

Input uncertainty analysis of the dynamic soil model SMART2 using Monte Carlo sampling

Katri Rankinen, Ilona Bärlund, Johanna Ahonen, Martin Forsius and Juha Kämäri

Finnish Environment Institute, P.O. Box 140, FIN-00251 Helsinki, Finland

Rankinen, K., Bärlund, I., Ahonen, J., Forsius, M. & Kämäri, J. 2001. Input uncertainty analysis of the dynamic soil model SMART2 using Monte Carlo sampling. *Boreal Env. Res.* 6: 147–158. ISSN 1239-6095

A dynamic soil model SMART2 has been developed to estimate long-term chemical changes in soil and soil water in response to changes in atmospheric deposition. The aim of this study was to rank the input parameters on the basis of their contribution to model uncertainty in order to determine which additional data would best improve the reliability of predictions. The Monte Carlo technique was used in combination with regression analysis. The uncertainty study was conducted for stream water pH and NO₃ concentration and for soil base saturation. Parameters defining nutrient mineralization in soil and plant uptake of nitrogen and base cations were also studied. Nitrogen uptake was mainly influenced by N concentration in stem and leaves, but also by parameters defining N mineralization in soil and N denitrification. Weathering rates and nutrient concentrations in vegetation appear to be the most important inputs explaining base saturation of mineral soil, NO₃ concentration and pH of stream water.

Introduction

Natural environmental systems are complex and modelling of the biogeochemical processes may lead to complex model structures and large numbers of parameters. Model parameters are often difficult to determine because data available for parameter estimation is often sparse in relation to the model complexity. Uncertainty analysis techniques can be used to evaluate the relative influences of different parameters on model output variables and to find out the key input parameters, by which the model performance can

be improved most. The Monte Carlo technique is often used for the sensitivity analysis and uncertainty assessment, recently for example by Soutter and Musy (1999) and Kuczera and Parent (1998). Kros *et al.* (1999) attempted to quantify the uncertainty in long term forecasts of soil acidification resulting from the uncertainty in input data. Forecasts were made by SMART2 in European scale.

The soil acidification model SMART (Simulation Model for Acidification's Regional Trends) was developed to relate the response of soil and soil water quality to atmospheric input (deVries

et al. 1989, Posch *et al.* 1993). The second version of the model, SMART2, has been extended to include processes of litter fall, root decay, mineralization and root uptake of nutrients, as well as canopy interactions (Kros 1995). A calibration and a description of the general behaviour of the model, applying it to a forested catchment in Finland, is described in Ahonen *et al.* (1998).

SMART2 was applied to a forested catchment in eastern Finland in order to study the effect of reduced atmospheric deposition and forest clearcutting on the ecosystem (Kämäri *et al.* 1998). In the study catchment, deposition was low and the forest was mature. Nutrient uptake has a more significant effect than deposition reductions on the state of the ecosystem at low deposition sites (Holmberg *et al.* 2000). Nitrogen is considered to be the growth-limiting factor in these types of terrestrial ecosystems. Low inputs by atmospheric deposition and the low leaching losses, generally less than a few kg N ha⁻¹ a⁻¹ (Gundersen and Bashkin 1994), indicate that conifer systems are very efficient in retaining nitrogen. The internal cycle of nitrogen in soil-plant systems is of great importance for nitrogen availability for vegetation. Internal cycling includes litter production of trees, litter decomposition in soil and mineralization of nutrients, as well as tree growth uptake of nutrients.

SMART2 is a relatively new model and the aim of this study was to analyse the effect of input uncertainty to SMART2 model output in order to become familiar with the model behaviour. The UNCSAM (Uncertainty analysis by Monte Carlo SAMpling techniques) software package (Janssen *et al.* 1992) was used to perform uncertainty analyses for calibration studies to determine which additional data or measurements would most improve the reliability of predictions. UNCSAM applies Monte Carlo sampling in combination with regression and correlation analysis to perform sensitivity and uncertainty analysis. Latin Hypercube Sampling technique (Iman and Conover 1982) was used to reduce the computation load. In particular, the uncertainty of parameters determining the internal nutrient cycle and nutrient uptake were evaluated, because they play an important role in

northern boreal forests and there is often insufficient data to calibrate them. Both mineralization and vegetation uptake of nitrogen and base cations were included in the input uncertainty analysis in order to identify the most important parameters in the internal cycle. Base saturation of mineral soil and litter layer, and pH and NO₃ concentration of stream water were included in the input uncertainty analysis, as they represent the main output variables of the model.

Materials and methods

Catchment description

The analysis of SMART2 was carried out by applying the model to the forested Kangasvaara catchment in eastern Finland (63°51'N, 28°58'E). It is one of the study catchments of the Finnish Forest Research Institute, and a description of vegetation, soil and water quality monitoring is presented in Finér *et al.* (1997). The main soil types of Kangasvaara are rather thin, weakly developed iron podzols, peaty podzols and shallow fibric histosols. The soils have developed on shallow (often < 2 m) stony to very stony till materials. The area of the catchment is 56 ha, and 8% of it is peatland. All of the land in the catchment is classified as forestry land and most of the catchment is covered by a 145 year-old forest. Dominant tree species are Norway spruce (54%), Scots pine (30%), birch and other deciduous trees (16%).

Meteorological data was obtained from an automatic weather station located in the Kangasvaara catchment. Bulk deposition is monitored with collectors installed close to the automatic weather station. Atmospheric deposition is generally low, only about 2 kg N ha⁻¹ a⁻¹. Tree stand variables were collected from a network of permanent circular measurement plots during 1990–1992. Soil sampling was carried out on the same measurement plots and runoff from the catchment was recorded at a stream discharge gauging station. Stream water samples were taken once a month during summer and winter and twice a month during spring and autumn. The input data used for the model calibration have been described in more detail by Finér *et al.* (1997).

SMART2 model

The SMART2 model (Kros *et al.* 1995, Mol-Dijkstra *et al.* 1998) is an extended version of the SMART model (De Vries *et al.* 1989), developed to estimate long-term chemical changes in two soil layers and in soil water in response to changes in atmospheric deposition. The model structure is based on the anion mobility concept, by incorporating the charge balance principle (Reuss *et al.* 1987). SMART2 can be defined as a simple, dynamic, process-oriented model, which takes into account the net element fluxes between the atmosphere, forest, forest soil and soil water, as well as the geochemical buffer processes in the soil, such as CO₂ equilibria, cation exchange and sulphate adsorption. The output of the model includes the soil base saturation and the concentrations of the major anions and cations in soil water and runoff water.

SMART consists of a set of mass balance equations which describe the soil input-output relationships for the major cations (Al³⁺, Ca²⁺, Mg²⁺, K⁺, Na⁺, NH₄⁺) and anions (SO₄²⁻, NO₃⁻, Cl⁻) and a set of equilibrium equations describing the equilibrium soil processes. The soil water chemistry depends solely on the net element input from the atmosphere and the geochemical interactions in the soil. The concentrations of HCO₃⁻ and Al³⁺ are determined by means of an equilibrium with H⁺, the concentration of which is given by the charge balance equation. The cation exchange reactions are described by the Gaines-Thomas equations. Sulphate adsorption/desorption reactions are described by a Langmuir isotherm. Dissociation of organic anions is described as a function of pH, but the weathering rate of base cations from silicates is independent of soil pH.

In SMART2, descriptions of the nutrient cycle and vegetation growth are included. The nutrient cycle consists of canopy interaction, litter fall, root decay, mineralization and root uptake of nutrients. The soil horizon is divided into litter layer and mineral layer. The nutrient uptake is driven by the growth function and it consists of maintenance uptake to supply leaves and roots and the net growth uptake in stems and branches.

The atmospheric input of element *X* to the

soil compartment consists of total deposition, X_{td} , corrected by foliar uptake, X_{fu} , of NH₄⁺ and H⁺, or by foliar exudation, X_{fe} , of K⁺, BC²⁺:

$$X_{\text{fu}} = X_{\text{fu-fr}} X_{\text{td}} \quad (1)$$

and

$$X_{\text{fe}} = X_{\text{fe-fr}} (\text{NH}_{4\text{fu}} + \text{H}_{\text{fu}}) \quad (2)$$

where $X_{\text{fu-fr}}$ and $X_{\text{fe-fr}}$ are the foliar uptake fraction and foliar exudation fraction of element *X*.

Input fluxes of nitrogen and base cations by litter fall are described as:

$$X_{\text{lf}} = (1 - X_{\text{re-fr}}) A_{\text{lf}} X_{\text{lv-ct}} \quad (3)$$

where A_{lf} is the amount of litter fall, $X_{\text{lv-ct}}$ is the content of element *X* in leaves and $X_{\text{re-fr}}$ are reallocation fractions for element *X*. *X* stands for N, BC²⁺ or K.

The root decay flux in the litter compartment is described as:

$$X_{\text{rd-lt}} = X_{\text{lf}} (\text{NCF}) F_{\text{rt-lt}} \quad (4)$$

where NCF is the nutrient cycling factor and $F_{\text{rt-lt}}$ is the fraction of fine roots in the litter layer.

The soil organic pool is divided into rapidly decomposing fresh litter and slowly decomposing old litter. Mineralization of nutrients in fresh litter is described as a fraction of nitrogen litter fall and root decay. The mineralization flux of *X* from fresh litter $X_{\text{mi-fl}}$ is described as a fraction of the input of *X* by litter fall and root decay in the litter compartment according to:

$$X_{\text{mi-fl}} = [X_{\text{le-fr}} + F_{\text{mi}} (1 - X_{\text{le-fr}})] X_{\text{lf}} \times [1 + (\text{NCF}) F_{\text{rt-lt}}] \quad (5)$$

where F_{mi} is a mineralization fraction and $X_{\text{le-fr}}$ is a leaching fraction. Leaching refers only to the release of base cations from fresh litter. Fresh litter that is not decomposed within one year is transferred to the old litter pool. The mineralization flux of nutrients from the old litter pool is described by first-order kinetics:

$$X_{\text{mi}} = k_{\text{mi-mx}} F_{\text{miPh}} F_{\text{miCN}} A_{\text{lt}} X_{\text{lt-ct}} \quad (6)$$

where $k_{\text{mi-mx}}$ is the maximum mineralization rate constant from old litter, A_{lt} is the amount of old litter and $X_{\text{lt-ct}}$ is the content of element *X* in old litter. Values are decreased by pH and C/N ratio.

Nitrification and denitrification are described as a fraction of the nitrogen net input:

$$\text{NH}_{4\text{ni}} = F_{\text{ni}}(\text{NH}_{3\text{td}} - \text{NH}_{4\text{gu}} - \text{NH}_{4\text{im}} + \text{NH}_{4\text{mi}}) \quad (7)$$

and

$$\text{NO}_{3\text{de}} = F_{\text{de}}(\text{NO}_{\text{xtd}} + \text{NH}_{4\text{ni}} - \text{NO}_{3\text{gu}} - \text{NO}_{3\text{im}}) \quad (8)$$

where F_{de} and F_{ni} are the denitrification and nitrification fractions, NO_{xtd} and $\text{NH}_{3\text{td}}$ the deposition, $\text{NO}_{3\text{gu}}$ and $\text{NH}_{4\text{gu}}$ the growth uptake, and $\text{NO}_{3\text{im}}$ and $\text{NH}_{4\text{im}}$ the immobilization fluxes. Immobilization of nitrogen is described as a rate limited equation, which depends on soil C/N ratio.

Nutrient uptake for NO_3 and NH_4 is described as a demand function:

$$X_{\text{ru}} = (N_{\text{lf}} - N_{\text{fu}} - N_{\text{gu}})(X_{\text{in}}/N_{\text{in}}) \quad (9)$$

where X stands for NO_3 or NH_4 , and N for NO_3 plus NH_4 , the subscript 'ru' for root uptake, 'lf' for litter fall, 'fu' for foliar uptake and 'gu' for growth uptake. For base cations (K, Mg, Ca), root uptake is described as:

$$X_{\text{ru}} = X_{\text{lf}} + X_{\text{fe}} + X_{\text{gu}} \quad (10)$$

Growth uptake flux is described as:

$$X_{\text{gu}} = [A_{\text{st}}(t) - A_{\text{st}}(t-1)]X_{\text{st-ct}} \quad (11)$$

where $A_{\text{st}}(t) - A_{\text{st}}(t-1)$ is the tree biomass (stems and branches) growth in the current year and $X_{\text{st-ct}}$ is the content of element X in stems.

These processes are included in the mass balance equations defining the nutrient concentrations of soil water. N fixation by pioneer plants was introduced to the model (Kämäri *et al.* 1998) in order to satisfy the nitrogen demand of new growing forest. A relation diagram of SMART2 is depicted in Fig. 1. The model processes are described in more detail in Ahonen *et al.* (1998).

UNCSAM

UNCSAM (UNCertainty analysis by Monte Carlo SAMpling techniques) applies Monte Carlo sampling in combination with regression and correlation analysis to perform sensitivity and uncertainty analysis. It assumes that variations and uncertainties in the parameters can be described by probability distributions and mutual

correlations. Sampling is performed from these distributions. Latin Hypercube Sampling technique (Iman and Conover 1982) was used to reduce the computation load.

Various statistics can be employed to quantify the input uncertainty contribution of the parameters to the model output. They are based on correlation or regression analysis. Two measures for sensitivity and uncertainty contribution, RTU (**R**oot **T** of **U**ncertainty) and SPC (**S**emi**P**artial **C**orrelation coefficient), were chosen in this study. RTU is based on correlation analysis and SPC on regression analysis. Good linear approximation is required in both.

In regression analysis approaches, the often complex relationship between model parameters and model output is approximated by a linear regression model:

$$\hat{y}(k) := \hat{\beta}_0 + \sum_{i=1}^p \hat{\beta}_i x_i(k) \quad (12)$$

where b_0 and b_i are coefficients and x_i is a model input parameter.

The goodness of the linear approximation can be assessed by the coefficient of determination:

$$R^2 := \frac{S_y^2}{S_y^2} = 1 - \frac{S_e^2}{S_y^2} \quad (13)$$

where S_e^2 is the estimated variance of the regression residuals, S_y^2 is the estimated variance of the model output and S_y^2 is the estimated variance of the output $\hat{y}(k)$ of the linear regression model.

The uncertainty in y (S_y^2) can be expressed in terms of $\hat{\beta}_i S_{x_i}$ and the correlation coefficients $r_{x_i x_j}$ between x_i and x_j :

$$S_y^2 = \sum_{i=1}^p \sum_{j=1}^p \hat{\beta}_i S_{x_i} \hat{\beta}_j S_{x_j} r_{x_i x_j} + S_e^2 \quad (14)$$

One way to handle the problem caused by correlation between the inputs was described by Janssen *et al.* (1992). The uncertainty contribution of x_i can be determined by expressing the relative

uncertainty change $\frac{\Delta S_y^2}{S_y^2}$ of the model response

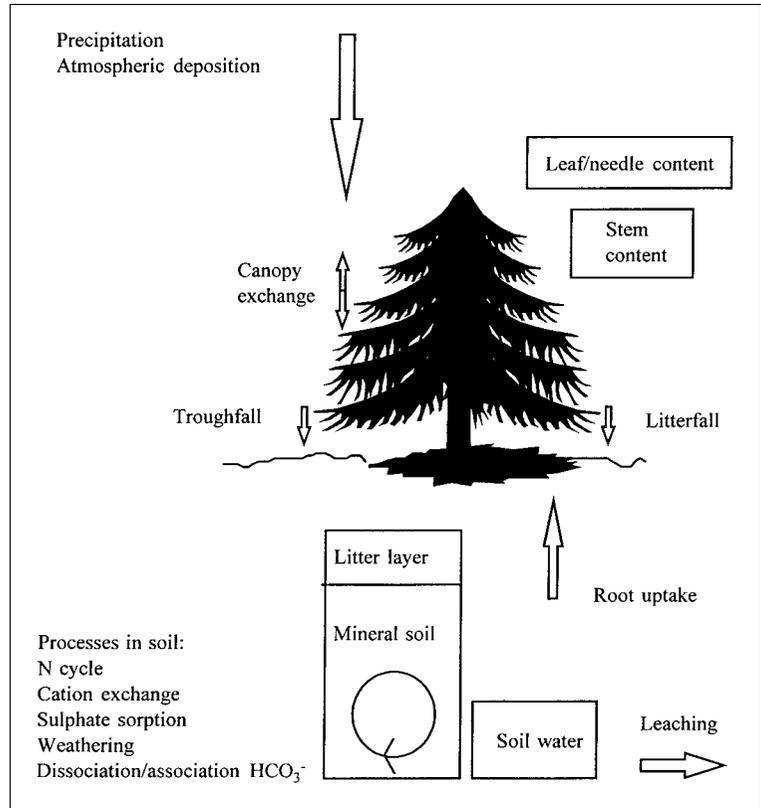


Fig. 1. Schematic diagram of the SMART2 model

y due to a relative uncertainty change $\frac{\Delta S_{x_i}^2}{S_{x_j}^2}$ of the individual x_i , thereby accounting for the induced change of the correlated inputs x_j ($j \neq i$):

$$\frac{\Delta S_y^2}{S_y^2} \approx \text{PUC}_i \frac{\Delta S_{x_i}^2}{S_{x_i}^2} \quad (15)$$

The resulting quantity PUC (**P**artial **U**ncertainty **C**ontribution) can be expressed as a combination of regression and correlation quantities (Janssen *et al.* 1992):

$$\text{PUC}_i := \sum_{j=1}^p \hat{\beta}_j^{(S)} r_{yx_j} r_{x_i x_j}^2 \quad (16)$$

RTU (**R**oot of **U**ncertainty) is the square root of the PUC:

$$\text{RTU}_i := \sqrt{|\text{PUC}_i|} \quad (17)$$

The key idea behind the correlation analysis ap-

proach is to measure the connection between the parameter x_i and the model output y . The simplest form is the linear correlation coefficient r_{yx_i} . If r_{yx_i} is close to 1 or -1 , y can almost be written as a linear function of x_i . If x_i is correlated to the other x_j , $j \neq i$, r_{yx_i} includes the influence of the other correlated parameters. SPC expresses the linear relation between model output and the corrected input parameter. In SPC_i the parameter x_i is first corrected for all linear effects of the remaining parameters x_j . This correction is made by regressing y and x_i linearly on all x_j ($j \neq i$). The corrected quantity \tilde{x}_i is correlated with the model output y :

$$\text{SPC}_i := r_{y\tilde{x}_i} \quad (18)$$

If the correlation between the sources is weak, SPC will be equal to the linear correlation coefficient. RTU takes into account the mutual correlations between all the sources. Due to this fact, it can occur that 'weak' components will be high in the ranking list, if they are correlated

with 'strong' components. The analyses are described in greater detail in Janssen *et al.* (1992) and in Heuberger and Janssen (1994).

Parameterization

The model was calibrated to observed vegetation growth and the measured soil and stream water quality data of 1993–1996 (Table 1), as

Table 1. Stream water quality, simulated values (1993) and measured values.

Variable	Unit	Simulated	Measured value
SO ₄ ¹⁾	μeq dm ⁻³	74.7	50.85 ± 3.8
NO ₃ ¹⁾	μeq dm ⁻³	3.52	0.65 ± 0.2
Na ²⁾	μeq dm ⁻³	53.77	52.9 ± 2.4
K ²⁾	μeq dm ⁻³	10.97	7.67 ± 1.9
Ca+Mg ²⁾	μeq dm ⁻³	76.3	85.4 ± 7.4
Cl ¹⁾	μeq m ⁻³	13.0	14.3 ± 1.4
pH ¹⁾		5.73	5.77
Base saturation, mineral ³⁾	%	42.8	43.7
Base saturation, litter ³⁾	%	49.2	51.6

¹⁾ Observations from years 1993–1996, ²⁾ Observations from years 1993–1995, ³⁾ Observation from year 1993.

reported in Finér *et al.* (1997). The output of the model includes soil base saturation and the major anions and cations in runoff water, but only base saturation of mineral soil and litter layer, and pH and NO₃ concentration of stream water were included in the input uncertainty analysis. The simulation period was 1850–2050 and the modelling time step was one year.

The mean value of precipitation was based on measurements (Finér *et al.* 1997), but variance and minimum and maximum values were based on long-term observations in north-east Finland (Alalammi 1987, Kuusisto 1986). Parameter values of weathering rate were based on calibration, but variance and the calibration range were derived from the literature (Lindroos *et al.* 1996). Chemical and physical properties of soil were based on measurements (Finér *et al.* 1997). Values for parameters defining nitrogen mineralization in soil were taken directly from the literature (Rankinen 1992), but the amount of mineralized nitrogen was calibrated to values found in the literature (Finér 1989). Nutrient concentrations in vegetation (Finér 1992) and reallocation of nutrients (Helmisaari 1990) were taken from the literature. Nutrient concentrations in vegetation were calculated as biomass-weighted averages and chemical and physical properties of soil as averages over the area.

Model input parameters and their distribu-

Table 2. Parameters and their distributions.

Parameter	Unit	Distribution	Mean	Variance	Min.	Max.
Precipitation	m	nor	0.54	0.02	0.2	1.0
Thickness of soil layer	m	nor	2.3	0.3	0.6	5
Bulk density of min. layer	g cm ⁻³	nor	1.0	0.06	0.2	1.9
Ca weathering	eq m ⁻² yr ⁻¹	nor	0.005	0.000015	0.001	0.016
Mg weathering	eq m ⁻² yr ⁻¹	nor	0.005	0.000015	0.001	0.016
K weathering	eq m ⁻² yr ⁻¹	nor	0.002	0.000002	0.0015	0.006
CEC in litter layer	meq kg ⁻¹	nor	146.97	2600	50	300
CEC in mineral layer	meq kg ⁻¹	nor	6.13	20	1	20
N conc. stems	%	nor	0.19	0.001	0.05	0.3
N conc. leaves	%	nor	1.6	0.02	0.7	2
K conc. stems	%	nor	0.05	0.0001	0.01	0.08
K conc. leaves	%	nor	0.55	0.03	0.05	1.6
BC ²⁺ conc. stems	%	nor	0.23	0.003	0.06	0.4
BC ²⁺ conc. leaves	%	nor	0.78	0.03	0.05	1.6
Denitrification fraction	–	nor	0.09	0.08	0.001	1
Fraction of nitrified N in litter layer	–	uni	0	1		
Mineralization rate	yr ⁻¹	nor	0.07	0.0004	0.001	1
Reallocation fraction	–	nor	0.4	0.02	0.1	0.8

tions and variances are presented in Table 2. Minimum and maximum values refer to physical boundaries. Parameters were assumed to be normally distributed, except for the parameters used in the Gaines-Thomas equation and the fractions of water and nutrients in litter layer, which were assumed to have uniform distribution. Mean values of parameters were used in calibration.

Relationships between parameters were described by mutual correlations. The correlation between nutrient concentrations in leaves and stem was assumed, as were correlations between mineralization parameters (Table 3). Habitat and environmental conditions were assumed to affect mineralization in a similar way in new and old litters and nutrients taken up were assumed to be distributed evenly between stem and leaves in a tree. Of the selected measures for sensitivity and uncertainty contribution, RTU is based on correlation analysis and can take correlation between parameters into account.

The deposition history and future scenarios were based on emission data and atmospheric transport models (Mylona 1993, Asman and Drukker 1988). Site-specific deposition values were derived by the model DEPUPT (Johansson *et al.* 1996), using forest growth information, bulk and through fall deposition measurements as well as future deposition scenarios modelled by DAIQUIRI (Syri *et al.* 1998).

Results

Soil base saturation

Simulated base saturation in mineral soil for the Kangasvaara catchment in 1994 was 43%. Simulated change in base saturation in mineral soil layer was best explained by soil thickness (thick), precipitation (precip), and weathering rates of Na, Ca and Mg (BC_{we}) (Fig. 2). Base saturation decreased 7.8% when precipitation increased 26% and increased 7.9% when soil thickness was assumed to increase up to 2.8 m (Table 4). The strong influence of soil thickness was explained by the fact that weathering rates are given per area (eq m^{-2}). Simulated change in base saturation in the thin litter layer was dependent on two

parameters used in the Gaines-Thomas equation, namely the exchange constant between Al and K ($\lg KAIBC$) in litter layer and between H and K ($\lg KHBC$) in mineral layer. Litter layer base saturation was also dependent on bulk density of litter layer (bulk_{ll}), CEC of litter layer (CEC_{ll}), precipitation (precip) and weathering of Mg and K (BC_{we}). Parameters defining nutrient mineralization in soil (k_{mi-mx} , F_{mi}), fraction of water and nutrients taken up in litter layer (F_{w-ll}) and fraction of roots in the litter layer (F_{rt-ll}) also have an influence on the simulated base saturation of litter layer (Fig. 2).

Nitrate and pH in stream water

NO_3 in stream water was best explained by nitrogen concentration in vegetation (N_{st-ct} , $N_{lf-mx-ct}$), precipitation (precip), CEC of mineral layer (CEC_{mi}) and nitrogen cycle parameters such as mineralization rate in soil (k_{mi-mx}), denitrification (F_{de}), reallocation (X_{re-fr}) and fraction of nitrified N in litter layer (N_{ll-fr}). Simulated NO_3 concentration was $3.7 \mu\text{eq dm}^{-3}$ in 1994. It decreased to $0.8 \mu\text{eq dm}^{-3}$ when nitrogen concentration in stem was increased from 0.19% up to 0.22% and further to $0.7 \mu\text{eq dm}^{-3}$ when nitrogen concentration in leaves was also increased from 1.6% to 1.74% (Table 4). The pH value was explained by thickness of soil layer (thick) and weathering rates of Na, Ca and Mg (BC_{we}). Stream water pH was also explained by two parameters used in the Gaines-Thomas equation, namely $\lg KAIBC$ and $\lg KHBC$ in mineral layer, as well as dissolution constant for Al-(hydr)oxide ($\lg KAlox$), K

Table 3. Correlations used in input uncertainty analysis.

Parameter	Parameter	Correlation
N concentration in stem	N concentration in leaves	0.7
K concentration in stem	K concentration in leaves	0.7
BC2 concentration in stem	BC2 concentration in leaves	0.6
N mineralization fraction in fresh litter	N mineralization rate in old litter	0.5

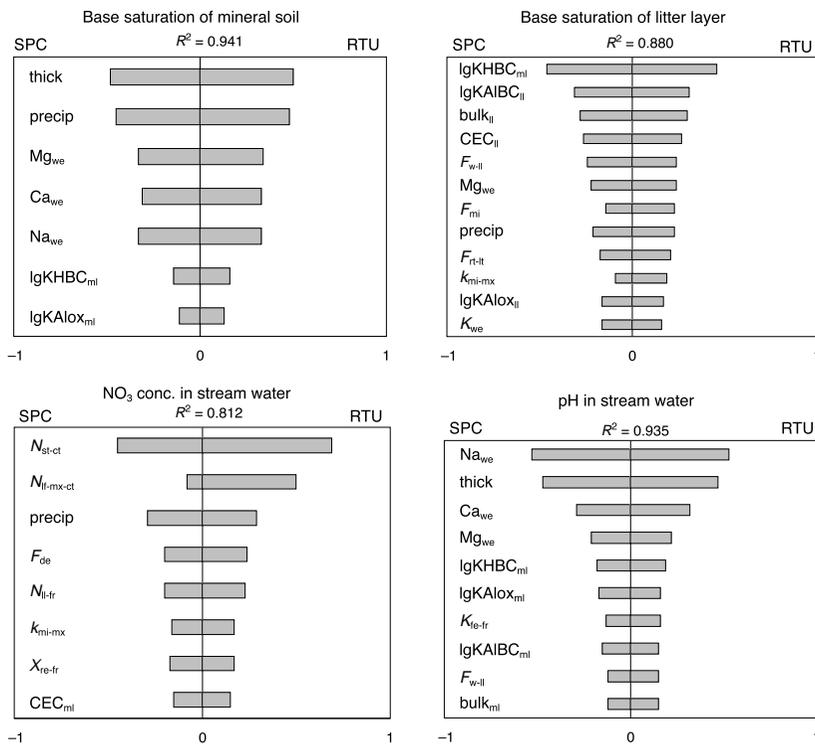


Fig. 2. Ranking of the most influential parameters on model main output variables according to RTU (Root of Uncertainty) and SPC (SemiPartial Correlation coefficient) measures for sensitivity and uncertainty contribution. The length of the bar shows the relative influence in scale 0–1, and the negative axis is used for SPC only for visual reasons. In the figure symbol thick stands for thickness of soil layer, precip for precipitation, Mg_{we}, Ca_{we}, K_{we} and Na_{we} for weathering rates of base cations, CEC_{ll} and CEC_{ml} for cation exchange capacity of litter layer and mineral layer respectively, bulk_{ll} and bulk_{ml} for bulk density of litter layer and mineral layer respectively, F_{mi} for mineralization fraction, k_{mi-mx} for mineralization rate, F_{de} for denitrification fraction, X_{re-fr} for reallocation fraction of nutrients, F_{rt-ll} for fraction of roots in the litter layer, N_{ll-fr} for fraction of nitrified N in litter layer, F_{w-ll} for fraction of water and nutrients taken up in litter layer, N_{st-ct} for N content in stems, N_{ll-mx-ct} for N content in leaves, lgKHBC_{ml}, lgKAIBC_{ml} and lgKAIBC_{ll} for exchange constants between Al and K and H and K in mineral soil and litter layer, and lgKAlOx_{ml} for dissolution constant for Al-(hydr)oxide.

Table 4. Influence of changes in model parameters to modelled soil base saturation and stream water NO₃ concentration in 1994.

Parameter	Mean value	Changed value	Orig. output	Changed output
Soil base saturation (%)				
Precipitation (m)	0.54	0.68	43.0	35.2
Soil thickness (m)	2.3	2.8	43.0	50.9
NO₃ concentration				
N conc. in stem (%)	0.19	0.22	3.7	0.8
N conc. leaves (%) ¹⁾	1.60	1.74	0.8	0.7

¹⁾N conc. in stem 0.22% + N conc. in leaves 1.74%

foliar exudation fraction ($K_{\text{re-fr}}$), fraction of water and nutrients taken up in litter layer ($F_{\text{w-l}}$), and bulk density of mineral soil (bulk).

Base cation and nitrogen mineralization and uptake

Nitrogen uptake was almost completely dependent on nitrogen concentration in vegetation ($N_{\text{st-ct}}$, $N_{\text{lf-mx-ct}}$). This was because in the Kangasvaara calibration, vegetation was assumed to fix atmospheric nitrogen. Nitrogen fixation was added to the model to supply nitrogen for growing forest in the beginning of the twentieth century when atmospheric deposition in the area was very low (Kämäri *et al.* 1998). Different tests gave a different emphasis for nitrogen concentration in leaves due to the correlation of nutrient concentration in stems and leaves. Base cation uptake was explained by mineralization ($k_{\text{mi-mx}}$, F_{mi}), concentration in stem and leaves ($\text{BC}_{\text{st-ct}}$, $\text{BC}_{\text{lv-ct}}$), weathering (BC_{we}) and thickness of rooting zone (thick) (Fig. 3). Base cation and nitrogen mineralization appear to be dependent on reallocation of nutrients ($X_{\text{re-fr}}$), but also on fraction of water and nutrients taken up in litter layer ($F_{\text{w-l}}$), fraction of roots in the litter layer ($F_{\text{rt-l}}$), thickness of rooting zone (thick_{rz}) and nutrient cycling factor (NCF).

Discussion and conclusions

The weathering rates, nutrient concentration of vegetation, precipitation and thickness of soil layer are the most important parameters explaining the key model output variables, namely base saturation of mineral soil and NO_3 concentration and pH of stream water. Precipitation has an influence on base saturation in mineral soil and on NO_3 concentration in stream water. The influence of the driving variable atmospheric deposition has a marked effect (Holmberg *et al.* 2000), but it was omitted in this study because deposition is included in the model as a time series and not as a parameter. The strong influ-

ence of precipitation indicates the importance of choosing representative years for calibration, because the use of particularly wet or dry years may lead to over- or underestimation of certain outputs. Precipitation was measured in years the 1992–1995 and this time series may have been too short to provide an accurate estimate of the actual precipitation in the area. The strong influence of weathering rates is often combined with the strong influence of thickness of soil layer, because in the model the weathering rates are given as units per area. Parameter values of weathering rate were based on calibration and on literature values, and more emphasis should be placed on narrowing the uncertainty in reported values. Vegetation uptake of nitrogen is explained almost solely by the concentration of nitrogen in stem and leaves, but vegetation uptake of base cations is also explained by parameters defining mineralization and weathering. Nutrient concentrations in vegetation in this study are based on values found in the literature. Tree stand measurements were carried out in the Kangasvaara catchment but the estimates of the element contents in stems, branches and leaves were not ready to be used in this study. This information would improve the reliability of simulated nutrient uptake as well as the reliability of the simulated NO_3 concentration in stream water. Selected tests gave different rankings for nutrient concentrations in leaves. The test based on correlation analysis, RTU, gives a higher ranking than the SPC test based on regression analysis, because of the correlation between nitrogen concentration in stems and leaves.

The model UNCSAM is rather easy to use, but it is DOS-based and needs a large amount of computation. The model gives the ranking of parameters according to their influence on a certain output, but it does not give an absolute value for the influence. SMART2 is a relatively simple dynamic model and all the input parameters were included in the input uncertainty analyses. If the UNCSAM software package is used with any model which needs a large number of input parameters, the parameters included in input uncertainty analysis should be chosen be-

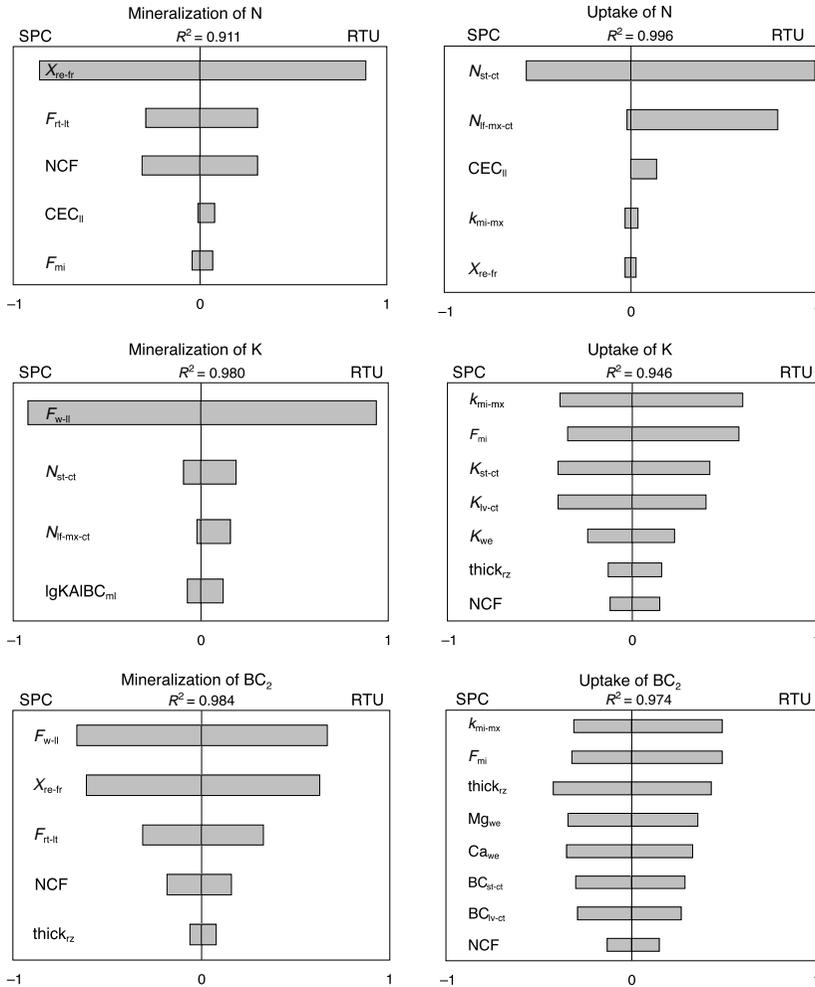


Fig. 3. Ranking of the most influential parameters on the nutrient cycle of the model according to RTU (Root of Uncertainty) and SPC (SemiPartial Correlation coefficient) measures for sensitivity and uncertainty contribution. The length of the bar shows the relative influence in scale 0–1, and the negative axis is used for SPC only for visual reasons. In the figure symbol $thick_{rz}$ stands for thickness of rooting zone, Mg_{we} , Ca_w and K_{we} for weathering rates of base cations, CEC_{ll} for cation exchange capacity of litter layer, F_{mi} for mineralization fraction, k_{mi-mx} for mineralization rate, X_{re-fr} for reallocation fraction of nutrients, F_{rt-lt} for fraction of roots in the litter layer, F_{w-ll} for fraction of water and nutrients taken up in litter layer, NCF for nutrient cycling factor, N_{st-ct} for N content in stems, $N_{lf-mx-ct}$ for N content in leaves, K_{st-ct} for K content in stems, K_{lv-ct} for K content in leaves, BC_{st-ct} for Mg and Ca content in stems, BC_{lv-ct} for Mg and Ca content in leaves, and $IgKAIBC_{mi}$ for exchange constants between Al and K in mineral soil.

forehand in order to reduce computation. Good linear approximation is required in both the measures for sensitivity and uncertainty contribution used in this study, and R^2 -values for different tests vary between 0.812 and 0.996. R^2 -value is the only parameter in the UNCSAM software package with which it is possible to test this approximation. A good graphical com-

ponent in the model to test linearity would improve the testing.

The aim of this study was to rank the input parameters on the basis of their contribution to model uncertainty in order to determine which additional data would best improve the reliability of predictions. This work provides an estimation of the uncertainty of the model results, but

an accurate uncertainty analysis would need considerable effort and would be worthy of reporting separately.

Acknowledgements: The authors thank the DYNAMO project (Dynamic models to predict and scale-up the impact of environmental change on biogeochemical cycling) of the European Commission (Contract: ENV4-CT95-0030) for financial support, Dr. Leena Finér and Sirpa Piirainen from The Finnish Forest Research Institute for providing data of the Kangasvaara catchment for model calibration and Hannu Sirviö from the Finnish Environment Institute for commenting on the statistical analyses.

References

- Ahonen J., Rankinen, K., Holmberg M., Syri S. & Forsius M. 1998. Application of the SMART2 model to a forested catchment in Finland: comparison to the SMART model and effects of emission reduction scenarios. *Boreal Env. Res.* 3: 221–233.
- Alalammi P. (eds.) 1987. *Atlas of Finland*. 131. National Board of Survey. Helsinki. 31 + 12 pp.
- Asman W. & Drukker B. 1988. Modelled historical concentrations and depositions of ammonia and ammonium in Europe. *Atmos. Environ.* 22(4): 725–735.
- DeVries W., Posch M. & Kämäri J. 1989. Simulation of the long-term soil response to acid deposition in various buffer ranges. *Wat. Air Soil Pollut.* 48: 349–390.
- Finér L. 1989. Biomass and nutrient cycle in fertilized and unfertilized pine, birch and spruce stands on a drained mire. *Acta Forestalia Fennica* 208, Helsinki, Finland. 63 pp.
- Finér L. 1992. Biomass and nutrient dynamics of Scots pine on a drained ombrotrophic bog. Finnish Forest Research Institute, *Research Papers* 420. Joensuu. 218 pp.
- Finér L., Ahtiainen M., Mannerkoski H., Möttönen V., Piirainen S., Seuna P. & Starr M. 1997. Effects of harvesting and scarification on water and nutrient fluxes. A description of catchments and methods, and results from the pretreatment calibration period. *The Finnish Forest Research Institute, Research Papers* 648, Joensuu Research Station. 38 pp.
- Gundersen P. & Bashkin V.N. 1994. Nitrogen cycling. In: Moldan B. & Cerny J. (eds.), *Biogeochemistry of small catchments: A tool for environmental research*. *SCOPE report* 51: 255–283. John Wiley & Sons, Chichester.
- Helmisaari H.-J. 1990. *Nutrient retranslocation within Pinus Sylvestris*. Academic dissertation. University of Joensuu. Joensuu, Finland.
- Heuberger P.S.C. & Janssen P.H.M. 1994. UNCSAM: a software tool for sensitivity and uncertainty analysis of mathematical models. In: Grasman P. & van Straten G. (eds.), *Predictability and non-linear modelling in natural sciences and economic*. Kluwer Academic Publishers, Dordrecht, pp. 362–376.
- Holmberg M., Rankinen K., Johansson M., Forsius M., Kleemola S., Ahonen J. & Syri S. 2000. Sensitivity of soil acidification model to deposition and forest growth. *Ecol. Mod.* 135(2–3): 311–325.
- Iman R.L. & Conover W.J. 1982. A distribution free approach to including rank correlations among input variables. *Communications in Statistics A9*: 1749–1842.
- Johansson M., Alveteg M., Walse C. & Warfvinge P. 1996. Derivation of deposition and uptake scenarios. In: Knoflacher M., Schneider J. & Soja G. (eds.), *International Workshop on Exceedance of Critical loads and levels, spatial and temporal interpretation of elements in landscape sensitive to atmospheric pollutants; Vienna 22–24 Nov 95*. Conference papers BD.15/VOL.15, Federal Environment Agency, Vienna.
- Janssen P.M.H., Heuberger P.S.C. & Sanders R. 1992. *UNCSAM 1.1: a Software package for sensitivity and uncertainty analysis*. Manual. RIVM-report nr. 959101004. Bilthoven, The Netherlands.
- Kros J., Reinds G.J., de Vries W., Latour J.B. & Bollen M.J.S. 1995. Modelling of soil acidity and nitrogen availability in natural ecosystems in response to changes in acid deposition and hydrology. DLO Winand Staring Centre for Integrated Land, Soil and Water Research, *Report* 95.
- Kros J., Pebesma E.J., Reinds G.J., Finke P.A. 1999. Uncertainty assessment in modelling soil acidification at the European scale: a case study. *J. Environ. Qual.* 28: 366–377.
- Kuczera G. & Parent E. 1998. Monte Carlo assessment of parameter uncertainty in conceptual catchment models: the Metropolis algorithm. *J. Hydrol.* 211: 69–85.
- Kuusisto E. 1986. Sadanta. In: Mustonen S. (ed.), *Sovellettu hydrologia*. Vesiyhdistys r.y., Mäntän Kirjapaino Oy, pp. 29–48.
- Kämäri J., Rankinen K., Finér L., Piirainen S. & Posch M. 1998. Modelling the response of soil and runoff chemistry to forest harvesting in a low deposition area (Kangasvaara, Eastern Finland). *Hydrol. Earth System Sci.* 2(4): 485–495.
- Lindroos A.-J., Starr M., Tarvainen T. & Tanskanen H. 1996. *Weathering rates in the Hietajärvi integrated monitoring area*. The 22nd Nordic Geological Winter Meeting, 8–11 January 1996, Turku, Finland.
- Mol-Dijkstra J.P., Kros H. & van der Salm C. Comparison of simulated forest soil response to acid deposition reduction with two models of differing complexity. *Hydrol. Earth System Sci.* 2(4): 473–483.
- Mylona S. 1993. Trends of sulphur dioxide emissions, air concentrations and depositions of sulphur in Europe since 1880. *EMEP/MSC-W Report 2/93*, Oslo, Norway.
- Posch M., Reinds G.J. & de Vries W. 1993. SMART — A simulation model for acidification's regional trends: Model description and user manual. *Mimeograph Series*

- ries of the National Board of Waters and the Environment no. 477, Helsinki, Finland. 43 p.*
- Rankinen K. 1992. Kosteuden vaikutus typen mineralisaatioon maaperässä [Effect of soil moisture on soil nitrogen mineralization]. M.Sc. thesis, Helsinki University of Technology, Espoo, Finland, 49 + xxvi pp. [In Finnish with English abstract].
- Reuss J.O., Cosby B.J. & Wright R.F. 1987. Chemical processes governing soil and water acidification. *Nature* 329: 28–31.
- Soutter M. & Musy A. 1999. Global sensitivity analyses of three pesticide leaching models using a monte-carlo approach. *J. Environ. Qual.* 28: 1290–1297.
- Syri S., Johansson M. & Kangas L. 1998. Application of nitrogen transfer matrices for integrated assessment. *Atmos. Environ.* 32: 409–413.

Received 7 February 2000, accepted 8 September 2000