Model description and Users guide SMART2 version 3.4
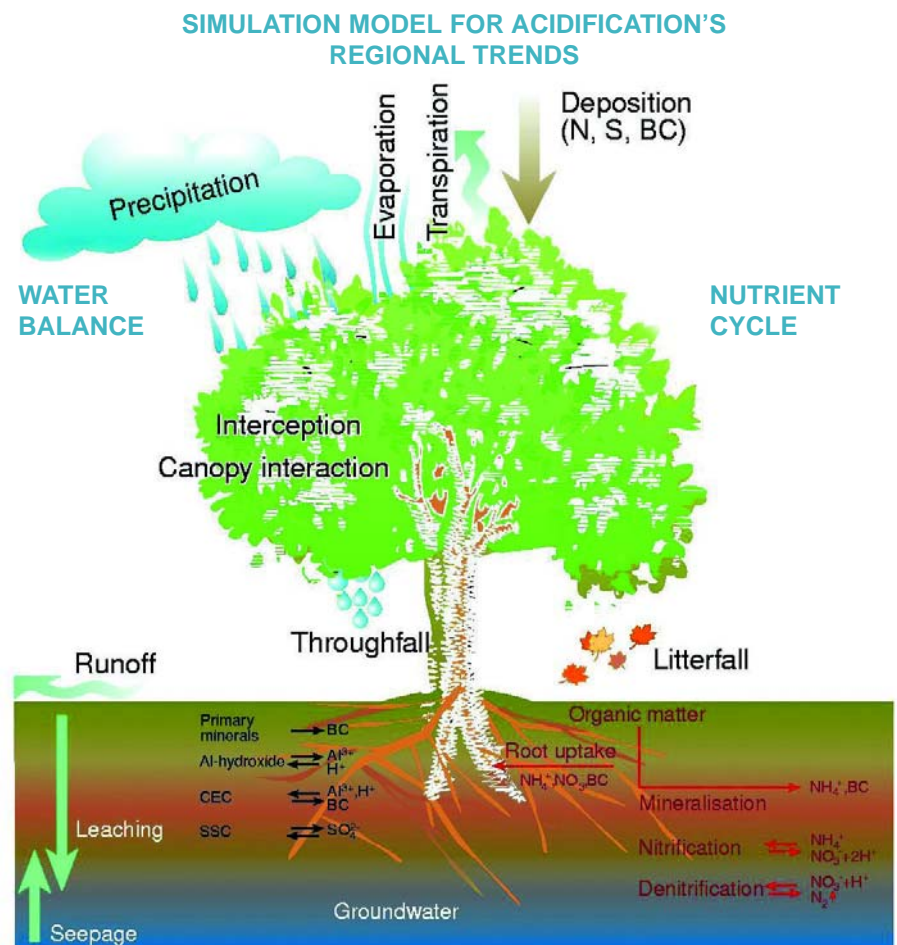
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SIMULATION MODEL FOR ACIDIFICATION'S REGIONAL TRENDS

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ABSTRACT

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This document gives a users guide and technical documentation of the stand alone version of the SMART2 model. It consists of a model description, input description, model use and a technical description for modellers. This version of SMART2 has Alterra quality control status A.

Keywords: SMART2, model, acidification

[Alterra-rapport 1425/12/2006]

Contents

Preface

In this report the soil acidification model SMART2 version 3.4 is described and instructions for installing and using this model are given. SMART2 stands for Simulation Model for Acidification's Regional Trends 2.

SMART2 is a simple, single-layer soil acidification and nutrient cycling model for terrestrial (semi-)natural ecosystems. It 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.

The model is not applicable to wet ecosystems and agricultural systems. Originally it was developed to examine effects of acid deposition on soil chemistry and soil acidification. Nowadays, it is often indrectly used to evaluate long term effects of deposition on plant diversity and carbon sequestration.

The described version is a so called 'stand-alone' version, which means that it performs calculations for a point. It runs with time steps of a year. Short abstracts of validation studies can be found in paragraph 2.4 of this document

Input for the model consists of a water balance, deposition fluxes, physical and chemical soil properties and vegetation data. The model produces time series of among other things soil solution concentrations, pH, nutrient availability, balances of cation and ion fluxes in the soil and biomass production.

The language of this documentation and interaction with the user within the model is English. The model was developed to run on a Intel based PC with Microsoft Windows (W98 or heigher).

The model is developed for researchers and for policy support. Basic knowledge about soil and vegetation ecosystems is needed. It is possible to obtain an executable version of the model by E-mailing to the contact person Janet Mol-Dijkstra. (janet.mol@wur.nl).

Summary

In this publication the soil acidification model SMART2 is described and instructions for installing and using this model are given. SMART2 stands for Simulation Model for Acidification's Regional Trends 2. The '2' means that this is an extended version of SMART, which means that a complete nutrient cycle has been included and that the modelling of the hydrology has improved.

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, divalent base cations (BC2=Ca+Mg), K, Na, NH4, NO3, SO4, HCO3 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.

It is possible to run the SMART2 model in combination with the successionmodel SUMO, which calculates vegetation growth dependent with a yearly back coupling of the availability of nitrogen and phosphorus. Without SUMO, the growth of vegetation is either constant or calculated from a predefined logistic growth curve.

1   Introduction

In this publication the soil acidification model SMART2 is described and instructions for installing and using this model are given. SMART2 stands for Simulation Model for Acidification's Regional Trends 2. The '2' means that this is an extended version of SMART, which means that a complete nutrient cycle has been included and that the modelling of the hydrology has improved. The development of the model has started as a collaborative effort between the Acid Rain project at the International Institute for Applied Systems Analysis in Laxenburg (Austria) and the Winand Staring Centre for Integrated Land Soil and Water Research in Wageningen (The Netherlands). Since 1989 model development continued at the Water and Environment Research Institute in Helsinki (Finland) (now SYKE), and from the mid ninetees onwards at RIVM-CCE and the Winand Staring Centre (now Alterra). For an overview of a first version of the model and some simulation results the reader is referred to the paper by de Vries et al. (1989). Since then the model has been enhanced by the inclusion of a description of (i) sulphate adsorption, (ii) organic anions, (iii) denitrification, and (iv) N-immobilisation. In addition, monovalent base cations and chloride are accounted for in the charge and mass balance (but they don't participate in the exchange reactions).

It is possible to run the SMART2 model in combination with the successionmodel SUMO, which calculates vegetation growth dependent with a yearly back coupling of the availability of nitrogen and phosphorus. Without SUMO, the growth of vegetation is either constant or calculated from a predefined logistic growth curve.

This manual consists of four chapters and three appendices. Chapter 2 outlines the modelling approach, the model structure and contains a description of the processes included in the model. Chapter 3, Model Code, describes the different subroutines in the program and their interaction. Chapter 4, Model Use, describes how to run the model, and. in Appendix A, the explanation of the symbols used in SMART2 is given. The method of solution of the model equations is described in Appendix B. Finally, the use of the graphic output software (MONITOR) is described in Appendix C.

2 Model description

2.1 Model structure

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, divalent base cations (BC2=Ca+Mg), K, Na, NH4, NO3, SO4, HCO3 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 (litterfall, 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 1 gives a schematic representation of the SMART2 model.
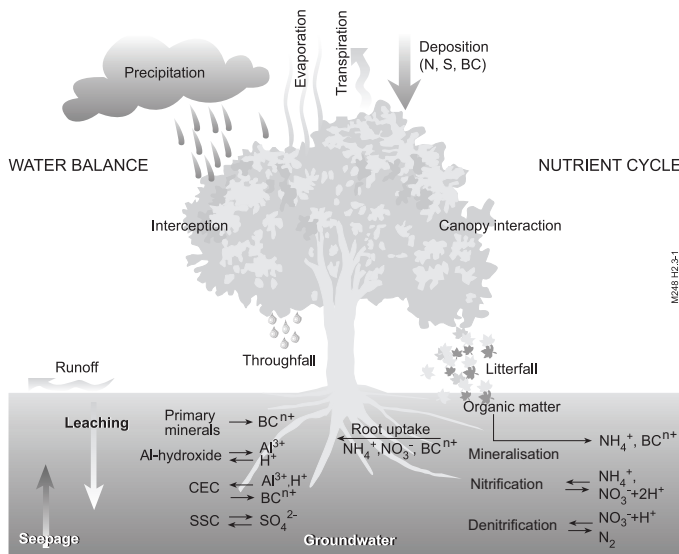

Figure 1 Schematic representation of the processes included in the SMART2 model

The included processes are summarised in Table 1.

Table 1 Overview of processes included in SMART2

Process	Element	Process description
Input:		
Total deposition	SO_4, NO_3, NH_4, BC2 [1], Na, K, Cl	Inputs; deposition fluxes are multiplied by an element- and vegetation-dependent filtering factor[2]
Upward seepage	SO_4, NO_3, NH_4, BC2 [1], Na, K, Cl	Inputs
Water Balance	-	Inputs: precipitation, upward seepage, evapotranspiration
Rate-limited reactions:		
Foliar uptake	NH_4	Linear function of total deposition
Foliar exudation	BC2 [1], K	Equals foliar uptake
Litterfall	BC2 [1], K, NH_4, NO_3	Logistic growth
Root decay	BC2 [1], K, NH_4, NO_3	Linear function of litterfall
Mineralisation	BC2 [1], K, NH_4, NO_3	First-order reaction and a function of pH, Mean Spring Water table (MSW) and C/N ratio of the litter
N immobilisation	NH_4, NO_3	Proportional to N deposition and a function of the C/N ratio soil organic matter
Growth uptake	BC2 [1], K, NH_4, NO_3	Logistic growth
Nitrification	NH_4, NO_3	Proportional to net NH_4 input and a function of pH, Mean Spring Water table (MSW) and C/N ratio
Denitrification	NO_3	Proportional to net NO_3 input and a function of pH, Mean spring water table (MSW) and C/N ratio
Silicate weathering	Al, BC2 [1], Na, K	Zero order reaction
Equilibrium reactions:		
CO_2 Dissociation	HCO_3	CO_2 equilibrium
Dissociation of organic acid	RCOO	Oliver equation
Carbonate weathering	BC2 [1]	Carbonate equilibrium
Al hydroxide weathering	Al	Gibbsite equilibrium
Cation exchange	H [3], Al, BC2 [1]	Gaines-Thomas equations
Sulphate and phosphate sorption	H [3], SO_4, PO_4	Langmuir equation

[1] BC2 stands for the sum of divalent base cations (Ca + Mg)
[2] The vegetation-dependent filtering factor takes the roughness length of the canopy into account
[3] Implicitly, H is affected by all processes. This is accounted for by the charge balance

SMART2 was constructed using a process-aggregated approach to minimise input data requirements for applications on a regional scale. This implied the following simplifying assumptions:
i. The various ecosystem processes have been limited to a few key processes:
   The soil solution chemistry in SMART2 depends solely on the net element input from the atmosphere (deposition), groundwater (upward seepage), nutrient cycling processes (uptake, litterfall, mineralisation and immobilisation) and the geochemical interaction in the soil ((de)nitrification, CO_2 equilibria, weathering of carbonates, silicates and/or Al-hydroxides and cation exchange). Processes that

are not taken into account, are: (i) N fixation and NH_4 exchange, (ii) uptake, immobilisation and reduction of SO_4 and (iii) complexation of Al with OH, SO_4 and RCOO.

ii. The included processes have been represented by simplified conceptualisations: Soil interactions are either described by simple rate-limited reactions (e.g. uptake and silicate weathering) or by equilibrium reactions (e.g. carbonate and Al-hydroxide weathering and cation exchange). Influence of environmental factors such as pH on rate-limited reactions and rate-limitation of weathering and exchange reactions are ignored. Solute transport is described by assuming complete mixing of the element input within one homogeneous soil compartment with a constant density and a fixed depth (at least the root zone). Because SMART2 is a single layer soil model neglecting vertical heterogeneity, it predicts the concentration of the soil water leaving the root zone. The annual water flux percolating from this layer is taken equal to the annual precipitation plus upward seepage minus evapotranspirations, which terms must be specified as a model input. The time step of the model is one year, so seasonal variations are not considered. Justifications for the various assumptions and simplifications have been given by De Vries et al. (1989).

2.2   Process descriptions

In this section an overview of the process descriptions used in SMART2 is given. An explanation of the symbols used is given in Appendix A.

Mass balances

For each of the cations (Na, K, BC2=Mg+Ca, NH_4, Al) and strong acid anions (SO_4, PO_4, NO_3, Cl) considered in SMART2 the mass balance equation for a compartment with depth z, is given by:

$$\frac{d}{dt} \cdot X_{tot}(z) = X_{in} + X_{int}(z) - PE(z) \cdot [X](z) + X_{sen}(z) \qquad (1)$$

where $X_{tot}(z)$ is the total amount of ion X in the soil solution (mol$_c$ m^{-2}) of a soil compartment with depth z (m). X_{in} is the sum of all input fluxes to the soil (mol$_c$ m^{-2} a^{-1}). $X_{int}(z)$ is the sum of all interaction fluxes (mol$_c$ m^{-2} a^{-1}) in the soil at depth z (m). $X_{sen}(z)$ is the net seepage flux (mol$_c$ m^{-2} a^{-1}) entering a soil compartment with depth z (see Eq. 6). $[X](z)$ is the concentration of ion X (mol$_c$ m^{-3}) in the soil compartment with depth z. In SMART2 the precipitation excess at depth z, $PE(z)$ is calculated as:

$$PE(z) = P \cdot (1 - f_{int}) - fr_{ru}(z) \cdot Tr \qquad (2)$$

where P is the precipitation, Tr the actual transpiration, f_{int} the interception fraction (-) and $fr_{ru}(z)$ the cumulative transpiration (water uptake by roots) fraction (-) in the root zone at depth z, which is calculated as:

$$fr_{ru}(z) = \begin{cases} 1 - \left(\dfrac{T_{rz} - z}{T_{rz}} \right)^{ru_{\exp}} & \text{for } z \leq T_{rz} \\ 1 & \text{for } z > T_{rz} \end{cases}$$ (3)

where T_{rz} is the thickness of the root zone (m) and $ru_{\exp}$ is an exponent determining the water uptake pattern.

Upward seepage

Upward seepage is included in the mass balance, Eq. (1), as a net term, i.e. the input of the upward seepage flux (X_{sen}) minus the lateral output flux (X_{la}). Figure 2 gives an overview of the water balance in the soil system, including seepage.
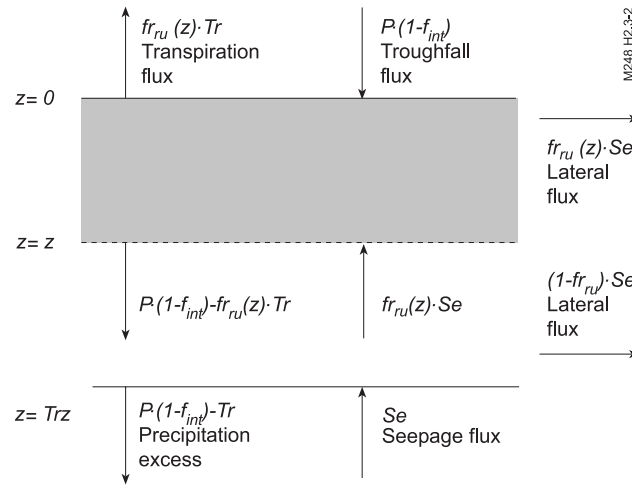
Figure 2 Water balance in SMART2

The input to the soil system consists of the throughfall flux, $P \cdot (1 - f_{int})$ and the upward seepage flux, Se. In SMART2, upward seepage is defined as the flux at the bottom of the root zone. The upward seepage flux is assumed to be reduced at shallower depth. For the sake of simplicity for seepage input into the root zone, the same reduction function with depth is used as for transpiration, i.e. $fr_{ru}(z)$, cf. Eq. (3). Consequently, the seepage input to the compartment with depth z equals: $fr_{ru}(z) \cdot Se$. The seepage flux of ion X is described as:

$$X_{se}(z) = fr_{ru}(z) \cdot Se \cdot [X]_{se}$$ (4)

where $[X]_{se}$ stands for the concentration of ion X in the seepage water (mol$_c$ m^{-3}) and Se the upward seepage flux (m a^{-1}). Because it is stated that the transpiration is independent of the upward seepage flux, Se, there must be a lateral output flux which equals the seepage input: $- fr_{ru}(z) \cdot Se$.

The concentration of ion X in the lateral output flux at depth z equals the concentration in the soil compartment, $[X](z)$. Consequently, the lateral output flux of ion X is described as:

$$X_{la}(z) = -fr_{ru}(z) \cdot Se \cdot [X](z) \tag{5}$$

where Se is the upward seepage flux (m a^{-1}). The net effect of seepage at depth z, $X_{sen}(z)$, is thus:

$$X_{sen}(z) = fr_{ru}(z) \cdot Se \cdot ([X_{se}] - [X](z)) \tag{6}$$

From Eq. (6) it follows that the influence of upward seepage on the concentration in the considered soil compartment is larger as the concentration of ion X in the upward seepage water deviates more from the concentration in the soil solution. Note that the remaining part of the upward seepage flux that does not reach depth z is draining laterally. This lateral flux equals: - $(1 - fr_{ru}(z)) \cdot Se \cdot [X_{se}]$.

Input fluxes

The external input by atmospheric deposition to the soil compartment is influenced by the total deposition (*td*), foliar uptake (*fu*), foliar exudation (*fe*) and mineralisation of litter (*mi*). Their presence depends on the component involved:

$$Al_{in} = 0 \tag{7}$$
$$BC2_{in} = BC2_{td} + BC2_{fe} + BC2_{mi} \tag{8}$$
$$K_{in} = K_{td} + K_{fe} + K_{mi} \tag{9}$$
$$Na_{in} = Na_{td} \tag{10}$$
$$NH_{4,in} = NH_{4,td} - NH_{4,fu} + N_{mi} \tag{11}$$
$$NO_{3,in} = NO_{3,td} \tag{12}$$
$$SO_{4,in} = SO_{4,td} \tag{13}$$
$$PO_{4,in} = P_{mi} \tag{14}$$
$$HCO_{3,in} = 0 \tag{15}$$
$$RCOO_{in} = 0 \tag{16}$$
$$Cl_{in} = Cl_{td} \tag{17}$$

And the input of H is calculated from the charge balance:

$$\begin{aligned} H_{in} = SO_{4,in} + PO_{4,in} + NO_{3,in} + HCO_{3,in} + Cl_{in} + RCOO_{in} - \\ - NH_{4,in} - Al_{in} - BC2_{in} - K_{in} - Na_{in} \end{aligned} \tag{18}$$

Canopy interactions

The canopy interactions included in SMART2 were taken from the RESAM model (De Vries *et al.*, 1995a). Foliar uptake of NH$_4$ and H is described as:

$$X_{fu} = frX_{fu} \cdot X_{td} \qquad (19)$$

where frX_{fu} is the foliar uptake fraction of H or NH$_4$. For H_{fu} the deposition of free H (H_{td}) is calculated from the charge balance:

$$H_{td} = SO_{4,td} + NO_{3,td} + Cl_{td} - NH_{4,td} - BC2_{td} - K_{td} - Na_{td} \qquad (20)$$

Foliar exudation of the cations (K, BC2) is taken equal to foliar uptake of NH$_4$ and H (cf. De Vries *et al.*, 1995a), and is assumed to be triggered by exchange with these ions (Roelofs *et al.*, 1985; Ulrich, 1983). The foliar exudation of each individual cation is calculated as:

$$X_{fe} = frX_{fe} \cdot (NH_{4,fu} + H_{fu}) \qquad (21)$$

with $X=K, BC2$, frX_{fe} is the foliar exudation fraction of K and BC2 (-), and sum of frK_{fe} and $frBC2_{fe}$ equals 1.

Litterfall and root decay

The inputs by litterfall and root decay in SMART2 affecting the mineralisation flux, were also taken from the RESAM model (De Vries *et al.*, 1995a). In SMART2, litterfall is the input to an organic pool containing N, P, BC2 and K. Contrary to RESAM, SMART2 does not include a physical litter layer in which a separate concentration is calculated. Only an organic pool is modelled, which has the same soil solution concentration as the mineral soil. Input fluxes of N, P, BC2 and K by litterfall, X_{lf} are described as:

$$X_{lf} = (1 - frX_{re}) \cdot Am_{lf} \cdot ctX_{lv} \qquad (22)$$

where Am_{lf} is the amount of litterfall (kg ha^{-1} a^{-1}), ctX_{lv} is the contents of element X in leaves (mol$_c$ kg^{-1}) and frX_{re} are reallocation fractions for element X in leaves (-). Reallocation of K and BC2 in leaves prior to litterfall is considered negligible (i.e. frK_{re} = $frBC2_{re}$ = 0). The amount litterfall is described by a logistic growth function (see Eq. 61). High contents of N in leaves and fine roots in Dutch forests are caused by the high N deposition level. To account for this effect, the N content in leaves is calculated as a function of the N deposition according to:

$$ctN_{lv} = \begin{cases} ctN_{lv,mn} & for\ N_{td} \leq N_{td,mn} \\ ctN_{lv,mn} + (ctN_{lv,mx} - ctN_{lv,mn}) \cdot \dfrac{N_{td} - N_{td,mn}}{N_{td,mx} - N_{td,mn}} & for\ N_{td,mn} < N_{td} < N_{td,mx} \\ ctN_{lv,mx} & for\ N_{td} \geq N_{td,mx} \end{cases} \quad (23)$$

where $ctN_{lv,mn}$ and $ctN_{lv,mx}$ are the minimum and maximum N content in leaves (mol$_c$ kg^{-1}) and $N_{td,mn}$ and $N_{td,mx}$ are the minimum and maximum total deposition levels of N (mol$_c$ ha^{-1} a^{-1}) between which the N content of leaves is influenced. For the Netherlands $N_{td,mn}$ = 1500 mol$_c$ ha^{-1} a^{-1} and $N_{td,mx}$ = 7000 mol$_c$ ha^{-1} a^{-1} were used. Contrary to RESAM the reallocation fraction (frX_{re}) is not considered as a function of the N content in the foliage, frX_{re} remains constant during the simulation period.

The dynamic turnover of fine roots is coupled with the amount of litterfall and divided between the litter compartment (depth independent) and the mineral soil (depth dependent). The root decay flux in the litter compartment ($X_{rd,lt}$) is described as:

$$X_{rd,lt} = X_{lf} \cdot ncf \cdot fr_{rt,lt} \quad (24)$$

where ncf is the nutrient cycling factor (-), which is defined as the ratio of the root turnover (related to nitrogen) and the above ground nitrogen cycle (litterfall flux), and $fr_{rt,lt}$ is the fraction of fine roots in the litter layer (-). The depth-dependent root decay flux in the mineral soil ($X_{rd,ms}(z)$) is described as:

$$X_{rd,ms}(z) = fr_{ru}(z) \cdot X_{lf} \cdot ncf \cdot (1 - fr_{rt,lt}) \quad (25)$$

Mineralisation

As with canopy interactions, litter fall and root decay, mineralisation in SMART2 is also taken from the RESAM model. For the simulation of the decomposition of above-ground organic matter (litter, including dead roots in the litter layer, and dead wood, which is computed by SUMO) a distinction is made between a rapidly decomposing pool of fresh litter (less than one year old) and a slowly decomposing pool of old litter (more than one year) (Janssen, 1984). The mineralisation flux of N (during mineralisation N is released as NH$_4$), P, K and BC2 (mol$_c$ ha^{-1} a^{-1}) from fresh litter, $X_{mi,fl}$, is described as a fraction of the input of X by litter fall and root decay in the litter compartment according to:

$$X_{mi,fl} = [frX_{le} + fr_{mi} \cdot (1 - frX_{le})] \cdot X_{lf} \cdot (1 + ncf \cdot fr_{rt,lt}) \quad (26)$$

where fr_{mi} is a mineralisation fraction (-) and frX_{le} is a litter leaching fraction (-). Leaching only refers to the release of BC2 (=Ca+Mg) and K from fresh litter just after litter fall, a process which is especially important for K. Litter leaching is a process which differs from mineralisation because organic matter is not decomposed.

Fresh litter which is not mineralised is transferred to the old litter humus pool. The mineralisation flux of NH_4, P, K and BC2 from this litter pool, $X_{mi,lt}$, and from dead wood, $X_{mi,dw}$, is described by first-order kinetics (Van Veen, 1977):

$$X_{mi,x} = k_{mi,x} \cdot Am_x \cdot ctX_x \qquad (27)$$

where x is lt for old litter and dw for dead wood, $k_{mi,x}$ is the mineralisation rate constant from old litter or dead wood (a^{-1}), Am_x is the amount of old litter or dead wood (kg ha^{-1}) and ctX_x is the content of element X in old litter or dead wood (mol$_c$ kg^{-1}). At present, mineralisation of organic matter in the mineral soil layers is not considered in SMART2, except for the mineralisation from root necro-mass, which is fed by root decay as described before. The total input by mineralisation (X_{mi}) in the litter layer consists of the sum of mineralisation of fresh litter, old litter, dead wood and the root decay in the litter layer:

$$X_{mi} = X_{mi,lt} + X_{mi,fl} + X_{mi,dw} + X_{rd,lt} \qquad (28)$$

Root decay in the mineral soil is considered to be mineralised completely. To simulate mineralisation on former agricultural soil, a humus pool was introduced. This pool consists of material built up in the agricultural history of the soil. The mineralisation fluxes from the humus pool are described according to Eq (27). The total mineralisation flux at depth z becomes equal to:

$$X_{mi,tot}(z) = X_{mi,lt} + X_{mi,fl} + X_{rd,lt} + X_{rd,ms}(z) + X_{mi,dw} + X_{mi,hu} \qquad (29)$$

The flux of organic anions, $RCOO_{mi,tot}$, produced during mineralisation from both fresh and old litter and from dead root (mol$_c$ ha^{-1} a^{-1}) is calculated from charge balance considerations:

$$RCOO_{mi,tot}(z) = N_{mi,tot}(z) + BC2_{mi,tot}(z) + K_{mi,tot}(z) \qquad (30)$$

Actual values for the mineralisation fraction ($fr_{mi,fl}$ and $fr_{mi,lt}$) and mineralisation rate constant ($k_{mi,fl}$ and $k_{mi,lt}$) are described in SMART2 as maximum values, which are reduced by factors such as soil moisture (water-table), pH and the C/N and C/P ratio. For all constituents the maximum value ($k_{mi,mx}$ and $f_{mi,mx}$) is influenced by the mean water-table during spring time (Mean Spring Water table, MSW) and the pH. The N and P mineralisation is also influenced by the C/N and C/P ratio:

$$fr_{mi} = fr_{mi,mx} \cdot rf_{mi,MSW} \cdot rf_{mi,pH} \cdot rf_{mi,CX} \qquad (31)$$

$$k_{mi} = k_{mi,mx} \cdot rf_{mi,MSW} \cdot rf_{mi,pH} \cdot rf_{mi,CX} \qquad (32)$$

where $rf_{mi,MSW}$, $rf_{mi,pH}$ and $rf_{mi,CX}$ are the reduction factors for water-table, pH and N or P content (C/N or C/P ratio) respectively (-). For BC2 and K, $rf_{mi,CX} = 1$. The reduction functions for water-table and pH were partly taken from RESAM (cf. De Vries *et al.*, 1988):

$$
rf_{mi,MSW} = \begin{cases} 0.25 & \textit{for } MSW \leq 0.45 \\ \log_{10}(4 \cdot MSW) & \textit{for } 0.45 < MSW < 2.50 \\ 1 & \textit{for } MSW \geq 2.50 \end{cases} \tag{33}
$$

$$
rf_{mi,pH} = \begin{cases} 0 & \textit{for } pH \leq 2.5 \\ \dfrac{pH - 2.5}{2} & \textit{for } 2.5 < pH < 3.5 \\ \dfrac{pH - 1}{5} & \textit{for } 3.5 \leq pH < 6 \\ 1 & \textit{for } pH \geq 6 \end{cases} \tag{34}
$$

The N and P mineralisation values are reduced at low N and P contents (high C/N and C/P ratios) to account for immobilisation by microbes according to (Janssen, 1984):

$$
rf_{mi,CX} = \begin{cases} 1 & \textit{for } CX_s \leq CX_{mo} \\ 1 - \dfrac{CX_s - CX_{mo}}{DA_{mo} \cdot CX_{mo}} & \textit{for } CX_{mo} < CX_s < (1 + DA_{mo}) \cdot CX_{mo} \\ 0 & \textit{for } CX_s \geq (1 + DA_{mo}) \cdot CX_{mo} \end{cases} \tag{35}
$$

where CX_{mo} is the C/N or C/P ratio of the micro-organisms decomposing the substrate (-), CX_s is the C/N or C/P ratio of the substrate (fresh litter ($s=fl$), old litter ($s=lt$)) and DA_{mo} is the dissimilation to assimilation ratio of the decomposing microbes (-). Values for DA_{mo} and CX_{mo} are related to fungi because they are mainly responsible for mineralisation of forest litter.

N immobilisation

Besides implicitly modelled immobilisation by mineralisation, SMART2 includes also a description of N immobilisation by soil organic matter, which has also been included in the SMART model (De Vries *et al.*, 1994b). The description of N immobilisation is based on the assumption that the amount of organic matter (carbon) is constant. Consequently, immobilisation of carbon and base cations is not accounted for the mineral soil.

N immobilisation is described by an increase in N content in organic matter. When the C/N ratio of the soil (CN_{om}) varies between a critical (CN_{cr}) and a minimum value (CN_{mn}), the immobilisation rate is assumed to decrease according to:

$$
N_{im} = \begin{cases} 0 & \textit{for } CN_{om} \leq CN_{mn} \\ (N_{td} - N_{gu} - N_{le,mn}) \cdot \dfrac{CN_{om} - CN_{mn}}{CN_{cr} - CN_{mn}} & \textit{for } CN_{mn} < CN_{om} < CN_{cr} \\ N_{td} - N_{gu} - N_{le,mn} & \textit{for } CN_{om} \geq CN_{cr} \end{cases} \tag{36}
$$

The minimum N leaching rate ($N_{le\ mn}$) is calculated by multiplying the precipitation excess by a natural background NO_3 concentration in drainage water of 0.02 mol$_c$ m^{-3} (Rosén, 1990). During the simulation, the C content is fixed whereas the N content is annually updated, by adding the amount of N immobilised during each time step to the N amount in the mineral topsoil. The C/N ratio is in turn updated by dividing the fixed C pool by the variable N pool according to:

$$CN_{om} = \frac{\rho_{rz} \cdot T_{iz} \cdot ctC_{iz}}{AmN_{iz} + N_{im}} \tag{37}$$

Because N immobilisation mainly occurs in the humus layer and the upper mineral soil (Tietema, 1992), the thickness of the zone where N immobilisation (T_{iz}) occurs is taken at 20 cm.

Interaction fluxes

The interaction fluxes for Al, BC2, P, K, Na, NH$_4$ and NO$_3$ accounted for in SMART2 are base cation and Al weathering (*we*), root uptake (*ru*), nitrification (*ni*), denitrification (*de*) and rootdecay in the mineral soil (*rd mi*). For nitrification and denitrification reduction functions as a function of pH and groundwater level are included (see Eq. 64 and 65). The interaction fluxes for a compartment with depth z are described as:

$$Al_{int}(z) = Al_{we} \cdot z \tag{38}$$
$$BC2_{int}(z) = BC2_{we} \cdot z - fr_{ru}(z) \cdot BC2_{ru} \tag{39}$$
$$K_{int}(z) = K_{we} \cdot z - fr_{ru}(z) \cdot K_{ru} \tag{40}$$
$$Na_{int}(z) = Na_{we} \cdot z \tag{41}$$
$$NH_{4,int}(z) = -fr_{ru}(z) \cdot (NH_{4,ni} + NH_{4,ru}) \tag{42}$$
$$NO_{3,int}(z) = fr_{ru}(z) \cdot (NH_{4,ni} - NO_{3,ru} - NO_{3,de}) \tag{43}$$
$$PO_{4int}(z) = P_{we} \cdot z - fr_{ru}(z) \cdot P_{ru} \tag{44}$$
$$SO_{4,int}(z) = 0 \tag{45}$$
$$HCO_{3,int}(z) = 0 \tag{46}$$
$$RCOO_{int}(z) = 0 \tag{47}$$
$$Cl_{int}(z) = 0 \tag{48}$$
$$\begin{aligned} H_{int}(z) = {} & SO_{4,int}(z) + PO_{4,int}(z) + NO_{3,int}(z) + HCO_{3,int}(z) + Cl_{int}(z) + \\ & RCOO_{int}(z) - NH_{4,int(z)} + Al_{int}(z) - BC2_{int}(z) - K_{int}(z) - Na_{int}(z) \end{aligned} \tag{49}$$

Mineral weathering

Weathering of divalent base cations (BC2=Ca+Mg) and monovalent base cations (Na, K) is included as a zero-order reaction. It is possible to make the weathering rate of base cations pH dependent according to:

$$BC_{we\ crit} = BC_{we\ field} * 10^{\alpha(pHref - pH)} \tag{50}$$

where BC_{we} and $BC_{we\ field}$ are the weathering fluxes at the reference pH (*pHref*) and the current pH of the soil solution respectively and α is the pH dependency of the weathering rate. Weathering rates of most minerals are independent of pH at values between 5 and 8 (c.f. Sverdrup, 1990), therefore a maximum value of 5 was used as the current pH in the soil solution. Values for α of pure minerals range from 0 to 1 (e.g. 1.0 for Adularia (Helgeson et al., 1984), 0.45 for albite (Chou and Wollast, 1985), 0.37 for muscovite (Knauss and Wolery, 1989), 0.7 for amphibole, chlorite and vermiculite (Sverdrup, 1990). On basis of these data, α was set to 0.5 for sandy soils in which feldspars are the predominant minerals and 0.6 for non-sandy soil in which the weathering of clay minerals contributes significantly to the observed weathering rates.

The weathering of Al is either related to BC2 weathering (Equation 51) or related to Ca, Mg, K and Na weathering according to (Eq 52):

$$Al_{we} = r_{BC2} \cdot BC2_{we} \tag{51}$$
$$Al_{we} = r_{Ca} \cdot Ca_{we} + r_{Mg} \cdot Mg_{we} + r_K \cdot K_{we} + r_{Na} \cdot Na_{we} \tag{52}$$

where r_X is the stoichiometric equivalent ratio of Al to X in the congruent weathering of silicates, with X = BC2, Ca, Mg, K or Na. In SMART2 the default value for r_{BC2} is 2, which is based on an average for Ca and Mg (cf. De Vries *et al.*, 1995a). Default values for r_{Ca}, r_{Mg}, r_K, and r_{Na} are resp. 3, 0.6, 3 and 3.

The weathering of P is related to BC2 weathering according to:

$$P_{we} = PBCrat \cdot BC2_{we} \tag{53}$$

where *PBCrat* is the stoichiometric equivalent ratio of P to BC2 in the congruent weathering of silicates.

Nutrient uptake

Nutrient uptake is taken from the MACAL model (De Vries *et al.*, 1994c). Total root uptake of NH_4, NO_3, P, BC2=Ca+Mg, K is described as a demand function, which consists of maintenance uptake, to re-supply the needles/leaves/shoots and roots (steady-state situation), and net (growth) uptake in stems and branches. The total root uptake fluxes for NH_4, NO_3, P, BC2 and K ($mol_c\ ha^{-1}\ a^{-1}$) are thus described as:

$$NO_{3,ru} = (N_{lf} - N_{fu} + N_{gu}) \cdot \frac{NO_{3,in}}{N_{in}} \tag{54}$$

$$NH_{4,ru} = (N_{lf} - N_{fu} + N_{gu}) \cdot \frac{NH_{4,in}}{N_{in}} \tag{55}$$

$$P_{ru} = P_{lf} + P_{gu} \tag{56}$$

$$BC2_{ru} = BC2_{lf} + BC2_{fe} + BC2_{gu} \tag{57}$$

$$K_{ru} = K_{lf} + K_{fe} + K_{gu} \tag{58}$$

where gu stands for growth uptake, and $N = NH_4 + NO_3$. In case of nutrient shortage the nutrient contents in the foliage are reduced according to the maximum available nutrients. However, the model does not include a feedback of nutrient shortage on growth.
Growth uptake is calculated as:

$$X_{gu} = (Am_{st}(t) - Am_{st}(t-1)) \cdot ctX_{st} \tag{59}$$

where $Am_{st}(t)$ - $Am_{st}(t\text{-}1)$ is the increment in amount stems for the current year (=time step) (kg ha^{-1} a^{-1}) and ctX_{st} is the content of element X in stems (mol$_c$ kg^{-1}). The current amount stems and branches is forced by a logistic growth function:

$$Am_{st}(t) = \frac{Am_{st,mx}}{1 + \exp(-k_{gl} \cdot (age_{vg} + t - t_{\frac{1}{2}}))} \tag{60}$$

where $Am_{st}(t)$ is the amount of stems (and branches) for simulation year t (kg ha^{-1}), $Am_{st,mx}$ the maximum amount of stems (kg ha^{-1}), age_{vg} the initial age of the vegetation (forest), $t_{\frac{1}{2}}$ the half life-time (a), k_{gl} is the logistic growth rate constant (a^{-1}).
In the model the amount of litterfall is linked to the stem growth parameters by assuming that the maximum amount of litterfall is reached with a three times higher growth constant than the maximum amount of stems:

$$Am_{lf}(t) = \frac{Am_{lf,mx}}{1 + \exp(-3 \cdot k_{gl} \cdot (age_{vg} + t - t_{\frac{1}{2}}))} \tag{61}$$

where $Am_{lf,mx}$ is the maximum amount of litterfall (kg ha^{-1} a^{-1}).

When SUMO is used, N and P uptake and growth and litter fall is calculated by SUMO. BC2 and K uptake is then calculated by SMART2, using the calculated growth and litterfall calculated by SUMO.

Nitrification and denitrification
Nitrification and denitrification for the complete soil layer (mol$_c$ ha^{-1} a^{-1}) are described in SMART2 as a fraction of the net input:

$$NH_{4,ni} = fr_{ni} \cdot \left(NH_{4,in} - NH_{4,ru} + \frac{NH_{4,in}}{N_{in}} \cdot \left(N_{mi,tot} - N_{im} \right) \right) \tag{62}$$

$$NO_{3,de} = fr_{de} \cdot \left(NO_{3,in} - NO_{3,ru} + NH_{4,ni} - \frac{NO_{3,in}}{N_{in}} \cdot N_{im} \right) \qquad (63)$$

where fr_{ni} and fr_{de} are the nitrification and denitrification fractions (-), $NH_{4,in}$ and $NO_{3,in}$ stand for the gross input fluxes of NH_4 and NO_3, respectively, cf. Eqs. (11) and (12), $NH_{4,ru}$ and $NO_{3,ru}$ stands for the root uptake fluxes of NH_4 and NO_3 respectively, cf. Eqs. (42) and (43), $NH_{4,im}$ and $NO_{3,im}$ stands for the immobilisation fluxes in the mineral soil of NH_4 and NO_3 respectively, Eq. (36), $N_{mi,tot}$ is the total mineralisation flux, cf. Eq. (29) and $NH_{4,ni}$ is the nitrification flux, cf. Eq. (62). As with mineralisation, the maximum values for the nitrification and denitrification rate constant, $fr_{ni,mx}$ and $fr_{de,mx}$, are adjusted by the mean water-table and pH:

$$fr_{ni} = fr_{ni,mx} \cdot rf_{ni,MSW} \cdot rf_{ni,pH} \qquad (64)$$

$$fr_{de} = fr_{de,mx} \cdot rf_{de,MSW} \cdot rf_{de,pH} \qquad (65)$$

where $rf_{ni/de,MSW}$ and $rf_{ni/de,pH}$ are the nitrification and the denitrification reduction factors for the water-table and pH respectively (-). Maximum values are reduced with a decreasing mean spring water-table for nitrification, because this process is restricted to aerobic conditions, whereas the opposite is true for denitrification. Both rate constants are also reduced with decreasing pH.
The nitrification reduction functions for mean spring water-table is described as:

$$rf_{ni,MSW} = \begin{cases} rf_{ni,MSW,mn} & \text{for } MSW \leq z_1 \\ rf_{ni,MSW,mn} + (rf_{ni,MSW,mx} - rf_{ni,MSW,mn})\dfrac{MSW - z_1}{z_2 - z_1} & \text{for } z_1 < MSW < z_2 \\ rf_{ni,MSW,mx} & \text{for } MSW \geq z_2 \end{cases} \qquad (66)$$

were $rfr_{ni,MSW,mn}$ is the soil dependent minimum value of the reduction function (-), and z_1 and z_2 are soil dependent MSW (m) values where the reduction function is changed.
The nitrification reduction function for pH is described as:

$$rf_{ni,pH} = \frac{1}{1 + \exp(4 \cdot (2.75 - pH))} \qquad (67)$$

The denitrification reduction function for mean spring water-table is described as:

$$rf_{de,MSW} = \begin{cases} rf_{de,msw,mx} & \text{for } MSW \leq 0m \\ rf_{de,msw,mx} + (rf_{de,msw,mn} - rf_{de,msw,mx}) \cdot \dfrac{MSW}{z_{de}} & \text{for } 0 < MSW < z_{de} \\ rf_{de,msw,mn} & \text{for } MSW \geq z_{de} \end{cases} \qquad (68)$$

where z_{de} (m) is the soil-dependent depth of the *MSW* below which the reduction by $rf_{de,MSW}$ (-).

The denitrification reduction function for mean pH is described as:

$$rf_{de,pH} = \begin{cases} 0 & for\ pH \leq 3.5 \\ \dfrac{pH - 3.5}{3} & for\ 3.5 < pH < 6.5 \\ 1 & for\ pH \geq 6.5 \end{cases} \tag{69}$$

Temperature effect

The temperature effect on mineralisation was included by using a response function described by Kirschbaum and Paul (2002), scaled to a reference temperature of 10°C

$$k_{(T)} = k_{(Tref)} \cdot e^{3.36\left(\frac{T-40}{T+31.79} - \frac{10-40}{10+41.79}\right)} \tag{70}$$

where k represents the mineralisation rate constant of old litter (a^{-1}), T is the temperature (ºC) and T_{ref} is the reference temperature (ºC).

Cation Exchange and chemical equilibria

Cation exchange is included for H, Al and BC2 described by Gaines-Thomas equations using concentrations instead of activities (cf. De Vries *et al.*, 1989):

$$\frac{fr\,H_{ac}^{\;2}}{fr\,BC2_{ac}} = KH_{ex} \cdot \frac{[H^+]^2}{[BC^{2+}]} \tag{71}$$

$$\frac{frAl_{ac}^{\;2}}{frBC2_{ac}^{\;3}} = KAl_{ex} \cdot \frac{[Al^{3+}]^{expH}}{[BC^{2+}]^3} \tag{72}$$

where *expH* is exponent of [H] in H-BC exchange. This is set to 2, which is a value for 'normal' Gaines-Thoams exchange, unless there are strong reasons to set to another value, which makes the KH_{ex} pH dependent.

The charge balance for the exchange complex requires that:

$$frH_{ac} + frBC2_{ac} + frAl_{ac} = 1 \tag{73}$$

Sulphate and phosphate adsorption is described by a Langmuir equation:

$$ctX_{ac} = \frac{XSC \cdot [X]}{C_{1/2} + [X]} \tag{74}$$

where ctX (mol_c kg^{-1}) is the sorbed amount of SO_4 or PO_4, XSC (mol_c kg^{-1}) the sorption capacity and $C_{1/2}$ the half-saturation constant (mol_c m^{-3}). The dissociation of CO_2, the dissolution of Ca carbonate (calcareous soils only) and the dissolution of Al hydroxide is described as (cf. De Vries *et al.*, 1988):

$$[HCO_3^-] = K_{CO_2} \frac{pCO_2}{[H^+]} \tag{75}$$

$$[BC^{2+}] = \frac{K_{Ca_{cb}} \cdot pCO_2}{[HCO_3^-]^2} \tag{76}$$

$$[Al^{3+}] = K_{Al_{ox}} \cdot [H^+]^{expAl} \tag{77}$$

Al dissolution is often described by a gibbsite equilibrium. Values for $log10$ K_{Alox} generally vary between 8.0 and 8.5. In general the Al concentration depends upon the H concentration and a site dependent exponent, *expAl*, as given in eq 77. Values for K_{Alox} and *expAl* a depend on the soil depth. Especially in forest topsoils, it is more accurate to use values for a that are lower than 3, and consequently also a different logK value. Regression analyses between the negative logarithm of the Al concentration (pAl) against the negative logarithm of the H concentration (pH), with concentrations in $mol.l^{-1}$ for nearly 300 Dutch forest stands give results as presented in Table 2. The data are based on measurements in approximately 200 sandy soils (Leeters and de Vries 2001) and in approximately 40 loess soils, 30 clay soils and 30 and peat soils (Klap et al. 1998). The results show that the standard gibbsite equilibrium constant and exponent of 3.0 is reasonable for clay soils. Very different values, however, are required for peat soils and to a lesser extent also for sandy and loess soils, especially at lower soil depths.

Table 2 Estimated values of KAlox and expAl based on regression between pAl and pH in the solution of Dutch soils (Van der Salm and De Vries, 2001)

Soil type	Depth (cm)	log KAl_{ox}	*expAl*	R^2_{adj}	n.
Sandy soils	0-10	-0.56	1.167	56.1	195
	10-30	2.37	1.88	82.8	348
	30-100	5.20	2.51	86.3	172
Peat	all depths	-1.06	1.31	81.2	116
Clay	all depths	7.88	2.65	87.3	116
Loess	0-10	-0.48	1.06	64.1	39
	10-30	3.29	1.90	87.9	39
	30-100	4.55	2.17	92.4	39

The dissociation of organic acids is modeled with varying complexity (see 0).
The H concentration is determined by charge balance, Eq. (18), because the model structure of SMART2 is based on the anion mobility concept (Reuss and Johnson, 1986). The charge balance for the soil solution concentrations equals:

$$[H^+] = [SO_4^{2-}] + [NO_3^-] + [HCO_3^-] + [Cl^-] + [RCOO^-] + [H_2PO4^-] - [BC^{2+}] - [NH_4^+] - [Na^+] - [K^+] - [Al^{3+}] \tag{78}$$

Concentrations of K, Na, NH_4, NO_3 and Cl are fully determined by the mass balance equation, cf. Eq. (1). The concentration of base cations in non-calcareous soils is determined by both the mass balance equation and a change in the adsorbed amount of base cations determined by cation exchange equilibrium reactions, Eqs. (71) and (72). The concentrations of HCO_3 and Al are determined by both the mass balance equations and an equilibrium with H, cf. Eqs. (75), (76) and (77). The concentration of divalent base cations in calcareous soils is determined by both the mass balance equation and a change in carbonate content. In these soils carbonate weathering is included, Eq. (76), but silicate weathering, Al hydroxide weathering and cation exchange are neglected (the Al concentration is thus set to zero). The dissociation of organic acids is modelled according to the description in 0. Sulphate and phosphate sorption is described by a Langmuir isotherm, Eq. (74). The pH is thus influenced by all rate-limited and equilibrium processes causing proton production or consumption.

The dissolved and adsorbed concentrations are calculated by solving fourteen equations with fourteen unknowns, i.e. ten concentrations ($[H^+]$, $[Al^{3+}]$, $[K^+]$, $[Na^+]$, $[BC^{2+}]$, $[SO_4^{2-}]$, $[H_2PO_4^-]$, $[NO_3^-]$, $[Cl^-]$, $[HCO_3^-]$, $[RCOO^-]$), three exchangeable fractions (frH_{ac}, $frBC2_{ac}$, $frAl_{ac}$) and adsorbed SO_4 ($ctSO_{4,ac}$). The numerical solution procedure is given in Solution method.

2.3   Input parameters

Most input parameters differ per soil type and vegetation type and are given in the chapter 4 (model use). Some parameters, however, are fixed in the source code (see Table 3). The column 'Equation' gives the equation number where the parameter is used in. Table 4 gives an overview of default values which are used when the parameters are not given in the input file.

Table 3 Fixed parameters in SMART2

Parameter	Description	Unit	Value	Equation
ru_{exp}	water and nutrient uptake parameter (expert judgement)	-	2.00	3
$ctclv$	50% C in leaves (basic assumption)	-	50.0	35[1]
CN_{mo}	C:N ratio micro-organism (Janssen, 1984)	-	15.0	35
CP_{mo}	C:P ratio micro-organism (Leeters and De Vries, 2002)	-	67.0	35
$caCN_{mn}$	minimum C:N ratio for calcareous soils (De Vries, 1994)	-	10.0	36
$caCN_{cr}$	critical C:N ratio for calcareous soils (De Vries, 1994)	-	20.0	36
$cnitmin$	min N-leaching concentration (Rosén, 1990)	mol_c m^3	0.02	36[2]
T_{iz}	top layer for N immobilisation	m	0.2	37
C_{om}	40% C in organic matter (basic assumption)	-	0.4	37[1]
$K_{Ca\,cb}$	dissolution constant for CaCO3		$10^{3.17}$	76
$midw$	mineralisation constant of dead wood (Zappeij, 1995)	y^{-1}	0.02	27
$ctbc2dw$	BC2 content in dead wood (= 0.1 * median of stem content)	-	0.008	27
$ctkdw$	K content in dead wood (= 0.1 * median of stem content)	-	0.005	27

[1] not directly used in the equation but used to calculate CN
[2] not directly used in the equation but used to calculate $N_{le,\,mn}$

Table 4 Default values for some parameters in SMART2

Parameter	Description	Unit	Value	Equation
expAl	exponent in [Al] = KAlox*[H]^expAl		3	77
expH	exponent of [H] in H-BC exchange (Gaines-Thomas only)		2	72
CN_{mn}	minimum C:N ratio for non-calc. soils (De Vries, 1994)	-	15.0	36
CN_{cr}	critical C:N ratio for non-calc. soils (De Vries, 1994)	-	40.0	36
Alox_0	initial Al buffer capacity	meq/kg	1e[9]	A31
f_ni			1	62
ratwAlBc	Stoichiometric equivalent ratio of Al to BC2	-	2	51
GVG	Means spring water table	m	100	
rat_asdi	dissimilation assimilation ratio (Kros et al., in prep)	-	5	35

[1] not directly used in the equation but used to calculate *CN*
[2] not directly used in the equation but used to calculate $N_{lk, mn}$

2.4 Model applications

The SMART2 model has been validated in several studies on different scales. Most of the described applications can be found in Kros (2002).

2.4.1 Local scale

On site scale, the model has been applied to a spruce site in Germany (Van der Salm et al., 1995), to a Douglas fir site in the Netherlands (Mol-Dijkstra et al, 1998), to a dwarf shrub vegetation in Norway (Mol-Dijkstra and Kros., 2001), to a chronosequence from bare formal agricultural soil to oak forest and a chronosequence with succession from bare sand to deciduous forest in the Netherlands, in combination with SUMO (Wamelink et al., 2001). In these applications, the model results are compared with measured data and with results of other models.

Spruce in Germany
From the application to the spruce site in Germany, where SMART2 was compared with more detailed acidification models RESAM (De Vries, et al., 1995) and NUCSAM (Groenenberg et al., 1995), was concluded that all models were able to simulate most of the concentrations during the examined period reasonably well. However, the one-layer model, SMART2, had some difficulties to simulate strong changes in soil solution concentrations due to a lower retardation in the soil system. RESAM simulated a somewhat stronger rise and fall in base cation and SO_4 concentrations in the subsoil.
Although both the seasonal and the interannual variation in the soil solution concentrations as modelled by the three models showed large differences, the long-term trends corresponded quite well and the leaching fluxes were almost similar. Generally it appeared that the uncertainty due to time resolution and vertical heterogeneity in long-term predictions was relatively small. So, the use of the

simplified model SMART2, that neglects seasonal variation and vertical heterogeneity, is in most aspects acceptable for the evaluation of long-term trends in soil and soil solution chemistry.

Spruce in the Netherlands
Both NUCSAM and SMART2 predicted soil solution concentrations within the 95 % confidence interval of the observed responses for both the ambient plot and the pristine plot at 90 cm depth. Despite the large seasonal and vertical (spatial) variation in soil solution chemistry, the trends in annual flux-weighted soil solution parameters, as predicted by SMART2 and NUCSAM corresponded quite well. The annual leaching fluxes below the root zone were similar, although differences exist for the topsoil. For the topsoil NUCSAM simulated the nutrients and acid related constituents better than SMART2. Both models overestimated the ammonium concentration at 10 cm depth. SMART2 underestimated BC2+ concentration at 10 depth, whereas NUCSAM overestimated BC2+ concentration at 90 cm depth. NUCSAM predicted the effect of deposition reduction on N concentrations well at both depths, whereas SMART2 underestimated the effect of deposition reduction at 10 cm depth. Both models calculated faster effects of deposition reduction on Al, SO_4 and base cations than observed. Generally it appeared that the differences were large during the period of profound deposition changes, whereas small differences occurred during slight variations in deposition level. It was concluded that a simpler model description does not have a significant impact on the model performance considering flux-weighted annual average concentrations at greater depth, whereas the performance decreases at a lower depth. Model improvements have to be focused on processes related to N-dynamics.

Dwarf shrub vegetation in Norway
This application is described in Mol-Dijkstra and Kros (2001) and in Kros (2002). To gain insight in long-term effects of acid deposition and elevated CO_2-levels, the SMART2 model was applied, using data from the catchment-scale experiments of the RAIN and CLIMEX projects, conducted on boreal forest ecosystems at Risdalsheia (southern Norway). These unique series of experiments at the ecosystem scale provides information on the short-term effects and interactions of N deposition and increased temperature and CO_2 on C and N cycling and especially the runoff chemistry. To predict changes in soil processes in response to climate change, the model was extended, by including the temperature effect on mineralisation, nitrification, denitrification, Al dissolution and mineral weathering. The extended model was tested on the two manipulated catchments at Risdalsheia and long-term effects were evaluated by performing long-time runs. The effects of climate change treatment, which resulted in increased N fluxes at both catchments, were slightly overestimated by SMART2. The temperature dependency of mineralisation was simulated adequately, but the temperature effect on nitrification was slightly overestimated. Monitored changes in base cation concentrations and pH, though were simulated quite well with SMART2. The long-term simulations, indicate that the increase in N runoff is only a temporal effect; on the long-term, no effect on total N-leaching is predicted. At higher deposition level the temporal increase in N-leaching

lasts longer than at low deposition level. Contrary to N leaching, a temperature increase leads to a permanent decrease in Al concentrations and pH.

Succesion from bare ground to forest, the Netherlands
This was the first application of SMART2 in combination with SUMO, described in Wamelink et al. (2001). The results were compared with results of NuCOM (Berendse, 1994). Concentrations in soil solution agreed well with measurements and NuCOM, but the C-pool in the soil were underestimated by SMART2-SUMO, resulting in low C:N ratios. The succession of vegetation was simulated quite well, although the dwarf shrub vegetation came a bit too early. Major outcome of this application was, that it was possible to reproduce a vegetation succession reasonably with the SMART2-SUMO model and that in principle effects of management measures could be evaluated.

Oak on former agricultural soil, the Netherlands
This application is done with the same version of SMART2-SUMO as used in the above described application and described in Wamelink et al. (2001). For this application, we put the organic matter from the agricultural soil in the old litter pool, resulting in high mineralisation rates in the begin years of the simulation. SMART2-SUMO underestimated nitrate and aluminium concentrations. Without SUMO, this underestimation was less. Biomass production was overestimated in the older stages.

2.4.2   Regional scale

On a national and European scale the model was applied in several studies. Although SMART2 was especially developed for application on a national to European scale, it still runs at a point support.

Scenario study in the Netherlands
This is described in Kros (2002). Model predictions on pH and Al concentration for deciduous forest showed a reasonable to good agreement with observations. Alternatively, the Al in concentration in poor sandy soils was overestimated. Model predictions for the NO3 and NH4 concentrations showed moderate relationship with the observations. A preliminary validation on N mineralisation fluxes, showed a reasonable agreement between calculated fluxes and measured fluxes available from literature. N mineralisation fluxes in forests are likely to be underestimated.

Calibration of SMART2 in the Netherlands with data on European scale
This is described in Kros (2002). SMART2 was applied in the Netherlands with data that are available on European scale. The prediction error of SMART2 was assessed before and after calibration, for the Al and NO3 concentrations on a block scale. Although SMART2 was especially developed for application on a national to European scale, it still runs at a point support. A 5×5 km^2 grid was used for application on the European scale. Block characteristic values were obtained simply by taking the median value of the point support values within the corresponding grid cell. In order to increase confidence in model predictions on larger spatial scales, the model was calibrated and validated for the Netherlands, using a resolution that is

feasible for Europe as a whole. Because observations are available only at the point support, it was necessary to transfer them to the block support of the model results. For this purpose, about 250 point observations of soil solution concentrations in forest soils were upscaled to a 5×5 km^2 grid map, using multiple linear regression analysis combined with block kriging. The resulting map with upscaled observations was used for both validation and calibration. A comparison of the map with model predictions using nominal parameter values and the map with the upscaled observations showed that the model overestimated the predicted Al and NO3 concentrations. The nominal model results were still in the 95% confidence interval of the upscaled observations, but calibration improved the model predictions and strongly reduced the model error. However, the model error after calibration remains rather large.

Level II plots in Europe to estimate C sequestration
This is described in Mol-Dijkstra et al. (in prep). SMART2 was applied to about 180 intensive monitoring plots (Level II) in Europe to estimate carbon sequestration. Mineralization constant, assimilation dissimilation ratio, exchange constants and N content in stems were calibrated to measured litter pool, C:N ratio in litter, pH and NO_3 concentrations. Compared to other calculation methods, SMART2 calculated very low C sequestration rates. The results of the discussed dynamic models and other concepts give rise to introduce in SMART2 a slower decomposable pool, with possibly a recalcitrant part (Mol-Dijkstra, et al., in prep).

2.5   Sensitivity analysis

Kros (2002) described a sensitivity analysis for an application on national scale. He found that the uncertainty in nitrate concentration originated dominantly from categorical vegetation data, which means that the vegetation type itself was the main predicting source of the variety in the model output nitrate concentration in soil solution. The nitrate concentrations was sensitive to continuous vegetation related parameters too. The aluminium concentrations in soil solution were most sensitive to the continuous soil related parameter above the soil types. Vegetation related parameters were unimportant for the calculation of aluminium concentrations.

A sensitivity analysis with version 3.4 was performed for one situation, i.e. deciduous forest on a poor sandy soil. In contrast to Kros (2002), we examined all input parameters for a run with standard options for the chosen situation. We use the term input parameter in this context for initial conditions of state variables, model inputs and model parameters. Each input parameter was sampled from a uniform distribution reaching from minus to plus ten percent of the nominal values for deciduous forest on a poor sandy soil. Table 5 gives a summary of the results of the sensitivity analysis for six model outputs. All the variables shown is this table, declare more than 5% of the output variance.

Table 5 Sensitivity of input parameters for six model outputs

Parameter*	Model output					
	N-availa-bility	P-availa-bility	pH	[NO$_3$]	[PO$_4$]	Amount of litter
Climate						
PE			*****	****	****	
T	*****		***	****	*****	*****
Deposition						
SO4$_{td}$			*****	***		
NOx$_{td}$			*****	****		
NH4$_{td}$			****	*****		
Vegetation						
fr$_{int}$			***		***	
Amlf	*****	***		***	***	*****
k$_{gl}$		***				
t$_{1/2}$		***		****	***	***
ctN$_{lv,mn}$	*****					
ctP$_{lv}$		***				
kr$_{mi}$		****				****
fr$_{mi}$						***
frN$_{re}$	****					
Ncf	***					
Soil						
KAl$_{ox}$			***			
Ca$_{we}$		***				
PBCrat		***				
fr$_{ni,mx}$			***			

* For explanations of symbols, see 0

It was concluded that the SMART2 model is very sensitive to the mineralisation process and therefore to all variables that affect mineralisation (*T*, *amlf*, *k$_{gl}$*, *t$_{1/2}$*, *kr$_{mi}$* and *fr$_{mi}$*), which are related to vegetation type. *ctN$_{lv,mn}$* and *ctP$_{lv}$*, have influence on N mineralisation and P mineralisation. The pH is less sensitive to mineralisation and is more affected by soil related parameters. This is in agreement with Kros (2002).

2.6 Model limitations

SMART2 is a soil acidification and nutrient cycling model for terrestrial (semi-) natural ecosystems. Originally it was developed to examine effects of acid deposition on soil chemistry and soil acidification. Nowadays, it is often indrectly used to evaluate long term effects of deposition on plant diversity and carbon sequestration.

The model is not applicable to wet ecosystems and agricultural systems.

Besides, there are some known conditions where the reach of the model is limited:
- The effect of calcareous seepage on calcareous soils is not modelled adequately. In the model, this has a pH-decreasing effect. It is not clear where this effect comes from, which has to be examined.
- When the Al-hydroxides are depleted, the mass balance is not zero.
- The P processes have to be validated in a detailed site application where the full mass balance is measured, so that each process can be validated. Until know, we just did a plausibility check and a comparison with STONE (Kros et al., 2006).

3   Model code

A schematic overview of the model is given in *Figure 3*. The model SMART2 is written in Fortran and consists of a main routine called RUNSMART that calls four different subroutines: SMART2IN, INFLUX2, SMART and MONITOR. For the use with SUMO, RUNSMART calls two extra subroutines: SUMOIN and SUMO. Each of the subroutines performs a specific task within the model. After the model is started, parameter values are read from a data file (subroutine SMART2IN and for the use with SUMO also SUMOIN). For a run with the use of SUMO, SUMO has to be initialised, which is done before the time loop. Then, a loop is started that runs from the first to the last time step specified. For each time step, all input fluxes are calculated (subroutine INFLUX2). For the use with SUMO, INFLUX2 is divided in two parts. The first part calculates nutrient availability, which is used by SUMO to calculate growth, uptake and litter fall. After SUMO is executed all fluxes are calculated in the second part of INFLUX2. Next, the soil solution chemistry is determined (subroutine SMART) and results are displayed (subroutine MONITOR). These subroutines, in turn, call some auxiliary subroutines and/or functions to perform their task. How the model equations are solved is described in Appendix B.
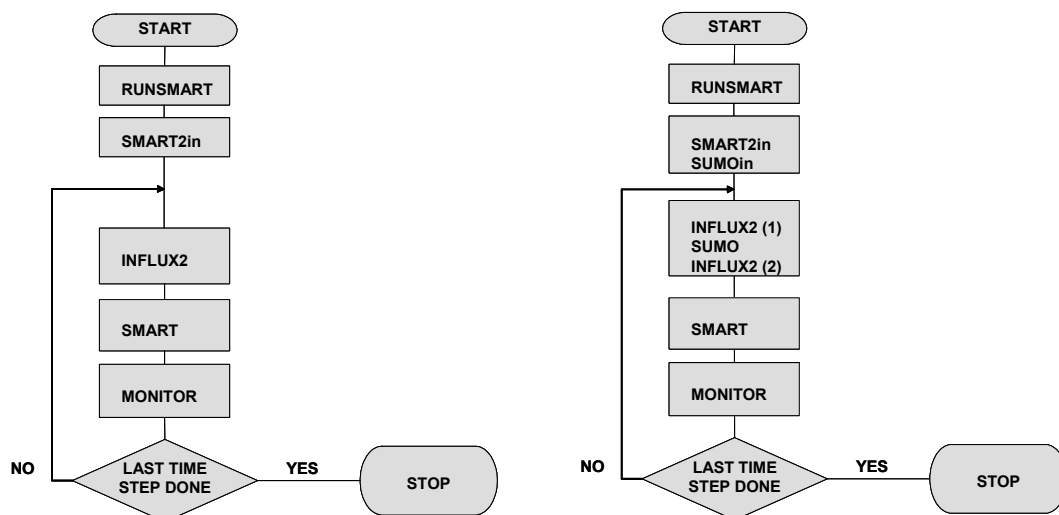
Figure 3: Flow diagram of the SMART2 (left) and SMART2-SUMO (right) model.

In the following sections each of the subroutines used in the model is described. Firstly, a short outline is given of what the subroutine does and secondly all input - and output parameters are listed and described. This description comprises the parameter name, a short description of its meaning, the units of measure and the variable type. Symbols used for variable types are:

I   integer*4
R   real*4
C*n   character*n (n=(*) for variable length character string)

L   logical
R(:)   real vector (one-dimensional array)

The subroutine MONITOR, used to display the results of SMART2, is described in 0.

3.1 Subroutine SMART2IN

The subroutine SMART2IN reads the necessary input data from the smart2.in file. Firstly, the user is asked to specify the name of the data file to be read (see par 4.2 and 4.3). From this data file a temporary data file is created (smart2.tmp), which is a copy of the original data file with all comment lines in the original data file left out. Finally, all input data are read from this temporary data file. The parameters needed in the data file are described in Section 4.2 together with the proper units of measure.

```
Input for subroutine SMART2IN
datfil ..... file with input data
msg ........ messagenumber
msgfil ..... file with message
IB ......... first index of time series vectors (-) (I)
IE ......... last index of time series vectors (-) (I)
```

```
Output of subroutine SMART2IN
iyrb ....... starting year for simulation (T) (I)
iyre ....... ending year for simulation (T) (I)
mstep ...... amount of steps within a year (-) (I)
sumo ....... logical for run with SUMO (true) or without (false)
(L)
nveg ....... number functional plant types
ioptu ...... uptake option (0=standard, 1=uptake prior to
immobilisation
           and denitrification)
ioptcl ..... critical load consistency option (0=standard,
1=compatible
           with CL: ctnitlv = constant)
iagevg ..... Age of present vegetation (T) (R)
igropt ..... Growth option (0 = constant growth, 1 = logistic
           growth curve) (I)
iagelt ..... Age of site (litter) (T) (R)
thick ...... thickness of the soil compartment (m) (R)
*thickrz ... thickness rooting zone (m)
cacarb0 .... initial amount of carbonates (meq/kg) (R)
cec ........ cation exchange capacity of the soil (meq/kg) (R)
theta ...... volumetric water content of the soil (m/m) (R)
rho ........ bulk density (g/cm3) (R)
rholt ...... bulk density litter layer (g/cm3)
Cpool0 ..... initial amount of C in topsoil (g/m2)
CNMin ...... C:N ratio (g/g) below which no time-dependent Nimm
CNMax ...... C:N ratio (g/g) above which all available N is
immobilised
*frrtlt .... Fraction of roots in litter layer (R)
ncf ........ Nutrient cycling factor (-) (R)
cnrat0 ..... initial C:N ratio in organic matter (R)
```

```
modexc ..... cation exchange model option: 1=Gaines-Thomas,
2=Gapon
KAlBC ...... log10 of selectivity constant for Al-BC exchange (R)
expH ....... exponent of [H] in H-BC exchange (Gaines-Thomas only)
KHBC ....... log10 of selectivity constant for H-BC exchange (R)
expAl ...... exponent in [Al] = KAlox*[H]^expAl
KAlox ...... log10 of gibbsite equilibrium constant (R)
Ebc0 ....... initial base saturation (-) (R)
fnitmx ..... nitrification factor (0<=fnit<=1) (R)
fdenmx ..... denitrification factor (0<=fden<=1) (R)
nimacc ..... constant rate of N immobilization (eq/m2/T)
*fmifl ..... Mineralization fraction fresh litter (-) (R)
*milt ...... Mineralization rate old litter (1/T) (R)
assdiss .... Assimilation dissimilation ratio of decomposing
microbes (-)
              (R)
alox0 ...... initial Al buffer capacity (meq/kg) (R)
sadmax ..... maximum SO4 adsorption capacity (meq/kg) (R)
sadh ....... "half-saturation" constant of SO4 adsorption (eq/m3)
 (R)
Padmax ..... maximum PO4 adsorption capacity (meq/kg) (R)
Padh ....... "half-saturation" constant of PO4 adsorption (eq/m3)
 (R)
modorg ..... protonity of organic acids:
             1,2,3; 0=Oliver mode; <0: not modelled
coacid ..... concentration of organic acids (m*TOC) (eq/m3) (R)
pkpar ...... 3 parameters for modeling pKa (R(:))
pkAlpar .... pK-values for organic Al-complexation
temp ....... soil temperature (øC, average over 1T)
prec ....... net precipitation (m/T) (R(:))
*fint ...... interception fraction (-) (R)
se ......... upward seepage (m/T) (R(:))
*tr ........ actual transpiration (m/T) (R(:))
gvg ........ mean spring groundwater-table (m) (R)
pco2 ....... CO2 pressure in soil solution,
             multiple of pCO2 (atm) in air (R(:))
We ......... weathering rate of X (eq/m3/T) (R)
             X = Ca, Mg, K, Na, PO4
alw ........ Al weathering (eq/m3/T) (R(:))
*fnh4fu .... Ammonium foliar uptake fraction (-) (R)
*fhfu ...... Proton foliar uptake fraction (-) (R)
*fkfe ...... K foliar exudation fraction (-) (R)
*fbc2fe .... BC2 foliar exudation fraction (= 1. - fkfe) (-) (R)
amlt0 ...... initial amount of litter (kg/m2) (R)
fre ........ Reallocation fraction (-) (R)
ctnitlvmn .. Minimum N content in litterfall (%) (R)
ctnitlvmx .. Maximum N content in litterfall (%) (R)
*ctbc2lv ... Content of BC2 in leaves (%) (R)
*ctklv ..... Content of K in leaves (%) (R)
ctPlv ...... Content of P in leaves (%) (R)
krgl ....... logistic growth rate constant (1/T) (R)
t05 ........ half time growth (T) (R)
amstmx ..... maximum stem mass or maximum standing biomass (kg/m2)
 (R)
amst0 ...... initial amount of stems (kg/m2) (R)
damst ...... stemwood increment (kg/m2/yr) (R(:))
```

```
amlf ....... amount of litterfall (kg/m2/T) (R(:))
ctnitst .... Content of N in stems (%) (R(:))
*ctbc2st.... Content of BC2 in stems (%) (R(:))
*ctkst ..... Content of K in stems (%) (R(:))
ctPst ...... Content of P in stems (%) (R(:))
cSe ........ concentration in seepage of X (eq/m3/T)
             X = Ca, Mg, K, Na, PO4
Nfix ....... fixation of N (eq/m2/T) (R)
DEP ........ deposition of ion X (eq/m2/T);
             X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
Iss ........ option for seasalt correction:
              =0: no seasalt correction
              =1: correct using Cl (i.e. Cl*=0)
              =2: correct using Na (i.e. Na*=0)
rfnigvgmn .. minimum nitrification reduction fraction for the
water-table
z1nit ...... lowest MSW for reduction of nitrification
z2nit ...... higest MSW for reduction of nitrification
rfdegvgmn .. minimum denitrification reduction fraction for the
water-
             table (-) (R)
z2den ...... soil dependent MSW for determination of rfdegvg
*ffso2 ..... filtering factor for SO2-deposition (-) (R)
*ffnh3 ..... filtering factor for NH3-deposition (-) (R)
*ffnox ..... filtering factor for NOx-deposition (-) (R)
*fdd ....... filtering factor for dry deposition (-) (R)
pHref ...... reference pH for BC2-weathering (-) (R)
alfa ....... exponent for calculation of pH dependent weathering
(-) (R)
PBcrat ..... P/BC2-ratio in minerals (-) (R)
amhu ....... amount of humus (former agricultural soil) (kg/m2)
(R)
ctnithu .... Content of N in humus (%) (R)
ctPhu ...... Content of P in humus (%) (R)
kmihu ...... Mineralization rate humus (1/T) (R)
fmilt ...... Mineralization fraction old litter (-) (R)
OBSv ....... Observations (R)
monfil ..... file for MONITOR (C)
balfil ..... file for SM2BAL (C)
errbyte .... byte-vector for error messages

* With SUMO, these variables have the type real vector with length
of nveg
```

3.2   Subroutine INFLUX2

This subroutine calculates the net influxes to the soil compartment At the first call
(time step) all variables used to compute the amount of N in organic matter and the
C/N ratio are initialised. Each time INFLUX2 is called (i.e. each time step), nitrogen
immobilisation is computed by eq. 35 and the C/N ratio is updated. Finally, the net
input fluxes are calculated as sum of the interaction fluxes (eqs.37-47) and the input
fluxes (eqs.7-17).

```
Input for subroutine INFLUX2
itask .... option for run with or without SUMO (-) (I)
start .... start flag; if true: compute parameters once
          for use in simulation; set to false afterwards
ioptu  ... uptake option (0=standard, 1=uptake prior to
immobilisation
          and denitrification)
ioptcl ... critical load consistency option (0=standard,
1=compatible
          with CL: ctnitlv = constant)
thick .... soil thickness (m)
thickrz .. thickness rooting zone (m)
ruexp .... uptake exponent
rho    ... bulk density mineral layer (g/cm3)
rholt .... bulk density litter layer (g/cm3)
Cpool .... initial amount of C in topsoil (g/m2)
CNmin .... C:N ratio (g/g) below which no time-dependent Nimm
CNmax .... C:N ratio (g/g) above which all available N is
immobilised
frrtlt ... fraction roots in litter layer (0<=frrtlf<=1)
ncf ...... nutrien cycling factor (Amrd/Amlf)
cacarb ... amount of carbonates in the soil (meq/kg)
amlt0 .... initial amount of litter (kg/m2)
temp ..... temperature (degrees celcius)
prec ..... precipitation (m/T)
fint ..... interception fraction (-)
se ....... upward seepage (m/T)
tr ....... actual transpiration (m/T)
gvg ...... mean spring groundwater-table (m)
Dep%X .... deposition of ion X (eq/m2/T);
           X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
We%X ...... weathering rate of X (eq/m3/T)
           X = Ca, Mg, K, Na, PO4
alw ...... Al weathering (eq/m3/T)
Se%X ...... concentartion in seepage of X (eq/m3/T)
           X = Ca, Mg, K, Na, PO4
ctkst .... potassium content in stems (eq/m2/T)
ctklv0 ... initial potassium content in leaves (%)
ctbc2st .. divalent base cation content in stems (eq/m2/T)
ctbc2lv0 . initial divalent base cation (=Ca+Mg) content in leaves
(%)
ctpst .... phosphate content in stems (eq/m2/T)
chplus ... H+ concentration (eq/m3)
ctnitst .. nitrogen content in stems (eq/m2/T)
fre ...... nitrogen reallocation factor for leaves (0<=fre<=1)
ctnitlvmn  minimum nitrogen content in leaves (%)
ctnitlvmx  maximum nitrogen content in leaves (%)
fnit ..... nitrification factor (0<=fnit<=1)
fden ..... denitrification factor (0<=fden<=1)
Nimacc ... minimum rate of N immobilization (if>supply) (eq/m2/T)
fmifl .... mineralization factor of fresh litter (0<=fmifl<=1)
fmilt .... transformation factor of old litter to humus
(0<=fmilt<=1)
kmiltref.. reference mineralization rate constant of old litter
(kmilt>=0) (1/T)
kmihu .... mineralization rate constant hunus (kmihu >= 0) (1/T)
```

```
assdiss .. assimilation-dissimilation ratio
fnh4fu ... ammonium foliar uptake fraction (0<=fnh4fu<=1)
fhfu ..... proton foliar uptake fraction (0<=fhfu<=1)
fkfe ..... potassium foliar exudation fraction (0<=fkfe<=1)
fbc2fe ... divalent base cation foliar exudation fraction (=1-
fkfe)
damst .... stemwood increment (kg/m2/yr)
amlf ..... amount of litterfall (kg/m2/T)
cut ...... sod cutting (1=yes, 0=no)
```

Output of subroutine INFLUX2
```
HU%X ..... amount and concentrations in humus
dDw%X .... amount and concentrations in deadwood flux
RD%X ..... amount and concentrations in dead roots
EX ........amount and concentrations in exrements
aNman  ... N flux manure
aPman .... P flux manure
cnrat .... C:N ratio in organic matter;
           Note: cnrat has to be initialized at first call!
LIT ...... amount and concentrations in Litter
thicklt .. thickness of litter layer (m)
nitlf .... nitrogen litterfall flux (eq/m2/T)
nitmi .... nitrogen mineralisation flux (eq/m2/T)
nitmiug .. above ground nitrogen mineralisation flux (eq/m2/T)
*tnitupt ..total root uptake of nitrogen (eq/m2/T)
*ctnitlv ..nitrogen content in leaves (%)
*ctplv ....phosphate content in leaves (%)
Influx%X .. Net input flux of ion X (eq/m2/T);
            X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
alin ..... input flux of aluminum (eq/m2/T)
oain ..... input flux of organic acids (m*TOC) (eq/m3)
ps ....... precipitation surplus (m/T)
no3ru .... nitrate root uptake (eq/m2/T)
nh4ru .... ammonium root uptake (eq/m2/T)
tbc2upt .. divalent base cations root uptake (eq/m2/T)
tkupt .... potassium root uptake (eq/m2/T)
*tpupt .... phosphate root uptake (eq/m2/T)
no3im .... nitrate immobilisation (eq/m2/T)
nh4im .... ammonium immobilisation (eq/m2/T)
no3de .... denitrification (eq/m2/T)
nh4ni .... nitrification (eq/m2/T)
bc2mi .... divalent base cation mineralisation (eq/m2/T)
kmi ...... potassium mineralisation (eq/m2/T)
pmi ...... phosphate mineralisation (eq/m2/T)
hfu ...... proton foliar uptake (eq/m2/T)
nh4fu .... ammonium foliar uptake (eq/m2/T)
bc2fe .... divalent base cation foliar exudation (eq/m2/T)
kfe ...... potassium foliar exudation (eq/m2/T)
tnituptmx  Nitrogen availability for root uptake (eq/m2/T)
tPuptmx .. Phosphate availability for root uptake (eq/m2/T)
errbyte .. byte-vector holding error messages;
           if char(errbyte(1)) not blank, there IS an
error(message)!
```

```
* with the use of SUMO, these variables are calculated by SUMO
```

3.3 Subroutine SMART

In the subroutine SMART the soil solution chemistry is determined by solving the appropriate equilibrium and charge balance equations valid for the buffer range of the soil-system (see Sections 1.2 and 1.3). After initialization of some variables at the first call, the concentrations of SO_4^{2-}, $H_2PO_4^-$, NO_3^-, NH_4^+, K^+, Na^+ and Cl^- are determined. The concentrations of H^+, BC^{2+}, Al^{3+} and $RCOO^-$ are determined depending on the buffer range: if the system contains free Ca carbonate, the soil is in the carbonate buffer range; if there are no carbonates left, but the system contains Al-(hydr)oxides, the soil solution composition is determined using aluminum dissolution and ion exchange. If all carbonates and Al (hydr)oxides are consumed by acidifying compounds, the system is only buffered by weathering of primary minerals and ion exchange. Before returning to the main routine, all variables are saved for use in the next time step.

```
Input for subroutine SMART
start ..... start flag; if true: compute variables and constants
once
           for use in simulation; set to false afterwards.
thick ..... soil thickness (m)
rho ....... bulk density (g/cm3)
theta ..... volumetric water content of the soil (m3/m3)
temp ...... soil temperature (øC)
ps ........ precipitation surplus (m/T)
pCO2 ...... partial CO2-pressure in soil solution (atm)
expAl ..... exponent in [Al] = KAlox*[H]^expAl
KAlox ..... Al equilibrium constant ((eq/m3)^(1-expAl))
modExc .... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
KAlBC ..... selectivity constant for Al-BC exchange
expH ...... exponent of [H] in H-BC exchange (Gaines-Thomas only)
KHBC ...... selectivity constant for H-BC exchange
Cacarb0 ... INITIAL amount of carbonates in the soil (meq/kg)
CEC ....... cation exchange capacity of the soil (meq/kg)
Alox0 ..... INITIAL amount of Al-(hydr)oxides (meq/kg)
Sadmax .... maximum SO4 adsorption capacity (meq/kg)
Sadh ...... "half saturation" constant for SO4 adsorption (eq/m3)
Padmax .... maximum PO4 adsorption capacity (meq/kg)
Padh ...... "half saturation" constant for PO4 adsorption (eq/m3)
modOrg .... protonity of organic acids:
           1,2,3; 0=Oliver mode; <0: not modelled
coacid .... total concentration of organic acids (m*DOC) (mol/m3)
KOrgv() ... parameters describing organic dissociation (<=3)
KAlOrgv() . parameters for Al-complexation
Influx%X .. Net input flux of ion X (eq/m2/T);
           X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
Alin ...... Net input of Al; not needed for calcareous soils
(eq/m2/T)
```

```
Output of subroutine SMART
cH ........ H+ concentration (eq/m3)
*Conc%X ....concentration of ion X (eq/m3);
           X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4;
           Conc%Ca=[Ca]+[Mg], Conc%Mg=0
```

```
cOrgv() ... concentrations of organic anions (eq/m3)
            cOrgv(0) = cOrgv(1)+...+cOrgv(modOrg)
*cAl ...... free Al concentration (eq/m3)
*cAlOrgv(). concentrations of complexed Al (eq/m3)
cHCO3 ..... bicarbonate concentration (eq/m3)
cANC ...... ANC concentration (as function of [H]) (eq/m3)
EH ........ exchangeable fraction of H
*EBC ...... exchangeable fraction of BC2+ (base saturation)
*EAl ...... exchangeable fraction of Al
*Cacarb ... amount of carbonates in the soil (meq/kg)
*Alox ..... amount of Al-(hydr)oxides (meq/kg)
errbyte ... byte-vector holding error messages;
             if char(errbyte(1)) not blank, there IS an
             error(message)!


*These variables have to hold the values from the previous
timestep UNLESS start=.true.: then they are initialized with
equilibrium/initial values (EBC only if <0).
```

Within the subroutine SMART several subroutines/functions are called to solve equilibrium and charge balance equations. The equations to be solved are defined as Fortran-functions. The name of the function is passed to the subroutine BRENTP as an argument; in BRENTP the equation with one unknown is solved by an iterative procedure (see Press et al., 1986). The subroutines/functions called by SMART are

fKCaCO3	Returns the Ca-carbonate equilibrium constant as a function of the temperature (in $^{\circ}C$)
fKHCO3	Returns the bicarbonate equilibrium constant
Brentio:	Subroutine that solves a (non-linear) equation with one unknown using Brent's method
Orgall:	Function that holds the equation to compute the concentration of organic anions
chbalSMA:	Function that holds the charge balance equation
AllEq0:	Function that holds the equation to compute the fraction base cations at the exchange complex in initialisation
AllEq:	Function that holds the equation to compute the fraction base cations at the exchange complex
fGTn:	Function with the equation for solving the Gaines-Thomas equations
G0:	Function that holds the equation to compute [H+] for soils in the carbonate buffer range

3.4   Subroutine SUMOIN

The subroutine SUMOIN reads the necessary input data from the input file. Firstly, the user is asked to specify the name of the data file to be read (see par 4.2 and 4.3). From this data file, that also includes the input for SMART2, a temporary data file is created (sm2s.tmp). This temporary file is a copy of the original data file with all comment lines in the original data file left out. Finally, all input data are read from this temporary data file. The parameters needed in the data file are described in Section 4.2 together with the proper units of measure.

Input for subroutine SUMOIN
```
datfil ..... file with input data
msg ........ messagenumber
msgfil ..... file with message
IB ......... first index of time series vectors (-) (I)
IE ......... last index of time series vectors (-) (I)
```

Output of subroutine SUMOIN
```
iyrb ....... starting year for simulation (T) (I)
iyre ....... ending year for simulation (T) (I)
mstep ...... amount of steps within a year (-) (I)
amlt0 ...... initial amount of litter (kg/m2) (R)
soil ....... soil type (-) (C)
vegtype .... vegetation structure type (-) (C)
beheer ..... management type (-) (I)
plaggen .... frequency of cutting (y) (I)
cut ........ switch for cutting (-) (I)
maaien ..... frequncy of mowing (y) (I)
bemesting .. amount of N manure (ton/ha/T) (R)
filenr ..... filenumber for reading vegetation data (-) (I)
larchfilenr  filenumber from Larchmap (-) (I)
cboom ...... climax tree species (-) (C)
pboom ...... pioneer tree species (-) (C)
nrdierha ... amount of animals per hectare
errbyte .... byte-vector for error messages
```

3.5   Subroutine SUMO

The subroutine SUMO calculates yearly growth, uptake of nitrogen and phosphorus and litter fall based on yearly nitrogen (and phosphorus) availability (calculated by INFLUX2) and light availability. It simulates biomass development for five 'functional plant types': grasses and herbs, dwarf shrubs, shrubs and two different tree species. Biomass development is affected by management, which may include mowing, sod cutting and forest management at various levels of intensity. The management measures remove biomass, and hence nitrogen and phosphorus from the system. SUMO is described in Wamelink (in prep). In this section, we describe the input (from INFLUX2) and output (to INFLUX2) of subroutine SUMO.

Input for subroutine SUMO (from subroutine INFLUX2)
```
tnituptmx  Nitrogen availability for root uptake (eq/m2/T) (R)
tPuptmx .. Phosphate availability for root uptake (eq/m2/T) (R)
nh4fu .... ammonium foliar uptake (eq/m2/T) (R)
*tr ...... transpiration (m/T) (R)
**gvg .... mean spring water table (m) (R)
*     tr is biomass weighted average of nominal values per
functional plant type
**    gvg is model input
```

Output of subroutine SUMO (to INFLUX2)
```
amlf ..... amount of litter fall (kg/m2/T)
RD%am .... amount of dead roots (kg/m2/T)
RD%ctN ... nitrogen content in dead roots (%)
```

```
RD%ctP ... phosphate content in dead roots (%)
ctnitlv .. nitrogen content in leaves (%)
ctplv .... phosphate content in leaves (%)
cut ...... switch for cutting (-) (I)
amst ..... amount of stems (kg/m2) (R)
tnitupt .. total root uptake of nitrogen (eq/m2/T)
iagelt ... Age of site (litter) (T) (R)
tPupt .... total root uptake of phosphate (eq/m2/T)
EX%am .... amount of excrements (kg/m2)
EX%ctN ... nitrogen content in excrements (%)
EX%ctP ... phosphate content in excrements (%)
dDW%am ... amount of dead wood (kg/m2)
dDW%ctN .. nitrogen content in dead wood (%)
dDW%ctP .. phosphate content in dead wood (%)
```

4 Model use

There are two executables for running SMART2 and SMART2SUMO: smart2.exe and sms.exe. Smart2.exe runs SMART2 only, sms.exe also includes (optionally) SUMO. The use of smart2.exe will be described first. The use of sms.exe will be described from paragraph 4.4

4.1 Model installation

For running SMART2 you need the files:
- Smart2.exe
- Cofu4all.dll
- Smart2.dll
- Smart.dll
- sm2.mon (default name for the 'monitor file' (see 0))

You can create an input file using a text editor and your are free to choose the name. In this manual we use the name 'smart2.in'; this file is described in paragraph 4.2.

In the 'monitor file' you can regulate how the graphical output will look like and whether output files will be saved (see 0).

In the file 'smart2.in', some parameters can be specified as files (e.g. for data on deposition, seepage, precipitation and for observations). If such input files with time-series of data are specified in the input file, they should also be available. It is advisable to store the program and input files in the same directory.

4.2 Model input

The main input parameter file is organised using labels. After each label a certain set of parameters is expected (Table 6). The order of the labels is not important. There can be comment lines, i.e. lines starting with an exclamation mark ('!'), anywhere in the file; they are ignored when reading the input data. The units of the parameters are given between square brackets. Many parameters get a default value if they are not specified in the input file. These default values are also given in Table 6 for the SMART2 input file.

Several input parameters (runoff, pCO_2, weathering rates and deposition fluxes) can be specified either as filenames, that refer to files with timeseries, or as (real) single values. These parameters are indicated with '(V/F)'. If a single value is given, the respective variable is assumed constant and equal to this value for the whole simulation period. If a filename is given, this timeseries file must contain on each line

at least two values: in the first column the time point (year) and in the next column(s) the value(s) of the variable for one time unit (year).

Table 6: An example of the main input parameter file (smart2.in) for SMART2

```
! This file contains the parameters for running SMART2:
!
! Lines with '!' in the first column are treated as comments and ignored
!
! The following parameters can be specified:
! (they can be in arbitrary order and they are case-sensitive)
! (V/F) means that either a constant value or a file can be specified
!       in the form [fac*]filename[#ncol]
! RF .... reduction function
! (I) ... integer value(s)
!
! With SUMO, the vegetation related parameters have to be given for the
!    five structural plant types. Sequence:
!    1) value for deciduous tree
!    2) value for spruce tree
!    3) value for pine tree
!    4) value for heather (shrub vegetation)
!    5) value for poor grassland (grasses and herbs)
!
! The labels are case sensitive
!
! period ..... starting and ending time of simulation [T T] (I)
! thick ...... thickness of the soil compartment [m]
! thickrz .... thickness of rooting zone [m]
! bulkdens ... bulk density [g/cm3]
! Theta ...... water content [m/m]
! Carbonat ... initial amount of carbonates [meq/kg];
!              if missing assumed zero
! CEC ........ cation exchange capacity [meq/kg]
! bsat_0 ..... initial base saturation;
!              if missing or -1 AND Carbonat=0 determined internally
! Excmod ..... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! lgKAlBC .... log10 of selectivity constant for Al-BC exchange [mol/l]
! lgKHBC ..... log10 of selectivity constant for H-BC exchange [l/mol]
! expAl ...... exponent for Al/BC exchange; if missing set to 3
! expH ....... exponent for H/BC exchange (default = 2);
!              only read if Excmod = 1
! Alox_0 ..... initial Al buffer capacity [meq/kg];
!              if missing assumed infinite (10**9)
! lgKAlox .... log10 of gibbsite equilibrium constant [(l/mol)**2]
! Nim_acc .... constant rate of N immobilization (eq/m2/T); if missing set to 0.
! Cpool_0 .... initial amount of C in topsoil (g/m2);
!              if missing assumed zero (no N-immobilization)
! CNrat_0 .... initial C:N ratio in organic matter;
!              not read if Cpool_0 <= 0. or missing
! CNratmin ... C:N ratio (g/g) below which no time-dependent Nimm;
!              if missing set to 15
! CNratmax ... C:N ratio (g/g) above which all available N is immobilised
!              if missing set to 40
! f_ni ....... nitrification fraction:
!              if 1 value: constant nitrification (0<=f_nit<=1)
!              if 4 values: defining RF for nitrification due to GVG (and pH):
!              1) fnitmx: overall maximum (0<=fnitmx<=1)
!              2) minimum value (0..1) of RF,
!              3) depth above which nitrification RF equals minimum value [m],
!              4) depth below which nitrification RF equals 1 [m];
!              not asked if NH3_dep<=0, if missing set to 1
! f_de ....... denitrification fraction:
!              if 1 value: constant denitrification (0<=f_de<=1)
!              if 3 values: defining RF for denitrification due to GVG (and pH):
!              1) fdenmx: overall maximum (0<=fdenmx<=1),
!              2) minimum value (0..1) of RF,
!              3) depth below which denitrification RF equals minimum value [m];
!              not asked if NOx_dep<=0, if missing set to 0
```

```
! SO4admax ... maximum SO4 adsorption capacity [meq/kg];
!               if missing assumed zero (no sulfate adsorption)
! SO4half .... half-saturation constant for SO4 adsorption [eq/m3];
!               not read if both SO4admax<=0 or missing
! PO4admax ... maximum PO4 adsorption capacity [meq/kg];
! PO4half .... half-saturation constant for PO4 adsorption
!               not read if both SO4admax<=0 or missing
! RCOOmod .... protonity of organic acids:
!               1,2,3; 0=Oliver mode; <0: not modelled
! RCOOpars ... parameters for modeling organic acids:
!               if RCOOmod = 0 (Oliver):
!                 1-3 parameters of (Oliver-type) mono-protic organics model:
!                 pK = par(1)+par(2)*pH-par(3)*pH^2
!               if RCOOmod 1, 2 or 3:
!                 give 1, 2 or 3 values
!               not read if cRCOO<=0 or missing
! cRCOO ...... total concentration of organic acids (m*TOC) [eq/m3];
!               if missing set to zero, no organic acids simulated
! AlApars .... pK-values for organic Al-complexation; read if RCOOmod is 2 or 3
! pCO2fac .... CO2 pressure in soil solution (multiple of pCO2[atm] in air) (V/F)
! TempC ...... Annual average soil temperature [øC] (V/F); if missing set to 7øC
! precip ..... precipitation [m/T] (V/F)
! f_inter .... fraction of precip intercepted by vegetation (0..1) (V/F);
!               if missing set to 0
!               with SUMO (default, not automaticcaly): 0.2 0.4 0.3 0.1 0.05
! seepage .... upward seepage [m/T] (V/F); if missing set to 0
! transpir ... transpiration of vegetation [m/T] (V/F); if missing set to 0
!               with SUMO (default, not automaticcaly):
!                                 0.326 0.296 0.276 0.335 0.15
! GVG ........ depth of mean spring groundwater table [m] (V/F);
!               if missing set to infinite (=100)
! Ca_we ...... weathering rate for Ca [eq/m3/T] (V/F); if missing set to 0
! Mg_we ...... weathering rate for Mg [eq/m3/T] (V/F); if missing set to 0
! K_we ...... weathering rate for K  [eq/m3/T] (V/F); if missing set to 0
! Na_we ...... weathering rate for Na [eq/m3/T] (V/F); if missing set to 0
! Al_we ...... weathering rate for Al [eq/m3/T] (V/F);
!               if missing ratwAlBC is asked
! ratAlwBC ... Al:BC ratio in silicate dissolution ;
!               if 1 value: Al:BC2 ratio (1<rat<3); if missing set to 2;
!               if 4 values: ratios for Ca, Mg, K and Na:
!               1) ratCa (default: 3),
!               2) ratMg (default: 0.6),
!               3) ratK (default: 3),
!               4) ratNa (default: 3);
! P_we ....... weathering rate for P [eq/m3/T] (V/F);
!               if missing PBCrat is asked
! PBCrat ..... P/BC2-ratio in minerals [-]
! cSO4_se .... conc. of SO4 in seepage [eq/m3/T] (V/F); if missing set to 0
! cNO3_se .... conc. of NO3 in seepage [eq/m3/T] (V/F); if missing set to 0
! cNH4_se .... conc. of NH4 in seepage [eq/m3/T] (V/F); if missing set to 0
! cCa_se ..... conc. of Ca in seepage [eq/m3/T] (V/F); if missing set to 0
! cMg_se ..... conc. of Mg in seepage [eq/m3/T] (V/F); if missing set to 0
! cK_se ...... conc. of K  in seepage [eq/m3/T] (V/F); if missing set to 0
! cNa_se ..... conc. of Na in seepage [eq/m3/T] (V/F); if missing set to 0
! cCl_se ..... conc. of Cl in seepage [eq/m3/T] (V/F); if missing set to 0
! SO2_dep .... deposition of SO2 [eq/m2/T] (V/F); if missing set to 0
! NOx_dep .... deposition of NOx [eq/m2/T] (V/F); if missing set to 0
! NH3_dep .... deposition of NH3 [eq/m2/T] (V/F); if missing set to 0
! Ca_dep ..... deposition of Ca [eq/m2/T] (V/F); if missing set to 0
! Mg_dep ..... deposition of Mg [eq/m2/T] (V/F); if missing set to 0
! K_dep ...... deposition of K  [eq/m2/T] (V/F); if missing set to 0
! Na_dep ..... deposition of Na [eq/m2/T] (V/F); if missing set to 0
! Cl_dep ..... deposition of Cl [eq/m2/T] (V/F); if missing set to 0
! age_site ... age of site (litter) [T] (I); not used with SUMO
! age_veg .... age of present vegetation [T] (I)
! F_growth ... forest (stem&leaves) growth specification:
!               4 values: parameters for logistic growth function:
!                 1) amst: maximum amount of biomass [kg/m2],
!                 2) krgl: logistic growth rate constant [1/T],
!                 3) t0.5: growth half-time [T],
!                 4) amlfmx: maximum amount of litterfall [kg/m2/T]
```

```
!                     2 values (if filenames then seperated by a ',' !!) :
!                        1) constant growth [m3/ha/yr] (V/F)
!                        2) constant litterfall [kg/m2/T] (V/F)
!                        not used with SUMO
! ioptu ...... uptake option (0=standard, 1=uptake prior to immobilisation and
!                 denitrification)
! ioptcl ..... critical load consistency option (0=standard, 1=compatible with CL:
!                 ctnitlv = constant)
! f_mifl ..... mineralization fraction of fresh litter (0..1)
!                 with SUMO (default, not automatically): 0.8 0.8 0.8 0.4 0.8
! r_miol ..... mineralization rate constant of old litter [1/T]
!                 with SUMO (default, not automatically): 0.05 0.05 0.05 0.3 0.3
! rat_asdi ... Assimilation dissimilation ratio of decomposing microbes (-) (R);
!                 if missing set to 5.
! f_rtll ..... fraction of roots in the litterlayer (0..1)
!                 with SUMO (default, not automatically): 0.25 0.25 0.25 0.75 0.75
! rat_rdlf ... nutrient cycling factor (Amrd/Amlf); not used with SUMO
! f_NH4fu .... ammonium foliar uptake fraction (0..1)
!                 with SUMO (default, not automatically): 0.3 0.3 0.3 0.4 0.3
! f_Hfu ...... proton foliar uptake fraction (0..1)
!                 with SUMO (default, not automatically): 0.3 0.3 0.3 0.4 0.3
! f_Kfe ...... fraction of K in foliar exudation of BC (0..1)
!                 with SUMO (default, not automatically): 0.66 0.63 0.63 0.65 0.50
! f_ralloc ... reallocation fraction of nutrients (0..1); not used with SUMO
! ctBC2lv .... content of BC2 in leaves [%]
!                 with SUMO (default, not automatically): 0.64 0.54 0.31 0.75 0.75
! ctKlv ...... content of K in leaves [%]
!                 with SUMO (default, not automatically): 0.92 0.61 0.6 0.25 0.70
! ctNlfmn .... minimum N content in litterfall [%]; not used with SUMO
! ctNlfmx .... maximum N content in litterfall [%]; not used with SUMO
! ctPlv ...... content of P in leaves [%]; not used with SUMO
! ctNst ...... content of N in stems [%] (V/F); not used with SUMO
! ctPst ...... content of P in stems [%] (V/F); not used with SUMO
! ctBC2st .... content of BC2 in stems [%] (V/F)
!                 with SUMO (default, not automatically): 0.06 0.08 0.11 0.06 0.75
! ctKst ...... content of K in stems [%] (V/F)
!                 with SUMO (default, not automatically): 0.12 0.04 0.05 0.12 0.7
! amlt_0 ..... initial amount of litter (kg/m2) (R)
!                 if missing set to -1, then amtl_0 is calculated from litter fall
!                 and age_site.
! humus ...... amount of humus [kg/m2]
! Nhumus ..... N-content in humus [%]
! fmilt ...... fraction of old litter into humus [-]
! kmihu ...... mineralization rate constant of humus [1/T]
! AlFe ....... Amount of AlFe(ox) [mmol/kg]; if missing set to 0
! Phumus ..... P-content in humus [%]
! pHref ...... reference pH for weathering (default = 5);
!                 if missing set to -1
! alfa ....... exponent for calculation of pH dependent weathering;
!                 only asked if pHref > 0
! ffso2 ...... filtering factor for SO2-deposition (-); if missing set to 0
!                 with SUMO (default, not automatically): 1.15 1.60 1.40 1.0 1.0
! ffnh3 ...... filtering factor for NH3-deposition (-); if missing set to 0
!                 with SUMO (default, not automatically): 1.10 1.50 1.30 1.0 1.0
! ffnox ...... filtering factor for NOx-deposition (-); if missing set to 0
!                 with SUMO (default, not automatically): 0.70 1.00 0.85 1.0 1.0
! fdd ........ filtering factor for dry deposition (-); if missing set to 0
!                 with SUMO (default, not automatically): 2.00 2.50 3.00 1.50 1.50
! N_fix ...... fixation of N (eq/m2/T); if missing set to zero
! SUMO
! soil ....... soiltype (SP, SR, SC, CS, CM, CH, CC, LS, LM, LH, PN, PS, PL, PM or
!                     PH)
! vegtype .... SUMO vegetation type (1.., see Wamelink ..)
! plaggen .... frequnecy of sod cutting (years)
! filenr ..... filenumber for SUMO vegetation parameters (1 ..57)
! pboom ...... pioneer tree (BER, EIK, etc)
! cboom ...... climax tree (BER, EIK, etc)
! larchfn .... larch file number for combination with Larchmodel
! Observations
! CNratobs ... oberservations for C:N-ratio
! Cpoolobs ... oberservations for C pool
```

```
! Nimobs ..... oberservations for  N immobilisation
! Ndeobs ..... oberservations for N denitrification
! bsatobs .... oberservations for base saturation (0-1)
! EAlobs ..... oberservations for fraction Al on CEC (0-1)
! EHobs ...... oberservations for fraction H on CEC (0-1)
! pHobs ...... oberservations for pH
! cHobs ...... oberservations for H+ concentration
! cSO4obs .... oberservations for SO4 concentration
! cNO3obs .... oberservations for NO3 concentration
! cNH4obs .... oberservations for NH4 concentration
! cBcobs ..... oberservations for base cation concentration
! cNaobs ..... oberservations for Na concentration
! cClobs ..... oberservations for Cl concentration
! cAlobs ..... oberservations for Al concentration
! cOrgobs .... oberservations for organic acid concentration
! cHCO3obs ... oberservations for HCO3 concentration
! cANCobs .... oberservations for ANC concentration
! AlBcobs .... oberservations for Al/Bc ratio
!
! monfile .... name of parameter file for 'monitor';
!              if missing monfile='smart2.mon'
! balfile .... name of file with balances per timestep;
!              if missing no balances
!------------------------------------------------------------------
period     1900 2400
thick      0.5
bulkdens   0.15 1.30
Theta      0.3
pCO2fac    30.
Carbonat   100.
CEC        50.
!bsat_0     0.694
lgKAlBC    1.0
lgKHBC     6.176
lgKAlox    8.77
Alox_0     75.
expH       2
Excmod     1
expAl      3
!Cpool_0    3361.425
CNrat_0    30.
f_nit      1.0
!f_den      0.8
!SO4admax   0.
SO4half    0.1
modorg     0
!RCOOpars    2.0  0.9   0.039  ! Santore transformed (3-protic)
!AlApars    -7.89  -12.86        ! Santore
cRCOO      0
TempC      10.
Ca_we      0.05
Mg_we      0.
K_we       0.
Na_we      0.
Al_we      0.
ratwAlBC   2.
N_fix      0.
SO2_dep    .\testset\dep.dat#1
NOx_dep    .\testset\dep.dat#2
NH3_dep    .\testset\dep.dat#3
Ca_dep     .\testset\dep.dat#4
```

```
Mg_dep      0.
Na_dep      0.
K_dep       0.
Cl_dep      0.
!pHref        5.
!alfa         0.6
monfile     .\testset\smart2.mon
balfile     .\testset\smart2.bal
!
! smart 2
!
thickrz     0.5
F_growth    25. 0.07 40.0 0.3
precip      0.6
age_veg     40   0
age_site    80
f_rtll      0.25
rat_rdlf    0.5
f_mifl      0.8
r_miol      0.05
f_inter     0.0
f_NH4fu     0.03
f_Hfu       0.02
f_Kfe       0.8
f_ralloc    0.36
ctNlfmn     1.0
ctNlfmx     3.
ctBC2lv     0.5
ctKlv       0.5
ctNst       0.1
ctBC2st     0.015
ctKst       0.0
seepage     0.
transpir    0.3
!gvg         10
ffSO2       1.
ffNOx       1.
ffNH3       1.
fdd         1.
!
! observations:
!
pHobs       .\testset\ph.obs/o
```

As an example, (Table 7 shows the 'dep.dat' file, with deposition flues for three points in time. The first line holds the deposition in year 0 of the simulation and the last line holds the deposition in the year 6000. One can specify as many points in time as desired, and between two time points the program interpolates linearly. The period specified in the deposition/uptake file has to contain the simulation period, i.e. the first time point (year) has to be earlier than or the same as the starting time of the simulation and the last time point later than or the same as the ending time. If this condition is not met, the program terminates with an error message.

Table 7 An example of a timeseries file (dep.dat, with constant deposition) for SMART2

```
!       SO2    NOx    NH3    BC2
1900  0.30   0.20   0.10   0.04
2400  0.10   0.20   0.10   0.04
6000  0.30   0.10   0.10   0.04
```

In the example input files described in this document (Table 6 and Table 7 the parameters are selected in such a way that SMART2 reproduces the pH-graph in Figure 4, see also De Vries et al. (1989). These input files can be used as a testset. This also means that the parameters are selected such that model enhancements that are added afterwards are `switched off'. In particular, (i) the organic matter content in the mineral top soil is set to zero, which means no N-immobilization, (ii) the denitrification factor is set to zero, meaning no denitrification, (iii) the maximum sulphate adsorption capacity is set to zero, meaning no sulphate adsorption, (iv) [RCOO] is set to zero, implying no organic anions in soil solution, and (v) the deposition of chloride and monovalent base cations as well as the uptake of monovalent base cations are set to zero. To test all extensions added to the basic model, a series of input files has been created, where the processes are switched on, one after the other.
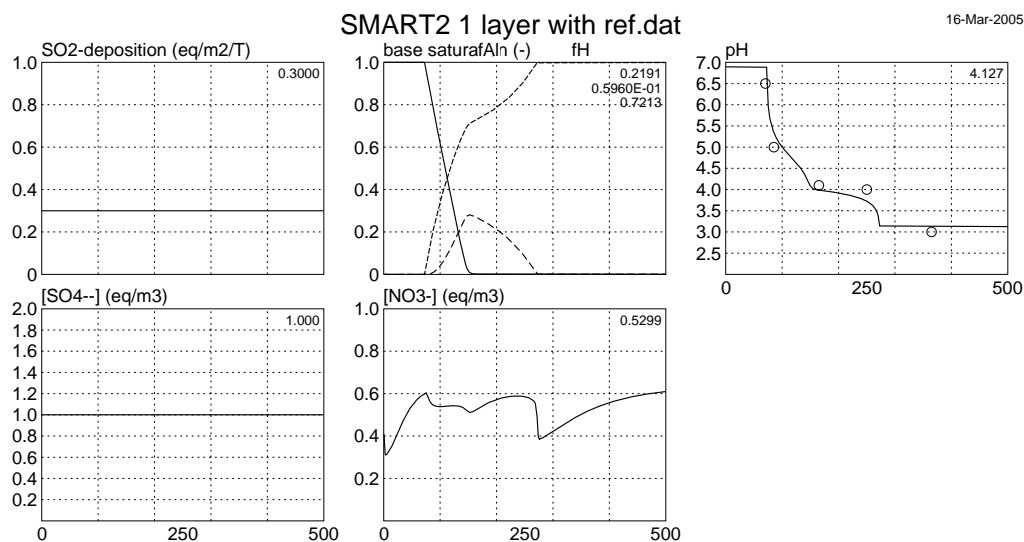
Figure 4 Results of a SMART2 run with the input parameters of Table 6 andTable 7.

One can force the model to use other input parameters by: (a) changing the contents of smart2.in, or, highly recommended (b) preparing another input file with different parameters and entering its name when the program prompts you for the input file To be able to reconstruct the original settings of the input parameters, one should not change smart2.in; instead, it is advised to copy smart2.in to another file and to change the contents of this new file.

In the input file smart2.in the user can specify the use, and location, of an observation file, a balance file and a monitor file. The use of an observation and balance file is optional, the use of the monitor file is mandatory. An observation file is an input file with measured values which can be displayed in the output graphs (see
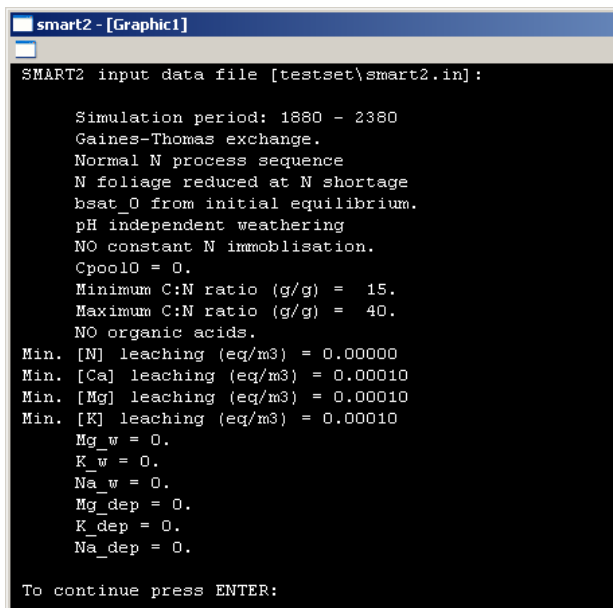
pH graph in Figure 4). Single observations can be specified using a keyword followed by the year and value of the observation. A balance file is an output file with yearly process balances of H, Al, BC2, K, Na, NH4, NO3, SO4, PO4, Cl, HCO3 and Org (see also paragraph 4.5). The monitor file is a input file for the subroutine MONITOR, the subroutine used for generating output for SMART2 (see also paragraph 4.5 and Appendix 0 for a complete description of MONITOR).

4.3   Running SMART2

The model SMART2 is run by double-clicking the smart2.exe. Firstly, the program will ask you to specify the file that holds the input parameters by displaying the line:

Input data file [testset\smart2.in]:

The file used in the previous run of SMART2 is shown between brackets. If ENTER is pressed, the program will use this input file. The first time the model is run there is no previous run, and therefore no filename will be displayed between the brackets (the same is true after booting). After selecting the input file and pressing ENTER the default values of those parameters not specified in the input file (and therefore defaulted) will be shown on the screen. See Figure 5.

```
smart2 - [Graphic1]

SMART2 input data file [testset\smart2.in]:

     Simulation period: 1880 - 2380
     Gaines-Thomas exchange.
     Normal N process sequence
     N foliage reduced at N shortage
     bsat_0 from initial equilibrium.
     pH independent weathering
     NO constant N immoblisation.
     Cpool0 = 0.
     Minimum C:N ratio (g/g) =   15.
     Maximum C:N ratio (g/g) =   40.
     NO organic acids.
Min. [N] leaching (eq/m3) = 0.00000
Min. [Ca] leaching (eq/m3) = 0.00010
Min. [Mg] leaching (eq/m3) = 0.00010
Min. [K] leaching (eq/m3) = 0.00010
     Mg_w = 0.
     K_w = 0.
     Na_w = 0.
     Mg_dep = 0.
     K_dep = 0.
     Na_dep = 0.

To continue press ENTER:
```

Figure 5 List of defaulted parameters

If these list is too long to be displayed in one window, press again ENTER to see the rest of the parameters. After pressing again ENTER the program will ask for the name of a PostScript file.

Postscript file [Testset\SMART2.eps]:

By entering a filename the a postscriptfile containing the output screen display is created (Figure 7 Example of the results (on screen) of a simulation run with SMART2). The file used in the previous run of SMART2 is shown between brackets. If ENTER is pressed, the program will use the same name for the newly constructed PostScript file. If ESC is pressed the name of the previous used file will be cleared and SMART2 does not generate a new PostScript file. The first time the model is run there is no previous run, and therefore no filename will be displayed between the brackets.

After pressing ENTER the program will ask for the name of an output (ASCII) file which might be useful for further processing of the model output:

Output file [/h] [fmt] [Testset\SMART2.out]

In this file all the selected and displayed output parameters will be printed. The file used in the previous run of SMART2 is shown between brackets. If ENTER is pressed, the program will use the name of this output file. If ESC is pressed the name of the previous used file will be cleared and SMART2 does not generate a output file. The first time the model is run there is no previous run, and therefore no filename will be displayed between the brackets. If after the filename the switch /h is used, the output file will also contain a header with the name of the selected variables. That can be followed by a Fortran format (between parentheses) specifying the output format (see example). If no format is specified, the default format '(2i6,99g12.4)' is used (thus avoiding over- or underflow).
For more details see also par 4.5 and 0.

After pressing ENTER the program will ask for the name of a comparison file.

Comparison file [testset\smart2_v33.out]

This file can be used for comparing the results of two different SMART2 runs. A comparison file normally is the name of a SMART2 output file from a previous run with different input parameters. The name of the comparisojn file used in the previous run of SMART2 is shown between brackets. If ENTER is pressed, the program will use this file for comparison. If ESC is pressed the name of the previous used file will be cleared and SMART2 does not use a comparison file. The first time the model is run there is no previous run, and therefore no filename will be displayed between the brackets. The data from the comparison file will be displayed in the output window (see Figure 7) as a black dotted line.

Finally, the program will ask to specify the variables for display on the screen and in an output file (Figure 6):

(More) Variable(s) for display/file (max 25; * observations available):

Your choice:
A list of 40 possible output variables is given
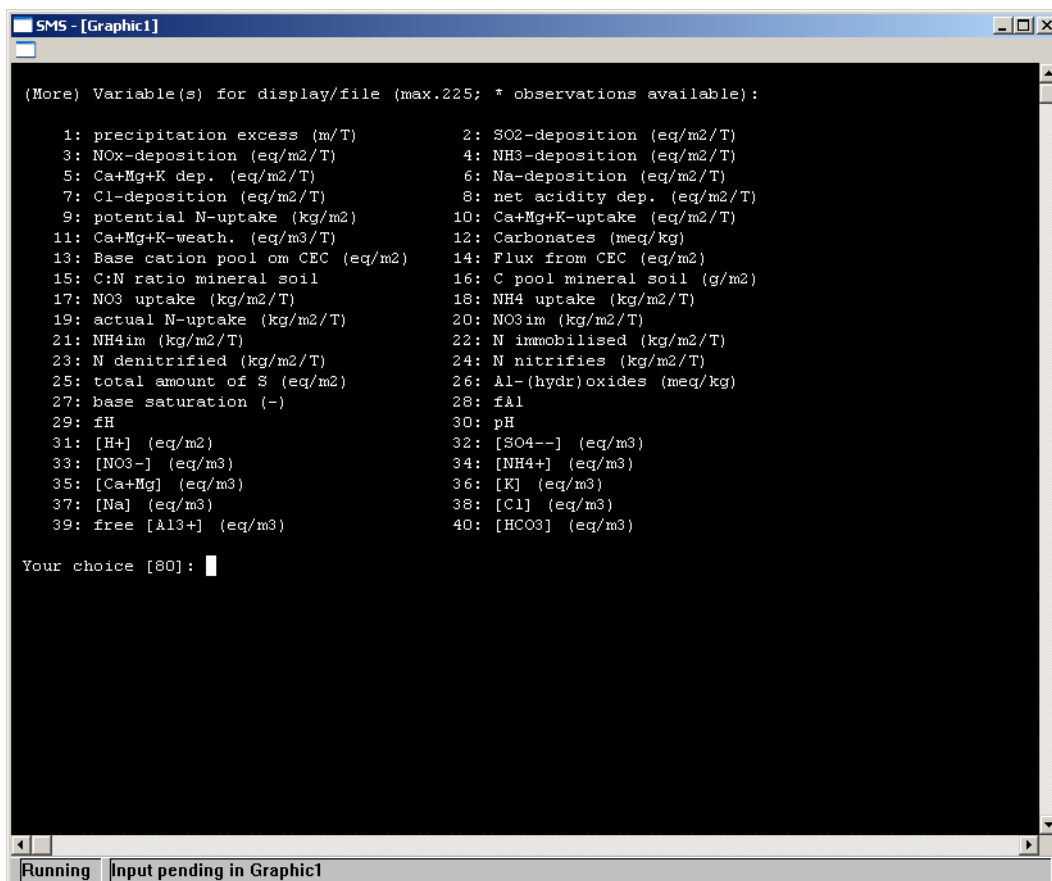
Figure 6 Screen with possible output variables.

The numbers used in the previous run of SMART2 are shown between brackets. If ENTER is pressed, the program will use these numbers (they don't have to be in ascending order) for displaying the results on screen or in an output file. Up to 25 variables can be displayed, if more then 25 variables are selected the programme displays an error message and terminates.

Variables for which an 'observation-file' has been specified (in the smart2.in file) are flagged with a star in front of the line. If there are more than 40 display variables to choose from, they are listed in "batches" of (maximal) 40 variables each. Numbers of variables chosen are 'remembered' and shown in subsequent runs [echoed between square brackets].

In order to plot/print the remembered variables, just press ENTER. There are several options for displaying the variables (Table 8. For more details see par 4.5 and 0, part A..

Table 8 Display options

Option	Description
u	If you want to *add* numbers of variables already chosen (=remembered), the first (non-blank) character of the additional choices has to be a 'u'
O	If you are happy with your (previous) choice of variables and want to prevent display of further screens (in case of many variables)
&	Up to 9 variables can be displayed in one window on the screen by linking their numbers with the '&'-sign.
i	If a variable is preceded by an 'i' (for **i**ntegrate), the running sum of that variable is displayed; it is reset to zero after every multiple of *module* steps (see above).

After selecting de output variables the program will start the simulation. Results are displayed on the screen during program execution (see Figure 7).
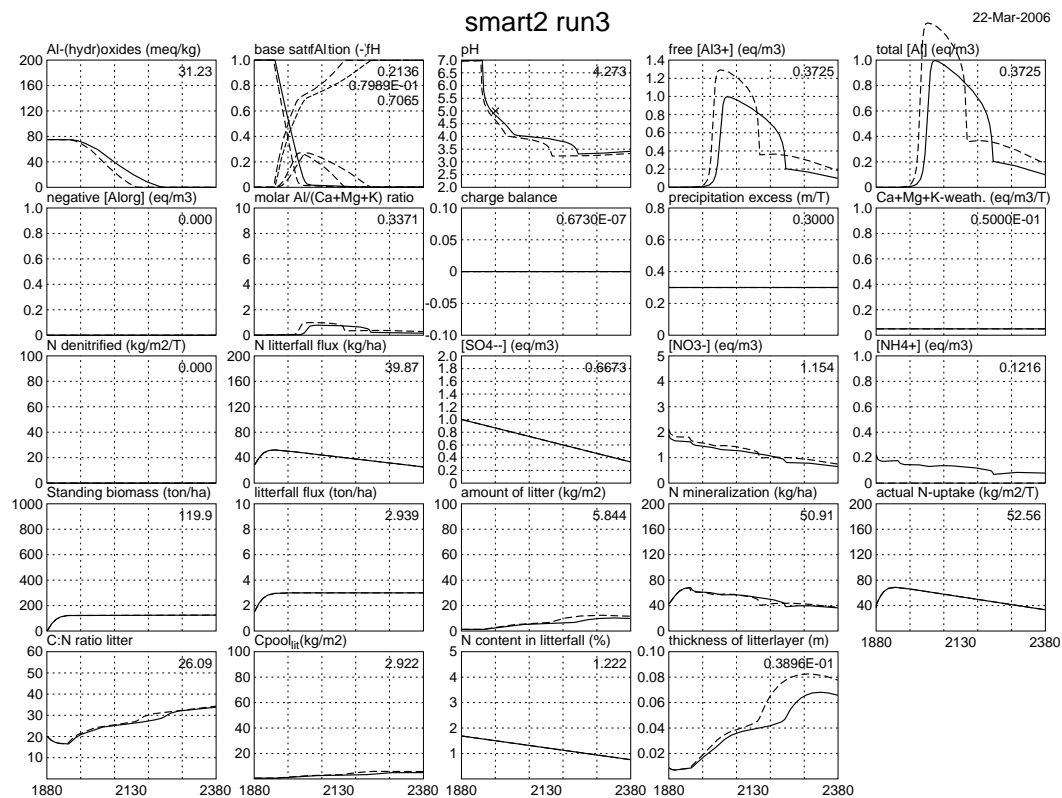
Figure 7 Example of the results (on screen) of a simulation run with SMART2

4.4 Running SMART2 with SUMO

To run SMART2 in combination with SUMO, you follow almost the same procedure as described in the previous paragraphs. You need some extra files and have to answer some extra questions in the interactive menu. Furthermore, the input file contains more parameters.

For running SMART2SUMO you need the files:

- Sms.exe
- Cofu4all.dll
- Smart2.dll
- Smart.dll
- Sumo_P_begr.dll
- sms.mon (name for the monitor file (see 0)

You can make the input file in a text editor and you are free in choosing a file name. In this manual we use the name 'sms.in' as an example of a SMART2SUMO input file. This file is described in paragraph 4.2. For running SMART2 in combination with SUMO you need extra input files besides the general input file. The extra SUMO input files, described in the SUMO manual (Wamelink, in prep), are:

- Biomini.txt,   with initial biomass data
- biommin.txt,   with biomass parameters for grazing
- boomparamete.txt,   with parameters for trees
- dunning.txt,   with parameters for thinning
- dunper.txt,   with parameters for thinning
- graas.txt,   with parameters about grazing behaviour of grazers
- lengteparam.txt,   with parameters for length growth
- poep.txt,   with parameters for excrements production
- terugtre.txt,   with parameters for reallocation
- transpiration.txt,   with potential transpiration per SUMO vegetation type

In the 'monitor file' you can regulate how the graphical output will look like and whether output files will be saved (see 0).

The file main input file 'sms.in' (Table 9) looks almost the same as the main input file 'smart2.in' for smart2.exe (see paragraph 4.2). The labels in the file are exactly the same, but for SUMO you need some extra labels: 'soil', 'vegtype', 'beheer', 'plaggen', 'filenr', 'pboom' and 'cboom', which are some general vegetation or site characteristics for a run with SUMO. For these input options of SUMO, is referred to tables in 0. Another important difference with the run without SUMO is that the vegetation related parameters have to be given for five vegetation types (see Table 9).

Table 9 : An example of an input parameter file (sms.in) for SMART2 in combination with SUMO

```
! This file contains the parameters for running SMART2:
!
! Lines with '!' in the first column are treated as comments and ignored
!
! The following parameters can be specified:
! (they can be in arbitrary order and they are case-sensitive)
! (V/F) means that either a constant value or a file can be specified
!       in the form [fac*]filename[#ncol]
! RF .... reduction function
! (I) ... integer value(s)
!
! With SUMO, the vegetation related parameters have to be given for the
!    five structural plant types. Sequence:
!    1) value for deciduous tree
!    2) value for spruce tree
!    3) value for pine tree
!    4) value for heather (shrub vegetation)
```

```
!   5) value for poor grassland (grasses and herbs)
!
! The labels are case sensitive
!
! period ..... starting and ending time of simulation [T T] (I)
! thick ...... thickness of the soil compartment [m]
! thickrz .... thickness of rooting zone [m]
! bulkdens ... bulk density [g/cm3]
! Theta ...... water content [m/m]
! Carbonat ... initial amount of carbonates [meq/kg];
!              if missing assumed zero
! CEC ........ cation exchange capacity [meq/kg]
! bsat_0 ..... initial base saturation;
!              if missing or -1 AND Carbonat=0 determined internally
! Excmod ..... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! lgKAlBC .... log10 of selectivity constant for Al-BC exchange [mol/l]
! lgKHBC ..... log10 of selectivity constant for H-BC exchange [l/mol]
! expAl ...... exponent for Al/BC exchange; if missing set to 3
! expH ....... exponent for H/BC exchange (default = 2);
!              only read if Excmod = 1
! Alox_0 ..... initial Al buffer capacity [meq/kg];
!              if missing assumed infinite (10**9)
! lgKAlox .... log10 of gibbsite equilibrium constant [(l/mol)**2]
! Nim_acc .... constant rate of N immobilization (eq/m2/T); if missing set to 0.
! Cpool_0 .... initial amount of C in topsoil (g/m2);
!              if missing assumed zero (no N-immobilization)
! CNrat_0 .... initial C:N ratio in organic matter;
!              not read if Cpool_0 <= 0. or missing
! CNratmin ... C:N ratio (g/g) below which no time-dependent Nimm;
!              if missing set to 15
! CNratmax ... C:N ratio (g/g) above which all available N is immobilised
!              if missing set to 40
! f_ni ....... nitrification fraction:
!              if 1 value: constant nitrification (0<=f_nit<=1)
!              if 4 values: defining RF for nitrification due to GVG (and pH):
!              1) fnitmx: overall maximum (0<=fnitmx<=1)
!              2) minimum value (0..1) of RF,
!              3) depth above which nitrification RF equals minimum value [m],
!              4) depth below which nitrification RF equals 1 [m];
!              not asked if NH3_dep<=0, if missing set to 1
! f_de ....... denitrification fraction:
!              if 1 value: constant denitrification (0<=f_de<=1)
!              if 3 values: defining RF for denitrification due to GVG (and pH):
!              1) fdenmx: overall maximum (0<=fdenmx<=1),
!              2) minimum value (0..1) of RF,
!              3) depth below which denitrification RF equals minimum value [m];
!              not asked if NOx_dep<=0, if missing set to 0
! SO4admax ... maximum SO4 adsorption capacity [meq/kg];
!              if missing assumed zero (no sulfate adsorption)
! SO4half .... half-saturation constant for SO4 adsorption [eq/m3];
!              not read if both SO4admax<=0 or missing
! PO4admax ... maximum PO4 adsorption capacity [meq/kg];
! PO4half .... half-saturation constant for PO4 adsorption
!              not read if both SO4admax<=0 or missing
! RCOOmod .... protonity of organic acids:
!                 1,2,3; 0=Oliver mode; <0: not modelled
```

```
! RCOOpars ... parameters for modeling organic acids:
!                 if RCOOmod = 0 (Oliver):
!                     1-3 parameters of (Oliver-type) mono-protic organics model:
!                     pK = par(1)+par(2)*pH-par(3)*pH^2
!                 if RCOOmod 1, 2 or 3:
!                     give 1, 2 or 3 values
!                 not read if cRCOO<=0 or missing
! cRCOO ...... total concentration of organic acids (m*TOC) [eq/m3];
!                 if missing set to zero, no organic acids simulated
! AlApars .... pK-values for organic Al-complexation; read if RCOOmod is 2 or 3
! pCO2fac .... CO2 pressure in soil solution (multiple of pCO2[atm] in air) (V/F)
! TempC ...... Annual average soil temperature [øC] (V/F); if missing set to 7øC
! precip ..... precipitation [m/T] (V/F)
! f_inter .... fraction of precip intercepted by vegetation (0..1) (V/F);
!                 if missing set to 0
!                 with SUMO (default, not automaticcaly): 0.2 0.4 0.3 0.1 0.05
! seepage .... upward seepage [m/T] (V/F); if missing set to 0
! transpir ... transpiration of vegetation [m/T] (V/F); if missing set to 0
!                 with SUMO (default, not automaticcaly): 0.326 0.296 0.276 0.335
!                                                          0.15
! GVG ........ depth of mean spring groundwater table [m] (V/F);
!                 if missing set to infinite (=100)
! Ca_we ...... weathering rate for Ca [eq/m3/T] (V/F); if missing set to 0
! Mg_we ...... weathering rate for Mg [eq/m3/T] (V/F); if missing set to 0
! K_we ....... weathering rate for K  [eq/m3/T] (V/F); if missing set to 0
! Na_we ...... weathering rate for Na [eq/m3/T] (V/F); if missing set to 0
! Al_we ...... weathering rate for Al [eq/m3/T] (V/F);
!                 if missing ratwAlBC is asked
! ratAlwBC ... Al:BC ratio in silicate dissolution ;
!                 if 1 value: Al:BC2 ratio (1<rat<3); if missing set to 2;
!                 if 4 values: ratios for Ca, Mg, K and Na:
!                 1) ratCa (default: 3),
!                 2) ratMg (default: 0.6),
!                 3) ratK (default: 3),
!                 4) ratNa (default: 3);
! P_we ....... weathering rate for P [eq/m3/T] (V/F);
!                 if missing PBCrat is asked
! PBCrat ..... P/BC2-ratio in minerals [-]
! cSO4_se .... conc. of SO4 in seepage [eq/m3/T] (V/F); if missing set to 0
! cNO3_se .... conc. of NO3 in seepage [eq/m3/T] (V/F); if missing set to 0
! cNH4_se .... conc. of NH4 in seepage [eq/m3/T] (V/F); if missing set to 0
! cCa_se ..... conc. of Ca in seepage [eq/m3/T] (V/F); if missing set to 0
! cMg_se ..... conc. of Mg in seepage [eq/m3/T] (V/F); if missing set to 0
! cK_se ...... conc. of K  in seepage [eq/m3/T] (V/F); if missing set to 0
! cNa_se ..... conc. of Na in seepage [eq/m3/T] (V/F); if missing set to 0
! cCl_se ..... conc. of Cl in seepage [eq/m3/T] (V/F); if missing set to 0
! SO2_dep .... deposition of SO2 [eq/m2/T] (V/F); if missing set to 0
! NOx_dep .... deposition of NOx [eq/m2/T] (V/F); if missing set to 0
! NH3_dep .... deposition of NH3 [eq/m2/T] (V/F); if missing set to 0
! Ca_dep ..... deposition of Ca [eq/m2/T] (V/F); if missing set to 0
! Mg_dep ..... deposition of Mg [eq/m2/T] (V/F); if missing set to 0
! K_dep ...... deposition of K  [eq/m2/T] (V/F); if missing set to 0
! Na_dep ..... deposition of Na [eq/m2/T] (V/F); if missing set to 0
! Cl_dep ..... deposition of Cl [eq/m2/T] (V/F); if missing set to 0
! age_site ... age of site (litter) [T] (I); not used with SUMO
! age_veg .... age of present vegetation [T] (I)
! F_growth ... forest (stem&leaves) growth specification:
!                 5 values: parameters for logistic growth function:
!                 1) gropt: 0: logistic growth 1: constant growth (= actual growth
!                    at t=age_veg)
!                 2) amst: maximum amount of biomass [kg/m2],
!                 3) krgl: logistic growth rate constant [1/T],
!                 4) t0.5: growth half-time [T],
!                 5) amlfmx: maximum amount of litterfall [kg/m2/T]
!                 not used with SUMO
! ioptu ...... uptake option (0=standard, 1=uptake prior to immobilisation and
!                 denitrification)
! ioptcl ..... critical load consistency option (0=standard, 1=compatible with CL:
!                 ctnitlv = constant)
! f_mifl ..... mineralization fraction of fresh litter (0..1)
!                 with SUMO (default, not automatically): 0.8 0.8 0.8 0.4 0.8
```

```
! r_miol ..... mineralization rate constant of old litter [1/T]
!              with SUMO (default, not automatically): 0.05 0.05 0.05 0.3 0.3
! rat_asdi ... Assimilation dissimilation ratio of decomposing microbes (-) (R);
!              if missing set to 5.
! f_rtll ..... fraction of roots in the litterlayer (0..1)
!              with SUMO (default, not automatically): 0.25 0.25 0.25 0.75 0.75
! rat_rdlf ... nutrient cycling factor (Amrd/Amlf); not used with SUMO
! f_NH4fu .... ammonium foliar uptake fraction (0..1)
!              with SUMO (default, not automatically): 0.3 0.3 0.3 0.4 0.3
! f_Hfu ...... proton foliar uptake fraction (0..1)
!              with SUMO (default, not automatically): 0.3 0.3 0.3 0.4 0.3
! f_Kfe ...... fraction of K in foliar exudation of BC (0..1)
!              with SUMO (default, not automatically): 0.66 0.63 0.63 0.65 0.50
! f_ralloc ... reallocation fraction of nutrients (0..1); not used with SUMO
! ctBC2lv .... content of BC2 in leaves [%]
!              with SUMO (default, not automatically): 0.64 0.54 0.31 0.75 0.75
! ctKlv ...... content of K in leaves [%]
!              with SUMO (default, not automatically): 0.92 0.61 0.6 0.25 0.70
! ctNlfmn .... minimum N content in litterfall [%]; not used with SUMO
! ctNlfmx .... maximum N content in litterfall [%]; not used with SUMO
! ctPlv ...... content of P in leaves [%]; not used with SUMO
! ctNst ...... content of N in stems [%] (V/F); not used with SUMO
! ctPst ...... content of P in stems [%] (V/F); not used with SUMO
! ctBC2st .... content of BC2 in stems [%] (V/F)
!              with SUMO (default, not automatically): 0.06 0.08 0.11 0.06 0.75
! ctKst ...... content of K in stems [%] (V/F)
!              with SUMO (default, not automatically): 0.12 0.04 0.05 0.12 0.7
! amlt_0 ..... initial amount of litter (kg/m2) (R)
!              if missing set to -1, then amtl_0 is calculated from litter fall
!              and age_site.
! humus ...... amount of humus [kg/m2]
! Nhumus ..... N-content in humus [%]
! fmilt ...... fraction of old litter into humus [-]
! kmihu ...... mineralization rate constant of humus [1/T]
! AlFe ....... Amount of AlFe(ox) [mmol/kg]; if missing set to 0
! Phumus ..... P-content in humus [%]
! pHref ...... reference pH for weathering (default = 5);
!              if missing set to -1
! alfa ....... exponent for calculation of pH dependent weathering;
!              only asked if pHref > 0
! ffso2 ...... filtering factor for SO2-deposition (-); if missing set to 0
!              with SUMO (default, not automatically): 1.15 1.60 1.40 1.0 1.0
! ffnh3 ...... filtering factor for NH3-deposition (-); if missing set to 0
!              with SUMO (default, not automatically): 1.10 1.50 1.30 1.0 1.0
! ffnox ...... filtering factor for NOx-deposition (-); if missing set to 0
!              with SUMO (default, not automatically): 0.70 1.00 0.85 1.0 1.0
! fdd ........ filtering factor for dry deposition (-); if missing set to 0
!              with SUMO (default, not automatically): 2.00 2.50 3.00 1.50 1.50
! N_fix ...... fixation of N (eq/m2/T); if missing set to zero
! SUMO
! soil ....... soiltype (SP, SR, SC, CS, CM, CH, CC, LS, LM, LH, PN, PS, PL, PM or
!              PH)
! vegtype .... SUMO vegetation type (see 0, Table 12)
! beheer ..... management type (see 0, Table 13), default = 0
! plaggen .... frequency of sod cutting (years)
! filenr ..... file number for SUMO vegetation parameters (see 0,
!              Table 14)
! pboom ...... pioneer tree (see 0, Table 11)
! cboom ...... climax tree (see 0, Table 11)
! larchfn .... larch file number for combination with Larch model
! Observations
! CNratobs ... oberservations for C:N-ratio
! Cpoolobs ... oberservations for C pool
! Nimobs ..... oberservations for  N immobilisation
! Ndeobs ..... oberservations for N denitrification
! bsatobs .... oberservations for base saturation (0-1)
! EAlobs ..... oberservations for fraction Al on CEC (0-1)
! EHobs ...... oberservations for fraction H on CEC (0-1)
! pHobs ...... oberservations for pH
```

```
! cHobs ...... oberservations for H+ concentration
! cSO4obs .... oberservations for SO4 concentration
! cNO3obs .... oberservations for NO3 concentration
! cNH4obs .... oberservations for NH4 concentration
! cBcobs ..... oberservations for base cation concentration
! cNaobs ..... oberservations for Na concentration
! cClobs ..... oberservations for Cl concentration
! cAlobs ..... oberservations for Al concentration
! cOrgobs .... oberservations for organic acid concentration
! cHCO3obs ... oberservations for HCO3 concentration
! cANCobs .... oberservations for ANC concentration
! AlBcobs .... oberservations for Al/Bc ratio
!
! monfile .... name of parameter file for 'monitor';
!              if missing monfile='smart2.mon'
! balfile .... name of file with balances per timestep;
!              if missing no balances
!----------------------------------------------------------------
------
period    1900 2400
thick     0.50
thickrz   0.5 0.5 0.5 0.2 0.2
bulkdens  0.15 1.30
Theta     0.30
Carbonat  100.
CEC       50.
!bsat_0      0.8
lgKAlBC   1.
lgKHBC    6.176
lgKAlox   8.77
Alox_0    75.
!Cpool     0.0
CNrat_0   30
f_nit     1.0
f_den     0.8
f_mifl    0.8 0.8 0.8 0.4 0.8
r_miol    0.05 0.05 0.05 0.3 0.3
f_rtll    0.25 0.25 0.25 0.75 0.75
!SO4admax  2.2
SO4half   0.1
cRCOO     0.
!RCOOpars  2.  0.9  0.039
precip    0.6
transpir  0.3 0.3 0.3 0.3 0.3
!f_inter   0.1 0.1 0.2 0.2 0.2
!seepage
!GVG        0.82
pCO2fac   30.
Ca_we     0.05
Na_we     0.
K_we      0.
Al_we     0.
!f_NH4fu   0.3 0.3 0.3 0.4 0.3
!f_Hfu     0.3 0.3 0.3 0.4 0.3
!f_Kfe     0.66 0.63 0.63 0.65 0.5
!ctBC2lv   0.64 0.54 0.31 0.75 0.75
!ctKlv     0.92 0.61 0.60 0.25 0.70
!ctBC2st   0.06 0.08 0.11 0.06 0.75
!ctKst     0.12 0.04 0.05 0.12 0.70
f_NH4fu   0.03 0.03 0.03 0.03 0.03
```

```
f_Hfu       0.02 0.02 0.02 0.02 0.02
f_Kfe       0.5 0.5 0.5 0.5 0.5
ctBC2lv     0.5 0.5 0.5 0.5 0.5
ctKlv       0.5 0.5 0.5 0.5 0.5
ctBC2st     0.15 0.15 0.15 0.15 0.15
ctKst       0. 0. 0. 0. 0.
SO2_dep     .\testset\dep.dat#1
NOx_dep     .\testset\dep.dat#1
NH3_dep     .\testset\dep.dat#1
Ca_dep      0.
Mg_dep      0.
K_dep       0.
Na_dep      0.
Cl_dep      0.
!cSO4_se    input\seep.dat#1
!cNO3_se    input\seep.dat#2
!cNH4_se    input\seep.dat#3
!cCa_se     input\seep.dat#4
!cMg_se     0.
!cK_se      input\seep.dat#5
!cNa_se     input\seep.dat#6
!cCl_se     input\seep.dat#7
frpp        0.
ffSO2       1.00 1.00 1.00 1.00 1.00
ffNOx       1.00 1.00 1.00 1.00 1.00
ffNH3       1.00 1.00 1.00 1.00 1.00
fdd         1.00 1.00 1.00 1.00 1.00
arable      0
!humus      27.42113
!Nhumus     1.989025
!fmilt      0.1
!kmihu      0.05
!P          0
!Pox        0.
!AlFe       0.
!AlFe       291.44
!kdif       0.
!N          0.
!N          0.022
!K_Fr       0.
!PO4half    0.
!PO4half    0.0002857
!PBCrat     0.
!Phumus     0.
monfile     .\testset\sms.mon
TempC       10.
pHref       5.
alfa        0.6
expH        2.
expAl       3.
! SUMO
soil        SC
vegtype     4
plaggen     30
filenr      27
pboom       BER
```

```
cboom      EIK
larchfn    B02
!
! observations:
!
pHobs      .\testset\ph.obs/o
```

The model SMART2 with SUMO is run by double-clicking the sms.exe. Firstly, the program will ask you if you want to run the model with or without SUMO (see Figure 8) by the line:

SUMO? (yes/no): [ ]:

Answer this question with yes (lowercase) followed by pressing ENTER if you want to use SUMO. **Note that answering 'Y' or 'y' is considered as no** and only SMART2 will be run (see 4.3).
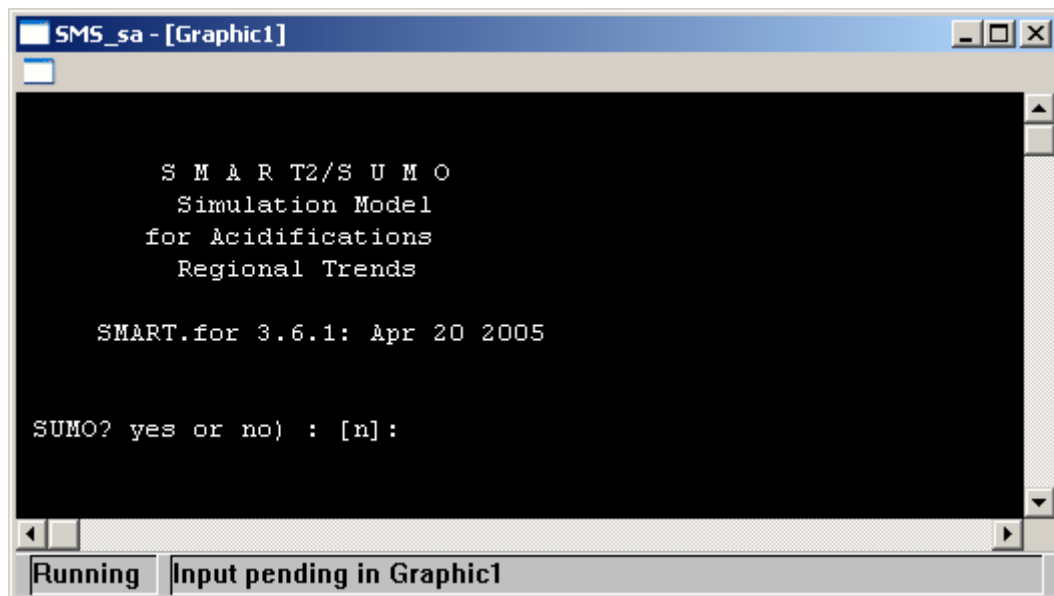
Figure 8 The SMS input screen

Secondly the program will ask you to specify the directory with the vegetation input files (the extra SUMO input files with extension '*.txt', given in the beginning of this paragraph) by displaying the line:

Directory with vegetation data (give also \): [testset\]:

Thirdly the program will ask you to specify the file that holds the input parameters by displaying the line:

Input data file [testset\sms.in]:

After this line the execution of the programme is identical as running it without SUMO.

4.5 Model output

The model SMART2(SUMO) can, by using the subroutine MONITOR, generate three types of output: output to the screen (see Figure 7), output (of the graphs shown on the screen) to a PostScript file and output (as data) to an (ASCII) file. A complete description of the subroutine MONITOR is available in 0 (see also paragraph 4.3).

Table 10 List with descriptions of SMART2 output variables that can be displayed

Output variables on screen	Explanation (if necessary)
1: precipitation excess (m/T)	
2: SO2-deposition (eq/m2/T)	
3: NOx-deposition (eq/m2/T)	
4: NH3-deposition (eq/m2/T)	
5: Ca+Mg+K dep. (eq/m2/T)	
6: Na-deposition (eq/m2/T)	
7: Cl-deposition (eq/m2/T)	
8: net acidity dep. (eq/m2/T)	
9: potential N-uptake (kg/m2)	
10: Ca+Mg+K-uptake (eq/m2/T)	
11: Ca+Mg+K-weath. (eq/m3/T)	
12: Carbonates (meq/kg)	
13: Base cation pool on CEC (eq/m2)	
14: Flux from CEC (eq/m2)	Flux of base cations
15: C:N ratio mineral soil (-)	
16: C pool mineral soil (g/m2)	
17: NO3 uptake (kg/m2/T)	
18: NH4 uptake (kg/m2/T)	
19: actual N-uptake (kg/m2/T)	
20: NO3 immobilisation (kg/m2/T)	
21: NH4 immobilisation (kg/m2/T)	
22: N immobilised (kg/m2/T)	
23: N denitrified (kg/m2/T)	
24: N nitrified (kg/m2/T)	
25: total amount of S (eq/m2)	
26: Al-(hydr)oxides (meq/kg)	
27: base saturation (-)	
28: fAl (-)	Al pool on CEC
29: fH (-)	H pool on CEC
30: pH	
31: [H+] (eq/m2)	
32: [SO4--] (eq/m3)	
33: [NO3-] (eq/m3)	
34: [NH4+] (eq/m3)	
35: [Ca+Mg] (eq/m3)	
36: [K] (eq/m3)	
37: [Na] (eq/m3)	
38: [Cl] (eq/m3)	
39: free [Al3+] (eq/m3)	
40: [HCO3] (eq/m3)	
41: [ANC] (eq/m3)	
42: [organic anions] (eq/m3)	

Output variables on screen	Explanation (if necessary)
43: [H2A-] (eq/m3)	Organic anions
44: [HA--] (eq/m3)	Organic anions
45: [A---] (eq/m3)	Organic anions
46: negative [Alorg] (eq/m3)	Complexed Al to organic anions
47: neutral [Alorg] (eq/m3)	Complexed Al to organic anions
48: positive [Alorg] (eq/m3)	Complexed Al to organic anions
49: total [Al] (eq/m3)	Total Al, anorganic and complexed
50: ratio org/total [Al] (-)	Ratio between complexed Al and total Al (-)
51: molar Al/(Ca+Mg+K) ratio (-)	
52: charge balance (-)	
53: [H2PO4-] (eq/m3)	
54: Adsorbed amount of P (meq/kg)	
55: N-leaching (kg/ha)	
56: N litter fall flux (kg/ha)	
57: N mineralization (kg/ha)	
58: amount of litter (kg/m2)	
59: thickness of litter layer (m)	
60: ctN in litter (ctN) (%)	N content in litter
61: Cpool_lit (kg/m2)	Cpool litter layer
62: C:N ratio litter (-)	
63: ctBC1 in litter (%)	BC1 content in litter
64: ctBC2 in litter (%)	BC2 content in litter
65: Standing biomass (ton/ha)	
66: litter fall flux (ton/ha)	
67: N content in litter fall (%)	
68: N availability (kg/ha)	
69: seepage (m/T)	
70: Cseq_soil (kg/ha/yr)	C sequestration in soil
71: Cseq_veg (kg/ha/yr)	C sequestration in vegetation
72: Cpool_tot(kg/ha/yr)	total C pool in soil
73: Npool_tot (kg/ha/yr)	total N pool in soil
74: total standing biomass (ton/ha)	Not used (same as 65)
75: P uptake (kg/ha/yr)	
76: P availability (kg/ha/yr)	
77: P desorption (kg/ha/yr)	
78: P weathering (kg/ha/yr)	
79: P mineralisation (kg/ha/yr)	
80: P content litterfall (%)	

If defined in the main input file, SMART2 can also produce a balance file (see Figure 9).

```
smart2.bal - Notepad
File  Edit  Format  View  Help

Process  /  Ion |    H      Al      BC2      K       Na      NH4      NO3      SO4      PO4      Cl      HCO3     Org
----------------------------------------------------------------------------------------------------------------------
deposition      |  3.596           0.400    0.000   0.000   1.000    2.000    2.996            0.000
seepage         |  0.000           0.000    0.000   0.000   0.000    0.000    0.000            0.000
foliar interac. | -0.072           0.020    0.082          -0.030
mineralisation  | -1.620           0.482    0.211           0.927                     0.000
nitrification   |  0.000                                    0.000    0.000
denitrification |  0.000                                             0.000
uptake          |  2.803          -0.635   -0.289          -1.897   -0.019            0.000
immobilisation  |  0.000                                    0.000    0.000
Ca dissolution  |-11.250          11.250
weathering      |  0.000   0.000   0.000    0.000   0.000                              0.000
exchange        |  0.000   0.000   0.000
bicarbonate     |  6.544                                                                                6.544
organic anions  |  0.000                                                                                         0.000
Al dissolution  |  0.000   0.000
adsorption      |  0.000                                             0.000    0.000
d/dt storage    |  0.000   0.000   0.088    0.000   0.000   0.000    0.111    0.001    0.000    0.000  -0.024    0.000
leaching        |  0.000   0.000 -11.605   -0.003   0.000   0.000   -2.092   -2.997    0.000    0.000  -6.519    0.000 ä=   0.000
----------------------------------------------------------------------------------------------------------------------
MASS BALANCE    |  0.000   0.000   0.000    0.000   0.000   0.000    0.000    0.000    0.000    0.000   0.000    0.000
======================================================================================================================
Process  /  Ion |    H      Al      BC2      K       Na      NH4      NO3      SO4      PO4      Cl      HCO3     Org
----------------------------------------------------------------------------------------------------------------------
deposition      |  3.592           0.400    0.000   0.000   1.000    2.000    2.992            0.000
seepage         |  0.000           0.000    0.000   0.000   0.000    0.000    0.000            0.000
foliar interac. | -0.072           0.020    0.081          -0.030
mineralisation  | -1.673           0.503    0.181           0.990                     0.000
nitrification   |  0.000                                    0.000    0.000
denitrification |  0.000                                             0.000
uptake          |  2.864          -0.655   -0.259          -1.960   -0.010            0.000
immobilisation  |  0.000                                    0.000    0.000
Ca dissolution  |-11.253          11.253
weathering      |  0.000   0.000   0.000    0.000   0.000                              0.000
exchange        |  0.000   0.000   0.000
bicarbonate     |  6.543                                                                                6.543
organic anions  |  0.000                                                                                         0.000
Al dissolution  |  0.000   0.000
adsorption      |  0.000                                             0.000    0.000
d/dt storage    |  0.000   0.000   0.028    0.000   0.000   0.000    0.034    0.002    0.000    0.000  -0.008    0.000
leaching        |  0.000   0.000 -11.549   -0.003   0.000   0.000   -2.024   -2.994    0.000    0.000  -6.535    0.000 ä=   0.000
----------------------------------------------------------------------------------------------------------------------
MASS BALANCE    |  0.000   0.000   0.000    0.000   0.000   0.000    0.000    0.000    0.000    0.000   0.000    0.000
======================================================================================================================
Process  /  Ion |    H      Al      BC2      K       Na      NH4      NO3      SO4      PO4      Cl      HCO3     Org
----------------------------------------------------------------------------------------------------------------------
deposition      |  3.588           0.400    0.000   0.000   1.000    2.000    2.988            0.000
seepage         |  0.000           0.000    0.000   0.000   0.000    0.000    0.000            0.000
foliar interac. | -0.072           0.020    0.081          -0.030
mineralisation  | -1.732           0.524    0.157           1.052                     0.000
nitrification   |  0.000                                    0.000    0.000
denitrification |  0.000                                             0.000
uptake          |  2.931          -0.674   -0.236          -2.022   -0.001            0.000
```

Figure 9 SMART2 balance file

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Appendix 1 List of symbols used in the process descriptions in the SMART2 model

Symbol	Explanation	Unit
θ	volumetric moisture content of the soil	$m^3\ m^{-3}$
ϱ_{lt}	bulk density of the mineral soil	$kg\ m^{-3}$
ϱ_{rz}	bulk density of the soil in the root zone	$kg\ m^{-3}$
age_{lt}	age of the site	a
age_{vg}	age of the vegetation	a
Am_{lt}	amount of litter	$kg\ ha^{-1}$
Am_{hu}	amount of humus	$kg\ ha^{-1}$
Am_{lf}	actual amount of litterfall	$kg\ ha^{-1}\ a^{-1}$
$Am_{lf,mx}$	maximum amount of litterfall	$kg\ ha^{-1}\ a^{-1}$
AmN_{iz}	amount of nitrogen in the zone where N immobilisation occurs	$mol_c\ kg^{-1}$
Am_{st}	actual amount of stems and branches	$kg\ ha^{-1}$
$Am_{st,mx}$	maximum amount of stems and branches	$kg\ ha^{-1}$
CEC	cation exchange capacity	$mol_c\ kg^{-1}$
CN_{cr}	critical C/N ratio of the soil	$g\ g^{-1}$
CN_{mn}	minimum C/N ratio of the soil	$g\ g^{-1}$
CN_{om}	C/N ratio of the soil	$g\ g^{-1}$
$ctAl_{ox}$	content of Al in secondary Al compounds in the soil	$mol_c\ kg^{-1}$
$ctCa_{cb}$	amount of Ca in carbonates in the soil	$mol_c\ kg^{-1}$
ctC_{iz}	organic carbon content in the zone where N immobilisation occurs	$mol_c\ kg^{-1}$
$ctN_{lv,mx}$	maximum N content in leaves	%
$ctN_{lv,mn}$	minimum N content in leaves	%
ctX_{lv}	nutrient content in leaves of ion X (N, K, BC2)	%
ctX_{sh}	nutrient content in shoot of ion X (N, K, BC2)	%
ctX_{hu}	nutrient content in humus ion X (N, K, BC2, P)	%
$C_{\frac{1}{2}}$	half-saturation constant for sulphate sorption	$mol_c\ m^{-3}$
DA_{mo}	dissimilation to assimilation ratio of decomposing microbes	-
dt	time step	a
fdd	dry deposition factor	-
fr_{de}	actual denitrification fraction	-
$fr_{de,mx}$	maximum denitrification fraction	-
fr_{int}	interception fraction	-
fr_{mi}	actual mineralisation fraction fresh litter	-
fr_{lt}	actual mineralisation fraction old litter	-
$fr_{mi,mx}$	maximum mineralisation fraction fresh litter	-
fr_{ni}	actual nitrification fraction	-
$fr_{ni,mx}$	maximum nitrification fraction	-
frN_{re}	reallocation of N fraction before litterfall	-
$fr_{rt,lt}$	fraction roots in the litter layer	-
fr_{ru}	cumulative transpiration fraction	-
frX_{ac}	fraction of ion X (BC2, Al, H) on the adsorption complex	-
frX_{fe}	foliar exudation fraction	-
frX_{fu}	foliar uptake fraction	-
frX_{le}	leaching fraction from fresh litter of ion K and BC2	-
frX_{le}	leaching fraction from fresh litter of ion K and BC2	-
K_a	dissociation constant for organic acids	$mol_c\ m^{-3}$
KAl_{ex}	selectivity constant for Al/BC2 exchange	$mol_c^{-1}\ m^3$
KAl_{ox}	dissolution constant for Al-hydroxide	$mol_c^{-2}\ m^6$
KBC_{cb}	dissolution constant for calcium carbonate	$(mol_c\ m^{-3})^3\ hPa^{-1}$
KCO_2	dissociation constant for CO_2	$mol_c^2\ m^{-6}\ hPa^{-1}$
k_{gl}	growth rate constant for logistic growth	$kg\ ha^{-1}\ a^{-1}$

Symbol	Explanation	Unit
KH_{ex}	selectivity constant for H/BC2 exchange	mol_c m^{-3}
kr_{mi}	actual mineralisation rate constant old litter	a^{-1}
$kr_{mi,mx}$	maximum mineralisation rate constant old litter	a^{-1}
kr_{hu}	actual mineralisation rate constant humus	a^{-1}
MHW	mean highest water-table	m
MLW	mean lowest water-table	m
ncf	nutrient cycling factor (ratio above ground N cycle/below ground N cycle)	-
N_{de}	denitrification flux	mol_c m^{-2} a^{-1}
N_{im}	N immobilisation flux	mol_c m^{-2} a^{-1}
$N_{le,mn}$	Minimum N leaching flux	mol_c m^{-2} a^{-1}
N_{ni}	nitrification flux	mol_c m^{-2} a^{-1}
$N_{td,mx}$	total N deposition above which $ctN_{lv} = ctN_{lv\,mx}$	mol_c m^{-2} a^{-1}
$N_{td,mn}$	total N deposition below which $ctN_{lv} = ctN_{lv\,mn}$	mol_c m^{-2} a^{-1}
OM	organic matter content	g g^{-1}
P	precipitation	m a^{-1}
$PBCrat$	stoichiometric equivalent ratio of P to BC2 in weathering	-
pCO_2	partial CO$_2$ pressure in the soil	hPa
PE	precipitation excess	m a^{-1}
r_X	Stoichiometric equivalent ratio of Al to X in congruent weathering of silicates	-
$rf_{mi,MSW}$	reduction fraction of the mineralisation rate for the water-table	-
$rf_{mi,CN}$	reduction fraction of the mineralisation rate for N content	-
$rf_{ni,MSW}$	reduction fraction of the mineralisation rate for the water-table	-
$rf_{de,MSW,mn}$	minimum denitrification reduction fraction for the water-table	-
$rf_{de,pH}$	reduction fraction of the denitrification fraction for pH	-
$rf_{de,MSW}$	reduction fraction of the denitrification fraction for the water-table	-
$rf_{ni,pH}$	reduction fraction of the nitrification fraction for pH	-
$rf_{ni,MSW,mn}$	minimum nitrification reduction fraction for the water-table	-
$rf_{mi,pH}$	reduction fraction of the mineralisation rate for pH	-
ru_{exp}	root uptake exponent	-
Se	upward seepage flux	m a^{-1}
$ctSO_{4,ac}$	Sulphate content at the adsorption complex	$mmol_c$ kg^{-1}
SSC	Sulphate adsorption capacity	$mmol_c$ kg^{-1}
t	time	a
$t_{1/2}$	half-life time parameter of logistic growth function	a
T	temperature	°C
T_{ref}	reference temperature	°C
T_{iz}	thickness of the zone where N mobilisation occurs	m
Tr	transpiration flux	m a^{-1}
T_{rz}	thickness of the root zone	m
X_{fe}	foliar exudation flux of ion X (K, BC2)	mol_c m^{-2} a^{-1}
X_{fu}	foliar uptake flux of ion X (NH$_4$, H)	mol_c m^{-2} a^{-1}
X_{gu}	growth uptake flux of element X (N, K, BC2, P)	mol_c m^{-2} a^{-1}
X_{in}	input flux of ion X (SO$_4$, NO$_3$, NH$_4$, Cl, RCOO, K, Na, BC2, HCO$_3$, Al, P)	mol_c m^{-2} a^{-1}
X_{int}	interaction flux of ion X (SO$_4$, NO$_3$, NH$_4$, Cl, RCOO, K, Na, BC2, HCO$_3$, Al, P)	mol_c m^{-2} a^{-1}
X_{la}	lateral output flux of ion X (SO$_4$, NO$_3$, NH$_4$, Cl, RCOO, K, Na, BC2, HCO$_3$, Al, P)	mol_c m^{-2} a^{-1}
X_{lf}	litterfall flux of ion X (NH$_4$, RCOO, K, BC2, P)	mol_c m^{-2} a^{-1}
X_{mi}	mineralisation flux fresh litter, old litter and the root decay in the litter layer of ion X (NH$_4$, RCOO, K, BC2, P)	mol_c m^{-2} a^{-1}
$X_{mi,lt}$	mineralisation flux old litter of ion X (NH$_4$, RCOO, K, BC2, P)	mol_c m^{-2} a^{-1}
$X_{mi,fl}$	mineralisation flux fresh litter of ion X (NH$_4$, RCOO, K, BC2,	mol_c m^{-2} a^{-1}

Symbol	Explanation	Unit
	P)	
$X_{mi,hu}$	mineralisation flux humus of ion X (NH$_4$, RCOO, K, BC2, P)	mol$_c$ m^{-2} a^{-1}
$X_{mi,tot}$	mineralisation flux fresh litter, old litter, humus and the total root decay of ion X (NH$_4$, RCOO, K, BC2, P)	mol$_c$ m^{-2} a^{-1}
$X_{rd,ms}$	root decay flux in the mineral soil of ion X (NH$_4$, RCOO, K, BC2, P)	mol$_c$ m^{-2} a^{-1}
$X_{rd,lt}$	root decay flux in the litter layer of ion X (NH$_4$, RCOO, K, BC2, P)	mol$_c$ m^{-2} a^{-1}
X_{se}	seepage flux of ion X (SO$_4$, NO$_3$, NH$_4$, Cl, K, Na, BC2, HCO$_3$, Al)	mol$_c$ m^{-2} a^{-1}
X_{sen}	net seepage flux of ion X (SO$_4$, NO$_3$, NH$_4$, Cl, RCOO, K, Na, BC2, HCO$_3$, Al)	mol$_c$ m^{-2} a^{-1}
X_{td}	total deposition of element X (SO$_4$, N, K, Na, BC2)	mol$_c$ m^{-2} a^{-1}
X_{we}	weathering flux of base cation X (Na, K, BC2, P)	mol$_c$ m^{-3} a^{-1}
$[X]$	concentration of ion X (SO$_4$, NO$_3$, K, Na, BC2, HCO$_3$, Al, P and H) in soil solution	mol$_c$ m^{-3}
z	depth	m
z_{ni1}	soil dependent depth of *MSW* for determination of $rf_{ni\,MSW}$	m
z_{ni2}	soil dependent depth of *MSW* determination of $rf_{ni\,MSW}$	m
z_{de}	soil dependent depth of *MSW* for determination of $rf_{de\,MSW}$	m

Appendix 2 Modelling the dissociation of organic acids

The dissociation of organic acids is modelled with varying complexity. *E.g.*, Driscoll *et al.* (1994) compare models for the following dissociation reactions (*A* stands for the organic anion):

Monoprotic model:
$$HA \quad \Leftrightarrow \quad H^+ + A^- \tag{79}$$

Diprotic model:
$$H_2A \quad \Leftrightarrow \quad H^+ + HA^-$$
$$HA^- \quad \Leftrightarrow \quad H^+ + A^{2-} \tag{80}$$

Triprotic model:
$$H_3A \quad \Leftrightarrow \quad H^+ + H_2A^-$$
$$H_2A^- \quad \Leftrightarrow \quad H^+ + HA^{2-}$$
$$HA^{2-} \quad \Leftrightarrow \quad H^+ + A^{3-} \tag{81}$$

These equations can be summarized for an *n*-protic model as:

$$H_{n-i+1}A^{(i-1)-} \rightarrow H^+ + H_{n-i}A^{i-}, \, i=1(1)n \tag{82}$$

where $H_nA^{0-}=H_nA$ and $H_0A^{n-}=A^{n-}$. Introducing the equilibrium constants K_i (mol/l), these chemical equations can be written in the following mathematical form:

$$\frac{[H^+][H_{n-i}A^{i-}]}{[H_{n-i+1}A^{(i-1)-}]} = K_i, \, i=1(1)n \tag{83}$$

The total concentration of organic acids is calculated as:

$$[H_nA]+[H_{n-1}A^-]+\ldots+[HA^{(n-1)-}]+[A^{n-}] = \sum_{j=0}^{n}[H_{n-j}A^{j-}] = m \cdot DOC \tag{84}$$

where DOC is the dissolved organic carbon concentration (molC/l) and *m* is the site density of organic solutes (mol/molC). To solve these *n*+1 equations (eqs.5,6), we first re-write eqs.5 as:

$$[H_{n-i}A^{i-}] = [H_{n-(i-1)}A^{(i-1)-}]\frac{K_i}{[H^+]}, \, i=1(1)n \tag{85}$$

Making this recursion explicit yields:

$$[H_{n-i}A^{i-}] = [H_nA]\frac{K_1 \cdot K_2 \cdot \ldots \cdot K_i}{[H^+]^i} = [H_nA]\prod_{l=1}^{i}(K_l/[H^+]) , \; i=1(1)n \tag{86}$$

Inserting this into eq.6 and solving for $[H_nA]$ we obtain:

$$[H_nA] = \frac{m \cdot DOC}{1+\sum_{j=1}^{n}\prod_{l=1}^{i}(K_l/[H^+])} \tag{87}$$

And from eq.8 thus for the organic anion concentrations:

$$[H_{n-i}A^{i}] = \frac{m \cdot DOC \cdot \prod_{l=1}^{i}(K_l/[H^+])}{1+\sum_{j=1}^{n}\prod_{l=1}^{i}(K_l/[H^+])} , \; i=1(1)n \tag{88}$$

The sum of organic anions is then given by summing the *n* expressions from eqs.10. Note that to obtain that sum in mol$_c$/l one has to multiply the *j*-th term by its charge *j*:

$$[\Sigma A^-] = \sum_{j=1}^{n} j \cdot [H_{n-j}A^{j-}] \; (mol_c/l) \tag{89}$$

In a software implementation to compute [ΣA⁻] one should first recursively calculate the denominator in eq.9, then the individual concentrations from eqs.7, and finally the sum according to eq.11.

Values for *m* and the pK_i=-$\log_{10}(K_i)$ were derived by Driscoll *et al.* (1994) from 1184 water samples from Adirondak lakes:

Model	m	pK$_1$	pK$_2$	pK$_3$
Monoprotic	0.135	4.45	-	-
Diprotic	0.082	4.02	6.04	-
Triprotic	0.055	2.64	5.66	5.94

Cosby *et al.* (1995) used values of pK_1=2.1, pK_2=5.6 and pK_3=7.0 for simulating both the soil and stream organic acids in two small catchments in Norway with a triprotic model.

Santore *et al.* (1995) describe a triprotic model for soil organic acids by the following equations:

$$
\begin{aligned}
A^{3-} + 3H^+ &\rightarrow H_3A \\
A^{2-} + 2H^+ &\rightarrow H_2A^- \\
A^- + H^+ &\rightarrow HA^{2-}
\end{aligned}
\tag{90}
$$

or, in general form:

$$A^{n-} + (n-i+1)H^+ \rightarrow H_{n-i+1}A^{(i-1)-}, i=1(1)n \tag{91}$$

which in its mathematical form reads

$$\frac{[H_{n-i+1}A^{(i-1)-}]}{[A^{n-}][H^+]^{n-i+1}} = K_i^{'}, i=1(1)n \tag{92}$$

Comparison with eqs.5 shows that

$$K_i^{'} = \frac{1}{K_i \cdot K_{i+1} \cdot \ldots \cdot K_n} = \prod_{l=i}^{n} \frac{1}{K_l} \Leftrightarrow K_i = \frac{K_{n+1}^{'}}{K_i^{'}} \text{ with } K_{n+1}^{'} = 1, i=1(1)n \tag{93}$$

or, expressed in pK-values:

$$-pK_i^{'} = -\sum_{l=i}^{n} pK_l \Leftrightarrow pK_i = pK_{i+1}^{'} - pK_i^{'} \text{ with } pK_{n+1}^{'} = 1, i=1(1)n \tag{94}$$

Santore *et al.* (1995) report values of *m* between 0.014 for topsoil samples and 0.044 mol/molC for a B-horizon in the Hubbard Brook experimental forest in New Hampshire. For the $pK_i^{'}$ they report $pK_1'=-13.71$, $pK_2'=-11.69$ and $pK_3'=-6.48$. Using eqs.16, this would result in $pK_1=2.02$, $pK_2=5.21$ and $pK_3=6.48$ for the Driscoll *et al.* (1994) formulation (compare with the Table above).

Instead of a model of higher protonity, Oliver *et al.* (1983) used a monoprotic model, i.e. (see eqs.10,11)

$$[\Sigma A^-] = \frac{m \cdot DOC \cdot K_1}{K_1 + [H^+]} \tag{95}$$

and fitted pK_1 with a quadratic function in pH:

$$pK_1 = a + b \cdot pH - c \cdot (pH)^2 \tag{96}$$

with *a*=0.96, *b*=0.90 and *c*=0.039 fitted from data (*m*=???). Driscoll *et al.* (1994) derived for the same model the parameters *m*=0.181 and *a*=0.15, *b*=1.41 and *c*=0.078.

References:

Cosby BJ, Wright RF, Gjessing E (1995) An acidification model (MAGIC) with organic acids evaluated using whole-catchment manipulations in Norway. *Journal of Hydrology* **170**:101-122.

Driscoll CT, Lehtinen MD, Sullivan TJ (1994) Modeling the acid-base chemistry of organic solutes in Adirondack, New York, lakes. *Water Resources Research* **30**:297-306.

Oliver BG, Thurman EM, Malcolm RL (1983) The contribution of humic substances to the acidity of colored natural waters. *Geochim. Cosmochim. Acta* **47**:2031-2035.

Santore RC, Driscoll CT, Aloi M (1995) A model of soil organic matter and its function in temperate forest soil development. In: WW McFee, JM Kelly (eds) *Carbon Forms and Functions in Forest Soils*. Soil Science Society of America, Madison, Wisconsin, pp.275-298.
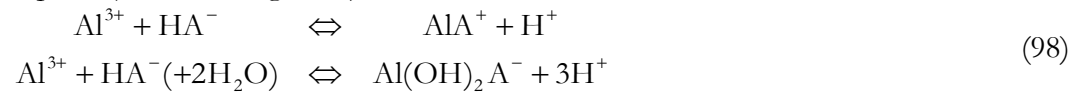
Appendix 3   Modeling the complexation of aluminum with organic acids

In the SMART model we consider the following complexation reactions of aluminum with (mono-,) di- and triprotic organic anions:

Monoprotic (to be done):

$$??? \Leftrightarrow ??? \tag{97}$$

Diprotic (Groenenberg 2000):

$$Al^{3+} + HA^- \qquad \Leftrightarrow \qquad AlA^+ + H^+$$
$$Al^{3+} + HA^- (+2H_2O) \quad \Leftrightarrow \quad Al(OH)_2 A^- + 3H^+ \tag{98}$$

Triprotic (Santore *et al.* 1995):

$$Al^{3+} + A^{3-} \qquad \Leftrightarrow \qquad AlA$$
$$Al^{3+} + A^{3-} + H^+ \quad \Leftrightarrow \quad AlHA^+ \tag{99}$$

In their mathematical form these equations read:

$$[AlA^+][H^+] = K_{21}[Al^{3+}][HA^-]$$
$$[Al(OH)_2 A^-][H^+]^3 = K_{22}[Al^{3+}][HA^-] \tag{100}$$
and
$$[AlA] = K_{31}[Al^{3+}][A^{3-}]$$
$$[AlHA^+] = K_{32}[Al^{3+}][A^{3-}][H^+] \tag{101}$$

where K_{21}, K_{22}, K_{31} and K_{32} are the respective equilibrium constants. Defining $pK=-\log_{10}(K)$ (with K expressed in mol/l or powers thereof), we find pK_{21}=-2.0, pK_{22}=8.1 (Groenenberg 2000) and pK_{31}=-7.89, pK_{32}=-12.86 (Santore *et al.* 1995). Note, that $[Al^{3+}]$ refers to the concentration of *free* aluminum. If this concentration (in addition to the pH and the concentrations of the organic anions) is known, the concentrations of the complexed Al-species can be readily computed from above equations.

From measurements, however, the only quantity often known is the concentration of *total* aluminum, $[Al_{tot}]=[Al^{3+}]+[\Sigma Al_{org}]$, where $[\Sigma Al_{org}]$ is the sum of the organically complexed Al-species (e.g., $[\Sigma Al_{org}]=[AlA]+[AlHA^+]$ in the case of the triprotic model). In this case the concentration of free aluminum is obtained as (cf. eqs.4,5):

$$[Al^{3+}] = \frac{[Al_{tot}]}{1+[HA^-](K_{21}/[H^+]+K_{22}/[H^+]^3)} \tag{102}$$
and
$$[Al^{3+}] = \frac{[Al_{tot}]}{1+[A^{3-}](K_{31}+K_{32}[H^+])} \tag{103}$$

References:

Groenenberg JE (2000) *pers. comm.*

Santore RC, Driscoll CT, Aloi M (1995) A model of soil organic matter and its function in temperate forest soil development. In: WW McFee, JM Kelly (eds) *Carbon Forms and Functions in Forest Soils*. Soil Science Society of America, Madison, Wisconsin, pp.275-298.

Appendix 4 Solution method

In order to solve the model equations, i.e. to compute the concentrations and total amounts of the different ions, we have to discretize the differential equations. The general form of a first order differential equation is given by

$$\frac{dy}{dt} = f(y(t),t)$$ (A1)

The simplest method of discretization is the so-called Euler first-order method:

$$y(t) = y(t - \Delta t) + f(y(t - \Delta t), t - \Delta t) \cdot \Delta t$$ (A2)

This method is explicit, i.e. the right-hand side of eq.A2 contains no terms at t, and of first-order accuracy. The method is very simple, but not always stable: To guarantee stability in the case of the mass balance equations the time step Δt has to be chosen such that (see, e.g., Potter 1973)

$$\Delta t \leq \frac{2\Theta Z}{Q_t}$$ (A3)

and this is not always the case. Therefore, in an earlier version of SMART the so-called implicit second-order method was implemented:

$$y(t) = y(t - \Delta t) + \left[f(y(t),t) + f(y(t - \Delta t), t - \Delta t) \right] \cdot \frac{\Delta t}{2}$$ (A4)

As an implicit method the desired $y(t)$ appears also on the right-hand side of the equation, which requires the solution of a (potentially non-linear) equation at every time step. The method is unconditionally stable and of second-order accuracy and for that reason it has been chosen earlier. However, as has been pointed out by a SMART user (J. Shindo from NIAES, Japan), if this equation is initialised away from the equilibrium solution, it takes many time steps to obtain reasonable accuracy.
Since the right-hand side of the differential equations is always simple in the SMART model, we use the following (almost obvious!) discretization (it could be called implicit first-order method):

$$y(t) = y(t - \Delta t) + f(y(t),t) \cdot \Delta t$$ (A5)

It can be shown that this method is stable for an arbitrary step size Δt as long as

$$\frac{\partial f}{\partial y} \leq 0$$ (A6)

and this is the case in all our equations.

For $X=NO_3$, NH_4, Na, K, Cl (we drop the indication of charges for convenience) the mass balance equation reads

$$\Theta Z \frac{d}{dt}[X] = X_{s,t} - Q_t[X] \tag{A7}$$

where $X_s = X_{in} + X_{int}$. Discretizing this equation according to eq.A5 yields

$$\Theta Z[X]_t = \Theta Z[X]_{t-\Delta t} + (X_{s,t} - Q_t[X]_t)\Delta t \tag{A8}$$

or, solving for $[X]_t$,

$$[X]_t = \frac{\Theta Z[X]_{t-\Delta t} + X_{s,t}\Delta t}{\Theta Z + Q_t\Delta t} \tag{A9}$$

Note that the subscript t stands for multiples of Δt. This equation is initialized (for all X) by

$$[X]_0 = X_{s,0} / Q_0 \tag{A10}$$

For sulfate the mass balance reads:

$$\Theta Z \frac{d}{dt}[SO_4] + \rho Z \frac{d}{dt} SO_{4,ad} = SO_{4,s,t} - Q_t[SO_4] \tag{A11}$$

or, after inserting $SO_{4,ad} = S_{max}[SO_4]/(S_{1/2}+[SO_4])$ and differentiating:

$$\left(\Theta Z + \frac{\rho Z S_{1/2} S_{max}}{S_{1/2} + [SO_4]^2} \right) \frac{d}{dt}[SO_4] = SO_{4,s,t} - Q_t[SO_4] \tag{A12}$$

which, after discretizing, becomes:

$$[SO_4]_t = [SO_4]_{t-\Delta t} + \frac{SO_{4,s,t} - Q_t[SO_4]_t}{\Theta Z + \dfrac{\rho Z S_{1/2} S_{max}}{(S_{1/2} + [SO_4]_t)^2}} \Delta t \tag{A13}$$

This non-linear equation is solved for $[SO_4]_t$ with Brent's method adapted from Press et al. (1992).

The computation of $[BC]_t$ and $[Al]_t$ is more involved, since equilibrium equations have to be fulfilled as well (see below).

1. Calcareous soils:
We assume no Al ions in the soil solution and therefore the charge balance equation reads:

$$[H]_t + [BC]_t - [HCO_3]_t - [RCOO]_t - [Oth]_t = 0 \tag{A14}$$

where

$$[Oth]_t = [SO_4]_t + [NO_3]_t + [Cl]_t - [NH_4]_t - [Na]_t - [K]_t \tag{A15}$$

is calculated from the mass balance equations (see above). $[BC]_t$, $[HCO_3]_t$ and $[RCOO]_t$ can be expressed as functions of $[H]_t$ from equilibrium equations:

$$[BC]_t = \frac{K_{cb}[H]_t^2}{K_{CO2}^2 p_{CO2}} \tag{A16}$$

$$[HCO_3]_t = \frac{K_{CO2} p_{CO2}}{[H]_t} \tag{A17}$$

and

$$[RCOO]_t = F_{org}([H]_t, \ldots) \tag{A18}$$

where F_{org} is a function of $[H]_t$ and other parameters (dissociation constants). Inserting eqs.A16-A18 into eq.A14 yields a non-linear equation for $[H]_t$ which is again solved by Brent's method. The quantities $[HCO3]_t$, $[BC]_t$ and $[RCOO]_t$ are then computed from eqs.A16-A18. The change in the total amount of base cations is computed from the mass balance equation:

$$\Theta Z \frac{d}{dt}[BC] + \rho Z \frac{d}{dt} BC_{carb} = BC_{s,t} - Q_t[BC] \tag{A19}$$

Discretized and solved for $BC_{carb,t}$ this becomes

$$BC_{carb,t} = BC_{carb,t-\Delta t} - \frac{\Theta}{\rho}([BC]_t - [BC]_{t-\Delta t}) + \frac{\Delta t}{\rho Z}(BC_{s,t} - Q_t[BC]_t) \tag{A20}$$

2. Non-calcareous soils:
The charge balance equation is given by:

$$[H]_t + [Al]_t + [\Sigma^+ Al_{org}]_t + [BC]_t - [HCO_3]_t - [RCOO]_t - [Oth]_t = 0 \tag{A21}$$

where $[Oth]_t$ is given by eq.A15. The equilibrium equations for $[HCO_3]_t$ and $[RCOO]_t$ are given by eqs.A17 and A18. For the concentration of free aluminum, $[Al]_t$, we assume a general relationship

$$[Al]_t = F_{AlH}([H]_t) \tag{A22}$$

and the sum of the concentrations of the net positively (i.e. positively minus negatively) charged organically complexed aluminium species, $[\Sigma^+ Al_{org}]_t$, are a function of $[H]_t$ and $[Al]_t$

$$[\Sigma^+ Al_{org}]_t = F_{AlA}^+([H]_t, [Al]_t, \ldots) \tag{A23}$$

In addition, we have the two exchange equations:

$$\frac{fAl_t^2}{fBC_t^3} = KAl_{exc}\frac{[Al]_t^2}{[BC]_t^3} \tag{A24}$$

$$\frac{fH_t^2}{fBC_t} = KH_{exc}\frac{[H]_t^\beta}{[BC]_t}, \; \beta > 0 \tag{A25}$$

with

$$fBC_t + fAl_t + fH_t = 1 \tag{A26}$$

The change in the total amount of base cations is given by:

$$\Theta Z \frac{d}{dt}[BC] + \rho ZCEC \frac{d}{dt} fBC = BC_{s,t} - Q_t[BC] \tag{A27}$$

which, discretized, can be written as:

$$fBC_t + \frac{\Theta Z + Q_t \Delta t}{\rho ZCEC}[BC]_t = fBC_{t-\Delta t} + \frac{\Theta Z[BC]_{t-\Delta t} + BC_{s,t}\Delta t}{\rho ZCEC} \tag{A28}$$

The solution of this set of equations can be reduced to the solution of a single non-linear equation in $[H]_t$ in the following way: Expressing fAl_t from eq.A24 (with $[Al]_t$ from eq.A22) and fH_t from eq.A25 yields after inserting them into eq.A26:

$$fBC_t + F_{AlH}([H]_t)KAl_{exc}^{1/2}\left(\frac{fBC_t}{[BC]_t}\right)^{3/2} + [H]_t^{\beta/2}KH_{exc}^{1/2}\left(\frac{fBC_t}{[BC]_t}\right)^{1/2} = 1 \tag{A29}$$

Furthermore, using the equilibrium equations (A17, 18, 22, 23), the charge balance (eq.A21) allows to express $[BC]_t$ as a function of $[H]_t$ alone, $[BC]_t = G([H]_t)$. Eq.A28 can then be used to express fBC_t as a linear function of $G([H]_t)$. Inserting these into eq.A29 yields a single equation in the unknown $[H]_t$ which can be solved by Brent's method.

Solving the above equations requires initial values for $[BC]_0$ and fBC_0 (in eq.A28). However, these two quantities are not independent:

(a) If $[BC]_0$ is known, the charge balance equation together with the equilibrium equations, yields initial concentrations for H and Al, and then eqs.A24-A26 yield initial exchangeable fractions.

(b) If fBC_0 is known, insert it into eq.A29 and solve for $[H]_0$; then $[BC]_0 = G([H]_0)$.

Finally, the change in the amount of Al_{ox} is computed from the mass balance for Al:

$$\Theta Z \frac{d}{dt}[Al_{tot}] + \rho Z CEC \frac{d}{dt} fAl + \rho Z \frac{d}{dt} Al_{ox} = Al_{s,t} - Q_t[Al_{tot}] \tag{A30}$$

which discretized and solved for Al_{ox} yields:

$$Al_{ox,t} = Al_{ox,t-\Delta t} - CEC(fAl_t - fAl_{t-\Delta t}) - \frac{\Theta}{\rho}([Al_{tot}]_t - [Al_{tot}]_{t-\Delta t}) +$$
$$\frac{\Delta t}{\rho Z}(Al_{s,t} - Q_t[Al_{tot}]_t) \tag{A31}$$

In these two equations $[Al_{tot}]_t$ denotes the sum of the concentrations of all aluminum species, which is a function of $[H]_t$ and $[Al]_t$ (compare eqs.A22 and A23):

$$[Al_{tot}]_t = [Al]_t + [\Sigma Al_{org}]_t = F_{AlH}([H]_t) + F_{AlA}([H]_t, [Al]_t, \ldots) \tag{A32}$$

The amount of Al-(hydr)oxides (pyrophosphate Al) is also used to update the equilibrium equation between [Al] and [H] (eq.A22) at every time step:

$$[Al]_t = F_{AlH}([H]_t) = KAl_{ox}[H]_t^\alpha \frac{Al_{ox,t-1}}{Al_{ox,0}} \quad (\alpha > 0) \tag{A33}$$

where the subscript '0' refers to the initial value.

References

Potter D (1973) *Computational Physics*. John Wiley & Sons, Chichester, UK, 304 pp.

Press WH, Teukolsky SA, Vetterling WT, Flannery BP (1992) *Numerical Recipes in FORTRAN*. 2nd edition. Cambridge University Press, 963 pp.

MONITOR

A subroutine for monitoring model output[*]

User Manual

Version 3.2 – October 2003

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Introduction

This manual describes the use of the Fortran subroutine *monitor*. This subroutine, which can be called from any Fortran program, displays up to 9 graphs each in maximal 25 frames on the screen of (interactively) selected variables during the course of a model run. In addition, it can produce (i) a PostScript file of the screen image, and (ii) an ASCII file containing the values of the selected variables. This allows the monitoring (*sic!*) of a model run, the production of high-quality graphs of model results, and the further processing of model outputs.

The manual consists of two parts: Part A is for users who have an executable program which calls *monitor*. It explains how to change parameters in the file that controls the output of *monitor*. For users, who are in the position to link the subroutine *monitor* to a program of their choice, Part B explains how to do just that.

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[*]MONITOR is a **P**ersonal **I**nformation & **S**imulation **S**ystem (PISS) program.

Part A: Running programs with built-in *monitor*

A program calling *monitor* requires also a parameter-file, which tells *monitor* what to display, plot and/or write. The name of that parameter-file is passed to the subroutine *monitor* in its argument list, and thus the user can change its name only if s/he can also change that argument. A typical parameter-file could look like this:

```
 ! Variables for display; if blank: interactive choice

 ! Screen display (blank, if none; '?' for interactive choice):
  yes
 ! Name of PostScript-file (blank/?):
  ?
 ! Name of output file [/h][(fmt)] (blank/?):
 model.out/h(i4,9f7.3)
 ! Name of input file for COMPARISON (blank/?):

 ! Title ('?' for interactive input):
  Testrun
 ! iyre, iyrb, intx, steps skipped ['averager' ['module' [line
 thickness]]]:
  0  0  6  0  0  1000 8
 ! File with definition of variables:
  yvars.dat
 ! Common name of variables (case-sensitive):
  Y
```

The order of the parameters is fixed; however, there can be comment lines, i.e. lines starting with an exclamation mark ('!'), anywhere in the file; they are ignored by *monitor*. In the following the line numbers refer to **non-commented** lines.

Line 1: Numbers of the variables selected for display and/or writing. If the line is blank, the variables are asked interactively. In this case the user is prompted with the list of variables which can be displayed and/or printed by *monitor*. The user can then select variables by typing their numbers (they don't have to be in ascending order and they can be repeated). Variables for which an 'observation-file' has been specified (see below) are flagged with a star in front of the number. The variables are displayed in the order in which they are selected.

It is possible to display up to 9 variables in one frame on the screen by linking them with a '&'-sign.

If a variable is preceded by an 'i' (for **i**ntegrate), the running sum (integral) of that variable is displayed; that sum is reset to zero after *module* steps (see below).

Up to 25 frames can be displayed on the screen. If no variable is selected, *monitor* does nothing. If more than 25 frames or more than 9 variables per frame are selected, *monitor* stops with an error message. If an invalid (too large) variable number is selected, *monitor* prints a warning message and asks for another choice.

On the **next 5 lines** *monitor* reads a filename (character string) in the following (consistent) manner: If a line is blank, no file/string is used (produced, read from, ...). If the line contains a single question mark ('?'), *monitor* will ask for the filename/string interactively.

Line 2: Screen display: Any non-blank character(s) (except '?') tells *monitor* to produce an on-line screen display. This is the primary function of *monitor*: to look at a model's output during a program's execution. If blank, no screen graphics is produced (screen remains in text mode).

Line 3: Name of a PostScript file (max. 128 characters) to be produced by *monitor* which images the screen display (in black-and-white).

Line 4: Name of an ASCII file (max. 128 characters) into which the time series of the selected variables are written.
If the filename is followed by the clause '/h' (like in our example), a header precedes the numerical output describing the variables printed.
That can be followed by a Fortran format (between parentheses) specifying the output format (see example). If no format is specified, the default format '(2i6,99g12.4)' is used (thus avoiding over- or underflow).
On the first line of such a file (numerical) codes are written, indicating which variables are written to this file. This information is only of relevance, if the file is used later for a comparison (see below).
If *nvar* is the number of variables selected, then the file contains 2+*nvar* columns of data written in the user-defined or default format. Column 1 contains the step number (counter), always starting at 0, column 2 contains the 'year', each repeated as many times as there are subdivisions of the 'year' in the simulation (here: 2). Columns 3 to 2+*nvar* contain the values of the variables (in the order selected by the user). The 'i'(=integral) in front of a variable number (see above) has no influence on the writing. The first lines written to the output file may look like this:

```
 T   9   2   7   4
!Testrun
!column  1: x-value (counter)
!column  2: x-value (year)
!column  3: pH
!column  4: N-deposition (eq/m2/yr)
!column  5: [SO4--] (eq/m3)
!column  6: fBC
  0  1800  6.960   .200  1.000  1.000
  1  1800  6.960   .200  1.000  1.000
  2  1801  6.960   .200  1.000  1.000
 .....
```

If Lines1-4 are all blank, i.e. none of the output modes is chosen, *monitor* does nothing (and the rest of the parameter file is not read). This allows to 'switch of' (i.e. not to use) *monitor*, even when it is linked to a program.

Line 5: Name of file for comparison (max. 32 characters; only asked/used if a screen display is chosen). This option allows the visual comparison with a previous model run. The file has to be in the form of a *monitor* output file (see above). The first line tells *monitor* whether there is a header ('T'[rue] or 'F'[alse]) and which variables there are. Graphs of those variables, which are chosen in the current model run, are displayed in the respective frames and written to a selected PostScript file as dotted lines.

Line 6: Title (max. 64 characters) for the graphical output; also written to the second line of the ASCII file, if the filename has the '/h' clause.

Line 7: Four to seven **integers**, say *iyrb*, *iyre*, *intx*, *nskip*[, *nav*[, *module*[, *ithick*]]], controlling the display/output:
The parameters *iyrb* and *iyre* can be used to determine the beginning and end 'year' of the display windows. If *iyrb*<*iyre* (i.e. they define a meaningful interval), they overrule the values *iyrb0* and *iyre0*, resp., from the argument list of *monitor* (thus, e.g., allowing to display only parts of a simulation), otherwise the default values *iyrb*=*iyrb0* and *iyre*=*iyre0* are used.
The 3-rd parameter, *intx*, is the number of intervals marked as thin dashed vertical lines in the graphical window of every selected variable. This parameter also controls the labeling of the horizontal axes: If *intx*=0 the horizontal axes are not labeled (and no vertical lines are plotted). If *intx*>0, the first and last time-interval of the lowest horizontal axes are labeled with *iyrb* and *iyre*; if *(iyrb+iyre)/2* is an even number, the central time-interval is also labeled.
The 4-th parameter, *nskip*, is the number of initial 'years' that are **not** displayed on the screen and/or written to a file, i.e. only data for 'years' ≥*iyrb0*+*nskip* and ≤*iyre0* are displayed (if they lie in the display windows). If the number of steps to be displayed is less than two, the program terminates with an error message.
The 5-th parameter, *nav*, controls the calculation of a "statistic" of the displayed variables. If *nav*>0, the sum of the displayed values for each variable is divided by *nav* at the last call to *monitor* and written in the upper right corner of the graph for that variable (i.e. if *nav*=1, the sum of the displayed variables is shown). If *nav*=0, the arithmetic mean of the displayed variables is shown. If *nav*=–1, the last value of the variable is displayed. If *nav*≤–2, nothing is shown (= default, if there are only 4 parameters on the line).
After each step, which is a multiple of the 6-th parameter, *module*, the integration of variables (i.e. those preceded by an 'i') is restarted from zero. If missing, *module* is set to a very large number.
The 7-th parameter, *ithick*, determines the thickness of the lines in the graphs (also comparison graphs); it is given by max{0.1*ithick*,0.12}/72 inches.

Line 8 holds the name of a file with the definitions of the variables that can be displayed with *monitor* (here 'yvars.dat'). Also in this file comment lines (i.e. lines starting with '!') are allowed.

Line 9 gives the common name of those variables (here 'Y') which is case-sensitive. The purpose of this name is explained in Part B.

The file *yvars.dat* could look like this:

```
 ! ...Y(n)...!% text; ymin ymax inty
[;[fac*]obsfile[#ncol][/style]]
 Y(1)!% SO2-deposition (eq/m2/yr); 0 0.4 4
 Y(2)!% N-deposition (eq/m2/yr); 0 0.4 4
 Y(3)!% BC-deposition (eq/m2/yr); 0 0.4 4
 Y(4)!% fBC; 0 1 5
 Y(5)!% fAl; 0 1 5
 Y(6)!% fH; 0 1 5
 Y(7)!% [SO4--] (eq/m3); 0 2 5
 Y(8)!% [NO3-] (eq/m3); 0 1 5
 Y(9)!% pH; 2 7 5; phm.obs/o
```

Every non-commented line contains the definition of one variable, which has to be of the following form:

(a) The variable identifier 'Y(n)' where 'Y' is identical to the character string given in Line 9 above and 'n' is the number of the variable. They don't have to be in ascending order. Also, any other characters are allowed before and after the variable; e.g. 'abcY(1)xyz' would be a valid construction instead of 'Y(1)'.

(b) Separated by '!%' from this, the "name" of the variable (max. 40 characters). This name is displayed when *monitor* interactively asks to select variables (see Line 1 above), and is also displayed on the screen on top of the graph of the corresponding variable. The user has to make sure that the identifier of the variable, Y(n), corresponds to the *n*-th variable passed by the calling program to *monitor* (there is no way for *monitor* to check this!).

(c) Separated by a semicolon (';') from this name follow 3 numbers specifying the scaling of the vertical axis of the graph of the corresponding variable. The first two numbers (real or integer) define the minimum and maximum value on the vertical axis, while the third number (an integer) defines the number of intervals to be plotted on the vertical axis.

(d) Optionally, separated by another semicolon, the name of a file can be specified which contains "observations" of the variable displayed, allowing model comparisons with these observations. The data in such a file are displayed at the first call to *monitor*, if their x-values fall within the display window given by *iyrb* and *iyre* (see above). An observation-file may contain comment lines, i.e. lines starting with an '!', anywhere in the file; they are ignored during reading. Each non-commented line of an observation file contains at least two (three, if there are 'months' defined) values (blank- or comma-separated); the first (and second) define the position on the horizontal axis (the 'time') and the following values are observations. The column to be displayed is chosen by appending the clause '#*n*', where *n* is the column number, directly to the filename. Note, that *n* refers to the *data* column number, i.e. not counting the first (and second) column. The default is *n*=1. Observations =-999 are treated as 'missing' and are not displayed. Furthermore, observations can be re-scaled

by a common factor, which can be specified by pre-pending the filename with *scal**,
where *scal* is an integer or real number; an exponential representation of *scal* (e.g.
1.e+6) is not allowed; obviously, the default is *scal*=1. The style of display can be
chosen by a clause '/z' after the column number, where 'z' can be one of the
following characters:

```
 s ... data points are connected by a (thin) solid line (default).
 w ... data points are connected by a thick line.
 d ... data points are connected by a dashed line.
 b ... data points are connected by a dashed thick line.
 l ... a vertical line connects each data point with the
horizontal axis.
 c ... each data point is marked with a cross (+).
 x ... each data point is marked with an 'x' (×).
 q ... each data point is marked with a square (□).
 v ... each data point is marked with a diamond (◊).
 t ... each data point is marked with a triangle (Δ).
 n ... each data point is marked with a nabla (∇).
 o ... each data point is marked with a circle (O).
```

For example, *0.001*obsfile#7/o* would be a valid construct for an observation file
'obsfil', and *monitor* would multiply the values in data column 7 (column 8 in the file!)
by 0.001 and display them as circles, if the corresponding value in column 0 lies
between *iyrb* and *iyre*.
Note that the line thickness affects Postscript output only; on screen all lines are of
equal thickness.

During running a program that calls *monitor* the interactive input depends on the
parameter file.

If there are more than 40 display variables to choose from, they are listed in
"batches" of (maximal) 40 variables each. Numbers of variables chosen are
remembered in subsequent calls [between square brackets]. In order to plot/print the
remembered variables, just press ENTER. If you want to *add* numbers of variables
already chosen (=remembered), the first (non-blank) character of the additional
choices has to be a 'u' (for **u**nion). If you are happy with your (previous) choice of
variables and want to prevent display of further screens (in case of many variables),
type 'q' (for **q**uit). Up to 9 variables can be displayed in one window on the screen by
linking their numbers with the '&'-sign. If a variable is preceded by an 'i' (for
integrate), the running sum of that variable is displayed; it is reset to zero after every
multiple of *module* steps (see above).

For every line in the parameter-file containing a single question mark ('?'), *monitor* will
ask for the filename/string interactively, and this string is remembered in subsequent
calls [between square brackets]. In order to invoke the same string, press ENTER; to
erase the previous choice without making a new one, press the ESC key (ASCII code
32) or the TAB key (ASCII code 9).

When a screen display is chosen and the last call to *monitor* is displayed, it produces the PostScript file (if chosen). During that period the message '... WAIT .....' appears in the upper left corner of the screen (on a yellow background). After finishing writing and closing open files the message 'To continue press ENTER' overwrites it. When ENTER is pressed, *monitor* closes the graphics library, clears the screen and resets it to text mode.

Below a sample plot of a PostScript file, generated by *monitor*, is shown for illustration. The file *phm.obs*, containing observation which are plotted as circles, looks like this:

```
1875   1   6.5
1890   2   5.0
1965   1   4.1
2100   2   3.9
```
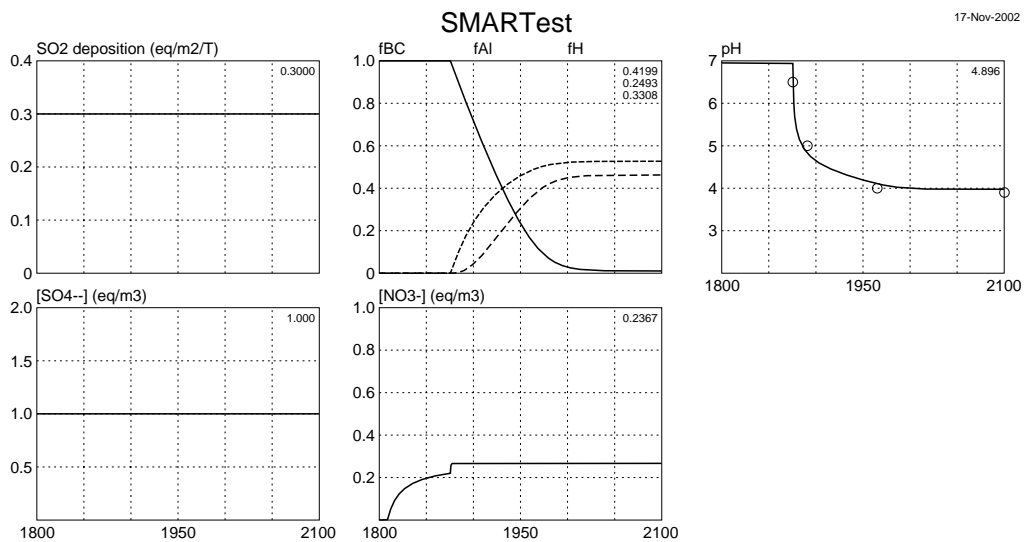
Part B: Including *monitor* into a Fortran program

In this part we describe how to include the subroutine *monitor* into a Fortran program, when it is provided as source-code or as object library (e.g. *monitor.lib*). It can be used with Fortran programs written (and compiled) in Visual Fortran 6.1(A) running on a PC under Windows.

Since *monitor* is designed to monitor a model's output in the course of a program execution, it has to be called within the loop, which updates the variables to be displayed. A typical program fragment could look like this:

```
  logical               start
  character             tmpdir*32 /'d:\temp'/
  real                  var(20)
  .....
  iyrb0 = 1800
  iyre0 = 2100
  mstep = 2
  start = .true.
  ntime = -1
  do iyr = iyrb0,iyre0
    do m = 1,mstep
      ntime = ntime+1
      .....
      call model (thick,rho,cacarb,alox,SO2dep,NOxdep,NH3dep,Bcdep,
 &                fBC,fAl,fH,cSO4,cNO3,cH)
      var(1) = SO2dep
      var(2) = NOxdep+NH3dep
      var(3) = Bcdep
      var(4) = fBC
      var(5) = fAl
      var(6) = fh
      var(7) = cSO4
      var(8) = cNO3
      var(9) = 3.-alog10(cH)  ! =pH
      call monitor
(start,tmpdir,'monitor.par',iyrb0,iyre0,mstep,ntime,var)
    end do
  end do
  .....
```

The arguments of *monitor* have the following meaning: *start* is a logical variable, which has to be set 'true' before the first call of monitor. At the first call *monitor* reads the file with the name given as the third argument (*monitor.par* in our example), determine which variables should be displayed and initialize the graphical output. After the first call *start* is set `false' by *monitor*. The character*32 variable *tmpdir* holds the name of a directory, into which *monitor* writes temporary files. The integer variables *iyrb0, iyre0* and *mstep* determine the time period (*iyre0-iyrb0*+1 'years' with *mstep* 'months' each) of the simulation and the (default) window to be displayed during the model run. The integer variable *ntime* is the time step counter starting at zero: $0 \leq ntime \leq (iyre0-iyrb0+1)*mstep-1$. Finally, the real vector *var* of arbitrary length holds the values of the variables to be displayed.

Before running a program calling *monitor* a parameter-file which tells *monitor* what to plot and/or write has to be prepared. The name of this file is arbitrary, and it is passed to *monitor* in its argument list (second argument *monitor.par*). An example of such a file and the description of its contents are given in Part A.

One frequent source of error is the mismatch between the variables as transferred to *monitor* from the calling program (via the vector *var*) and the variable list read in by *monitor* (file 'yvars.dat' in Part A). A possible remedy is to use the source-code of the calling program also as the file defining the variables. For the program fragment listed above it could look like this:

```
  .....
  ntime = -1
  do iyr = iyrb0,iyre0
    do m = 1,mstep
      ntime = ntime+1
      .....
      call model (thick,rho,Cacarb,Alox,SO2dep,NOxdep,NH3dep,Bcdep,
&                 fBC,fAl,fH,cSO4,cNO3,cH)
      var(1) = SO2dep         !% SO2-deposition (eq/m2/yr); 0 0.4 4
      var(2) = NOxdep+NH3dep  !% N-deposition (eq/m2/yr); 0 0.4 4
      var(3) = Bcdep          !% Bc-deposition (eq/m2/yr); 0 0.4 4
      var(4) = fBC            !% fBC; 0 1 5
      var(5) = fAl            !% fAl; 0 1 5
      var(6) = fH             !% fH; 0 1 5
      var(7) = cSO4           !% [SO4--] (eq/m3); 0 2 5
      var(8) = cNO3           !% [NO3-] (eq/m3); 0 1 5
      var(9) = 3.-alog10(cH)  !% pH; 2 7 5; phm.obs/o
      call monitor (start,tmpdir,'monitor.par',iyrb0,iyre0,mstep,ntime,
var)
    end do
  end do
  .....
```

Putting the source code file (e.g. 'model.for') on Line 8 of the parameter file for *monitor* and defining 'var' (instead of 'Y') on Line 9 allows to use a single file for all the information on the variables to be displayed. Note that the variables don't have to be in ascending order, nor do all indices have to be assigned a value. Variable indices not assigned any value are displayed as '(NOT USED)' when asked interactively.

Acknowledgements

Appendix 6   Input options for SUMO

Table 11. Tree species modelled by SUMO.

Code	Species
GEE	no tree species
BER	birch
BEU	beech
EIK	Oak
AME	northern red oak
ES	ash tree
ELS	Alder
WIL	Willow
POP	Poplar
DOU	Douglas
FIJ	Spruce
GRO	Pine
LAR	Larch

Table 12. Vegetation types modelled (vegtype) in SUMO

Vegetation type number	Vegetation type
1	Grassland
2	heath land
3	dark coniferous forest
4	light deciduous forest
5	light coniferous forest
6	dark oak beech forest
7	dark beech forest
8	structure rich deciduous forest
9	reed
10	Shrub
11	salt marshes
12	peat bog
13	Swamp
14	no vegetation
15	-
16	Road verge with trees
17	Wooded bank

Table 13. Management options in SUMO.

Code	Option
0	No management
1	Mowing
2	Turf stripping
4	Natural forest management
5	Production forestry management
6	Coppice management
7	Turf stripping combined with mowing (once a year)
8	Road verge management
9	Turf stripping combined with removal of shrubs and trees
10	Burning

Table 14 Possible combinations of vegetation type, file number, vegetation type number, stand age and climax tree species for SUMO. Pioneer species can be chosen freely from the species pool given in Table 11, the given species is the dominant one, containing the major part of the biomass. The explanation for the vegetation type number is given in Table 12.

Vegetation type	File number	Vegetation type number	Initial age	Climax tree species
dune shrub	1	10	50	GEE
dune open vegetation	2	2	20	GEE
salt marsh	3	11	50	GEE
reed	4	9	10	GEE
Rough land	5	1	10	GEE
managed grassland	6	1	10	GEE
natural grassland	7	1	10	GEE
heath <75% grass	8	2	10	GEE
heath >75 % grass	9	2	25	GEE
peat bog	10	12	50	GEE
no vegetation	11	2	1	GEE
natural vegetation	12	1	10	GEE
Swamp	13	13	10	GEE
northern red oak <40 years	14	4	30	AME
northern red oak 40-80 years	15	4	60	AME
northern red oak 80-120 years	16	4	100	AME
northern red oak >120 years	17	4	130	AME
beech <40 years	18	7	30	BEU
beech 40-80 years	19	7	60	BEU
beech 80-120 years	20	7	100	BEU
beech >120 years	21	7	140	BEU
douglas <40 years	22	3	30	DOU
douglas 40-80 years	23	3	60	DOU
douglas 80-120 years	24	3	100	DOU
douglas >120 years	25	3	130	DOU
oak <40 years	26	4	30	EIK
oak 40-80 years	27	4	60	EIK
oak 80-120 years	28	4	100	EIK
oak >120 years	29	4	140	EIK
alder <40 years	30	4	30	ELS
alder 40-80 years	31	4	60	ELS
alder 80-120 years	32	4	100	ELS
alder >120 years	33	4	130	ELS
scots pine <40 years	34	5	30	GRO
scots pine 40-80 years	35	5	60	GRO
scots pine 80-120 years	36	5	100	GRO
scots pine >120 years	37	5	130	GRO
larch <40 years	38	5	30	LAR
larch 40-80 years	39	5	60	LAR
larch 80-120 years	40	5	100	LAR
larch >120 years	41	5	130	LAR
poplar <40 years	42	4	30	POP
poplar 40-80 years	43	4	60	POP
poplar 80-120 years	44	4	100	POP
wilow <40 years	45	4	30	WIL
wilow 40-80 years	46	4	60	WIL

Vegetation type	File number	Vegetation type number	Initial age	Climax tree species
wilow 80-120 years	47	4	100	WIL
wilow >120 years	48	4	130	WIL
new forest	49	8	20	GEE
timber-felling	50	8	1	Any tree
alder coppice	51	8	50	ELS
willow coppice	52	8	50	WIL
oak coppice	53	8	50	EIK
ash tree coppice	54	8	50	ES
Road verge with newly planted trees	55	8	2	Any tree
Road verge with trees <40 years	56	8	30	Any tree
Road verge with trees 40-80 years	57	8	60	Any tree
Road verge with trees 80-120 years	58	8	100	Any tree
Road verge with trees >110 years	59	8	110	Any tree