate input file named ‘atmospheric.CO2’.
- Three files for management events related to soil, extensions .sme, .smm, .snp.

The required and optional content of these input files is given in the next paragraphs of this chapter. There is one flag that initiates simulation of nitrogen-limited crop growth; this flag is given in the SWAP main input file with extension .swp (see paragraph 8.1.2).
To describe the input files in this paragraph, we have used data that originate from a field experiment in Argentina location Zavalla (Rotundo et al., 2014).

8.1.1 CO_2-changes

To simulate the impact of CO_2 on crop growth one has to:

1. Activate a flag in the input file with extension .crp (Box 8.1.1.1).
2. Enter crop-specific relations in input file with extension .crp (Box 8.1.1.2).
3. Enter the actual CO_2 concentration in the atmosphere in an input file with extension .CO2 (Box 8.1.1.3).

*Box 8.1.1.1 CO2-concentration defined in the input file *.CRP, Section CO2.*

```
** CO2-impact:
FLCO2 = .TRUE. ! Switch/flag for application of CO2 correction [Y=.TRUE.]
```

Box 8.1.1.2 Relations between CO2 and Amax, Eff and Tra defined in the input file *.CO2, Section part ...

```
* correction of photosynthesis as a function of atmosph. CO2 concentration (-)
* correction of radiation use efficiency as a function of atmosph. CO2concentration (-)
* correction of transpiration as a function of atmosph. CO2 concentration (-)
* values for C3 crops (potatoes, grassland, soybean)
CO2AMAXTB  =  40.,  0.0,   ! multiplication factor for AMAX
             360.,  1.0,  ! to account for an increasing CO2 concentration
             720.,  1.6,
            1000.,  1.9,
            2000.,  1.9

CO2EFFTB   =  40.,  0.00,   ! multiplication factor for EFF
             360.,  1.00,  ! to account for an increasing CO2 concentration
             720.,  1.11,
            1000.,  1.11,
            2000.,  1.11

CO2TRATB   =  40.,  0.0,   ! multiplication factor for maximum transpiration rate TRAMX
             360.,  1.0,  ! to account for an increasing CO2 concentration
             720.,  0.9,
            1000.,  0.9,
            2000.,  0.9
**  actual CO2 concentration in atmosphere [ppm] in separate file  Atmosferic.co2
```

Box 8.1.1.3 ! actual CO2 concentration in atmosphere [ppm] in this input file with the name atmospheric.CO2

```
* ---------------------------------------------
* Filename: Atmosferic.co2
*
* Contents: CO2 (micromol/mol or ppm per year)
*           for each simulation year a value must be given.
* Source:
* 1. from 1959-2015 :
*    NOAA (www.esrl.noaa.gov/gmd/ccgg/trends/)
*    Manua Loa observations
*    Data from March 1958 through April 1974 have been obtained by C. David Keeling
*    of the Scripps Institution of Oceanography (SIO) and were obtained from the
*    Scripps website (scrippsco2.ucsd.edu).
*
*    The estimated uncertainty in the annual mean is the standard deviation
*    of the differences of annual mean values determined independently by
*    NOAA/ESRL and the Scripps Institution of Oceanography.
*
* ---------------------------------------------
 CO2year CO2ppm   CO2unc
  1959   315.97     0.12
  1960   316.91     0.12
  1961   317.64     0.12
  1962   318.45     0.12
  1963   318.99     0.12
  1964   319.62     0.12
  1965   320.04     0.12
  1966   321.38     0.12
  1967   322.16     0.12
  1968   323.04     0.12
  1969   324.62     0.12
  1970   325.68     0.12
  1971   326.32     0.12
  1972   327.45     0.12
  1973   329.68     0.12
  1974   330.18     0.12
  1975   331.08     0.12
  1976   332.05     0.12
  1977   333.78     0.12
  1978   335.41     0.12
  1979   336.78     0.12
  1980   338.68     0.12
  1981   340.10     0.12
  1982   341.44     0.12
  1983   343.03     0.12
  1984   344.58     0.12
  1985   346.04     0.12
  1986   347.39     0.12
  1987   349.16     0.12
  1988   351.56     0.12
  1989   353.07     0.12
  1990   354.35     0.12
  1991   355.57     0.12
  1992   356.38     0.12
  1993   357.07     0.12
  1994   358.82     0.12
  1995   360.80     0.12
  1996   362.59     0.12
  1997   363.71     0.12
  1998   366.65     0.12
  1999   368.33     0.12
  2000   369.52     0.12
  2001   371.13     0.12
  2002   373.22     0.12
  2003   375.77     0.12
  2004   377.49     0.12
  2005   379.80     0.12
  2006   381.90     0.12
  2007   383.76     0.12
  2008   385.59     0.12
  2009   387.37     0.12
  2010   389.85     0.12
  2011   391.63     0.12
  2012   393.82     0.12
  2013   396.48     0.12
  2014   398.61     0.12
  2015   400.83     0.12
```

8.1.2 Nitrogen in crop and soil

To simulate the carbon and nitrogen in soil one has to:

1. Activate a flag in the input file with extension .swp (Box 8.1.2.1).
2. Enter crop-specific parameters in input file with extension .crp (Box 8.1.2.2).

Box 8.1.2.1 Switch for simulation of Nitrogen in Crop and Soil defined in the input file *.SWP, CROP Section

```
* flag for nitrogen in crop and soil ***
flCropNut = .TRUE.
```

Data for parameters related to nitrogen use by the crop can be found in the database belonging to Lintul4 (http://models.pps.wur.nl/models, see also Wolf, 2012).

Box 8.1.2.2 Parameters for simulation of Nitrogen in Crop defined in the input file *.CRP, MANAGEMENT Section.

```
** nitrogen use
* Data from: Linutl4,  http://models.pps.wur.nl/models
*                         param values from SOY0902.DATo
*       reference:     Wolf, J. (2012). Users guide for LINTUL4 and LINTUL4V:
*                       Simple generic model for simulation of crop growth under
*                       potential, water limited and nitrogen limited conditions.
*                       WUR-PPS report (Vol. 4).
RDRNS    = 0.05     ! max. relative death rate of leaves due to N stress
DVSNLT   = 2.0      ! development stage above which no crop nitrogen uptake does occur
DVSNT    = 0.8      ! development stage above which nitrogen translocation to storage organs does occur
FNTRT    = 0.15     ! nitrogen translocation from roots as a fraction of total N amount translocated from leaves and
stems
FRNX     = 0.5      ! optimal N concentration as fraction of maximum N concentration
LRNR     = 0.50     ! maximum N concentration in roots as fraction of maximum N concentration in leaves
LSNR     = 0.50     ! maximum N concentration in stems as fraction of maximum N concentration in leaves
NLAI     = 1.0      ! coefficient for the reduction due to N stress of the LAI increase (during
juvenile phase)
NLUE     = 1.1      ! coefficient for the reduction of RUE due to  Nitrogen stress
NMAXSO   = 0.062    ! maximum N concentration (= 1.6*min. N conc.) in storage organs [kg N kg-1 dry
biomass]
NPART    = 1.0      ! coefficient for the effect of N stress on leaf biomass reduction
NSLA     = 0.5      ! coefficient for the effect of N stress on SLA reduction
RNFLV    = 0.00933  ! residual N fraction in leaves [kg N kg-1 dry biomass]
RNFST    = 0.00467  ! residual N fraction in stems [kg N kg-1 dry biomass]
RNFRT    = 0.00467  ! residual N fraction in roots [kg N kg-1 dry biomass]
TCNT     = 10.0     ! time coefficient for N translocation to storage organs [days]
NFIXF    = 0.80     ! fraction of crop nitrogen uptake by biological fixation [-]
NMXLV    =  0.0, 0.06,   ! maximum N concentration in leaves as function of development stage [kg N kg-1 dry
biomass]
            0.4, 0.040,
            0.7, 0.035,
            1.0, 0.030,
            2.0, 0.0293,
            2.1, 0.0293

! Harvest losses of organic matter ! [0.0..1.0 kg.kg-1 DM, R]
FraHarLosOrm_lv = 0.5   ! fraction harvest losses of organic matter from leaves
FraHarLosOrm_st = 0.5   ! fraction harvest losses of organic matter from stems
FraHarLosOrm_so = 0.01  ! fraction harvest losses of organic matter from storage organs
```

8.1.3 Maturity groups in soybean

To simulate phenological conditions using the concept of maturity groups, one must:

1. Activate a switch in the input file with extension .crp (Box 8.1.3.1).
2. Enter crop-specific parameters in input file with extension .crp (Box 8.1.3.2).

Box 8.1.3.1 Switch for use of Maturity Groups in the input file *.CRP

```
* Part 2: Maturity group, special for soybean  SWSOYBEAN = [0,1], 0=No, 1=Yes

  SWSOYBEAN = 1
```

Box 8.1.3.2 Parameters for us of Maturity Groups defined in the input file *.CRP

```
* Part 2.1: Maturity group parameters, specifically for soybean (SWSOYBEAN=1)

  MG =  4.5            ! select Maturity Group MG [0.5..6.0,-, R]
  DVSI =     0.0       ! Initial development stage [0.0 .. 2.0,- , R]
  DVRMAX1 =  0.0545    ! max development rate from emergence to anthesis [0.0..1.0,C/d, R]
  DVRMAX2 =  0.0221    ! max development rate from anthesis to maturity [0.0..1.0,C/d, R]
  TMAXDVR = 40.0       ! maximum temperature development rates [0.0 .. 45.0, C, R]
  TMINDVR =  7.0       ! minimum temperature development rates [0.0 .. TMAX, C, R]
  TOPTDVR = 31.0       ! optimum temperature development rates [TMIN .. TMAX, C, R]
  DVSEND =   2.00      ! development stage at harvest [-]
  ANGLE =   -0.83      ! solar elevation angle [-3.0..0.0, degr, R]
```

8.1.4 Management events related to soil

The Soil-N module requires three input files additional to the files for a regular SWAP / WOFOST run:

1. Soil Management Event parameters in an input file with extension .sme (Box 8.1.4.1).
2. Soil Management Materials in an input file with extension .smm (Box 8.1.4.2).
3. Soil Nitrogen Parameters in the input file *.snp (Box 8.1.4.3).

The filename should correspond to the project-name defined in the general input file with extension .swp (Kroes et al., 2009; Kroes et al, in prep)).

The ‘project’.sme file contains information about soil management events, such as the date of a fertilization event, the material number, the dosage and the fraction of the ammonium volatilised. A further explanation of the input is given as comment in the text box 8.1.4.1.

Box 8.1.4.1 Define Soil Events in the input file *.sme

```
**********************************************************************************
* Comment:
* Case: Zavalla - field 25e
* An example with input values that are beyond the simulation period
* In this there are no soil management events (no tillage soybean)
* and the fertilizer is not applied because the dates are later then
* the end of the simulation period
**********************************************************************************

* Soil management events:
* (smedate(1) must be after start of simulation !!)
    smedate    MatNum Dosagekgha VolatFraction
     01-nov-2023    10    25.    0.0
     01-dec-2023    10    50.    0.0
     01-jan-2024    10    25.    0.0
!  smedate:       date (dd-mmm-yyyy) of fertilizer application or amendment of a
!                 certain material (organic waste, residue) preferably in ascending
!                 order. Take notice: specification of events out of the range of
!                 the simulation period can cause errors. If different materials are
!                 amended, specify them on individual records. Multiple records for
!                 the same day can be specified.
!  Matnum:        Number of the material amended at the date specified. The number
!                 refers to the definition of materials in the snm-file
!  Dosagekgha:    dosage (kilogram per hectare) of the application
!  VolatFraction: fraction of the ammonium-N that is lost at the time of application
!                 by volatilization. Take notice of the fact that volatilization
!                 afterwards is not included in the model. If volatilization is
!                 expected to occur, it should be described as an instantaneous
!                 process at the time of application.
!                 If the ammonium-N content of the material equals zero, a dummy-
!                 value should be specified.
* End of input file .sme!
```

The ‘project’.smm file contains parameters to characterise the materials involved in additions to the soil. The file has a comma-separated layout. A further explanation of the input is given as comment in the text box 8.1.4.2.

Box 8.1.4.2 Definition of Materials in the input file *.smm

```
**********************************************************************************
* Filename: Zavalla.smm
* Contents: Soil Management Material Definitions
**********************************************************************************
* Comment area:
* Case: Zavalla - soybean
**********************************************************************************
* soil management material definitions
MatNum ,   MatName              , AppAge,OrgMatFrac, OrgNFrac,  NH4NFrac,NO3NFrac
    1  ,  'Cattle manure'       ,  3.16  ,  0.150  ,  0.035  ,  0.0012  ,  0.0000
    2  ,  'Pig manure'          ,  1.36  ,  0.161  ,  0.037  ,  0.0015  ,  0.0000
    3  ,  'Poultry manure'      ,  1.36  ,  0.376  ,  0.058  ,  0.0024  ,  0.0000
    4  ,  'Cattle slurry'       ,  3.16  ,  0.064  ,  0.034  ,  0.0022  ,  0.0000
    5  ,  'Pig slurry'          ,  1.36  ,  0.060  ,  0.050  ,  0.0042  ,  0.0000
    6  ,  'Poultry slurry'      ,  1.36  ,  0.093  ,  0.047  ,  0.0058  ,  0.0000
    7  ,  'Compost'             ,  1.96  ,  0.190  ,  0.041  ,  0.0008  ,  0.0000
    8  ,  'Champost'            ,  1.36  ,  0.220  ,  0.025  ,  0.0003  ,  0.0000
    9  ,  'Urea'                ,  0.00  ,  0.460  ,  0.000  ,  0.4600  ,  0.0000
   10  ,  'Mineral N fertilizer',  0.00  ,  0.000  ,  0.000  ,  0.5000  ,  0.5000
   11  ,  'Green leaves'        ,  0.92  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   12  ,  'Overground crop res.',  0.99  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   13  ,  'Root + stubble res.' ,  1.57  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   14  ,  'Grass shoots'        ,  0.92  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   15  ,  'Grass roots'         ,  1.20  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   16  ,  'Tree leaves'         ,  2.25  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000
   17  ,  'Spruce needles'      ,  3.34  ,  1.000  ,  0.000  ,  0.0000  ,  0.0000

! MatNum      Number of the material. In the sme file for specification of events
!             and dosages, the material is referred to MatNum in this snm-file.
! MatName     Name of the material. This character string is used for assisting the
!             user and for clarification of materials and events in the model output
! AppAge      Apparent Age parameter (year) in the Janssen's one parameter organic
!             matter decay model.
! OrgMatFrac  Organic Matter weight fraction of the material defined. (kilogram
!             organic matter per kilogram total weight)
! OrgNFrac    Nitrogen fraction of the organic matter (kilogram nitrogen per
!             kilogram organic matter)
! NH4NFrac    Ammonium-N fraction of the material defined. (kilogram Ammonium-N per
!             kilogram total weight). Nearly all crop residues do not contain
!             Ammonium-N.
! NO3NFrac    Nitrate-N fraction of the material defined. (kilogram Nitrate-N per
!             kilogram total weight). Most of the organic fertilizers does not
!             contain nitrate, but most of the mineral fertilizers contain nitrate.
!             Grass shoots of heavily fertilized grassland can contain a small
!             quantity of nitrate in the fresh biomass
* End of input file .smm!
```

The ‘project’.snp file comprises the initial values of the state variables, boundary concentrations and parameters.
The file has a SWAP compliant layout that can be read by TTUTIL procedure.
An example for the soybean case in Zavalla is given in Box 8.1.4.3.
A description of input of soil schematisation, soil organic matter and soil nitrogen input is given for an example in Annex A.

Box 8.1.4.3 Define Soil Nitrogen Parameters in the input file *.snp

```
* Filename: Zavalla.snp
* Contents: Soil Nutrient Parameters
**********************************************************************************
* Comment area:
*
* Case: Zavalla - field xxx
*
**********************************************************************************
* soil nutrient parameters

* initial state variables of soil organic matter pools,
* ammonium-N liquid concentration and nitrate-N liquid concentration

FOM1_t = 0.0476
FOM2_t = 0.2141
FOM3_t = 0.0238
FOM4_t = 0.0238
FOM5_t = 0.3093
FOM6_t = 0.3569
FOM7_t = 0.3093
FOM8_t = 0.3093
Bio_t    = 0.3093
Hum_t    = 21.8868
cNH4_t   = 0.001
cNO3_t   = 0.010
!-----------------------------------------------------------------------------------------
!             Pool     Assimilation value   N-content value      Proposed initial fraction
!                                                                    of Soil Organic Matter
!-----------------------------------------------------------------------------------------
!   FOM1_t    DPM      Minimum              Minimum              0.2%
!   FOM2_t    DPM      Minimum              Maximum              0.9%
!   FOM3_t    DPM      Maximum              Minimum              0.1%
!   FOM4_t    DPM      Maximum              Maximum              0.1%
!   FOM5_t    RPM      Minimum              Minimum              1.3%
!   FOM6_t    RPM      Minimum              Maximum              1.5%
!   FOM7_t    RPM      Maximum              Minimum              1.3%
!   FOM8_t    RPM      Maximum              Maximum              1.3%
!   BIO_t     BIO                                                1.3%
!   HUM_t     HUM                                               92.0%
!-----------------------------------------------------------------------------------------
! FOM1_t ..FOM8_t, Bio_t and  Hum_t are expressed in kg organic matter per m3 soil
! The sum of FOM1_t until FOM8_t + Bio_t + Hum_t should be equal to Soil Organic Matter
!             content (expressed in kg SOM per kg soil) multiplied by dry bulk density
!             (kg soil per m3 soil volume)
! Initially,  the total of the organic matter present in soil should be attributed to the
!             ten pools.
! Then, a pre-run is advised by which the model simulates the distribution of organic
!             matter, as expressed by the pools' contents.
! The final distribution is given in the PROJECT_nut.end file.
! The pre-run can be repeated a number of times. If the fractional distribution of the
!             pools seems to be stable, the repetition of pre-runs can be stopped.
! This final fractional distribution can be used to assign the initial values.

! cNH4_t :    NH4-N concentration in soil moisture (kg per m3 water volume)
! cNO3_t :    NO3-N concentration in soil moisture (kg per m3 water volume)
! If the method of pre-runs is applied, as proposed for organic matter pools, the final
! concentrations as given in the PROJECT_nut.end file can be used.
```

```
*** boundary concentrations

cNH4N_top  = 0.0025 ! half of annual N-deposition input as NH4N in rain
cNH4N_lat  = 0.0
cNH4N_seep = 0.0
cNO3N_top  = 0.0025 ! half of annual N-deposition input as NO3N in rain
cNO3N_lat  = 0.0
cNO3N_seep = 0.0

! cNH4N_top : NH4-N total deposition expressed by the NH4-N concentration in rain. This
!             concentration should be calculated from the total NH4-N deposition divided
!             by the precipitation amount.
!             If the NH4-N deposition is specified by mol nitrogen per hectare per year
!             and the precipitation amount by millimeter per year, the concentration is
!             calculated by: cNH4N_top = 0.0014 * NH4-N deposition / precipitation amount.
!             If only the total nitrogen deposition is known, we propose to take half of
!             the total deposition.
! cNH4N_lat : NH4-N concentration in lateral inflowing water from irrigation canals, or
!             upstream adjacent fields.
!             If no surface irrigation is applied, or runon from  upstream adjacent fields
!             appears, this boundary condition variable can be set to zero.
! cNH4N_seep: NH4-N concentration in upward seeping water at the bottom the root zone
!             profile. In this simulation module, the depth of the root zone is specified
!             by dz_WSN.
!             Take notice that the capillary rise also transports solutes from the deeper
!             soil layer to the root zone profile. If no information is available about
!             this concentration, the value can be set to zero, but it is advised to check
!             for the NH4-N concentrations in leaching water in periods which precede the
!             periods in which the capillary rise occurs. Check for NH4_out, divided by
!             WFl_Out, in the PROJECT_nut.csv file.
! cNO3N_top : NO3-N total deposition expressed by the NO3-N concentration in rain:
!             cNO3N_top = 0.0014 * NO3-N deposition / precipitation amount.
!             If only the total nitrogen deposition is known, we propose to take half of
!             the total deposition.
! cNO3N_lat : NO3-N concentration in lateral inflowing water from irrigation canals, or
!             upstream adjacent fields.
!             If no surface irrigation is applied, or runon from  upstream adjacent fields
!             appears, this boundary condition variable can be set to zero.
! cNO3N_seep: Similar to cNH4N_seep, cNO3N_seep is the concentration in upward seeping
!             water (incl. capillary rise) at the bottom the root zone profile. If no
!             information is available about this concentration, the value can be set to
!             0, but check for NO3_out, divided by WFl_Out, in the PROJECT_nut.csv file.

*** Coefficients and rate constants
Temp_ref          = 10.0
SorpCoef          = 0.0005
RateConNitrif_ref = 1.0
RateConDenitr_ref = 0.06

! Temp_ref :  Reference temperature at which the transformation rates have been
!             stablished. The temperature response of transformation rates is accounted
!             for by an equation given by Rijtema et al (1999). The response factor reads
!             as:
!             Response factor = { 1/(1+exp(-0.26*(Temp-17.0))) - 1/(1+exp(-0.77*(Temp-
41.9))) } /
!                             {1/(1+exp(-0.26*(Temp_ref-17.0)))-1/(1+exp(-0.77*(Temp_ref-
41.9)))}
!             If no information is available, the mean annual air temperature can be taken
!             as a default. The variable can be established by an optimization procedure.
! SorpCoef :  Ammonium sorption coefficient. Ammonium sorption is described by a linear
!             relation. The coefficient is expressed in m3 soil water per kg soil. The
!             retardation of the ammonium-N migration in soil is expressed as
!             Retardation = 1 + sorption coefficient * dry bulk density / moisture volume
fraction
!             Values of SorpCoef = 0.0005, dry bulk density = 1200 kg per m3 soil and
!             moisture volume fraction = 0.3 leads to Retardation = 3. This value is
!             somewhat high, but within the range of expected values. If the retardation
!             of ammonium migration is soils is known, then the coefficient can be
```

```
!             calculated from:
!             Sorption coefficient = (Retardation - 1) * moisture volume / dry bulk density
!             Simulation results appear to have a minor sensitivity to this coefficient.
! RateConNitrif_ref : Nitrification rate constant established at the reference
!             temperature, expressed in 1/day
! RateConDenitr_ref : Denitrification rate constant established at the reference
!             temperature, expressed in 1/day

*** Response function parameters

WFPSCrit   = 0.95
WFPScrit2  = 0.7
CdissiHalf = 0.001

! WFPSCrit :  critical water filled pore space value for organic matter transformation. At
!             very wet conditions (water filled pore space > WFPScrit) the transformation
!             rate is reduced. Between WFPS = WFPScrit and WFPS = 1, the  response
!             function is expressed by a second order polynomial. At WFPS = WFPScrit the
!             response function takes the value 6.*WFPS**2/(1.+9.*WFPS**4) and at WFPS = 1
!             it takes the value 0.01.
! WFPScrit2 : critical water filled pore space value for the denitrification rate. At WFPS
!             > WFPScrit2 the response function is calculated according to:
!             ((WFPS-WFPScrit2)/(1.0d0-WFPScrit2))**2. For values smaller than WFPScrit2,
!             the response values is set to zero.
! CdissiHalf : parameter in the denitrification response function for the respiration
!             activity in soil, expressed in kilogram carbon per m2. When the
!             dissimilation rate of soil organic matter is low, the demand for
!             nitrate-oxygen is also low and the denitrification rate is limited by the
!             dissimilation rate. The dissimilation rate is calculated from the
!             transformations of the organic matter pools. The response function reads as:
!             response = carbon dissimilation / (parameter + carbon dissimilation).
!             It should be noted that the parameter is specified in kg carbon per 2.
!             The choice for other values of the depth of the effective soil layer dz_WSN
!             influences the response values.

*** Soil supply uptake parameter

TCSF_N = 0.15
! TCSF_N :    Transpiration concentration stream factor. When the ammonium concentration
!             in soil moisture is rate limiting, the NH4-N uptake by plant roots is
!             calculated according to:
!             Uptake = TCSF_N * (moisture volume fraction + dry bulk density * SorpCoef) /
!             (moisture volume fraction) * transpiration flux * ammonium concentration,
!             expressed in kg per m2
!             When the ammonium concentration in soil moisture is rate limiting, the NH4-N
!             uptake by plant roots is calculated according to:
!             Uptake = TCSF_N * transpiration flux * ammonium concentration, expressed in kg
per
!             m2. The vlaue for TCSF_N is dependent on soil type and the rooting pattern
!             of the crop. For the simulation of nitrogen uptake responses to the
!             availability of nitrogen (fertilization field trials), this parameter is
!             calibrated.
!LaiCritNupt = 0.1
! LaiCritNupt : Critical LAI value to calculate uptake rate based on the ammonium
availability
!              For the simulation of nitrogen uptake responses to the availability of
nitrogen
!               (fertilization field trials), this parameter may be calibrated.
!              This parameter is optional and may be left out if the hydrological and crop
!              growth submodels are well tuned or if uptake at very low transpiration rates
is
!              unlimited
!
* Effective depth of soil layer
dz_WSN = 1.0
! dz_WSN :    Thickness of the soil layer considered for the simulation of the soil
!             organic matter and nitrogen dynamics. The model is based on a single layer
!             approach and it should be noted that stratification of properties and
```

```
!             process rates cannot be accounted for in this approach. The thickness mainly
!             depends on the crop type. For high production grassland dz_WSN could be set
!             to 0.3, whereas for winter wheat this parameter is much larger (e.g. 1.0 m).
!             Water balance items resulting from the SWAP model are aggregated and
!             recalculated for the single layer model.
* End of input file .snp!
```

8.2 Model outputs

8.2.1 Crop dry matter

The biomass organic matter (OM) balances (par. 5.2) of the crops are exported to two output files with extensions *.om1 and *.om2.

The *.om1 file provides information about the dry matter increase per time step of different plant parts. The header information is given in Records 1-8. From Record 9 until the end of the file, the information is given in a comma separated value layout. The output comprises:

- Date (dd-mmm-yyyy)
- Daynr: Julian day number (-)
- Daycrp: Day number after the start of the crop (-)
- DVS: crop development stage (-)
- TSUM: Temperature sum from cropstart (^{o}C d)
- Gass: Gross assimulation (kg ha^{-1})
- mres: Total maintenance respiration for actual crop (kg ha-1)
- OMroots: Dry matter increase of living roots (kg ha^{-1})
- OMleaves: Dry matter increase of leaves (kg ha^{-1})
- OMstems: Dry matter increase of stems (kg ha^{-1})
- OMstorage: Dry matter increase of storage organs (kg ha^{-1})
- Dmi: dry matter increase (kg ha^{-1})
- cvf: factor used in wofost to calculate the increase in biomass (dmi) from the net assimilation of the whole plant (asrc); dmi = cvf*asrc.
- OMcheck: balance deviation (kg ha^{-1})

The *.om2 file provides information about cumulative amounts of dry matter in different plant parts and increments. The layout of file is similar to the *.om1 file. The following items are given for each record:

- Date (dd-mmm-yyyy)
- Daynr: Julian day number (-)
- Daycrp: Day number after the start of the crop (-)
- DVS: crop development stage (-)
- TSUM: Temperature sum from cropstart (^{o}C d)
- storagediff (kg ha^{-1}): (wlv+wst+wso+wrt) at new time level - (wlv+wst+wso+wrt) at previous time level
- wlv: weight of leaves (kg ha^{-1})
- wst: weight of stems (kg ha^{-1})
- wso: weight of storage organs (kg ha^{-1})
- wrt: weight of roots (kg ha^{-1})
- grlv: growth rate of leaves (kg ha^{-1} d^{-1})
- grst: growth rate of stems (kg ha^{-1} d^{-1})
- grso: growth rate of storage organs (kg ha^{-1} d^{-1})
- grrt: growth rate of roots (kg ha^{-1} d^{-1})
- ombalan (kg ha^{-1}) : balance checked by difference of (wlv+wst+wso+wrt) = (grlv+grst+grso+grrt)*delt – (drlv+drst+drso+drrt)*delt
- drlv: death rate of leaves (kg ha^{-1} d^{-1})
- drst: death rate of stems (kg ha^{-1} d^{-1})
- drso: death rate of storage organs (kg ha^{-1} d^{-1})
- drrt: death rate of roots (kg ha^{-1} d^{-1})

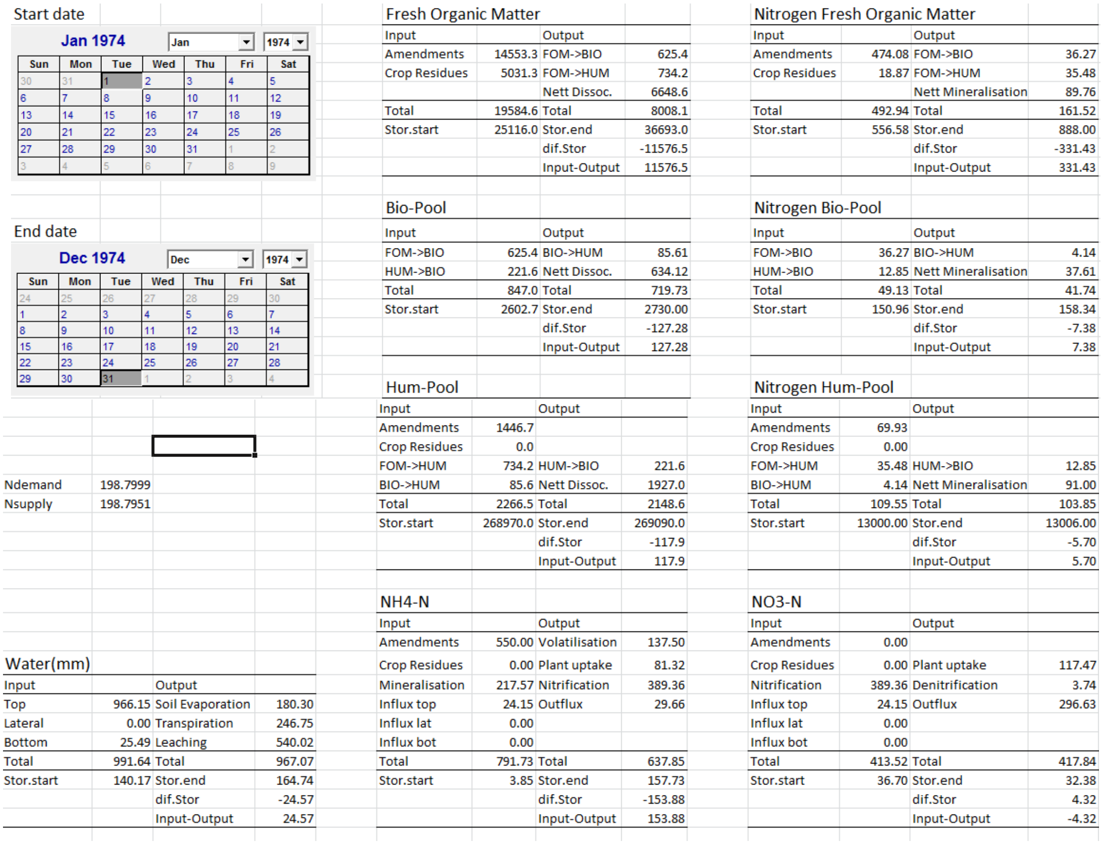
8.2.2 Soil nutrient balances

The resulting organic matter and nitrogen balance of the soil is given in a file with extension *_nut.csv. The header information is given in Records 1-7. From Record 8 until the end of the file, the information is given in a comma separated value layout. The output comprises the following variables:

Date	date (dd-mmm-yyyy)
Day	Julian daynumber (-)
Dcum	day number since start of simulation (-)
FOM_old	amount fresh OM at start of time step
FOM_end	amount fresh OM at end of time step (kg ha^{-1})
FOM_dif	FOM_old – FOM_end (kg ha^{-1})
FOM_add	fresh OM amended as manure / fertilizer (kg ha^{-1})
FOM_cres	fresh OM amended as crop residue (kg ha^{-1})
FOM2Bio	transformation of fresh OM into BIO pool (kg ha^{-1})
FOM2Hum	transformation of fresh OM into BIO pool (kg ha^{-1})
FOM_dis	total Fresh OM dissociation (kg ha^{-1})
Bio_old	amount BIO-pool at start of time step (kg ha^{-1})
Bio_end	amount BIO-pool at start of end step (kg ha^{-1})
Bio_dif	Bio_old – Bio_end (kg ha^{-1})
Bio2Bio	transformation of BIO pool into BIO pool (kg ha^{-1})
Bio2Hum	transformation of BIO pool into HUM pool (kg ha^{-1})
Bio_dis	total Bio-pool dissociation (kg ha^{-1})
Hum_old	amount HUM-pool at start of time step (kg ha^{-1})
Hum_end	amount HUM-pool at start of time step (kg ha^{-1})
Hum_dif	Hum_old – Hum_end (kg ha^{-1})
Hum_add	Manure/fertilizer amendment to Hum-pool (kg ha^{-1})
Hum_cres	Crop residue amendment to Hum-pool (kg ha^{-1})
Hum2Bio	Transformation of HUM into BIO-pool (kg ha^{-1})
Hum2Hum	Transformation of HUM into HUM-pool (kg ha^{-1})
Hum_dis	Total dissociation of HUM-pool (kg ha^{-1})
cDissi	Carbon dissimilation of combined pools (kg ha^{-1} C)
NFOM_old	Fresh organic matter nitrogen at t_0 (kg ha^{-1} N)
NFOM_end	Fresh organic matter nitrogen at $t_0+\Delta t$ (kg ha^{-1} N)
NFOM_dif	NFOM_old – NFOM_end (kg ha^{-1} N)
NFOM_add	NFOM amended by manure/fertilizer (kg ha^{-1} N)
NFOM_cres	NFOM amended by crop residues (kg ha^{-1} N)
NFOM2Bio	N released from NFOM incorpor. in BIO (kg ha^{-1} N)
NFOM2Hum	N released from NFOM incorpor. in HUM (kg ha^{-1} N)
NFOM_min	NFOM mineralised to NH_4-N (kg ha^{-1} N)
NBio_old	Bio-pool nitrogen at t_0 (kg ha^{-1} N)
NBio_end	Bio-pool nitrogen at $t_0+\Delta t$ (kg ha^{-1} N)
NBio_dif	NBio_old – NBio_end (kg ha^{-1} N)
NBio2Bio	N released from BIO incorpor. in BIO (kg ha^{-1} N)
NBio2Hum	N released from BIO incorpor. in HUM (kg ha^{-1} N)
NBio_min	NBio mineralised to NH_4-N (kg ha^{-1} N)
NHum_old	Hum-pool nitrogen at t_0 (kg ha^{-1} N)
NHum_end	Hum-pool nitrogen at $t_0+\Delta t$ (kg ha^{-1} N)
NHum_dif	NHum_old – NHum_end (kg ha^{-1} N)
NHum_add	NHum amended by manure/fertilizer (kg ha^{-1} N)
NHum_cres	NHum amended by crop residues (kg ha^{-1} N)
NHum2Bio	N released from HUM incorpor. in BIO (kg ha^{-1} N)
NHum2Hum	N released from HUM incorpor. in HUM (kg ha^{-1} N)
NHum_min	NHum mineralised to NH_4-N (kg ha^{-1} N)
Nminer	N-mineralisation of combined pools (kg ha^{-1} N)

NH4_old	NH_4-N amount in soil at t_0 (kg ha^{-1} N)
NH4_end	NH_4-N amount in soil at $t_0+\Delta t$ (kg ha^{-1} N)
NH4_dif	NH4_old - NH4_end (kg ha^{-1} N)
NH4N_amend	NH_4-N amended by manure/fertilizer (kg ha^{-1} N)
NH4N_cres	NH_4-N amended by crop residues (kg ha^{-1} N)
NH4_intop	NH_4-N influx at top of soil layer (kg ha^{-1} N)
NH4_inlat	NH_4-N lateral influx into soil layer (kg ha^{-1} N)
NH4_inbot	NH_4-N influx at bottom of soil layer (kg ha^{-1} N)
NH4_upt	NH_4-N plant uptake from soil layer (kg ha^{-1} N)
NH4_out	NH_4-N outflux from soil layer (kg ha^{-1} N)
NH3N_volat	NH_4-N lost by volatilisation (kg ha^{-1} N)
NH4_nitrif	NH_4-N nitrified to NO_3-N (kg ha^{-1} N)
NO3_old	NO_3-N amount in soil at t_0 (kg ha^{-1} N)
NO3_end	NO_3-N amount in soil at $t_0+\Delta t$ (kg ha^{-1} N)
NO3_dif	NO3_old – NO3_end (kg ha^{-1} N)
NO3N_amend	NO_3-N amended by manure/fertilizer (kg ha^{-1} N)
NO3N_cres	NO_3-N amended by crop residues (kg ha^{-1} N)
NO3_intop	NO_3-N influx at top of soil layer (kg ha^{-1} N)
NO3_inlat	NO_3-N lateral influx into soil layer (kg ha^{-1} N)
NO3_inbot	NO_3-N influx at bottom of soil layer (kg ha^{-1} N)
NO3_upt	NO_3-N plant uptake from soil layer (kg ha^{-1} N)
NO3_out	NO_3-N outflux from soil layer (kg ha^{-1} N)
NO3_denitr	NO_3-N denitrified to gaseous N_2 (kg ha^{-1} N)
Ndemand	Demand of crop for mineral N (kg ha^{-1} N)
Nsupply	N supplied from soil to meet demand (kg ha$^{-1)}$
WVol_old	Soil water volume per areal unit at t_0 (mm)
WVol_end	Soil water vol. per areal unit at $t_0+\Delta t$ (mm)
WVol_dif	WVol_old - WVol_end (mm)
WFl_inTop	Water inflow at top in time increment (mm)
WFl_inLat	Lateral water inflow in time increment (mm)
WFl_inBot	Water inflow at bottom in time increment (mm)
WFl_Eva	Water outflow by soil evaporation (mm)
WFl_Tra	Water amount extracted by crop (mm)
WFl_Out	Water outflow over soil layer boundaries (mm)
Idwrt	Org. matter amendm. by dead roots (kg ha^{-1})
Idwlv	Org. matter amendm. by dead leaves (kg ha^{-1})
Idwst	Org. matter amendm. by dead stems (kg ha^{-1})
iNLOSSL	Nitrogen amendment by dead leaves (kg ha^{-1})
iNLOSSR	Nitrogen amendment by dead roots (kg ha^{-1})
iNLOSSS	Nitrogen amendment by dead stems (kg ha^{-1})
idwso	Org. matter amendm. by dead st.org. (kg ha^{-1})
iNLOSSO	Nitrogen amendment by dead st.org. (kg ha^{-1})
WFPS	Water filled pore space of soil layer (-)
red_T	Soil temperature response on process rates (-)
red_W	Moisture response on OM transformation (-)
red_W_Nit	Moisture response on nitrification (-)
red_W_Den	Moisture response on de-nitrification (-)
red_Resp	Respiration response on de-nitrification (-)

A spreadsheet is available that uses this output file to generate mass balances for Water, Organic Matter (FOM, Bio, Hum), Nitrogen in Organic Matter pools and for NH_4-N and NO_3-N. Mass Balances can be made for user defined periods (see Figure 12: Start Date and End Date).
In addition, different R-procedures are available to analyse to content of this output file.



Start date

Jan 1974 Jan 1974

Sun	Mon	Tue	Wed	Thu	Fri	Sat
30	31	1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31	1	2
3	4	5	6	7	8	9

End date

Dec 1974 Dec 1974

Sun	Mon	Tue	Wed	Thu	Fri	Sat
24	25	26	27	28	29	30
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31	1	2	3	4

Ndemand	198.7999
Nsupply	198.7951

Water(mm)

Input		Output	
Top	966.15	Soil Evaporation	180.30
Lateral	0.00	Transpiration	246.75
Bottom	25.49	Leaching	540.02
Total	991.64	Total	967.07
Stor.start	140.17	Stor.end	164.74
		dif.Stor	-24.57
		Input-Output	24.57

Fresh Organic Matter

Input		Output	
Amendments	14553.3	FOM->BIO	625.4
Crop Residues	5031.3	FOM->HUM	734.2
		Nett Dissoc.	6648.6
Total	19584.6	Total	8008.1
Stor.start	25116.0	Stor.end	36693.0
		dif.Stor	-11576.5
		Input-Output	11576.5

Nitrogen Fresh Organic Matter

Input		Output	
Amendments	474.08	FOM->BIO	36.27
Crop Residues	18.87	FOM->HUM	35.48
		Nett Mineralisation	89.76
Total	492.94	Total	161.52
Stor.start	556.58	Stor.end	888.00
		dif.Stor	-331.43
		Input-Output	331.43

Bio-Pool

Input		Output	
FOM->BIO	625.4	BIO->HUM	85.61
HUM->BIO	221.6	Nett Dissoc.	634.12
Total	847.0	Total	719.73
Stor.start	2602.7	Stor.end	2730.00
		dif.Stor	-127.28
		Input-Output	127.28

Nitrogen Bio-Pool

Input		Output	
FOM->BIO	36.27	BIO->HUM	4.14
HUM->BIO	12.85	Nett Mineralisation	37.61
Total	49.13	Total	41.74
Stor.start	150.96	Stor.end	158.34
		dif.Stor	-7.38
		Input-Output	7.38

Hum-Pool

Input		Output	
Amendments	1446.7		
Crop Residues	0.0		
FOM->HUM	734.2	HUM->BIO	221.6
BIO->HUM	85.6	Nett Dissoc.	1927.0
Total	2266.5	Total	2148.6
Stor.start	268970.0	Stor.end	269090.0
		dif.Stor	-117.9
		Input-Output	117.9

Nitrogen Hum-Pool

Input		Output	
Amendments	69.93		
Crop Residues	0.00		
FOM->HUM	35.48	HUM->BIO	12.85
BIO->HUM	4.14	Nett Mineralisation	91.00
Total	109.55	Total	103.85
Stor.start	13000.00	Stor.end	13006.00
		dif.Stor	-5.70
		Input-Output	5.70

NH4-N

Input		Output	
Amendments	550.00	Volatilisation	137.50
Crop Residues	0.00	Plant uptake	81.32
Mineralisation	217.57	Nitrification	389.36
Influx top	24.15	Outflux	29.66
Influx lat	0.00		
Influx bot	0.00		
Total	791.73	Total	637.85
Stor.start	3.85	Stor.end	157.73
		dif.Stor	-153.88
		Input-Output	153.88

NO3-N

Input		Output	
Amendments	0.00		
Crop Residues	0.00	Plant uptake	117.47
Nitrification	389.36	Denitrification	3.74
Influx top	24.15	Outflux	296.63
Influx lat	0.00		
Influx bot	0.00		
Total	413.52	Total	417.84
Stor.start	36.70	Stor.end	32.38
		dif.Stor	4.32
		Input-Output	-4.32

Figure 12 *Microsoft Excel® spreadsheet presentation of the results written to the output file *_nut.csv*

9 Field studies

The newly developed crop and soil nitrogen sub-models, implemented in Swap-Wofost version 3.2.59, were tested using data sets from local scale field experiments in The Netherlands and Argentina. Results of these tests are described in the subsequent paragraphs. This description is given as an example of input and output involved in the application of the sub-models and not intended to present an optimum result. The results require further testing (calibration, validation, etc.) when applied in a new study. Results of a test of SWAP-WOFOST by means of a comparison with pyWOFOST are given in Annex 1.

9.1 Maize crop on sandy soils: Cranendonck16

9.1.1 Experimental set-up and data acquisition

To test the leaching of nitrate-N under different fertilizer regimes we selected a nine-year field experiment described by Schröder (1985a). Cattle slurry was applied with yearly doses of 50 – 300 tons slurry per hectare each year. Six fields, each with different applications, were simulated.

Observed values of yield and N-uptake were given by Schröder (1985a). The observed NO3-N surplus was based on observed NO3-N concentrations at a depth of 1m (in suction cups) multiplied by calculated downward water flux at the same depth to estimate amounts in kg/ha N. Observations are given in Table 6.

Table 6 *Fertilizer treatments and observed dry matter and nitrogen yields for 6 field trials*

Field nr	Cattle slurry applied (1000 kg/ha)	N-application by cattle slurry (kg/ha N)	Observed Yield ` (kg/ha DM)	Observed N-uptake (kg/ha N)	NO_3-N surplus (kg/ha N)
18	50	318	11358	147	148
15	100	505	12288	165	161
13	150	758	13240	181	243
17	200	979	13583	199	376
16	250	1199	13788	198	525
14	300	1420	13553	201	589

Lower boundary conditions were derived from an observation well in the neighbourhood of the experimental plot. The observation well results are stored in the national database (DINO, 2015) for the Netherlands. The observations were adjusted for differences of field elevation and were imposed as hydraulic heads in deep groundwater.

The crop parameter values for the dry matter simulation were taken from the standard data set File MAG201.CAB: Grain maize (Zea mays L). The nitrogen crop parameters are taken from: Linul (http://models.pps.wur.nl/models). Data were taken from the file MAG202.DATo, as described by Wolf (2012).

9.1.2 Results

Simulation results for field nr 16 are presented for groundwater levels, dry matter yields, nitrogen yields and nitrate leaching.

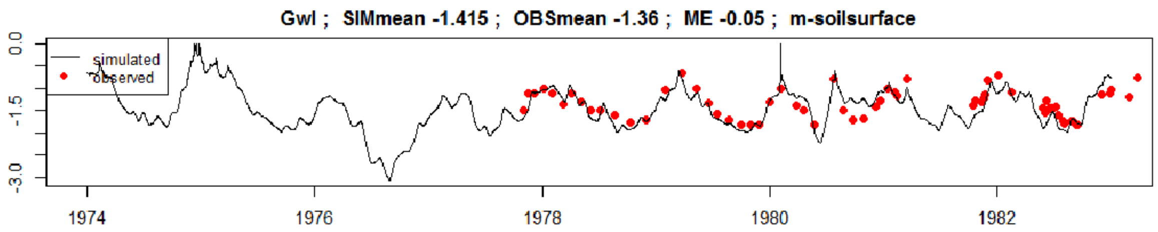


Figure 13 *Observed and simulated groundwater levels for field 16 in Maarheze/Cranendonck of a fertilization field experiment (Schröder, 1985a)*

The groundwater levels (Fig 13) were simulated using a bottom boundary condition where the flux is calculated from an average hydraulic head in the underlying aquifer. The values for the hydraulic head were taken from the Dutch national database DINO (https://www.dinoloket.nl/en).
Simulation results were compared with observed groundwater levels and showed a good comparison with a mean error of 5 cm.

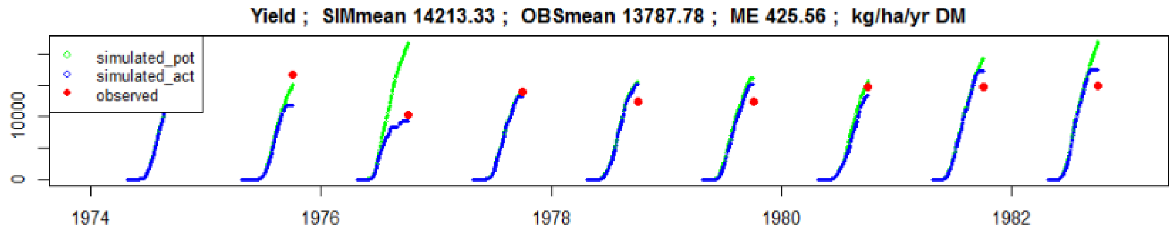


Figure 14 *Observed and simulated dry matter yields for field 16 in Maarheze/Cranendonck of a fertilization field experiment (Schröder, 1985a)*

The simulated yields (Fig 14) were compared with observed values and showed a slight underestimation of 426 kg/ha N, which was regarded as acceptable.
Simulated uptake of nitrogen (Fig. 15) and leaching of nitrate-N (Fig. 16) was also compared with observations. Yearly fluctuations were less accurate, but results were regarded as satisfactory, if one looks at the average values for the longer term.

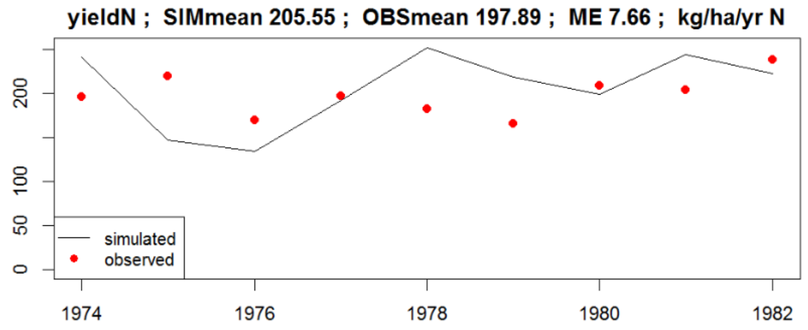


Figure 15 *Observed and simulated nitrogen yields for field 16 in Maarheze/Cranendonck of a fertilization field experiment (Schröder, 1985a)*

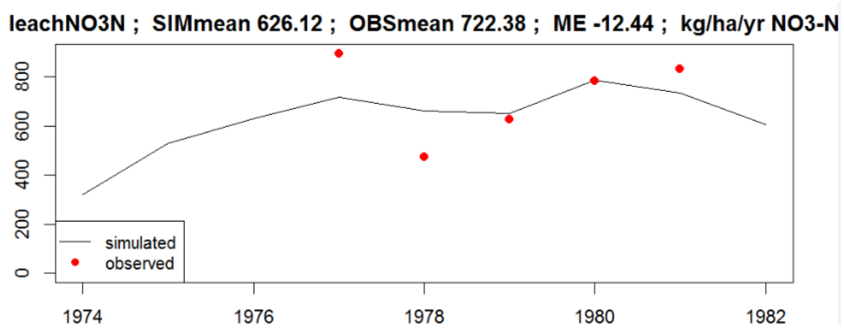


Figure 16 *Observed and simulated nitrate leaching fluxes for field 16 in Maarheze/Cranendonck of a fertilization field experiment (Schröder, 1985a)*

9.2 Soybean in Zavalla, Argentina

9.2.1 Calibration of phenological parameters

The observations from INTA covering the years 2012, 2013 and 2014 for Zavalla were used to estimate the phenological parameters DVRMAX1 and DVRMAX2. Calibration was carried out by minimizing RMSE between the observed and simulated R1 and R8 stages using all experiments for the Zavalla site for the given years (Table 7).

Table 7 *Calibrated values of DVRMAX1 and DVRMAX2 for Zavalla*

	DVRMAX1	DVRMAX2	RMSE [days]
Zavalla_a	0.0545	0.0221	13.81
Zavalla_b	0.041	0.0223	

Moreover, the scatter plots (Figure 17) of simulated *versus* observed days with R1 and R8 demonstrate that the variability in both the R1 and R8 stage can be reproduced reasonably well. The experiments of Zavalla contain two different groups of cultivars which are reflected in both graphs (Figure 17 left and right). Therefore calibration on each cultivar group will improve results (example: Table 7, Zavalla_b, Figure 18 bottom).

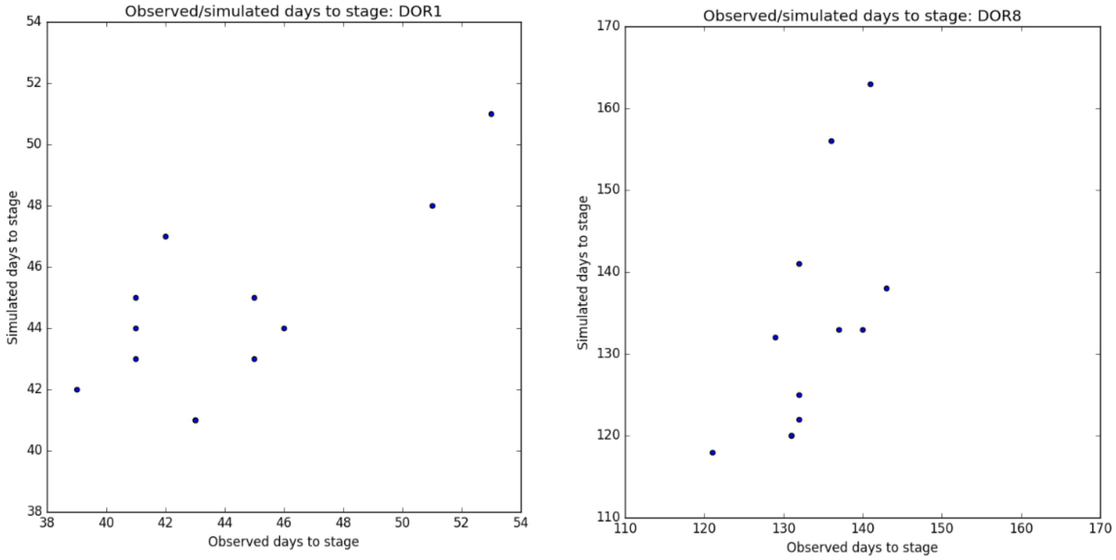


Figure 17 *Observed vs. simulated R1 stage (left) and R8 stage (right) for all experiments at the Zavalla site.*

9.2.2 Experimental setup and data acquisition

Simulations were carried out for one field in Argentina, field 35e, in which soybean was grown during the growing season 2013-2014.

9.2.3 Results

Some results are given to illustrate some of the possible results:

- simulated and observed yield in the year 2014 is given in Figure 18.
- simulated gross assimilation (gass), maintenance respiration (mres) and production rates of plant parts for the growing period in 2013/2014 is given in Figure 19.
- simulated partitioning of produced dry matter and nitrogen to plant parts is given in Figures 20 and 21.
- simulated nitrogen rate variables are given in Figure 22.

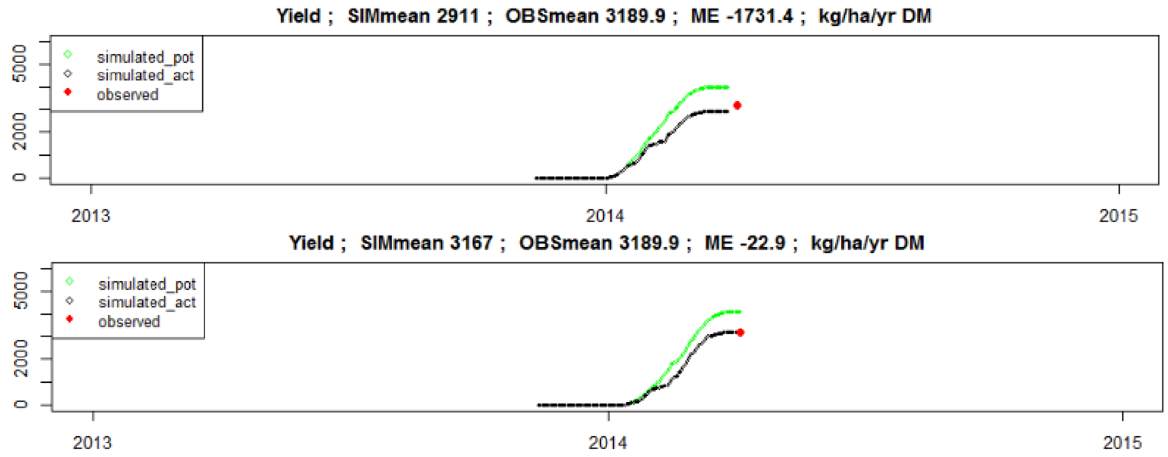


Figure 18 *Observed and simulated dry matter yields of a soybean crop in field 35e during the growth period 2013/2014 in Zavalla, Argentina, with DVRMAX1=0.0545 and DVRMAX2=0.0221 (top, Zavalla_a) and with DVRMAX1=0.041 and DVRMAX2=0.0223 (bottom, Zavalla_b)*

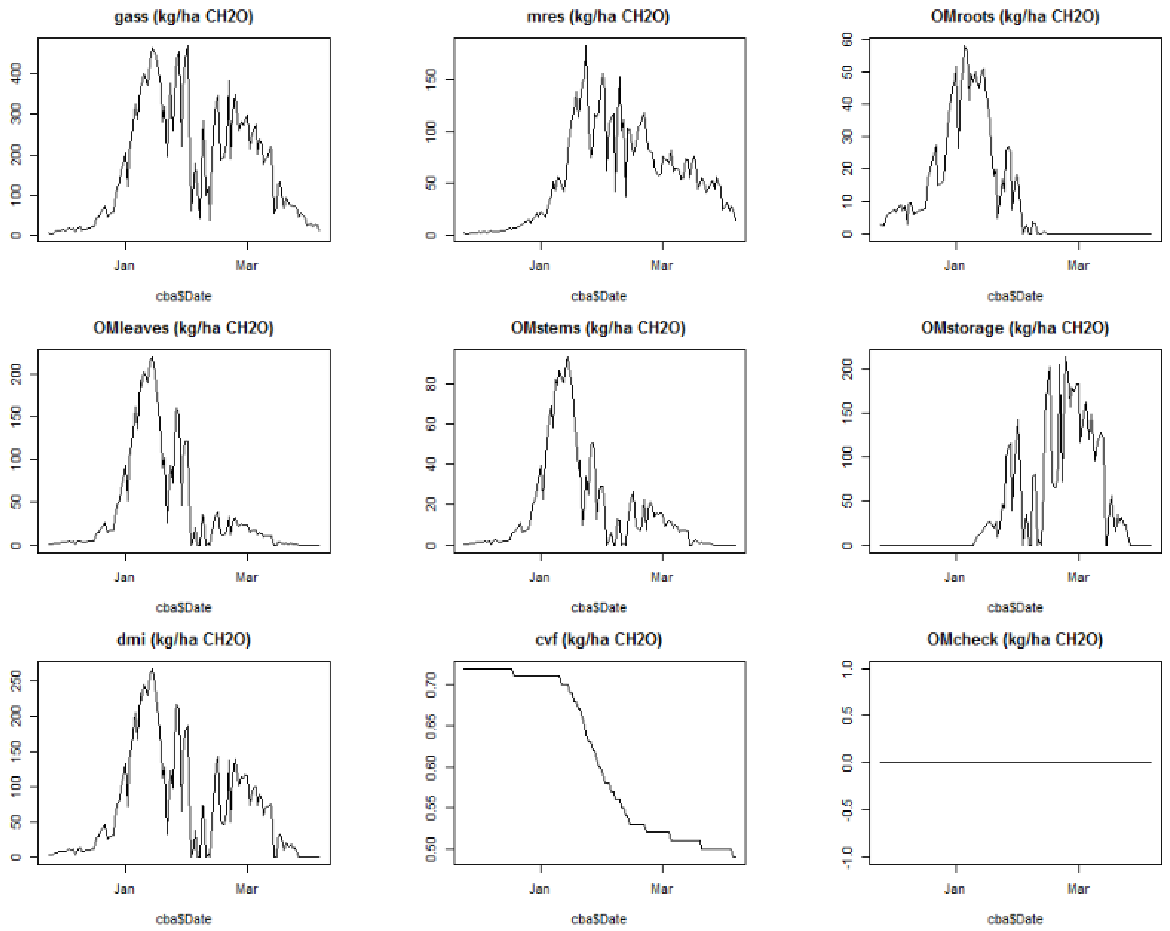
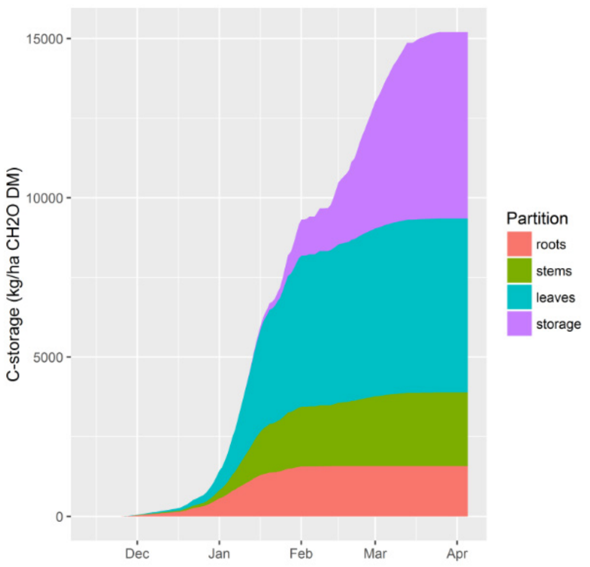


Figure 19 *Simulated gross assimilation (gass) and maintenance respiration (mres), production rates of plant parts for a soybean crop in Zavalla, Argentina in 2013/2014.*



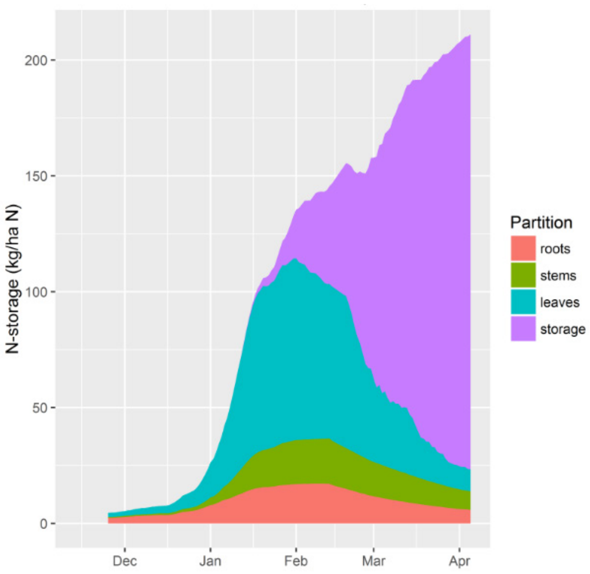


Figure 20 *Simulated partitioning of produced dry matter to plant parts of soybean, Zavalla*

Figure 21 *Simulated partitioning of produced nitrogen to plant parts of soybean, Zavalla*

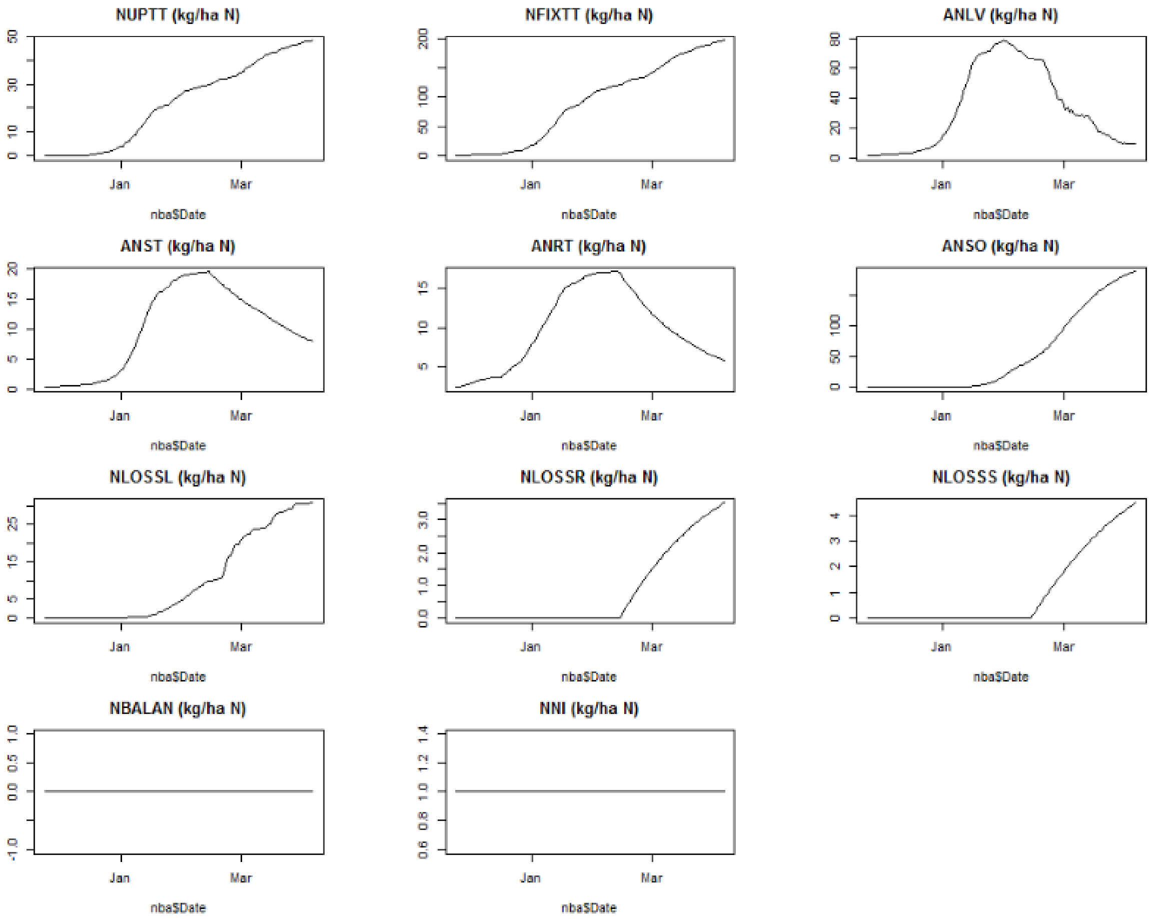


Figure 22 *Simulated nitrogen rate variables for a soybean crop, Zavalla, Argentine in 2013-2014*

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Annex 1 Comparison of SWAP/WOFOST and pyWOFOST

A comparison of SWAP/WOFOST and pyWOFOST was conducted for potential circumstances. DVS-values, LAI-values, above ground productions and weights of storage organs were compared for:

- A maize crop in Yucheng, China (2003).
- A winter wheat crop in Yucheng, China (2004).
- A soybean crop in Zavalla, Argentina (2014).

Details of the experimental setup of the test cases are given by Boogaard, 2016 (in prep.).

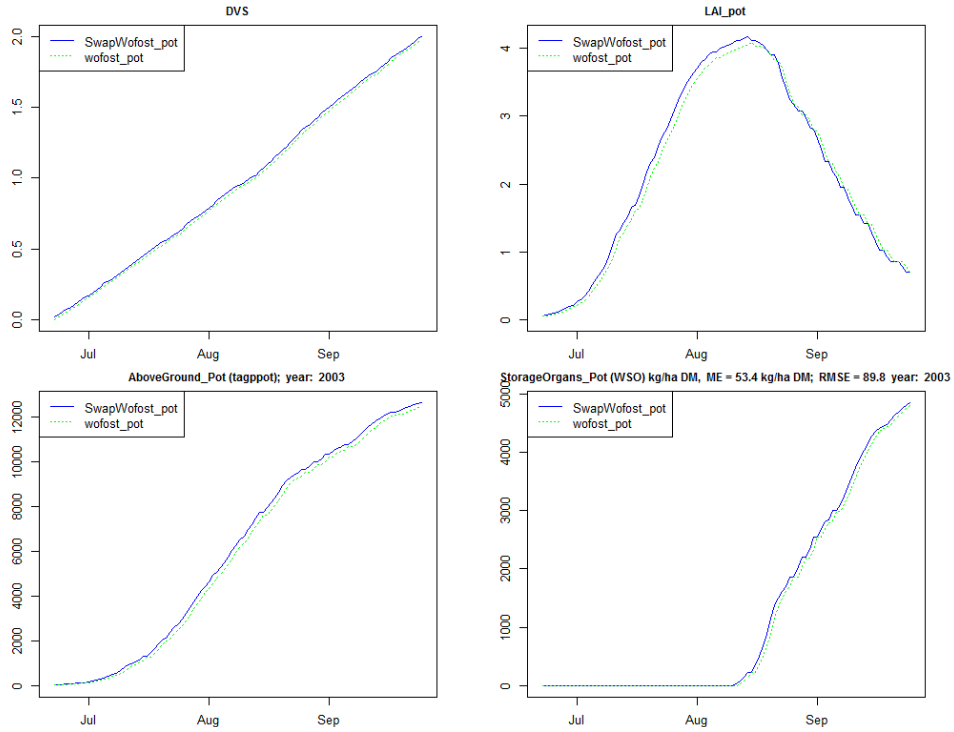

Figure 23 *Simulated DVS, LAI, above ground production and weight of storage organs by SWAP/WOFOST and pyWOFOST for a maize crop in Yucheng, China*

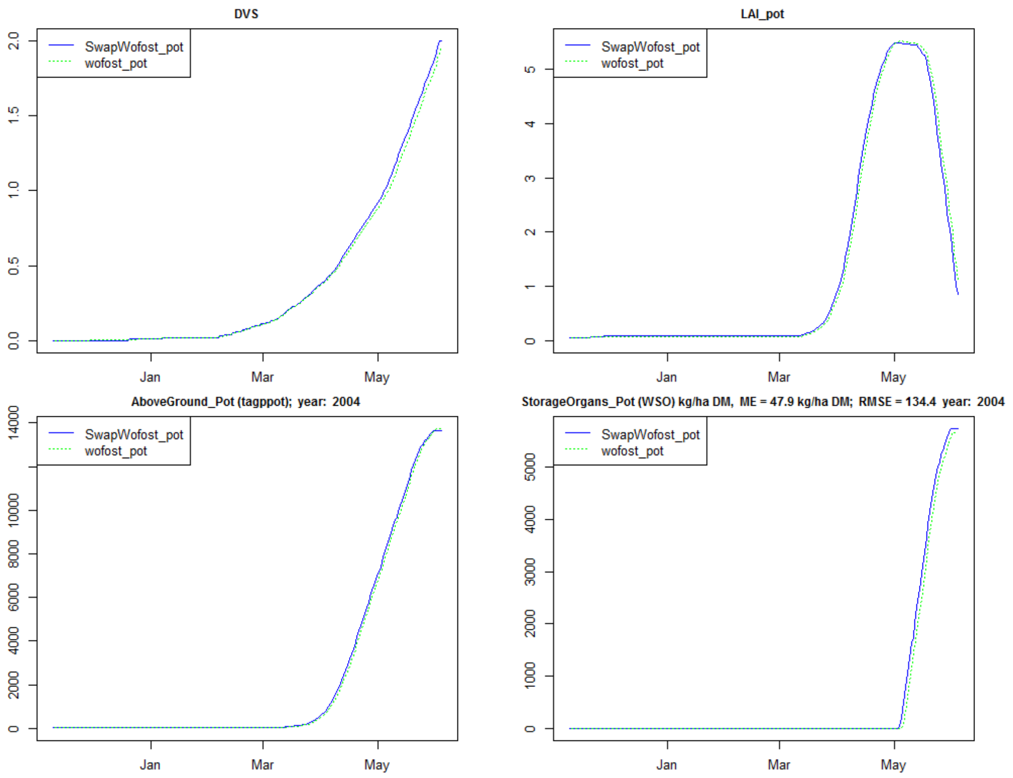

Figure 24 *Simulated DVS, LAI, above ground production and weight of storage organs by SWAP/WOFOST and pyWOFOST for a winter wheat crop in Yucheng, China*

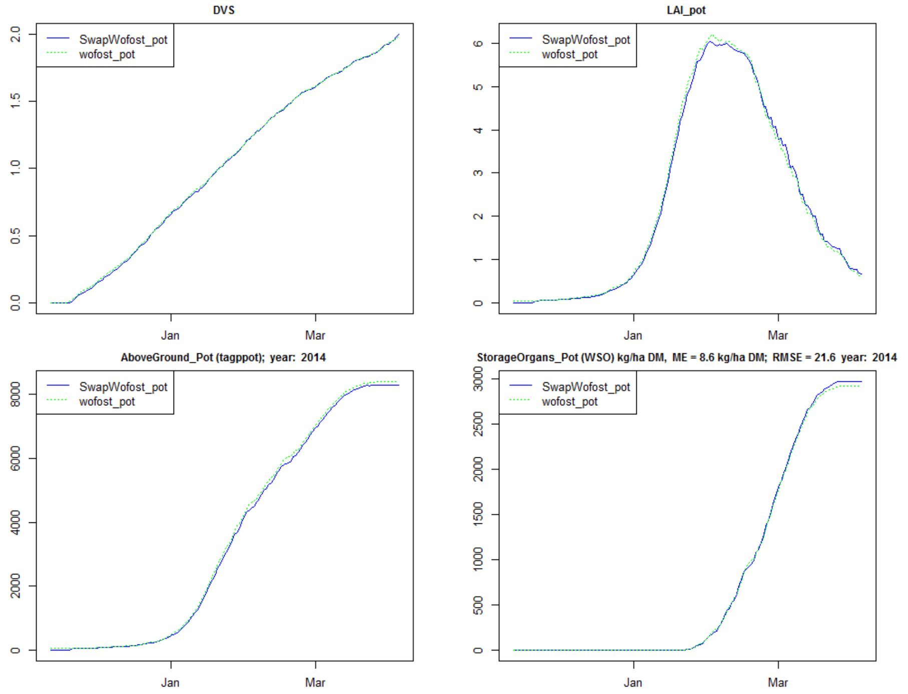

Figure 25 *Simulated DVS, LAI, above ground production and weight of storage organs by SWAP/WOFOST and pyWOFOST for a soybean crop in Zavalla, Argentine*

A maximum difference in simulated yields of 1% was regarded as acceptable and is probably caused by minor differences in schematisation, numerical solution technique and I/O differences.

Annex 2 Input of soil schematisation, soil organic matter and soil nitrogen using an example from Argentina

This Annex describes the schematisation and corresponding input of soil organic matter and soil nitrogen as required Soil Input data for SWAP-WOFOST.
Soil schematisation and parameterisation are described, using an example from Argentina: soil SERIE CAPITÁN SARMIENTO (Sm) [1]

1. Define vertical discretization in *.swp-file

The number of soil horizons (ISOILLAY) and the thickness and number of model compartments (HCOMP and NCOMP) are defined in Part 4 of the file *.swp. The values are based on the soil description for the field that is to be simulated.

```
* Part 4: Vertical discretization of soil profile
* Specify the following data (maximum MACP lines):
* ISOILLAY = number of soil layer, start with 1 at soil surface, [1..MAHO, I]
* ISUBLAY  = number of sub layer, start with 1 at soil surface, [1..MACP, I]
* HSUBLAY  = height of sub layer, [0.0..1000.0 cm, R]
* HCOMP    = height of compartments in this layer, [0.0..1000.0 cm, R]
* NCOMP    = number of compartments in this layer (= HSUBLAY/HCOMP), [1..MACP, I]
 ISOILLAY ISUBLAY  HSUBLAY    HCOMP    NCOMP
     1       1       18.0      1.0       18  ! A (A1+A2) 0-18 cm
     2       2       12.0      1.0       12  ! BA  from 18-30 cm
     3       3       15.0      1.0       15  ! Bt1 from 30-45 cm
     4       4       55.0      1.0       55  ! Bt2 from 45-100 cm
     5       5       50.0      1.0       50  ! BC  from 100-150 cm
     6       6      450.0     10.0       45  ! C   from 150-600 cm
* end of table
```

2. Define Soil hydraulic properties in *.swp-file

Several options exist to define soil hydraulic properties to the defined soil layers:

- As functions specifying for each soil layer: ORES,OSAT,ALFA, NPAR,KSAT,LEXP.
- As Table: use this option in case you have observed values (switch SWSOPHY = 1).

For the functions, you may use pedotransfer functions, as given by Hypress (Wösten, et al. 2001), UNSODA (Nemes et al.), ROSETTA (Schaap et al,) or StaringSeries (Wosten et al., 2014), see [3] .. [11].
Preferably, try to find data sources from the area/field you try to simulate. For example: Hodnett and Tomasella (2002) developed ptf's for water-retention curves of tropical soils and Wosten et al (2013) applied them in a study in South Africa. However, caution is required, because these ptf's often require simplification and are only valid for the domain they were developed for. It also may require a simplification for hydraulic conductivity values.

For this example, we applied tables using a data set described by Wosten et al. (2001).
We used eq. 16 from Keller & Håkansson (2010) to estimate bulk density from soil particle size distribution and soil organic matter content.

```
Part 5: Soil hydraulic functions
* as table or as function
 SWSOPHY = 0   ! Switch for use of tables or functions[tables=1, functions=0]
* If SWSOPHY = 1 then supply input data for tables (see manual)

* If SWSOPHY = 0  Specify for each soil layer (maximum MAHO):
* ISOILLAY1 = number of soil layer, as defined in part 4 [1..MAHO, I]
* ORES   = Residual water content, [0..0.4 cm3/cm3, R]
* OSAT   = Saturated water content, [0..0.95 cm3/cm3, R]
* ALFA   = Shape parameter alfa of main drying curve, [0.0001..1 /cm, R]
* NPAR   = Shape parameter n, [1..4 -, R]
* KSAT   = Saturated vertical hydraulic conductivity, [1.d-5..1000 cm/d, R]
* LEXP   = Exponent in hydraulic conductivity function, [-25..25 -, R]
* ALFAW  = Alfa parameter of main wetting curve in case of hysteresis, [0.0001..1 /cm, R]
* H_ENPR = Air entry pressure head [-40.0..0.0 cm, R]

* For this example data were taken from the StaringSeries using indications from the
* soil profile description, such as Eq.humedad (%) and particle size distribution:
* using Staring Series from NL (Wosten et al.,1994)
  ISOILLAY1,  ORES,  OSAT,  ALFA,  NPAR,  KSAT,   LEXP,   ALFAW  H_ENPR
       1  ,   0.0100,0.4500,0.0152,1.4120,17.8100,-0.2130,0.0304,0.0000   ! B3
       2  ,   0.0100,0.4500,0.0152,1.4120,17.8100,-0.2130,0.0304,0.0000   ! B3
       3  ,   0.0100,0.4200,0.0163,1.5590,54.8000, 0.1770,0.0326,0.0000   ! B4
       4  ,   0.0000,0.6000,0.0243,1.1110, 5.2600,-5.3950,0.0486,0.0000   ! B11
       5  ,   0.0000,0.4100,0.0291,1.1520, 5.4800,-6.8640,0.0582,0.0000   ! O6
       6  ,   0.0000,0.4100,0.0291,1.1520, 5.4800,-6.8640,0.0582,0.0000   ! O6

* --- end of table
```

3. Define Soil Organic Matter and Soil Organic nitrogen In *.snp-file

The sub-model for carbon and nitrogen in the soil uses a one-layer approach. The thickness of this layer should be defined as the input parameter dz_WSN. The value represents the thickness of the rootable zone and serves to interact between soil hydrology (defined by SWAP-modules) and roots for crop uptake and growth (defined by WOFOST-modules).

The value in the example is the rootable zone for soy beans in the soil series Capitan Sarmiento (Sm):

```
* effective depth of soil layer

dz_WSN = 0.6
```

The organic matter content should be given for different soil organic matter pools [1].

The sum of these pools should be equal to the observed value. The observed value for the rootable zone is input and can be derived from observations by taking the weighted average of the values for the different soil layers/horizons.

Be aware of the units: values for soil organic matter in the file *.snp are expressed in kg soil organic matter (SOM) per m^3 soil.

In the example of the soil series Capitan Sarmiento (Sm) the weighted mean SOM value will be 2.42 % (= kg SOM / kg soil), assuming a dry bulk density of 1300 kg/m3 soil volume), then the input value for SOM becomes 31.46 kg SOM per m^3 soil.

Initially, the total of the organic matter present in soil should be attributed to the ten pools. The total SOM value should be distributed over the SOM-pools as indicated by [1]: 92 % in pool HUM_t and the rest in the remaining SOM-pools.

Table A.1 *Initial distribution of Soil Organic Matter: 10 values of the SOM-pools*

		%	kg SOM/m^3 soil
FOM1_t	DPM	0.20%	0.0629
FOM2_t	DPM	0.90%	0.2831
FOM3_t	DPM	0.10%	0.0315
FOM4_t	DPM	0.10%	0.0315
FOM5_t	RPM	1.30%	0.4090
FOM6_t	RPM	1.50%	0.4719
FOM7_t	RPM	1.30%	0.4090
FOM8_t	RPM	1.30%	0.4090
BIO_t	BIO	1.30%	0.4090
HUM_t	HUM	92.00%	28.9432
		100.00%	31.4600

Then, a pre-run is advised by which the model simulates the distribution of organic matter, as expressed by the pools' contents. The final distribution is given in the PROJECT_nut.end file.
The pre-run can be repeated a number of times. If the fractional distribution of the pools seems to be stable, the repetition of pre-runs can be stopped. This final fractional distribution can be used to assign the initial values.
Soil organic nitrogen requires no additional input.

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Wageningen Environmental Research
Report 2721
ISSN 1566-7197

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