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Modelling approach and data requirements

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ABSTRACT

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This study determines the most suitable model and required model improvements to link atmospheric deposition of nitrogen and other elements in the Netherlands to measurements of nitrogen and other elements in the upper groundwater. The deterministic model SMARTml was found to be the most suitable model. The model requires an improved C&N modeling, improved forest growth modeling, linking forest growth to hydrology and an explicit dispersion calculation. A large number of independent data are available for validation of the improved model. Application of the model to sites of the 'National monitoring network on nitrate concentrations in the upper groundwater under nature areas' requires assumptions on soil properties, hydrology, deposition of base cations and chloride.

Keywords: nitrogen, deposition, leaching, groundwater, nature, modelling, forest, acidification

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Summary

RIVM runs the national monitoring networks on (i) nitrate concentrations in the upper groundwater under nature areas (Trendmeetnet Verzuring; TMV) and (ii) deposition of reduced and oxidized nitrogen species in nature areas and at background stations in the Dutch Air Quality Monitoring Network. Currently, both networks are designed, sampled, reported and interpreted separately.

The aim of this project is to determine the most suitable model that is currently available to link data form both monitoring networks, i.e. atmospheric deposition and concentrations in the upper groundwater, to investigate which improvements of this model are required, to determine the data requirements for the improved model and to assess which data are currently available for model validation and application.

The model SMARTml combined with the hydrological model SWAP was found to be the most suitable model. This model has been developed from the soil acidification model SMART2, is a multilayer model and can in principle be used to calculate element concentrations till groundwater levels.

The following improvements of the model are required to optimize it for calculating N concentrations:

- an improved model for organic matter dynamics and nitrogen mineralisation;
- the model EFISCEN to estimate forest growth, litter fall and root distribution;
- a coupling of vegetation growth and hydrology;
- vegetation growth is related to nutrient deposition levels;
- explicit calculation of dispersion in the solute transport.

A great number of data are available for validation and calibration of an improved version of SMARTml.

To apply the model at the TMV plots the following assumptions need to be made:

- Initial calculations will be performed for sites with information on soil properties and soil acidity: 20 sites included in LMB and 78 locations on non-calcareous sand. Missing information will be taken from national soil datasets and qualitative soil properties of the TMV plots.
- Site specific hydrology calculations will be performed to obtain hydrology.
- Deposition data at a 5x5 km grid and more detailed data if available will be used, thereby taking into account the local surface roughness of the vegetation. Later, filter factors for plots at or near forest edges will be used.
- Total deposition of Ca, Mg, Na, K, and Cl will be estimated from wet deposition.
- The age of the forest stands and management measures shoud be collected.

1 Introduction

1.1 Background

RIVM runs the national monitoring networks on (i) nitrate concentrations in the upper groundwater under nature areas (Trendmeetnet Verzuring; TMV) and (ii) deposition of reduced and oxidized nitrogen species in nature areas and at background stations in the Dutch Air Quality Monitoring Network. Currently, both networks are designed, sampled, reported and interpreted separately. Combining and integrating the measurements and interpretation of nitrate leaching and deposition can be profitable for the understanding of observed nitrate concentrations and trends in the observations in relation to policy measures regarding N emissions and N deposition.

At this moment nitrate concentrations in upper groundwater are interpreted statistically by relating the concentration levels to soil characteristics, geographical information about the locations of the nature areas and nitrogen deposition data. The latter data are based on a combination of model calculations and measurements. These statistical relationships explain 35% of the variance in the observed nitrate concentration levels in groundwater. Only a weak relation is found between nitrogen deposition and nitrate concentrations. (Boumans et al., 2004). It is expected that the relationships can be considerably improved when using more detailed deposition estimates. At this moment no good estimates of nitrate concentrations can be made for sites without deposition measurements.

A drawback of a statistical model is that it is not suitable for a good forecast of future nitrate levels, because it lacks process based information and it is not guaranteed that even a largely predictive statistical model for the present situation holds for the future. This hampers the use of such a model for policy support. The use of deterministic process based models relating N deposition to nitrate concentrations in the groundwater allows such a forecast of nitrate levels in the future and can be calculated as long as the input data to the models are available. At WUR (Alterra) a number of models are available that describe the interactions between atmosphere, vegetation and soil.

1.2 Goal

The aim of this project is to determine the most suitable model that is currently available to link atmospheric deposition to groundwater concentrations, to investigate which improvements of this model are required, to determine the data requirements for the improved model and to assess which data are currently available for model validation and application.

The model and the improvements are directed to a better understanding of the link between the atmospheric deposition levels and the concentration levels of elements in the upper groundwater by a combination of process based and statistical models. With the model it should be possible to (i) make accurate maps of element concentration levels in upper groundwater and (ii) predict effects of different scenarios for climate change and air pollution policies on the element concentration levels at a national scale. The emphasis in the improvements lies on nitrogen (specifically nitrate).

1.3 Contents of the report

In Chapter 2 we discuss the selection of the most appropriate model to link (N) deposition to (N) concentrations in the groundwater (section 2.1) and the required model improvements (section 2.2). Furthermore, the required input data for running the model are given (section 2.3). Chapter 3 describes the datasets that are available for calibrating and validating the model (section 3.1) and those for model application (section 3.2), including the Trend Monitoring Network Acidification (section 3.2.1) and deposition calculations (section 3.2.2). Next, an overview is given of the data that are currently missing to run the model and how these data can be obtained (section 3.3). Finally, chapter 4 gives the most important conclusions and recommendations.

2 Model development

2.1 Model selection

The aim of this study is to determine the most suitable model that is currently available to link atmospheric N deposition to groundwater concentrations and to investigate which improvements of this model are required. A model that is able to calculate interactions between deposition and groundwater concentrations should meet the following requirements:

- the model should include hydrology and chemistry of the soil and soil solution till a depth of at least the groundwater table;
- it should include interactions between organic carbon turnover and nitrogen immobilisation and mineralisation. Only then effects of nitrogen storage within the soil system can be accounted for;
- the model should be able to be run on a national or regional scale, which means that input should be available from datasets on a national or regional scale.

At Alterra, several models are available that describe the interactions between atmosphere, vegetation and soil, like VSD(+) (Posch & Reinds, 2009), SMART2 (Kros, 2002) and SMARTml. These are all soil acidification models that focus on a fully balanced calculation of all major elements in soil solution (SO_4, Cl, HCO_3, NO_3, NH_4, Ca, Mg, K, Na, Al and Fe) and the pH. Both VSD+ and SMART2 model are single layer models that are limited to the upper soil zone (approximately up to 1 m), whereas SMARTml is the only multilayer model that can be used to calculate soil chemistry till depths below the groundwater table. Consequently, SMARTml is the only appropriate model to use when concentrations in groundwater have to be predicted. Additionally, SMARTml has the advantage over the other models that it can use time steps smaller than one year, which makes it possible to calculate yearly variations in the N concentrations.

Both SMARTml and the other models need input from a hydrological model to calculate the transport of solutes in the soil profile. Momentarily SMARTml uses output of the 1-dimensional hydrological model SWAP (Kroes et al., 2008).

So far, SMARTml has only been applied on a site scale and not on a regional scale. However, the hydrological model SWAP has been used on a national scale to calculate nutrient and heavy metal emissions to surface waters (e.g. Bonten & Groenenberg, 2009). This facilitates the use of SMARTml on a national scale (which is the aimed scale to calculate effects of policy measures).

Concluding, the SMARTml model is suitable to calculate N concentrations in groundwater both on site scale to calculate N concentrations at sampling points of the 'Trendmeetnet Verzuring' and at national scale to calculate effects of policy measures. However, the model in its current form can not directly by applied to calculate N concentrations in groundwater, because SMARTml:

- lacks a good description of the interaction between carbon and nitrogen which is crucial for an adequate estimate of the concentrations of NH_4 and NO_3;
- uses a constant vegetation biomass in the hydrological modelling, which means that water uptake and evaporation by the vegetation are not related to the development stage (specifically relevant for forests) and management practices of the vegetation.

To make the model SMARTml suitable for calculating N concentrations in groundwater, we propose some changes in the model which are described in the next section.

2.2 Changes in selected model

2.2.1 C-N interactions

Currently, in mineralisation calculations with SMARTml, it is discriminated between fresh litter, old litter and humic matter. Old litter and humic matter are produced due to the decomposition of fresh litter and old litter respectively. In this approach nitrogen has no effect on the decomposition rates of the litter. Only N mineralisation/immobilisation itself due to decomposition of old litter and humic material is dependent on the C/N ratio of these organic matter fractions, i.e. at high C/N ratios N mineralisation is reduced and N is retained within the organic matter.

To improve the interaction between carbon and nitrogen, which is crucial for a good estimate of N concentrations, a different C/N model is required. While there are numerous models that calculate only C-dynamics, there are only a few models that calculate both C and N dynamics. Of these models, DNDC is the most advanced and complex model, describing in detail all processes with respect to C and N dynamics in soil systems (Li et al. 1994).

For modelling carbon dynamic we propose a simplified approach of the DNDC model. The proposed model is a four compartment C-model, containing: 1) easily decomposable fresh litter (Cfe), 2) recalcitrant fresh litter (Cfs), 3) microbial biomass (Cmb) and 4) slowly degradable humic material (Chu). Each compartment has its own first order mineralisation and turnover rate and its own fixed C/N ratio. Because litter fall is distributed over two types of fresh litter, different kinds of plant residues depending on vegetation type can be defined (e.g. less degradable residues will have a higher fraction in the recalcitrant fresh litter compartment). Mineralisation and turnover rates are dependent on temperature, pH and moisture content. Figure 1 shows a schematic representation of the CN-model.

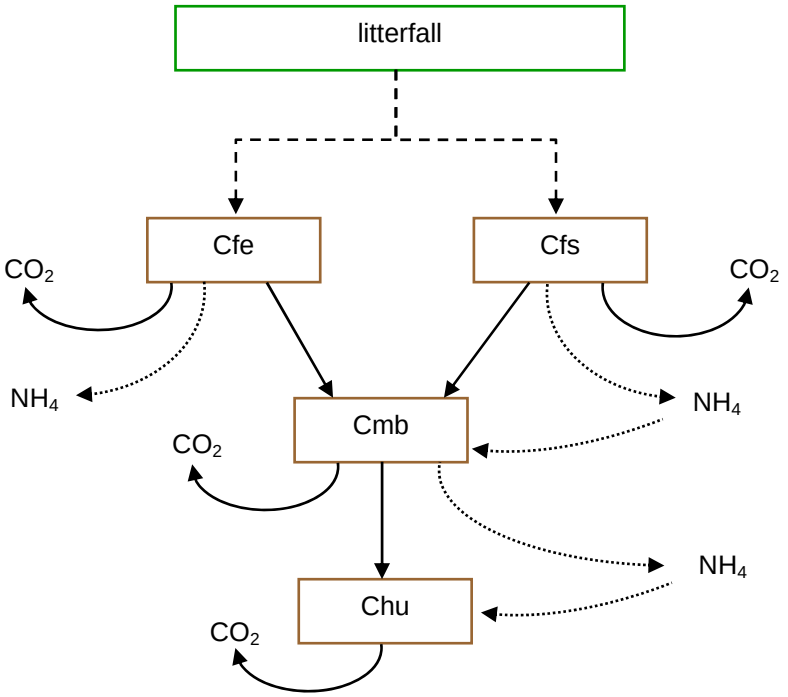

Figure 1. Schematic representation of CN-model

Figure 2 gives an overview of all N soil processes that are included in the model. The deposition of NH_4 and NO_3 refers to throughfall. The difference between throughfall and total wet and dry deposition, i.e. canopy interactions, are taken into account in plant uptake. The numbers indicate the calculation sequence of all N processes.

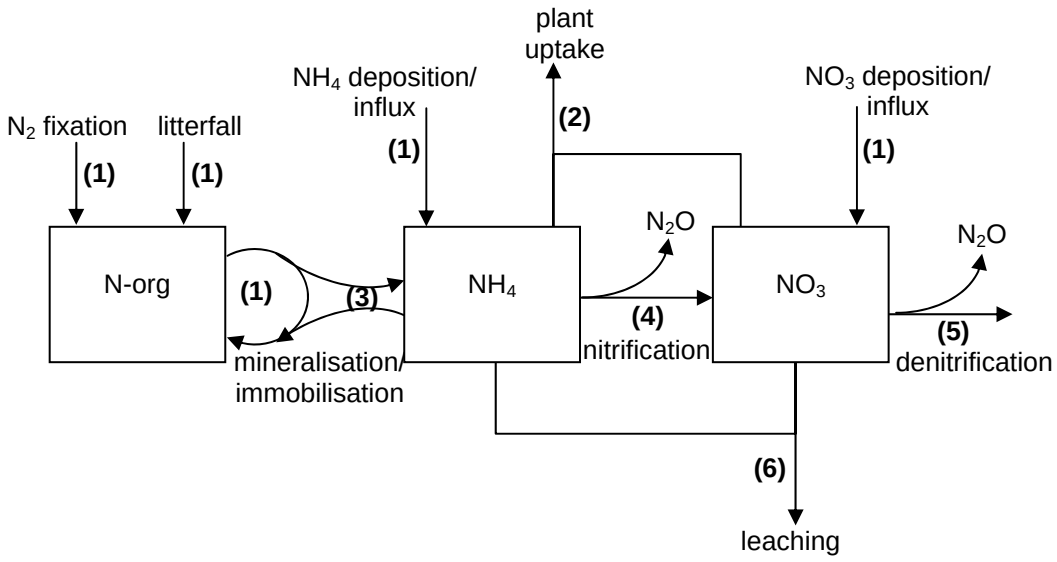

Figure 2.Overview of N processes

2.2.2 Forest growth and forest management

Currently, SMARTml contains a simple nutrient cycling model for short vegetation, by including data on the (constant) productivity of heathlands and natural grasslands and assuming that a fraction of this production is recycled by above and below ground biomass turnover (Kros, 2002). This approach is considered adequate for this study. For forests, it uses a simple logistic growth model to calculate stem growth and litter fall. This model has not been calibrated for most forest types. This model also contains no information about important processes like root distribution and turnover of roots, stems and branches.

At Alterra, the model EFISCEN (Schelhaas et al, 2007) has been developed to simulate the growth of forest and to calculate the spatial distribution of forest development stages and how these distribution change in time. EFISCEN is a database model based on field data of vegetation growth. Because the model EFISCEN can relatively easily be coupled to SMARTml, we propose to use this model instead of the simple and non-calibrated model that has currently been implemented. An alternative would be the use of models such as SUMO (Wamelink, 2007) that explicitly include N uptake and release by the forest understory growth. Inclusion of this would lead to a strong increase in model complexity, whereas the impact of this kind of nutrient cycling in the topsoil is nearly negligible on the nutrient leaching.

Figure 3 shows a graphical presentation of the scheme that is used in EFISCEN to calculate forest growth, litter fall and the leaf area index. The latter is important for use in the hydrology calculations.

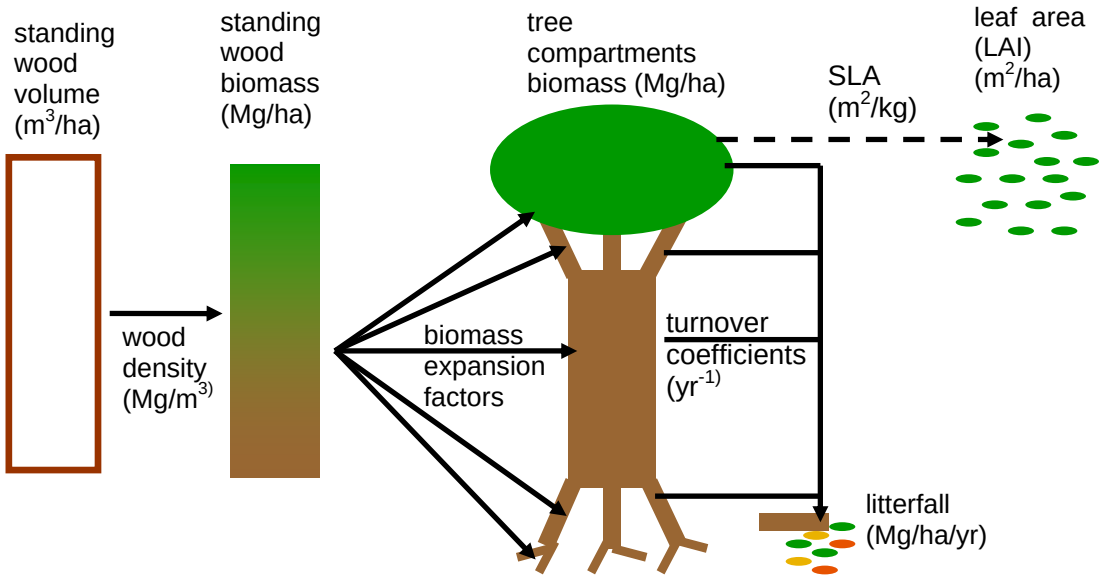

Figure 3. Calculation scheme for calculation of litter fall and leaf area.

First, the standing wood volume is calculated by a logistic growth function. The parameters of this growth function are dependent on the type of tree species. Then, the standing wood biomass ($Mg \cdot ha^{-1}$) is calculated by multiplying the standing wood volume with the wood density ($Mg \cdot m^{-3}$). The distribution of biomass over the different compartments is given by biomass expansion factors (BEF). Litter fall is calculated by multiplying the amount of biomass in each compartment ($Mg \cdot ha^{-1}$) with a turnover coefficient for each compartment. The leaf area index (LAI) can be calculated from the amount of foliage by multiplying this with the specific leaf area ($m^2 \cdot kg^{-1}$).

The distribution of the roots with depth is mainly dependent on the tree species and on soil type. For SMARTml we will use one distribution for each species, because the difference between the different soil types is relatively small. Because no data are available for the development of rooting depth in time, but only for full grown forests, we will use these distributions also for young developing forests. As for all species most roots are present in the upper 60 cm, the error that is made with this assumption will be small.

A more detailed description of the model EFISCEN is given in Appendix 2.

For use of EFISCEN in SMARTml it is not possible to discriminate between every type of tree species. Therefore we will use four different forest types, broad leaf I (willow, poplar, and birch), broad leaf II (oak and beech), evergreen pine (pine and larch) and evergreen spruce (spruce, fir and Douglas-fir). EFISCEN does not include understory vegetation. Including of this requires more complex vegetation models like SUMO, with the previously mentioned disadvantages (see also section 2.2.3). Furthermore we expect the including nutrient cycling by understory vegetation has very little effect on the nutrient leaching. The effects of the omission of understory vegetation on leaching will be tested when determining the model sensitivy for uncertainties in model input.

2.2.3 Coupling vegetation growth and hydrology

At this moment we assume a constant biomass in the hydrological modelling, which means that water uptake and evaporation by the vegetation are not related to the development stage of the forest. This is not a problem for a full-grown forest and most short vegetations, but for most Dutch forests the potential evaporation by the vegetation will increase in time because of forest growth. Furthermore, standard forest management practices like clearance or thinning will affect (i.e. reduce) the potential evaporation. Finally, during forest growth tree roots will penetrate deeper into the soil and take up water from these deeper soil layers as well. To include these changes in vegetation a coupling is required between vegetation growth, forest management and hydrological calculation.

Currently, SMARTml uses the hydrology from model SWAP (Kroes et al., 2008). Within SWAP it is possible to provide changes in vegetation parameters as an input

for the hydrology calculations. However, SWAP requires different vegetation parameters than SMARTml. Therefore, to couple vegetation growth and hydrology we need to relate vegetation growth (i.e. litter fall rates, stem growth, root growth) to input for SWAP (i.e. leaf area index, soil cover, root distribution). Changes in the SWAP parameters because of vegetation growth and/or forest management will then be used as input for SWAP.

In the coupling as described above, we assume that forest growth is only dependent on factors that are known beforehand, like average climate, vegetation type, soil type, etc. When this is the case, hydrology calculations can be performed prior to the SMARTml calculations. In some cases however, the outcome of the SMARTml calculation might determine forest growth, e.g. a low nutrient status of the soil that limits forest growth, thereby influencing hydrology. The two main options to account for effects of a low nutrient status include:

- a direct coupling between SMARTml and SWAP, where both models run simultaneously and exchange data on a real-time basis. The major disadvantage of this option is that it is very difficult to implement;
- to relate vegetation growth to nutrient inputs (here: deposition). Now hydrology can still be calculated prior to SMARTml calculations. The disadvantage is that nutrient availability is limited to atmospheric inputs, neglecting the nutrient stock in the soil. Consequently, vegetation growth will response relatively fast to changes in N deposition.

Use of the first option would only be relevant when including a real growth model such as SUMO, but this would lead to a strong increase in model complexity whereas the lack of data would most likely not lead to an increase in model performance. This together with the technical complexity of the first option, the second option will be implemented.

2.2.4 Solute transport

Transport of solutes in SMARTml is currently calculated with the model Transol version 2.1 (Kroes, 1991). Within this model dispersion is calculated implicitly by assuming that the numerical dispersion of the model is equal to the actual dispersion. This means that the thicknesses of the soil layers in the model are defined by the chosen dispersion lengths. A thicker model layer will lead to a larger calculated dispersion. However, it is very much desirable that dispersion is not linked to the schematisation of the soil profile but can be calculated independently. Then, schematisation of the soil profile can be based on the properties of the soil profile and the distribution of soil horizons.

A more recent version of Transol (version 2.9) offers the possibility to calculate dispersion using dispersion coefficients that are provided as input instead of setting dispersion equal to the numerical dispersion of the model. Therefore version 2.9 of the Transol model will be included within SMARTml.

2.3 Data requirements

The following input is required to run the SMARTml model and the hydrological model SWAP including the proposed changes from section 2.2. Input parameters that are in principle generic like chemical equilibrium parameters are not included in this list.

- deposition:
  - deposition of NH_3, NO_x, Ca, Mg, K, Na, Cl and SO_2
- vegetation:
  - vegetation type
  - vegetation age
  - vegetation management
- soil properties (for each horizon till groundwater level):
  - organic matter
  - clay
  - CEC (can be estimated from OM and clay)
  - soil density (can be estimated from OM and clay)
  - CN ratio of OM
  - thickness and CN of litter layer
  - $CaCO_3$
  - pH/base saturation
  - Fe and Al-hydroxides
  - S and P adsorption isotherms (can possibly be estimated from Fe/Al-ox)
- hydrology:
  - meteorology (precipitation, temperature, potential evaporation)
  - physical soil properties (can be estimated from chemical soil properties using Staring reeks)
  - bottom boundary conditions
  - lateral boundary conditions

3 Data

3.1 Datasets for model calibration and validation

There are several datasets available for calibration and validation of the improved SMARTml model. Most datasets however contain no information about groundwater concentrations but only about soil solution concentrations. The following datasets contain information about both groundwater and soil solution quality:

- a set of 12 evergreen forest stands containing soil moisture concentrations of all macro-elements (NO_3, NH_4, PO_4, SO_4, Ca, Mg, K, Na, Cl, pH, DOC) for four soil horizons till a depth of 1 m for the period 1992 till 2000, and groundwater concentration of all macro-elements for the period 1992 till 1996. This set has originally been described in De Vries et al. (1994). Soil moisture and groundwater was sampled once a year;
- a set of 150 forest stands on non-calcareous sand containing soil moisture concentrations of all macro-elements for two soil depths (0-30 cm and 60-100cm) in 1990 (de Vries & Leeters, 2001) and groundwater concentrations of all macro-elements at a subset of 78 stands in 1990 (Boumans and Beltman, 1991; De Vries and Jansen, 1994)
- a set of 63 forest stand in the catchment of the river 'Drentse Aa', containing soil solution concentration of two soil horizon till a depth of 60 cm and groundwater concentrations of all macro-elements in 1994 (Klap et al., 1997).

For all of these datasets, however, deposition is only available from modelling but not from measurements.

Furthermore, the following datasets contain both deposition measurements and time series of very frequently sampled soil moisture, but no groundwater concentrations:

- a Norway spruce site in Solling (Germany) containing soil solution concentrations at six depths till 90 cm for the period 1969 (or later at some depths) till 2003;
- measurements from the international monitoring network of ICP forests with data on meteorology, atmospheric deposition, assessed from bulk deposition and throughfall, accounting for canopy exchange, soil and soil solution chemistry at approximately 200 sites in Europe (De Vries et al., 2003). Soil solution has been sampled weekly to monthly since 1997 and data are available at Alterra up to 2002. On three Dutch plots (Hardenberg, Zeist and Dwingeloo) soil moisture was sampled from 2003 till 2006 (Leeters et al., 2007).

Besides these datasets, the following datasets can also be used for calibration and validation, but these contain only soil solution concentrations, which are measured once:

- a set of 100 forest stands on silt, peat and clay soils containing soil moisture concentrations of all macro-elements for four soil depths (0-10 cm, 10-30 cm, 30-60 cm and 60-100cm) measured in 1992 (Klap et al., 1999);

- a set of 48 locations on non-calcareous sand in the dunes containing soil solution concentrations of four soil horizons till a depth of 60 cm measured in 1991 (De Vries, 1993);
- a set of 200 forest stands on non-calcareous sand containing soil moisture concentrations of all macro-elements for the organic horizon and two soil depths (0-10 and 10-30 cm) in 1995 (Leeters & de Vries, 2001).

3.2 Data sets for model application

3.2.1 Trend Monitoring Network Acidification

Introduction

Deposition of sulphurdioxide, sulphate and nitrogenous components affect terrestrial and aquatic ecosystems. In the "Trendmeetnet Verzuring" (TMV) the quality of the uppermost groundwater under nature areas on sandy soil in the Netherlands is determined. TMV is run by the National Institute of Public Health and the Environment (Dutch acronym RIVM).

The objectives of TMV are:

- to determine the changes in groundwater quality in nature areas (forest and heather) on sandy soil;
- and to describe and explain the quality and the changes in relation to environmental pressures (atmospheric emissions) and policy measures (measures to limit emissions).

Sampling and analysis

A total of 155 locations on sandy soil have been selected (see Figure 4). Sites were selected where the groundwater level always occurs within 6 metres below soil surface. This implies that no sites have been selected in the largest nature areas, the Veluwe where groundwater levels exceed even 40 m below soil surface.

At each location, 10 sampling points are chosen. These sampling points are located along a straight 50 metres transect. If the transect is less than 450 metres long the rest of the sampling points are placed along the perpendicular bisector of the transect. Sampling points are always located at least 20 metres from the edge of the forest or the heather.

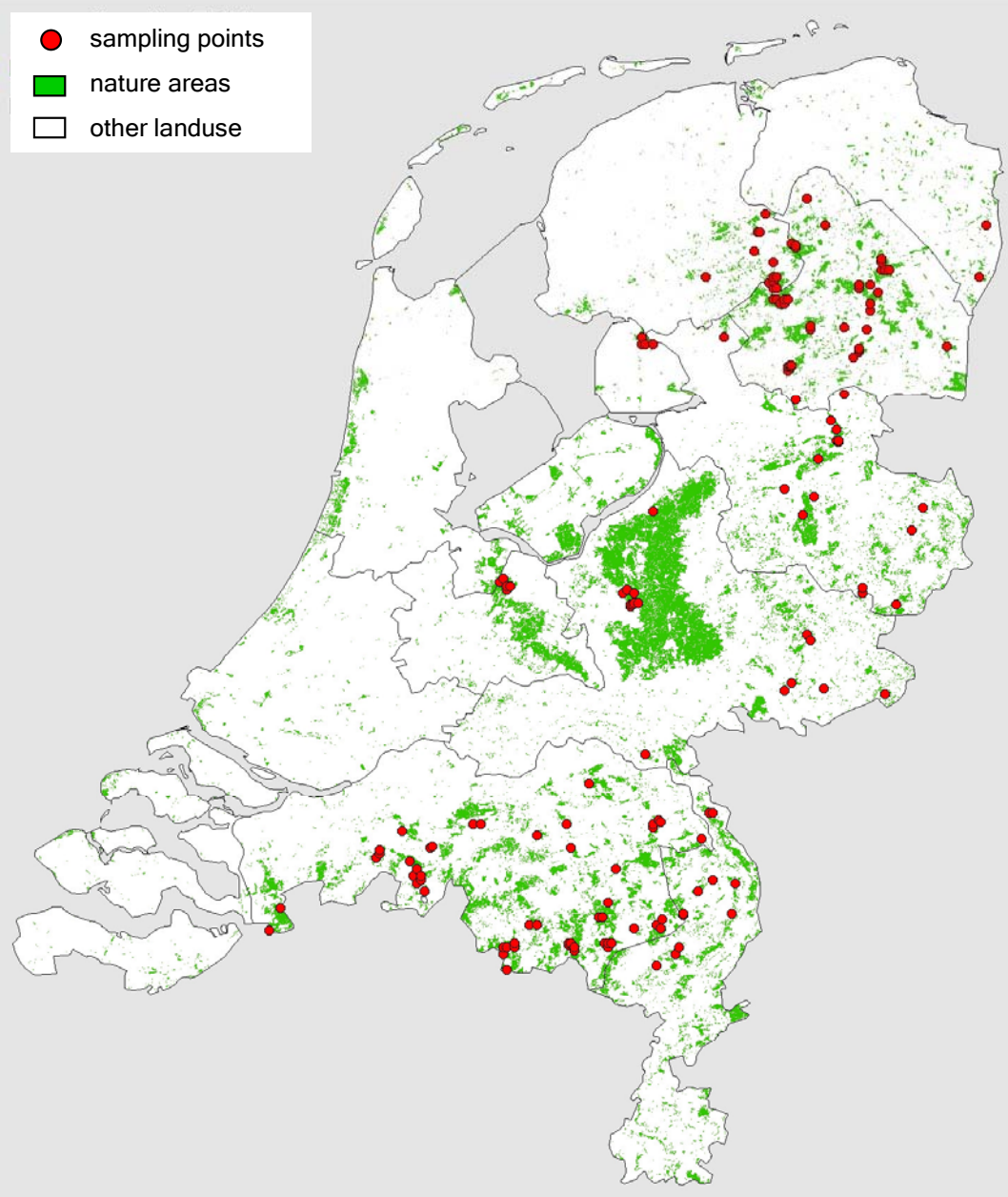

Figure 4. Monitoring locations of the Trend Monitoring Network Acidification

So far, the locations have been sampled four times, in 1989/1990, 2001/2002, 2003/2004 and 2006/2007. In principle sampling takes place in the period September to December with a possible extension to January/February. Half of the samples is taken in the first year, the other half in the second year.

This sampling involves collecting the uppermost groundwater from each of the 10 sampling points at a location, which is then combined into a single mixed sample at the laboratory. This mixed sample is analysed for a large number of components. In the individual groundwater samples several parameters are determined in the field.

Furthermore, a description of the sampling points has been made during the sampling rounds of 1989/1990 and of 2006/2007 (local factors). The type of landscape is recorded and within a sample circle with a radius of four metres the following is described: the ground cover type, main tree species, crown coverage, tree height, shrub layer coverage, herbaceous layer coverage and forest litter thickness.

Also, a qualitative description of the soil profile of each sampling point has been made (in terms of e.g. a slightly peaty sand or a moderately clayey peat, etc.)

The open borehole method is used to sample the uppermost groundwater. An Edelman hand-drill is used to drill to a depth of about 50 cm below the groundwater level and subsequently a filter lance is placed. The groundwater is then pumped up with a peristaltic pump and filtered.

The groundwater samples are analysed in the field, for:
- acidity (pH);
- electrical conductivity (EC);
- oxygen concentration;
- nitrate concentration (via colour reaction).

Additionally the groundwater level and exact location of the sampling point in the field are recorded.

In the laboratory mixed samples of the 10 sampling points for each location are analysed for:
- pH, EC and dissolved organic carbon (DOC);
- nutrients (total P, ortho-phosphate, total N, NH_4, Cl, NO_3, SO_4 and K);
- other macro-elements (Al, Ba, Ca, Fe, Mg, Mn, Na and Sr);
- heavy metals (As, Cd, Cr, Cu, Pb, Ni and Zn).

Results of TMV are published by Boumans and Beltman (1991), Boumans and Fraters (1993), Boumans et al. (2004), Boumans et al. (2009), and Van Elzakker et al. (2009). The latter publication gives a detailed overview of 75 locations sampled in the period October 2006 until the end of January 2007.

3.2.2 Deposition data

The deposition of nitrogen to nature areas is obtained from model calculations with the OPS-model of RIVM/PBL (van Jaarsveld, 2004). The OPS model represents a combination of a Gaussian plume model for local-scale application and a trajectory model for long-range transport (Van Jaarsveld, 2004). The model is used for issues on acidification/eutrophication as well as on heavy metals and persistent organic pollutants. Furthermore, the model has been successfully applied to deduce SO_2 and NO_x trends from measurements of ambient concentrations. An early version of the OPS model (called TREND model) has taken part in a number of model

intercomparison studies (Derwent et al., 1989, Gusev et al., 2000). More recently, results of the OPS model were compared to detailed measurements of ammonia in the Netherlands (van Pul et al., 2004) and compared with results of the EMEP unified model on the issue of, among others, ammonia and ammonium concentrations and deposition in the Netherlands (Velders et al., 2003).

Especially in the case of ammonia the local scale plume model allows for a detailed approach of the low level release height in combination with near-source deposition. Dry and wet deposition for both NH_3 and the secondary product, NH_4^+ are calculated with a spatial resolution mainly dependent on the resolution of the emission data.

The model calculations are based on emission inventories by the Emission Registration of PBL and on actual meteorological information. Time series of yearly deposition are calculated at a 5x5 km resolution for the National Environmental and Nature Balance reporting. In several projects, nitrogen deposition is calculated at higher resolutions, e.g. 1x1 km in the study on optimizing ammonia emissions at the scale of provinces (van Dam et al., 2001), but no time series on a national scale are available on this resolution.

In the deposition calculation, the spatial distribution of sources in the vicinity of nature areas is taken into account. Specific characteristics of the nature areas themselves, like surface roughness affecting the dry deposition velocity, are only partly taken into account and are dependent on the resolution of the calculations. In the OPS model the following nature types are considered: evergreen forest, deciduous forest and other areas (mostly considered to be grasslands including heather and dune vegetation). If more than 50% of the area in a grid cell is covered with nature it is considered as a nature area and the cell obtains the specific deposition characteristics for nature area. Because of this a different land use and land cover is attributed to small nature areas. So typically larger nature areas such as forest areas are considered in the maps in which for instance specifically the surface roughness is taken into account.

Time series of deposition on a national scale are available for NH_3, NO_x and SO_2 at a 5x5 km resolution. For other elements (Ca, Na, Mg, K, Cl) only data are available for wet deposition, i.e. rainwater concentrations, and not for dry deposition. Wet deposition data are available on a monthly basis for 11 locations in the Netherlands.

3.3 Mismatch between data requirements and availability at TMV plots

3.3.1 Missing data

A comparison between the data required for running the SMARTml model (section 2.3), the data available from TMV (section 3.2) and from deposition calculations (section 3.2.2) shows that the following required input data are not directly available:

- soil properties, like organic matter content and clay content;
- nutrient status (i.e. C/N ratio) of the soil organic matter and the litter layer;
- acidity of base saturation of the soil;
- the age and history of the vegetation;
- input for hydrology calculations;
- deposition of base cations (Ca, Mg, K, Na) and chloride.

Soil properties, nutrient status and acidity

Soil properties have been determined in TMV only qualitatively, but a quantitative description of the soil profile is required as input for SMARTml. Information about the nutrient status of the soil profiles are probably the most important missing data for calculating element (and specifically nitrate) concentrations in groundwater. The nutrient status determines how much nitrogen can potentially be released for leaching. Something similar holds for the pH or base saturation, because the pH is important for the rates of many soil processes like organic matter decomposition, N mineralisation, nitrification and denitrification, while the base saturation determines the capacity to buffer the pH.

Fortunately, soil properties, nutrient status and acidity have been determined for a number of locations of TMV in other monitoring programs:

- 20 locations of TMV are included in the National Monitoring Program on Soil Quality (LMB). Here, the topsoil (0-10 cm) and the subsoil (30-50 cm) are sampled and analysed for a great number of parameters, including organic matter and clay content, CEC and pH. The nutrient status is not determined in LMB;
- 78 forest stands on non-calcareous sand, sampled in 1990, which are a subset of 150 stands that have been mentioned in section 3.1 (De Vries and Jansen, 1994). Information on the chemical soil composition below those stands is given in Vries & Leeters (2001) for the humus layer and the mineral topsoil (0-30 cm). Parameters, include organic matter content and total contents of C, N, P, S, Ca and Mg and K , CEC, exchangeable cation contents and pH. At 12 plots, being a subset of the 78 plots, those parameters have been determined in four layers up to 100 cm (0-10 cm, 10-30 cm, 30-60 cm and 60-100 cm).

For deeper soil layers and for locations for which no measurement are available soil properties can be estimated by converting qualifications like slightly peaty or moderately clayey to estimates of the organic matter content and clay content by using information of the soil map of the Netherlands and/or the Soil Information System.

The nutrient status and the acidity can also be estimated using the Soil Information System. Additionally, for locations for which superficial soil samples are available, the pH or base saturation can be estimated by interpolation using the pH measured in TMV in the groundwater and the pH or base saturation in the soil samples.

Vegetation

Within TMV, information about the vegetation has been collected during the first and last sampling rounds. This information, however, does not include the age of the forest stands and forest management measures. The age of a forest stand is important because it determines the growth of the stands and with that the uptake of nutrients from the soil and the input through litter fall to the soil. Information of management measures is important because the removal of trees or clear-cut of a stand can lead to increased leaching of nitrogen because of reduced uptake of nitrogen and increased mineralisation of roots left in the soil. The suggested approach to assess those data is to collect these data within the framework of TMV.

Hydrology

The hydrology at the TMV locations (i.e. water fluxes, evaporation and groundwater level) is required to calculate the leaching rates of nitrogen (and other elements) to the groundwater. However, the measurements in TMV contain no information on physical soil properties. Further, there is only little information on hydrological boundary conditions or groundwater dynamics, besides the groundwater levels during the sampling of the groundwater.

In general, there are two options to obtain hydrological information for the TMV sites:

- The first option is to use the hydrology from available hydrological calculations on a national scale;
- The second option is to perform site specific calculations.

For the first option, hydrological calculations from the STONE model are the most suitable to use. Then a STONE plot will be selected which most closely resembles the properties of the TMV site with respect to soil properties, vegetation, meteorology and groundwater levels. The disadvantage of this approach is that effects of forest growth and forest management practices can not be accounted for, because STONE uses a constant vegetation biomass. Furthermore, the uncertainties in the variations of the groundwater levels at the TMV sites are very large, because the groundwater levels have been determined only four times. Because of this, the chances of selecting a STONE plot with a wrong hydrology are large.

When performing site specific hydrology calculations, forest growth and forest management can be included. Physical soil properties can be attributed to the soil profile using the 'Staring reeks' and the chemical soil properties that have previously been attributed to the soil profile can be used (see above). A fixed groundwater level, e.g. the average of the groundwater levels determined during the sampling rounds, can be used as hydrological boundary condition. The disadvantage of this approach is that effects of fluctuating groundwater levels on nitrate concentrations are not accounted for.

Concluding, for the hydrology we will perform site specific calculations, which allows us to include forest growth and forest management practices. Then the variations in

groundwater level are neglected, but we consider this less important, because uncertainties in these variations are very large when selecting the hydrology of a STONE plot.

Deposition of other elements
Because SMARTml calculates on a fully balanced calculation of all major elements in soil solution the inputs of these elements to the soil system are required. Deposition of NH_3, NO_x and SO_2 are available from OPS calculations. For deposition of cations (Ca, Mg, K, and Na) and chloride only concentrations in rainwater are available. Dry deposition of these elements is not measured and calculated on a national scale. However, a method to calculate dry deposition and, thus, total deposition based on wet deposition has been described in Van Jaarsveld (*in prep.*).

3.3.2 Difference in scale of data

When modelling N leaching to groundwater, all input data should be available on the same spatial scale, because this largely determines to which spatial scale the model outcome can be applied.

The data from the TMV monitoring network refer to a very small, local, scale. This is demonstrated by the fact that the measurements of nitrate concentrations show sometimes great variations with changes in vegetation or land use, e.g. across forest edges. On the other hand, the deposition data are calculated with a model on a national scale at a 5x5 km grid scale. This means that depositions at a certain location are average values for the whole grid cell based on the most dominant land use type of that grid cell.

Further, deposition can be greatly increased at forest edges due to the filtering effect of trees at the edge. The deposition to small nature areas and the effects of a high heterogeneity in land use on the deposition is not yet considered. This means that data from the deposition are most likely not representative for TMV locations in a heterogeneous landscape or locations at or near forest edges. This requires either a correction of the deposition for changes in vegetation, like forest edges, or that modelling calculation are only performed for TMV plots that are located in a large area with homogeneous vegetation. In the SOR Nitrogen project RIVM will investigate whether simple correction factors can be applied for the deviation of the deposition to small areas and to heterogeneous vegetation e.g. forest edges.

Because of these differences in scale of the model inputs, the model outcomes can not be directly compared with the measured nitrate concentrations at the TMV plots. Therefore we propose to not only perform a plot by plot comparison on model outcomes and measurements but also by using frequency distributions and by focusing on changes in nitrate concentrations instead of exact concentrations themselves.

The model SMART will not only be applied on a local scale to calculate nitrate concentration in the groundwater at the TMV plots, but also at a national scale to estimate effect of policy measures. Then input like soil properties and hydrology can be taken from existing national scale datasets. For the calculations on a national scale, it is easier to ensure that all input data have a similar scale.

3.3.3 Recommendations for obtaining missing data

We can not directly apply the model SMARTml for calculating nitrate concentrations at the TMV plot, because not all required input data are available (see section 3.3.1) and model and inputs have different scales (section 3.3.2). To overcome these conflicts between data requirements and data availability we propose the following:

- Initially calculations will only be performed for sites at which information on soil properties and soil acidity is available. These are the 20 locations of TMV that are also included in LMB and 78 locations on non-calcareous sand which were sampled in 1990 and for which soil solution chemistry data are available as well. For soil layers for which no information is available we will use information from national soil datasets and qualitative soil properties of the TMV plots. For these calculations, TMV locations where major changes have occurred (forest clearance, land use changes, etc.) will not be included in these calculations. Later, the model will be run on all other locations using information from national soil datasets.
- To obtain the hydrology at the TMV locations, we will perform site specific hydrology calculations using the SWAP model, which allows to include forest growth and forest management practices.
- We will use the deposition data at a 5x5 km grid and the data on a more detailed grid (most likely 500x500m) if available. The deposition figures will be corrected in case the vegetation in a specific grid cell differs from the actual vegetation of the TMV plot in that grid cell. This correction will be made for the surface roughness of the vegetation. In case a TMV plot contains two different vegetations, two separate calculations will be carried out for that plot with two different deposition figures. Later, deposition figures for plots at or near forest edges can be improved with filter factors, if necessary.
- The total deposition of Ca, Mg, Na, K, and Cl will be estimated from the wet deposition.
- To correctly include litter fall and nutrient uptake, the model requires information about the age of the forest stand and about management measures. We suggest that these data will be collected within the framework of TMV.

4 Conclusions and recommendations

The goal of this study is to determine the model and data requirements to link atmospheric N deposition to groundwater concentrations in the Netherlands. Therefore we looked at

- what is the most suitable currently available model,
- which improvements of this model are required,
- what are the input requirements of the improved model,
- and which data are currently available for model validation and application.

4.1 Model selection

Most models that can describe interactions between atmosphere, vegetation and soil, are single-layer models and are limited to the upper soil layer. The model SMARTml, which has been developed from the soil acidification model SMART2, is a multilayer model and can in principle be used to calculate element concentrations till groundwater levels. Therefore we propose to use SMARTml, in combination with the hydrological model SWAP, to calculate effects of inputs on groundwater concentrations.

4.2 Required changes in the model

Because SMARTml has been derived from a soil acidification model, it is not optimised for calculating N concentrations. Therefore we propose the following improvements of the model:

- an improved model for organic matter dynamics including effects on nitrogen mineralisation;
- the model EFISCEN will be used to improve estimations of forest growth, litter fall and root distribution;
- to couple vegetation growth and hydrology, growth (i.e. litter fall rates, stem growth, root growth) will be related to input for SWAP (i.e. leaf area index, soil cover, root distribution);
- reduction of vegetation growth due to a limited nutrient availability will incorporated by relating growth to nutrient deposition levels;
- dispersion will be calculated explicitly using the model Transol 2.9, which enables that the vertical schematisation of soil properties can be done independent of the schematisation of the hydrological model.

4.3 Data for calibration and validation

A great number of data from sites both in the Netherlands and in other countries are available for validation and calibration of an improved version of the SMARTml model of which three datasets contain not only soil solution concentration but also groundwater concentrations of all major elements.

4.4 Data availability and recommendation for additional data collection

- Initial calculations will be performed for sites at which information on soil properties and soil acidity is available. These are 20 sites that are also included in LMB and 78 locations on non-calcareous sand which were sampled in 1990 and for which soil solution chemistry data are available as well. TMV sites with major changes will be excluded from these first calculations. Missing information will be taken from national soil datasets and qualitative soil properties of the TMV plots. Later, the model will be run on all other locations using information from national soil datasets.
- Site specific hydrology calculations will be performed to obtain hydrology at the TMV sites.
- The official deposition data at a 5x5 km grid and more detailed deposition data will be used, whereby the local surface roughness of the vegetation of the TMV plot is taken into account. Later, we will use filter factors to improve deposition figures for plots at or near forest edges.
- Total deposition of Ca, Mg, Na, K, and Cl will be estimated from wet deposition.
- We recommend that the age of the forest stands and management measures are collected for the TMV sites, in order to correctly include litter fall and nutrient uptake.

4.5 Model application

Model outcomes and measurements at TMV sites will be compared by a site by site comparison and by using frequency distributions and focusing on changes in nitrate concentrations.

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Appendix 1 SMARTml

SMARTml is a multilayer model for the calculation of acidification and nutrient behaviour. It is based on the one-layer model SMART2. The major difference with the original SMART2 model is the use of more soil layers with variable depth. This enables simulation of transport of compounds through a soil profile and calculation of leaching to surface waters.

SMART2 is a simple, single-layer soil acidification and nutrient cycling model for terrestrial (semi-)natural ecosystems. It includes the major hydrological and biogeochemical processes in the vegetation, litter and mineral soil. The model simulates changes in H, Al, Ca, Mg, K, Na, NH_4, NO_3, SO_4, HCO_3 and Cl concentrations in the soil solution. In addition, it simulates changes in solid phase characteristics connected to the acidification status, i.e. carbonate content, base saturation and amorphous Al precipitates. The SMART2 model consists of a set of mass balance equations, describing the soil input-output relationships, and a set of equations describing the rate-limited and equilibrium soil processes. SMART2 is an extension of the SMART model (De Vries et al., 1989). Since the (original) SMART model does not include a complete nutrient cycle, it is not suitable for calculating N availability. Furthermore, it does not include upward solute transport. Therefore, the model SMART was extended with a nutrient cycle (litter fall, mineralisation and uptake) and an improved modelling of hydrology, including runoff, upward and downward solute fluxes. Most of the extensions were derived from the dynamic multi-layer model RESAM (De Vries et al., 1995a) and the steady-state multi-layer model MACAL (De Vries et al., 1994c). Figure A1.1 gives a schematic representation of the SMARTml model.

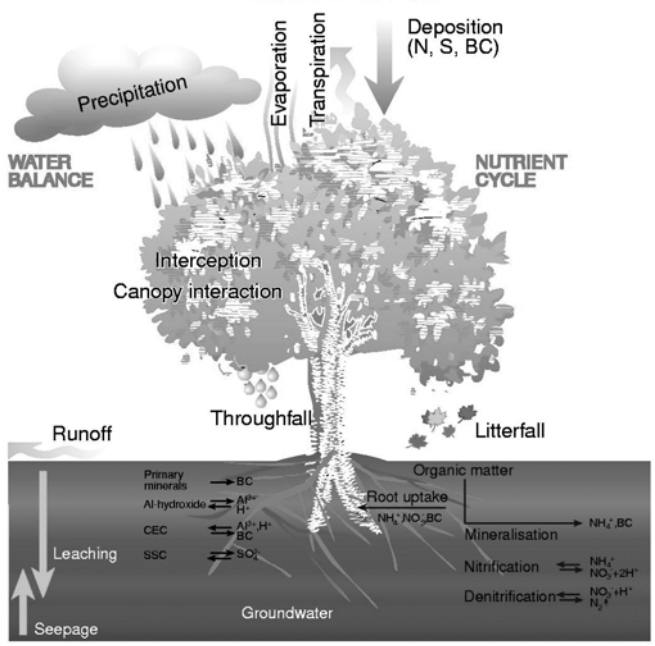

Figure A1.1. Schematic representation of the processes included in the SMARTml model

The included processes are summarised in Table A1.1.

Table A1.1. Overview of processes included in SMARTml

Process	Element[1)]	Process description
Input:		
Total deposition	SO_4, NO_3, NH_4, Ca, Mg, Na, K, Cl	Inputs
Upward seepage	SO_4, NO_3, NH_4, Ca, Mg, Na, K, Cl	Seepage concentrations are inputs
Water Balance	-	Inputs (from SWAP): precipitation, water fluxes between soil layers, upward seepage, evapotranspiration
Rate-limited reactions:		
Foliar uptake	NH_4	Linear function of total deposition
Foliar exudation	Ca, Mg, K	Linear function of total deposition
Litter fall	Ca, Mg, K, NH_4, NO_3	Logistic growth
Root decay	Ca, Mg, K, NH_4, NO_3	Linear function of litter fall
Mineralisation	Ca, Mg, K, NH_4, NO_3	First-order reaction and a function of pH, moisture content, temperature
N immobilisation	NH_4, NO_3	Function of the C/N ratio soil organic matter
Growth uptake	Ca, Mg, K, NH_4, NO_3	Logistic growth
Nitrification	NH_4, NO_3	Michaelis-Menten kinetics as function of NH_4 concentrations and dependent on pH, moisture content, and temperature
Denitrification	NO_3	Michaelis-Menten kinetics as function of NO_3 concentrations and dependent on pH, moisture content, and temperature
Silicate weathering	Al, Ca, Mg, Na, K	Zero order reaction
Equilibrium reactions:		
CO_2 Dissociation	HCO_3	CO_2 equilibrium
Dissociation of organic acid	RCOO	Oliver equation
Carbonate weathering	Ca, Mg	Carbonate equilibrium
Al hydroxide weathering	Al	Gibbsite equilibrium
Cation exchange	H [1)], Al, Ca, Mg	Gaines-Thomas equations
Sulphate and phosphate sorption	SO_4, PO_4	Langmuir equation

[1)] Implicitly, H is affected by all processes. This is accounted for by the charge balance

Appendix 2 EFISCEN

Forest growth

The standing wood biomass (M_{wood}) is calculated according to the Richards' (1959) equation:

$$M_{wood} = \rho_{wood} \cdot A_{max} \cdot (1 - e^{-\kappa \cdot age})^{\gamma} \quad \text{(Eq 1)}$$

where M_{wood} is the standing wood biomass ($Mg \cdot ha^{-1}$); ρ_{wood} is wood density ($Mg \cdot m^{-3}$); A_{max} is the maximum standing wood volume ($m^3 \cdot ha^{-1}$); age is the age of the standing trees (yr).

The values for coefficients are given in Table A2.1.

Table A2.1. Coefficients to calculate standing wood biomass

Species	ρ_{wood} (Mg/m^3)	A_{max} (m^3/ha)	κ (yr^{-1})	γ (-)
Alnus glutinosa	0.55	214.01	0.0454	2.176
Betula pendula	0.51	209.71	0.0389	2.176
Betula pubescens	0.51	210.29	0.0327	2.176
Fagus sylvatica	0.58	426.29	0.0196	2.176
Fraxinus excelsior	0.55	353.16	0.0224	2.176
Larix leptolepis	0.46	317.89	0.0437	2.176
Picea abies	0.40	711.73	0.0189	2.176
Pinus nigra	0.42	691.47	0.0224	2.176
Pinus sylvestris	0.42	323.64	0.0257	2.176
Populus x euroamericana	0.40	395.55	0.0414	2.176
Pseudotsuga menziesii	0.45	382.83	0.0366	2.176
Quercus robur	0.58	300.59	0.0246	2.176
Quercus rubra	0.58	252.61	0.0220	2.176

The distribution of biomass over the different compartments is given by biomass expansion factors (BEF). For instance, foliar biomass is calculated according to:

$$M_{foliar} = M_{wood} \cdot BEF_{foliar} \quad \text{(Eq 2)}$$

These BEFs depend on the age of the forest and species (see Figure A2.1 and Figure A2.2).

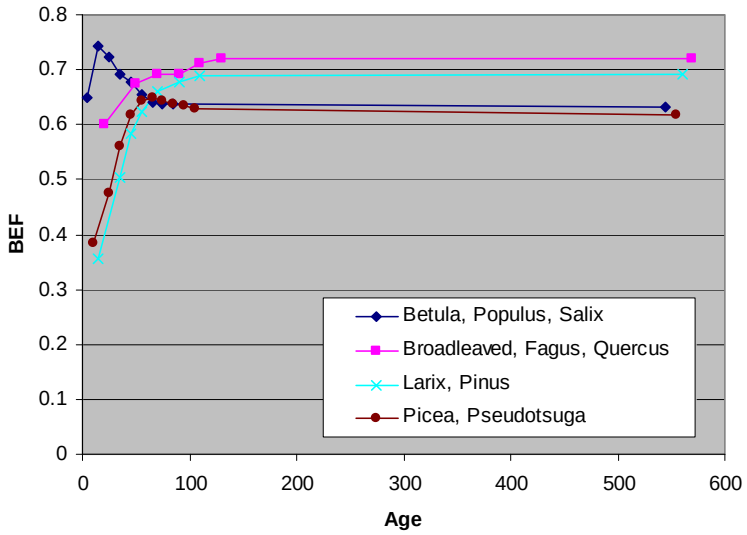

Figure A2.1. BEF of stems for the different tree species

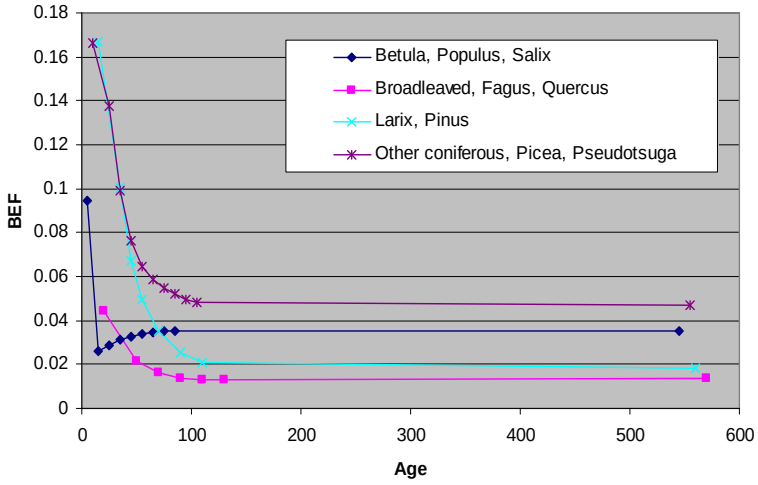

Figure A2.2. BEF of foliar for the different tree species

Leaf area index

The leaf area index (LAI) is calculated from the amount of foliar biomass and the specific leaf area (SLA) according to:

$$LAI = M_{foliar} * SLA \qquad \text{(Eq 3)}$$

Table A2.2. SLA in EFISCEN per tree species:

Species	SLA
Abies	5
Acer	20
Betula	20
Fagus sylvatica	22
Fraxinus excelsior	22
Larix decidua	8
Picea abies	5
Pinus sylvestris	5
Pseudotsuga menziesii	5
Quercus	15
Quercus petraea	15
Quercus robur	15
Quercus rubra	15
Salix	20

Litter fall

To calculate litter production, EFISCEN uses turnover coefficients (r) per compartment, given in Table , according to:

$$\text{Litterfall} = \sum_{compartments} M_{compartment} * r_{compartment} \qquad \text{(Eq 4)}$$

Table A2.3. Turnover coefficients (yr⁻¹)

Tree type	Branches	Coarse roots	Fine roots	Foliage	Stem
Broadleaved	0.025	0.025	0.641	1	0.0087
Coniferous	0.027	0.027	0.641	0.25*	0.0043

* For Larix, the turnover coefficient of foliage is 1 and for Pinus 0.5.

Root distribution

Figure A2.3 to Figure A2.6 show the rooting depths of Douglas fir, poplar and beech for different soil types.

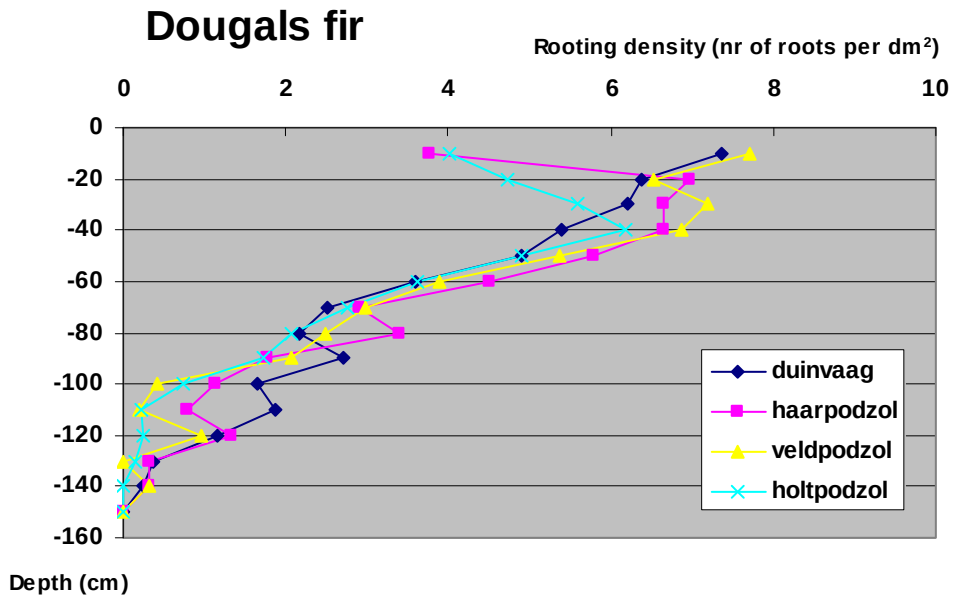

Figure A2.3. Rooting depth of Douglas fir in four different soil types

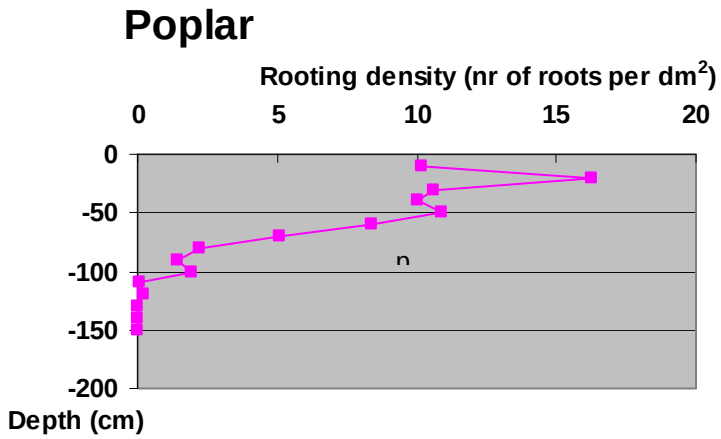

Figure A2.4. Rooting depth of Poplar

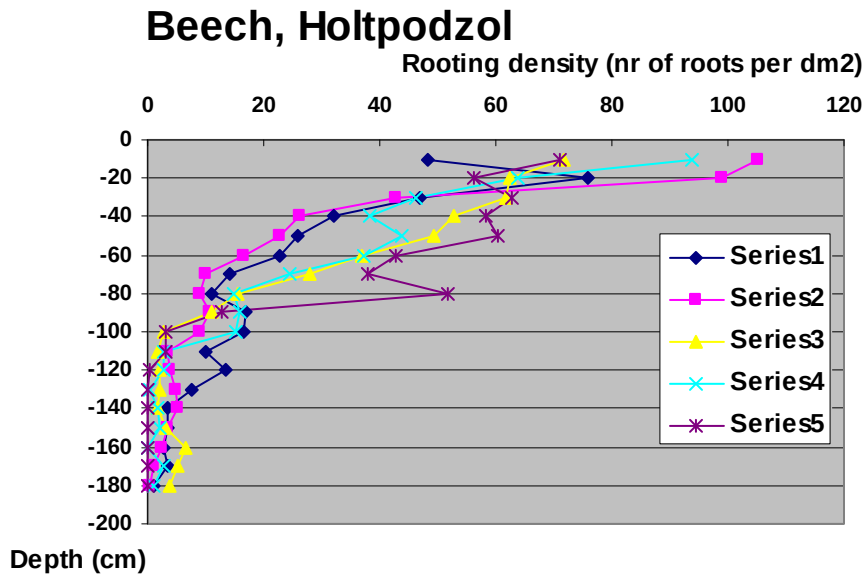

Figure A2.5. Rooting depth of Beech on "Holtpodzol"

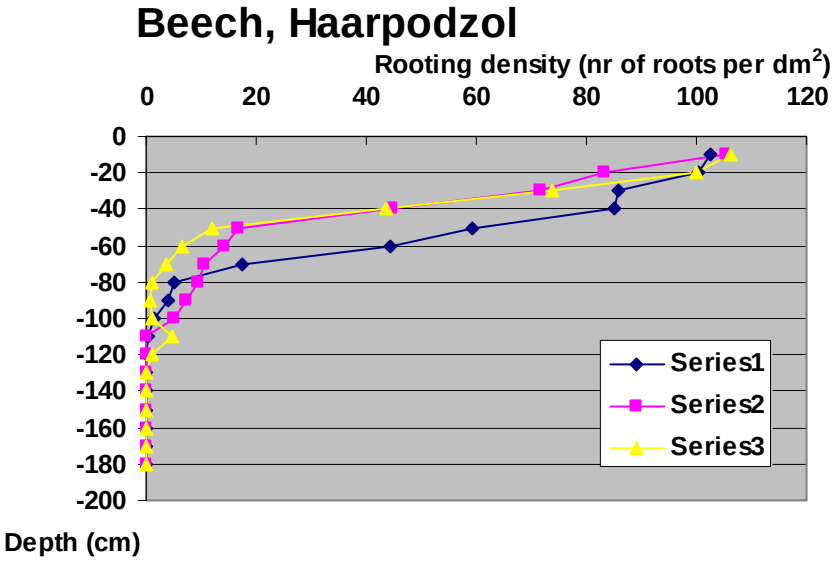

Figure A2.6. Rooting depth of Beech on "Haarpodzol"