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THE NUTRIENT CYCLING MODEL (NuCM)

USER MANUAL

by

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Summary: The Nutrient Cycling Model (NuCM) is a dynamic process orientated model which simulates the atmospheric, hydrologic, plant and soil processes affecting a forest ecosystem. This NuCM User manual describes the hydrological and chemical process equations in detail. It is intended as a more detailed supplement to the original manual (Munson et al., 1992). It contains many useful hints for preparing input files and parameters. Parameters are listed with their program code name and in which equations they are used. A layman's guide to the program description of the chemistry simulation is included.

Sammendrag: NuCM er en dynamisk prosessorientert modell som simulerer de atmosfæriske, hydrologiske, samt plante- og jord-prosesser som påvirker et skogøkosystem. Denne NuCM manualen beskriver detaljert de hydrologiske og kjemiske prosess-ligninger. Dens hensikt er å være et detaljert supplement til den opprinnelige manual (Munson et al., 1992). Den inneholder mange nyttige råd om hvordan man setter opp filer og parametre. Parameterlister viser deres kode navn i programmene og i hvilke ligninger de er brukt. En elementær veiledning til beskrivelsen av den kjemisk simuleringen er inkludert.

4. Emneord, norske

1. NuCM
2. Modell
3. Næringssirkulasjon
4. Prosess-beskrivelse

Prosjektleder:

Per Jørgensen

4. Emneord, engelske

1. NuCM
2. Model
3. Nutrient Cycling
4. Process Description

For administrasjonen:

Steinar Abrahamson

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Introduction

The NuCM model stands for the **Nutrient Cycling Model**. It was developed as part of the Integrated Forest Study (IFS) initiated in 1986 by the American Electric Power Research Institute (EPRI). The IFS's goal was to evaluate the effects of atmospheric deposition on nutrient cycling in forest ecosystems (Johnson et al., 1992). The \$15 million project included field measurements of atmospheric inputs and quantification of nutrient pools and fluxes at 17 forest sites, 15 in the USA, 1 in Canada and 1 in Norway (Nordmoen).

NuCM is a dynamic process orientated model which simulates the atmospheric, hydrologic, vegetation and soil processes which alter the composition of deposition as it moves through the tree canopy and down the soil profile.

NuCM has evolved from the ILWAS model (Goldstein et al., 1984; Gherini et al., 1985) and in comparison has simplified hydrological processes, more complex canopy interactions and similar soil chemical processes.

The program was written by the firm, Tetra Tech, inc. in Microsoft FORTRAN 5.0 and C, 6.0 and runs on IBM compatible computers. The code is distributed in executable form so no FORTRAN/C compilers are required, although a coprocessor is necessary.

The model separates the hydrology and chemistry simulations. The hydrology simulation must be run first and always uses a daily time step. However the time step specified for the chemistry simulation can be daily, weekly, monthly or yearly. Hence the hydrology simulation will summarise the necessary hydrological data in a monthly, weekly or daily format in file, SITENAME.H2O, for the chemistry simulation.

NuCM has a manual (Munson et al., 1992), which I am very grateful for and henceforth refer to as the original manual. Few forest-soil-atmosphere models have available documentation (6 of 16) according to Tiltak and van Grinsven, 1995, although many plan to produce it (8 of 16). However through working with NuCM, I have found the present manual and the HELP screens far from complete. This is probably quite a common experience of modellers working with models created by others (Tiltak et al., 1995 (Ch. 6)). I soon found that it was necessary to find the names of the parameters in the code and use a textsearcher to find the equations involved. As I am most interested in the canopy and soil processes, I have concentrated mainly on the chemistry simulation and to a lesser degree on the hydrology simulation. I am neither a FORTRAN nor C programmer and have used considerable time and effort tracing parameters, equations and processes. I still do not understand a vast proportion of the C programs used, see the chemistry equilibrium section. However it is important that people using models purely at the computer screen/manual level are at least aware of the vast amount of work that lies behind the programming. For NuCM, many equations, parameters, data are included there, which are never mentioned in the manual or HELP screens. Some of these missing equations are too simple to waste space on in a manual but others are not and are important. I therefore now present the results of my labour in an improved and more complete NuCM manual. It is my hope that this manual will prevent others experiencing the many delays I had while preparing, inputting and calibrating data for NuCM.

Hydrology Simulation

Parameters used in atmospheric and hydrological processes

Table 1 shows the order of physiographic parameters required if one simulates a forest stand without a stream or understory but with snow. These parameters are mainly used to simulate the hydrological processes but can also be used in the chemistry simulation. The parameter is input in the units shown although within the program unit conversions often occur. The name of the parameter in the program code, the participation of a parameter in the equations described in the manual and the menu number for parameter input are also shown.

Table 1. Parameters required to simulate atmospheric and hydrological processes

No.	Description	Units	Parameter name in program code	Used in equation	Menu no.
1	stand area	m ²	starea	3,4,27,28	p10
2	hydrological catchment area	m ²	tarea		p10
3	number of soil layers (max 10)		layers (L ¹)		p10
4	bedrock elevation, lowest point	m	belev		p20
5	latitude		xlat	10	p20
6	longitude		xlon		p20
7	mean catchment/stand width	m	scwidth	20,24	p20
8	aspect (0-360 °)		aspect	12,13,14	p20
9	Average surface slope (decimal fraction)		sslope		p20
10	Manning's n for overland flow (0.1-0.6)		nn	20	p20
11	Maximum surface depression storage	cm	dtsmax	20	p20
12	Canopy monthly leaf area index (Jan.-Dec.)	m ² m ⁻²	lai/d/c/o ² (36)	4,5,27,283 2, 98	p30
13	Areal % of canopy type (deciduous, coniferous and open)		pcdec pcconf pcopen (3)	18,33,41,7 7,98	p40
14	Max. canopy interception storage	cm	d/c/oimax (3)	5	p40
15	Monthly mean relative humidity (%) (Jan.- Dec.)		rh (12)	9	p50
16	Coefficient to adjust evaporation up/down		ecoeff	12	p50
17	Coefficient to adjust seasonal variation of evaporation (skew<1 or flatten>1)		scoeff	8	p50
18	Multiplier for the heat convection parameter for soil-air interface		rkcfac		p50
19	Multiplier for the heat convection parameter for soil-snowpack interface		sncfac		p50
20	Atmospheric CO ₂ levels v. time curve	ppm	co2atm		p55
21	Soil layer areal extent	m ²	scarea (L)	21,33,40, 41,77,98, 101,103	p60

22	Soil layer thickness	cm	thick (L)	22,40, 101	p60
23	Fraction of roots in layer		etwght (L)	77	p60
24	Saturated moisture content (0.1-0.6)		thets (L)	23,25	p60
25	Field capacity moisture content (0-0.4)		thefc (L)	23,25	p60
26	Initial moisture content (0-0.6)		theta (L)	23,25	p60
27	Hydraulic conductivity	cm s ⁻¹	perm (L)	23	p70
28	Initial soil temperature	°C	soltmp (L)	45,68,70, 74	p70
29	Initial Chloride concentration	μmol _c l ⁻¹	solion (L)		p70
30	Temperature below which precipitation is snow	°C	snotmp	1,13,14,15	p80
31	Sublimation rate (0.005)	cm day ⁻¹	snosbo/f ³ (2)	18	p80
32	Initial depth of snow	cm water	snodep		p80
33	Snow melt rate coefficient (0.05-0.1)	cm water °C ⁻¹ day ⁻¹	osmrat fsmrat ³ (2)	13,14	p80
34	Max. moisture holding capacity of snow (%)		pcstor	17	p80
35	Air temp. at which snow begins to melt	°C	tcoef	13	p80
36	Rain induced snow melt rate (0.001-0.01)	°C ⁻¹	rsmrat	15	p80
37	Snowmelt leaching coefficient (0-4)		ckmelt		p90
38	Ion concentrations in snowpack at beginning of simulation NH ₄ , AL _v , Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , DOC(mg/l), SiO ₂ (mg/l)	μmol _c l ⁻¹	snoion (max12)		p90

Notes

1. L denotes the number of soil layers and hence the number of values required for certain soil layer parameters

2. There can be 3 areas in the catchment/forest stand:

- deciduous canopy, denoted by suffix/prefix d
- coniferous canopy denoted by suffix/prefix c
- open area, denoted by suffix/prefix o

Parameter numbers 12, 13 and 14 require 36, 3 and 3 values for this reason.

When an equation involves these parameters, the same equation is repeated for each of the areas and the total is then summed for the 3 areas e.g. equations 18 and 19.

3. Parameters 31 and 33 involved in snow melting equations have 2 values, o denoting open areas and deciduous canopy (bare in winter and so like open) and f denoting coniferous areas.

The use of parameters in table 1, where no equation is referred to in the "Used in equation" box is briefly described now.

The hydrological catchment area (2) is used to calculate fluxes for the output files and graphs. The number of soil layers (3) is obviously a vital parameter, which decides the number of values needed for parameters 21 - 29 and other chemical parameters and the number of times many equations are repeated in the program codes.

The lowest point in the bedrock elevation (4) is used as zero datum to calculate water table slopes.

The longitude (6) is only used in HYDRO3.FOR, which computes heat exchange terms for the lake.

The average surface slope (9) is used in various slope calculations, e.g. lateral flow. **N.B.** Even if one is simulating a **flat forest stand** or **lysimeters**, it is **vital to include a small slope** to ensure the hydrology simulation runs. Also the **evapotranspiration** is **very sensitive** to the **combination** of mean catchment width (**scwidth**) and average surface slope (**sslope**) chosen. The multiplier for heat convection parameters between the soil and air (18) and soil and snow interfaces (19) are used to calculate the temperature of the top layer of soil. They are given the respective values 1.0E-8 and 1.0E-4 in HYDRO1.FOR.

The atmospheric CO₂ levels(20) although asked for in the physiographic data menus is not used in the hydrology submodule.

The initial soil temperature (28), chloride concentration (29) and depth of snow (32) are starting values for various integration calculations.

The snowmelt leaching coefficient (37) is used to increase the leaching of chloride and other ions from the snowpack within a timestep, while ions in the snowpack (38) are only required if starting the simulation with a snowpack.

Information on systematic method of writing parameter/filename

Parameters in table 1, and tables 5 - 8 are always written in lower-case. These input parameters are only described in the tables. Additional parameters which crop up in most equations are written in large capitals. These additional parameters are either file input data or more usually descriptive parameters used in the calculation of processes. These parameters are either defined in the text nearby the equation or the most frequently mentioned parameters are defined below. File names are always written in small capitals.

P_T = total amount of precipitation (cm day⁻¹) daily input meteorological file

R = amount of rainfall (cm day⁻¹)

S = amount of snowfall (cm day⁻¹)

T_{MAX} = max. temperature (°C) daily input meteorological file

T_{MIN} = minimum temperature (°C) daily input meteorological file

T_{MEAN} = mean ambient temperature of day (°C) calculated from meteorological file

T = amount of throughfall (cm day⁻¹)

TIMSTP = current timestep (s)

M_{AX} = ambient air concentration of ionic species x (μmol_cm⁻³) monthly input in air file

TLFD/C = total annual litterfall (g cm⁻² year⁻¹)

File details

Meteorological and depositional input data to NuCM are given in the form of 2 Ascii files; SITENAME.MET, the meteorology file and SITENAME.AIR, the deposition file (air file).

An example of the set-up of the meteorology file is shown in table 2. Daily values of precipitation quantity (cm), minimum air temperature (°C), maximum air temperature (°C), cloud cover (decimal fraction), dewpoint (°C), atmospheric pressure (mbars) and wind speed (m s⁻¹) are required. The **29th February in leap years is not defined** in NuCM, so it should not be included in the SITENAME.MET file.

Table 2. The set-up of the meteorology file, NORDMOEN.MET .

Description	date	precipit. quantity	minimum air temp.	maximum air temp.	cloud cover	dew point temp.	atmos. pressure	wind speed
Units		cm	°C	°C	decimal fraction	°C	mbar	m s ⁻¹
FORTTRAN format	10x,3I2	7F8.3	7F8.3	7F8.3	7F8.3	7F8.3	7F8.3	7F8.3
Data	11087	.00	1.50	12.40	.10	2.10	999.999	1.20
	21087	.00	.40	9.20	.70	1.10	999.999	1.00
	31087	.00	3.40	11.20	.50	3.80	999.999	2.20
	41087	.00	2.10	10.80	.50	3.60	999.999	2.50
	51087	.00	2.80	8.50	.80	2.70	990.80	.90
	61087	1.35	6.80	9.50	.80	6.20	973.60	1.70
	71087	1.79	7.70	11.40	.40	6.50	965.90	4.70
	81087	2.45	7.40	8.80	.80	7.80	963.00	4.40
	91087	2.24	7.30	11.50	.50	6.50	971.00	2.40
	101087	.50	6.60	11.60	.70	4.90	985.30	2.40

It is important to note the FORTRAN format, which is in reality different from that recommended on p.3-3 in the original manual. This means that atmospheric pressures >999.999 mbar do not fit into this format. The manual recommends to generate this file by writing a computer program (FORTRAN, C or another language) or by using a spreadsheet program. I used Excel to generate 1 year of data, but found it a frustrating although possible process converting the excel file into an ASCII file with the correct format.

The necessity of the precipitation quantity and the maximum and minimum temperatures is obvious from glancing through the equations shown in this manual for atmospheric and hydrologic processes. However the need for daily values of the other meteorological data is less clear. Looking through the FORTRAN files in the Hydrology submodule of the source code, it became clear that cloud cover, dewpoint, atmospheric pressure and wind speed are mainly used in HYDRO3.FOR, which computes heat exchange terms for the lake. Dewpoint is mentioned in CLDMAIN.FOR, where if the dewpoint temperature (DPT) > Tmean, Tmean = DPT. Wind speed is used in the file CLD4.FOR where it is used in equations calculating heat dynamics between the snow/soil layer. Otherwise wind speed is used in some stream and lake calculations. Therefore, when one is only simulating a forest stand without stream or lake, only precipitation quantity, maximum and minimum temperatures are strictly necessary. Dewpoint and wind speed would be useful to have if available, whereas cloud cover and atmospheric pressure are not required. However at the present time, values for all meteorological data in the correct format are necessary, even if one inserts an average pressure and cloud cover for the whole simulation period.

The format for the deposition file as shown in the original NuCM manual is shown in table 3. The manual again suggests to generate this file by programming or spreadsheet. New data can also be input in the base case options menu when running the NuCM program or by altering the original example file, (TOWER.AIR) in an ASCII editor. The FORTRAN format is not column based and therefore difficult to translate from a spreadsheet file to an ASCII file, so I recommend the last 2 alternatives.

Although the manual suggest unit options: ME mmol_cl⁻¹ or MG mg l⁻¹, I strongly recommend to use the options selected in TOWER.AIR, i.e. ME units for both precipitation and air quality. I originally used the MG option for NORDMOEN.AIR (Nordmoen is the site I am simulating) and got far too large results for soil Cl concentration as a result. I therefore suspect an error in the

conversion equation when using the MG option. The DOC concentration should always be input as mg l^{-1} .

Table 3. The format for the Deposition data file.

Component	FORTTRAN format	Constituents
Date	10x,3I2	Day ¹ , Month, Year
Precipitation quality	6x,A2,9(1PE8.2)/ 8x,9(1PE8.2)	OP ² , SO _x , NO _x , H, NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , ANC, DOC, DIC, Al ₀ , SiO ₂
Ambient Air Quality	6x,A2,9(1PE8.2)/ 8x,9(1PE8.2)	OP ² , SO _x , NO _x , H, NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , ANC, DOC, DIC, Al ₀ , SiO ₂
Cloud Interception	6x,A2,9(1PE8.2)/ 8x,9(1PE8.2)	OP ² , QC ³ , NO _x , H, NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , ANC, DOC, DIC, Al ₀ , SiO ₂

1. This value is always 1 for this file (monthly data)

2. OP stands for unit option:

precipitation quality: MG = mg l^{-1} ; ME = $\text{mmol}_c\text{l}^{-1}$

Ambient air quality: MG = $\mu\text{g m}^{-3}$; ME = $\mu\text{mol}_c\text{m}^{-3}$

Cloud interception: MG = mg l^{-1} ; ME = $\text{mmol}_c\text{l}^{-1}$

3. Cloud interception (cm)

Atmospheric Processes

The quantity of precipitation is a daily input. During the winter, NuCM partitions mixed precipitation into rain and snow with the following equation:

$$R = P_T \left\{ (T_{\text{MAX}} - \text{snotmp}) / (T_{\text{MAX}} - T_{\text{MIN}}) \right\} \quad 1$$

This equation only comes into operation when $T_{\text{MIN}} < \text{snotemp}$. When $T_{\text{MAX}} < \text{snotmp}$, all precipitation is snow and when $T_{\text{MIN}} > \text{snotmp}$, all precipitation is rain

Amount of snow in mixed precipitation:

$$S = P_T - R \quad 2$$

The wet deposition of a given solute x is given in equation 3:

$$R_W = 0.01 P_T * P_{\text{CX}} * \text{starea} \quad 3$$

where

R_W = wet deposition ($\mu\text{mol}_c\text{s}^{-1}$)

P_{CX} = concentration of solute x in precipitation ($\mu\text{mol}_c\text{l}^{-1}$) monthly input in air file

Equation 3 is also used to calculate deposition from cloud water, P_T being replaced by the amount of water being condensed from clouds (monthly input in air file) and P_{CX} being the concentration of solute x in cloud water (monthly input in air file).

Dry deposition is given in equation 4;

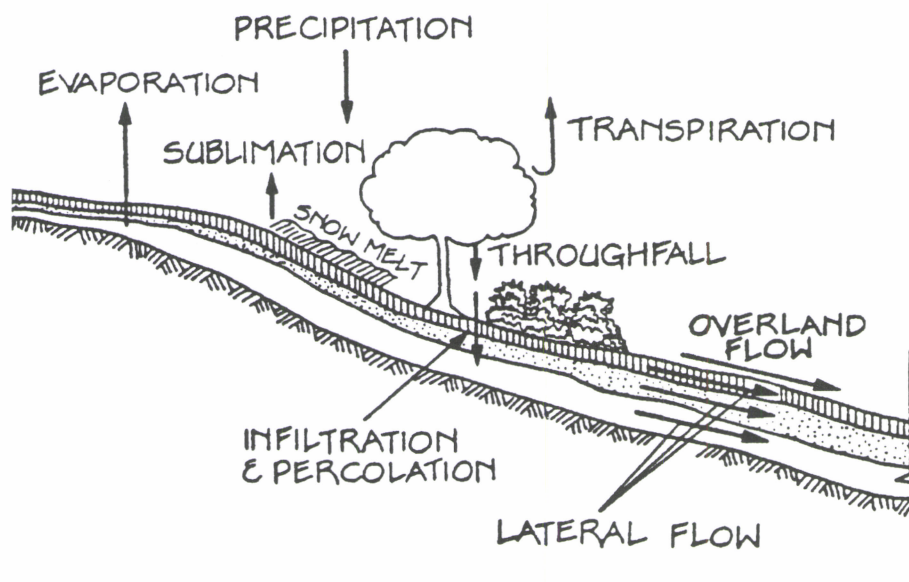
$$R_D = 0.01 * coelfc * partdv * M_{AX} * laic * starea \quad 4$$

where

R_D = deposition rate ($\mu\text{mol}_c\text{s}^{-1}$)

Hydrological Processes

Figure 1. Overview of hydrological processes simulated by NuCM (after Munson and Gherini, 1991)



Interception and Throughfall

The first surface the precipitation hits is the tree canopy. Rainfall can be intercepted and stored on the canopy allowing chemical reactions to occur. Snowfall is assumed not to be intercepted or stored and is routed straight to the soil in NuCM. The potential interception storage defines the canopy's capacity to hold water and is given in equation 5:

$$S_I = (laic/LAIC_{MAX})cimax \quad 5$$

where

S_I = potential interception storage (cm day^{-1})

$LAIC_{MAX}$ = maximum leaf area index in year (max. value of lai)

If rainfall(R) is intercepted by the canopy and some is retained by the canopy at the end of the previous time step, the actual amount of water intercepted is:

$$S_A = S_I - S_T \quad 6$$

where

S_A = actual amount of water that can be intercepted (cm day⁻¹)

S_T = amount of interception storage retained at time t (cm day⁻¹)

If rainfall is greater than S_A , throughfall (T) will result:

$$T = R - S_A \quad 7$$

The interception storage is then updated to account for the additional increment.

Potential Evapotranspiration

Potential evapotranspiration is defined as the maximum evapotranspiration possible for a given timestep under the prevailing meteorological conditions. It is based on work by Hargreaves, 1974 and is given in equation 8:

$$ET_p = (F_{et}/n)(T_{MEAN} * s_{coeff} * H_c) \quad 8$$

where

ET_p = daily potential evapotranspiration (mm day⁻¹)

F_{et} = evapotranspiration factor for the month (mm °F⁻¹ month⁻¹) see equations 10-11

n = number of days in month

H_c = humidity correction factor (unitless) see equations 9

$$H_c = 0.166 (100 - rh)^{0.5} \quad (\text{for } H \geq 64\%) \quad 9$$

$$H_c = 1 \quad (\text{for } H < 64\%)$$

F_{et} is a function of latitude and the season of the year. The mean annual value F_{et} is given in equation 10a & b:

$$F_{et} = 2.322 - 0.0115 \text{ xlat}, \text{ xlat} \leq 35 \text{ °N} \quad 10a$$

$$F_{et} = 3.434 - 0.0434 \text{ xlat}, \text{ xlat} > 35 \text{ °N} \quad 10b$$

F_{et} for each month can be calculated using a Fourier model.

$$F_{et} = \bar{F}_{et} + \sum_{k=1}^2 [A(K) \cos((\pi MK) / P) + B(K) \sin((\pi MK) / P)] \quad 11$$

where

k = harmonic number 1 or 2

M = month of year

P = total number of months

The Fourier coefficients are a function of latitude and are determined using the following relationships.

$$\begin{aligned} A(1) &= 0.037 - 0.03238 \text{ xlat, if xlat} > 35 \text{ }^\circ\text{N} \\ A(1) &= 0.8235 - 0.0034 \text{ xlat, if } 35 \text{ }^\circ\text{N} \leq \text{xlat} \leq 45 \text{ }^\circ\text{N} \\ A(1) &= -1.741 + 0.0118 \text{ xlat, if xlat} \geq 45 \text{ }^\circ\text{N} \end{aligned}$$

$$\begin{aligned} A(2) &= -0.1042 + 0.0033 \text{ xlat, if xlat} < 29 \text{ }^\circ\text{N} \\ A(2) &= -0.2332 + 0.0077 \text{ xlat, if xlat} \geq 29 \text{ }^\circ\text{N} \end{aligned}$$

$$\begin{aligned} B(1) &= -0.57 - 0.0015 \text{ xlat} \\ B(2) &= -0.045 + 0.0017 \text{ xlat} \end{aligned}$$

ET_p can then be adjusted up or down by an evaporation calibration coefficient (ecoeff) which accounts for local microclimatological characteristics such as wind, elevation etc. The aspect angle (aspect) of the forest stand is also taken into account as shown in equation 12.

$$ET_{p(\text{adj})} = ET_p * \text{ecoeff} * (0.4 + \sin(\text{aspect} * \pi/360)) \quad 12$$

A southward facing slope with aspect = 180 ° gives the sine function a maximum, whereas a northward facing slope gives a minimum.

As mentioned previously, this potential evapotranspiration will be satisfied first from intercepted water stored on the canopy and if still unsatisfied, from uninfiltreated water on soil surface and then from the soil layers.

All soil moisture (thet) above field capacity (thetfc) is available for the process of evapotranspiration. The distribution of evapotranspiration among the soil layers is determined by the fraction of roots in each layer (physiographic parameter). When the soil moisture is below field capacity, the actual evapotranspiration is reduced exponentially between field capacity and zero moisture content:

Snowpack

The formation of a snowpack slows down the infiltration of water into the soil system. Abiotic and microbial reactions take place in the soil under the snowpack, but since the flow of water into the soil is limited, the concentrations of the products of these reactions increase. These products are rapidly leached from the soil when snowmelt occurs.

Both increasing air temperature and rainfall can cause snow to melt. The rate of air temperature induced snow melting is given in equation 13 for open areas and deciduous forest (M_O) and in equation 14 for coniferous forest (M_C):

$$M_O = \text{osmrat} ((T_{\text{MEAN}} + \text{tcoef}) - \text{snotmp})^{1.25} (0.4 + \sin(0.00087\text{aspect})) \quad 13$$

$$M_C = \text{fsmrat} (T_{\text{MEAN}} - \text{snotmp})^{1.25} (0.4 + \sin(0.00087\text{aspect})) \quad 14$$

Rain induced melting is shown in equation 15:

$$M_R = \text{rsmrat}((T_{MAX} - \text{snotmp})/2) T \quad 15$$

where

M_R = rain induced melting rate (cm day⁻¹)

The water equivalent depth of the snow pack is calculated in equation 16:

$$D_S = S_E + S - (S_S + S_M) dt \quad 16$$

where

D_S = water equivalent snowpack depth (cm water)

S_E = water equivalent snowpack depth at end of previous time step (cm water)

S_S = snow sublimation rate (cm day⁻¹)

S_M = rate of snowmelt (cm day⁻¹) see equation 17

$$S_M = (M_O^* + M_R) - ((pcstor - \theta)/dt) S_E \quad 17$$

where

θ = liquid water content of snow in decimal fraction of total volume

M_O^* either M_O or M_C .

As the air induced snow melting is calculated differently for open/deciduous and coniferous areas, an average value of S_M must be calculated for a heterogeneous stand and then used in equation 16.

The general equation for snow sublimation S_S is the physiographic parameter snow sublimation rate for open, deciduous or coniferous area multiplied by the timestep multiplied by the fraction of area covered with open, deciduous or coniferous forest. An example of snow sublimation from a coniferous area is given in equation 18, which is taken straight out of program file CLD4.FOR.

$$\text{SUBC} = \text{DMIN1}(\text{SNOCOV}, \text{snosbf} * \text{TIMSTP}) * \text{pcconf} \quad 18$$

where

SUBC = sublimation of snow in coniferous canopy during this timestep (cm³ cm⁻²)

DMIN1 is a FORTRAN command to take the smallest value of (x1, x2)

SNOCOV = net snowcover thickness on ground expressed in terms of water content per unit area (cm³ cm⁻²)

$$S_S = \text{SUBO} + \text{SUBD} + \text{SUBC} \quad 19$$

where

S_S = total sublimation

Surface runoff occurs when the top soil layer is frozen or saturated. When the depth of water on the surface (D) exceeds the maximum detention storage on the land surface (D_O), surface runoff is generated :

$$R_S = (\text{scwidth}(D - \text{dtsmax})^{5/3} S^{1/2})/nn \text{ for } D > D_0 \quad 20$$

where

$$R_S = \text{surface runoff (cm}^3\text{s}^{-1}\text{)}$$

The mass balance equation for surface runoff is:

$$T_M - R_S = \text{scarea (dD/dt)} \quad 21$$

where

$$T_M = \text{throughfall + snowmelt (cm}^3\text{s}^{-1}\text{)}$$

Soil Hydraulics

The movement of water through the system is simulated using the continuity equation, Darcy's equation for permeable media flow and Manning's equation for free surface flow. Water that infiltrates the soil (see figure 2) can contribute to

- increase soil moisture
- become lateral flow
- satisfy evapotranspiration
- percolate to the next layer

The model divides the soil up into layers (maximum 10). For the Lth layer, conservation of mass (continuity equation) requires that:

$$\text{scarea(L) thick(L) dTHET(L)/dt} = \text{scarea (L-1)P(L-1)} - \text{scarea(L)*(ET}_p\text{(L) + P(L))} - \text{L(L)} \quad 22$$

where

THET(L) = average volumetric moisture content of layer L

P(L-1) = percolation from layer over L (cm s⁻¹) (see equation 23)

L(L) = lateral flow from layer L (cm³s⁻¹) (see equation 24)

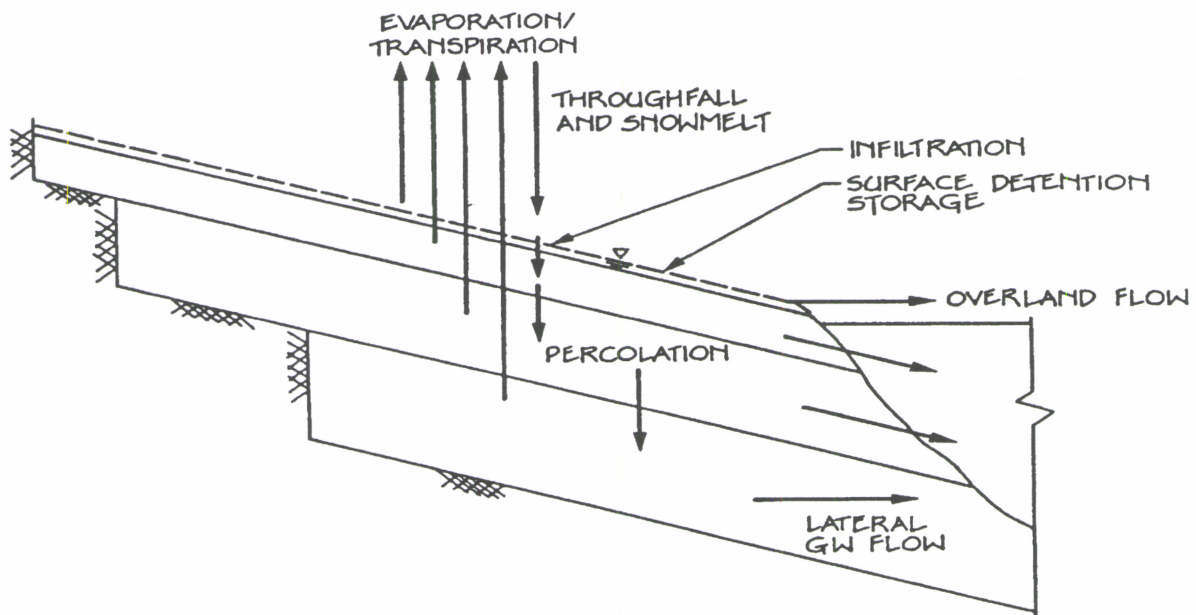
*

Percolation (P) is described by the following equation:

$$P(L) = \text{perm(L) * ((THET(L) - thetfc(L))(thets(L) - thetfc(L)))} \quad 23$$

This equation is a simplified version of Darcy's law. P(L) = 0, when soil moisture is equal to or lower than field capacity. In-between field capacity and saturation, percolation is an increasing fraction of the saturated hydraulic conductivity. When soil moisture equals saturated moisture content, the percolation becomes equal to the saturated hydraulic conductivity.

Figure 2. Idealised representation of hydrologic flow routing in NuCM (after Gherini et al., 1985)



Lateral flow is generally only occurring when soil moisture is over saturation. However it is possible for the soil moisture to be distributed nonuniformly with depth in the soil layer. For example, if there is a large reduction of surface areas between layers and a saturated condition in the next lower layer, then although the average moisture content of layer L is less than θ_{fc} , a temporary saturated zone may be formed:

$$L(L) = \text{perm}(L) * \text{scwidth} * F_R * Z_S \quad 24$$

where

F_R = vertical depth over the horizontal distance for flow

Z_S = equivalent saturation depth approximated in next equation

$$Z_S = \text{thick}(L) * ((\theta(L) - \theta_{fc}(L))(\theta_{s}(L) - \theta_{fc}(L))) \quad 25$$

Equation 25 is established for each soil layer. $P(L-1)$ is the infiltration rate for the very top soil layer. If the bedrock is assumed to be impermeable, then the value for $P(L)$ in

the bottom layer is zero. If $P(L)$ is higher than the potential in the next lower layer to receive water, iterative corrections need to be made in overlying layers since equation 22 is not coupled between soil layers.

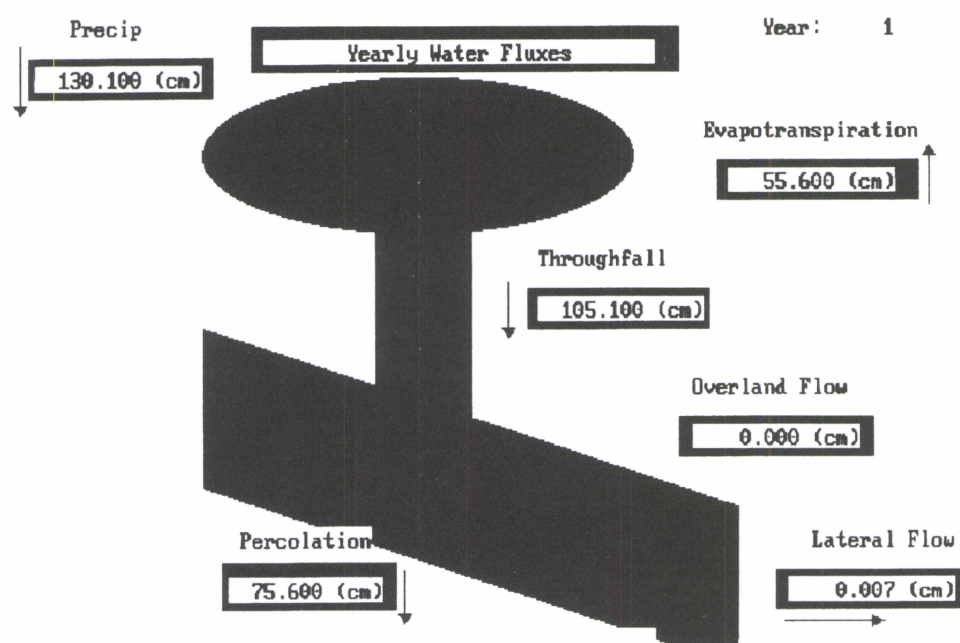
Hydrology Simulation results

NuCM shows the following list of output diagrams and files (see table 4). The hydrological tree is a summary of the hydrology for a year (see figure 3). The soil solution chloride concentration versus time plot shows how downward percolation is simulated. The idea is to compare observed soil Cl concentration data with the simulation. However one hardly ever measures daily chloride concentrations in soil. In addition chloride is not conservative over short time periods. Soils with high porosity can keep chloride until soil is totally saturated, while other chloride percolates down through macropores. It is therefore necessary to check the hydrology result file, (the H2O file) for more details of the hydrology simulation.

Table 4. Hydrology Output Options

1	Tree
2	Instantaneous lateral flow vs. time plot
3	Instantaneous stream flow vs. Time plot
4	Soil solution chloride concentration vs. Time plot
5	Stream chloride concentration vs. time plot
6	Observed and simulated vs. Time plot
7	Store output data to ASCII file for subsequent analysis

Figure 3. Example of hydrology tree diagram showing annual results



A print out of the hydrological result file, NORDMOEN.H2O is shown in figure 4. for a monthly timestep. One should note that the format is different for October (no snow) and November (snow occurs).

Figure 4. A printout of the first 2 months of NORDMOEN.H2O.

OCTOBER

```
2.179E+01 0.000E+00 0.000E+00 1.211E+01 0.000E+00 2.179E+01 2.082E+01
2.179E+01 2.082E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
9.990E+02
3.834E+03 1.225E+04 7.388E-01 1.300E-04 5.817E+00 3.853E-01 4.497E-01
2.878E-01 3.532E-01 3.712E-01 2.048E+01 2.043E+01 2.035E+01 2.031E+01
0.000E+00
```

NOVEMBER

```
1.102E+01 1.162E-01 0.000E+00 1.457E+01 0.000E+00 1.102E+01 1.102E+01
1.102E+01 1.112E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
5.000E-03
2.074E-02 6.065E+03 4.293E+03 0.000E+00
2.084E+03 6.675E+03 1.332E-04 7.161E-05 1.308E+01 3.904E-01 4.475E-01
2.876E-01 3.527E-01 3.956E-01 1.112E+01 1.114E+01 1.116E+01 1.119E+01
0.000E+00
```

October's results are listed below, for the numbering read each row left to right. The block letter acronym is the name for the result used in the chemistry model program codes.

Results 1 -11 are depths of water (cm)

1. PREC, Precipitation on canopy
2. SNOC, snowfall on canopy
3. DI(1), Overstory canopy storage (deciduous)
4. CI(1), Overstory canopy storage (coniferous)
5. OI(1), Overstory canopy storage (open)
6. AD(1), Overstory throughfall (deciduous)
7. AC(1), Overstory throughfall (coniferous)
8. AO(1), Overstory throughfall (open)
9. PWATER, Infiltration
10. OVFLOW, Overland flow
11. DTSTOR, Surface detention

12-14 stream results

15. 9.99 E+05 is shown, which signalises there is no snow cover and snow results 16-19 are missing

20- 24 FLOW, Lateral flow volume (cm³) Layer 1 - 5

25 - 29 THETA, Volumetric water content of each layer (%) Layer 1 - 5

30 - 34 INFIL, Percolation (cm) Layer 1-5

October and November are identically set up apart from the snow results 15 - 20.

15. SNOCOV, Snow cover (cm water equivalent)

16. SUBLIM, Sublimation (cm)

17. PAKVOL, Gross snowpack volume (cm³)/1000

18. SNOOUT, Total volume of snow melted in a timestep (cm³)/1000

19. FWCONT, Residual volume of melted water remaining trapped in the snowpack (cm³)/1000.

Comments on the Hydrology Simulation

One cannot evaluate the hydrology simulation in detail, without analysing the H2O file. This file is intended as a summary of hydrological information to run the chemistry simulation and is therefore set up in a very user unfriendly format. However it is possible to change values here. For example, I changed percolation monthly values to those simulated by the SOIL model.

I have been running the chemistry simulation on a monthly timestep, as my lysimeter data is at this timestep. However the snow results seem to be accumulated wrongly for a month and for sites with snow, it is probably better to simulate at a daily chemical timestep.

Chemistry Simulation

Parameters used in Chemical processes

The following parameters are required as input for the chemistry simulation. Table 5 shows biomass characteristics, Table 6 soil chemistry characteristics, Table 7 equilibrium constants and Table 8 rate coefficients. The same presentation form is used as described in the text above Table 1.

Table 5. Biomass Characteristics.

No.	Description	Units	Parameter name in source code	Used in equation	Menu no.
39	Standing biomass	kg m ⁻²	stand/d/c/o (3)		b10
40	Root biomass	kg m ⁻²	rtbio/d/c/o (3)		b10
41	Conversion factor from leaf surface area to leaf dry weight	g cm ⁻²	const/d/c/o (3)	28,32,98	b10
42	Active respiration	mgC cm ⁻² s ⁻¹	resp/dg/cg/og (3)	76	b10
43	Maintenance respiration	mgC cm ⁻² s ⁻¹	resp/dm/cm/om (3)	76	b10
44	Monthly uptake of trees (Jan. - Dec.)	year ⁻¹	udist/d/c/o (36)	33,76	b20
45	Monthly litterfall rate (Jan. - Dec.)	kg m ⁻² month ⁻¹	lf/d/c/o (36)	41	b25
46	Fraction of annual translocation for the month (Jan. - Dec.)		tdis/d/c/o (36)	31	b30
47	Fraction of current ion storage to be translocated N, Ca, Mg, K, Na, S, Cl, P		tlloc/d/c/o (8)	32	b30
48	Dry surface collection efficiency		colef/d/c/o (3)	4	b40
49	Wet surface collection efficiency		(3)		b40

50	Leaf chemical composition N, Al, Ca, Mg, K, Na, S, Cl, P, C, S	mg g ⁻¹	lfcmp/d/c/o (33)	28,34,98	b50
51	Bole chemical composition N, Al, Ca, Mg, K, Na, S, Cl, P, C, S	mg g ⁻¹	trcmp/d/c/o (33)	35	b55
52	Root chemical composition N, Al, Ca, Mg, K, Na, S, Cl, P, C, S	mg g ⁻¹	rtcmp/d/c/o (33)	36	b56
53	Uptake limits for nutrients		uplimit lowlimit		b60
54	Monthly particle deposition velocities (Jan. - Dec.)	cm s ⁻¹	partdv (12)	4	
55	NO _x & SO _x monthly deposition velocity (0-2) (Jan. - Dec.)	cm s ⁻¹	gasdv (12)	4	b70
56	NO _x & SO _x monthly uptake velocity (0-2) (Jan. - Dec.)	cm s ⁻¹	gasuv (12)	27	b70
57	Deposition loading factors		depfac		b80

Table 6. Soil Chemistry characteristics

No.	Description	Units	Parameter name in source code	Used in equation	Menu no.
58	Fraction of immediately leachable ions in litterfall		frlch(1)		s5
59	Fraction of S & N that mineralise when fine litter/humus decomposes into humus/fulvic acid, i.e. fraction not incorporated into organic acid		frlch(2)		s5
60	Fraction of S & N that is incorporated into organic acid during humus decay		frlch(3)	54	s5
61	Amount of N in organic acid	mole N mol ⁻¹ acid	oaln	53,55	s5
62	Amount of S in organic acid	mole S mol ⁻¹ acid	oals	(53)	s5
63	Amount of C in organic acid	mole C mol ⁻¹ acid	oalc	(53),96	s5
64	Weight fraction of litter in top soil layer		xlit	40,63,99	s5
65	Weight fraction of fine litter in top soil layer		fines	(40,63), 99	s10
66	Weight fraction of humus in top soil layer		humus	(40,63)	s10
66	number of primary minerals (max.4)		nmnrls (4)		s10
67	Mineral molecular weight	g mol ⁻¹	mnmwt (4)	80	s10
68	Dissolution Stoichiometry NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , DOC, DIC, SiO ₂	mmol _c mol ⁻¹ weathered	mnwth (52)	81	s20
69	CEC	mmol _c 100g ⁻¹	cec (L)	58,85	s30

70	Bulk density of soil layer	g cm^{-3}	dnsity (L)	40	s30
71	% by weight of each mineral type		slcomp (4*L)	64,79	s30
73	Decide gibbsite dissolution/precipitation option		naloh3		s40
74	Soil CO ₂ gas concentration factor		pco2 (L)		s40
75	Uptake distribution of nutrients in layer NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , SiO ₂		disun (11*L)	38,39	s50
76	Cations % held on CEC NH ₄ , H, Al, Ca, Mg, K, Na		adscat (7*L)	58, 83-85	s60
77	Adsorbed anions, SO ₄ , PO ₄ , DOC	$\text{mmol}_c \cdot 100\text{g}^{-1}$ $\text{mg } 100\text{g}^{-1}$	adscat (3*L)	86-89	s60
78	Dissolved ions in soil solution NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , NO ₃ , Cl, PO ₄ , SiO ₂ , DOC, DIC	$\mu\text{mol}_c \cdot \text{l}^{-1}$ mg l^{-1}	solion (12*L)	56,57,67, 69,78,82 -89	s70

Table 7. Equilibrium constants.

No	Description	Units	Parameter name in source code	Used in equation	Menu no.
79	Carbonate equilibrium constants H ₂ CO ₃ *, pka HCO ₃ , pka H ₂ O, pkw Henry's Law constant, CO ₂ (g), logkH	mol l^{-1} mol l^{-1} mol l^{-1} atm	kc1 kc2, kw kh		E10
80	Aluminium equilibrium constants Gibbsite solubility constant, logkso Al ³⁺ + H ₂ O = Al(OH) ²⁺ + H ⁺ , logk1 Al ³⁺ + 2H ₂ O = Al(OH) ₂ ⁺ + 2H ⁺ , logk2 Al ³⁺ + 4H ₂ O = Al(OH) ₄ ⁻ + 4H ⁺ , logk4 AlR = Al ³⁺ + R ³⁻ , logkR		kso kal1 kal2 kal4 kar1	90 92 (92) (92) 93	E20
81	Organic acid equilibrium constants, pka H ₃ R = H ₂ R ⁻ + H ⁺ H ₂ R ⁻ = HR ²⁻ + H ⁺ HR ²⁻ = R ³⁻ + H ⁺		kr1 kr2 kr3	94	E30
82	Cation exchange coefficients			83	E40
83	SO ₄ adsorption, C half saturation constant Emax, max. adsorption capacity		b2(L) emax (L)	86	E50
84	PO ₄ adsorption- linear constant				E60
85	Organic anion adsorption- linear constant				E60

Table 8. Rate coefficients

No.	Description	Units	Parameter name in source code	Used in equation	Menu no.
86	Annual vegetation growth v. time	kg m ⁻² year ⁻¹	grow/d/c/o (3)		R10
87	Number of years to stand closure	years	close/d/c/o (3)		R15
88	Current stand age	years	age/d/c/o (3)		R15
89	Foliar exudation rate (jan-dec)	day ⁻¹	beta/d/c/o (36)	28	R20
90	Foliar exudation amplification factor NH ₄ , Al, Ca, Mg, K, Na, SO ₄ , Cl, PO ₄ , SiO ₂		exdamp, excamp, exoamp (30)	28	R30
91	Foliar leaching rate constant	year ⁻¹	leach/d/c/o (3)	29	R40
92	Foliar leaching rate dependence on H ⁺ ion (0-0.5)		alfa/d/c/o (3)	29	R40
93	litter breakdown rate constant	year ⁻¹	lbrate	45	R50
94	fine litter to humus breakdown rate constant	year ⁻¹	fbrate	(45)	R50
95	humus to fulvic acid breakdown rate constant	year ⁻¹	hbrate	(45)	R50
96	organic acid breakdown rate constant	year ⁻¹	oarate	68	R50
97	Microbial C:N ratio (5-80)		mcton	47	R50
98	Nitrification rate on canopy	day ⁻¹	vnh4	26	R60
99	Denitrification rate for soil	day ⁻¹	fdnit	74	R60
100	Nitrification rate for soil	day ⁻¹	ckvnh4	70	R60
101	Snowmelt nitrification rate	day ⁻¹	snitr		R60
102	rate dependence of the weathering rate on H ⁺ ion (n)		wexp (5*L)	79,91	R70
103	specific reaction rate constant	(year ⁻¹)* (L μmol _c ⁻¹) ⁿ	ckmnr1 (5*L)	79	R70

In addition, the following symbols are used frequently in the description of the chemical processes.

L = layers, 1-?, decided by parameter inputs

NMI = number of minerals

I = element/ion

ALK refers to alkalinity

OACD refers to total organic acid/DOC (H2ORG)

MOACD refers to **mass** of total organic acid/DOC (H2ORG)

OAAL refers to organic Al

Chemical Processes

Canopy Processes

The tree canopy is the first surface where chemical and biological reactions can occur that alter the dry and wet intercepted deposition and produce the resulting throughfall. The following processes are described in the order given in CLDLEAF.FOR.

Foliar oxidation/nitrification

Ammonium deposited on the canopy can be oxidised to form nitrate as shown below:



A first order rate expression is used to simulate this nitrification process:

$$-d(\text{NH}_4^+)/dt = -v_{\text{nh4}} * 1.02^{(\text{T}_{\text{MEAN}} - 20)} * \text{NH}_4^+ \quad 26$$

where

left hand term is the decrease of ammonium on the canopy in $\mu\text{mol}_c\text{day}^{-1}$

NH_4^+ = amount of ammonium present on canopy (μmol_c)

The amount of ammonium oxidised is subtracted from the original NH_4^+ present, added to the original NO_3^- present and twice this amount is subtracted from the alkalinity present (production of 2 hydrogen ions).

Dry and Wet Deposition Accumulation

Equation 4 described under atmospheric processes is calculated next. The monthly deposition velocities are of 2 types, one for the gases NO_x and SO_x and the other for all other particles. Wet deposition is calculated by equation 3 and then pH is calculated by the pHSILLEN procedure. The sum of each species is calculated from the nitrification, wet and dry depositions.

Exudation

SO_x and NO_x gases are first absorbed from the atmosphere into the canopy in the form of NH_4 and SO_4 using a similar equation to equation 4.

$$\text{Absorbed X} = (0.01 * \text{gasuv} * \text{laic} * \text{timstp} * \text{starea} * M_{\text{AX}}) / 1 + \text{E06} \quad 27$$

where

Absorbed X = amount of SO_x or NO_x absorbed (μmol_c)

This absorbed NH_4 and SO_4 is first used to satisfy the potential uptake associated with the leaves (litterfall) and then to satisfy the sum of the potential uptake for the bole and roots. If there is any left after this, it will be added to the amount exuded.

Exudation is thought to be driven by internal processes taking place within the leaf. The rate of exudation is a proportional to the chemical composition of the leaf, a chemical species amplification factor, and the leaf area index.

$$E(I) = (\text{betac} * \text{excamp}(I) * \text{lfcmpc}(I) * \text{constc} * \text{laic} * \text{starea})/86400 \quad 28$$

where

$E(I)$ = the exudation rate of ionic species I ($\mu\text{mol}_c \text{ s}^{-1}$)

The exuded amount of a species (EXU) in a timestep is the minimum of the leaf content or EXU. The final section of the exudation procedure adjusts the biomass alkalinity to account for exudation.

Foliar Leaching

Intercepted water is stored on leaf surfaces before being evaporated. Depending on the length of time of storage and the acidity of the stored solution, it is possible for some of the nutrients to be actively leached from the leaves.

The LEACH.FOR procedure must first calculate the pH of the water stored on the leaves.

NuCM uses a rate expression dependent on the hydrogen ion concentration to represent foliar leaching.

$$\text{TLCH}(I) = 10^{-3} * \text{leachc} * [\text{H}^+]^{\text{alfad}} * \text{BIOSTc}(I) \quad 29$$

where

TLCH = foliar leaching of species I (mmol_c)

BIOSTc = biomass associated with leaf (mmol_c) (see equation 98)

The exuded and leached amounts are added to the previously accumulated values.

The amount of a species I washing off in the throughfall (WASH(I)) in a coniferous stand:

$$\text{WASH}(I) = (\text{ACCC}(I) * \text{AC})/\text{CTH2O} \quad 30$$

where

ACCC = accumulated amount of species I on leaf

AC = throughfall depth at this time step ($\text{cm}^3\text{cm}^{-2}$)

CTH2O = total water depth available = AC + CI (water storage on canopy)

The total throughfall and wet deposition fluxes are then calculated. The pH is then determined in the throughfall by the pHILLEN procedure. Finally CO_2 absorption by the intercepted water is accounted for.

Translocation

The subroutine TRANSL removes nutrients from leaves during senescence and before abscission. Nutrients are stored in a reserve, TRANSD. This subroutine only works for **deciduous** trees, although this important fact is omitted in the manual and help screens.

$$\text{DECD} = \text{tdistd} * \text{TIMSTP} * \text{TLFD} \quad 31$$

$$\text{TFRACT}(I) = \text{DECD} * \text{tlocd}(I) * \text{BIOSTd}(I)/(\text{laid} * \text{constd}) \quad 32$$

where

BIOSTd = mass of ion associated with leaf (mmol_c) (see equation 98)

The charge balance of the biomass and stored translocation reserve is checked. This monthly amount of translocated ion, which is removed from the litterfall (TFRACT) is stored in the reserve, TRANSD and is subtracted from BIOSTd.

In the subroutine TBACK, nutrients, if available are taken from the translocation reserve. If the potential uptake for leaf (ULIFD) is less than TRANSD, the remaining TRANSD after the timestep = TRANSD - ULIFD and the new ion leaf biomass = ULIFD + BIOSTd. Otherwise if potential uptake > TRANSD, the entire TRANSD reserve is used up and the new ion leaf biomass = TRANSD + BIOSTd.

Uptake

The potential uptake is calculated by the subroutine CALUPD.FOR for each of the 3 areas, deciduous, coniferous and open. The calculation of the coniferous potential uptake (fraction of yearly uptake) is given as an example.

$$\text{CONF} = \text{udistc}(\text{MNTH}) * \text{timstp} * \text{pconf} * \text{scaea} \quad 33$$

Potential leaf uptake for individual species I, ULIFC(I) to satisfy litterfall, foliage growth and exudation (EXUC):

$$\text{ULIFC}(\text{I}) = (\text{CONF} * \text{TLFC} * \text{lfcmpc}(\text{I})) + (\text{XGROWC} * \text{lfcmpc}(\text{I})) + \text{EXUC}(\text{I}) \quad 34$$

where

XGROWC = growth factor for coniferous foliage (calculated in GROW.FOR subroutine)

The potential uptake to satisfy bole (UGTRC) and root growth (UGRTC) are calculated in similar ways:

$$\text{UGTRC} = \text{CONF} * \text{PRODC} * \text{BOLEC} * \text{trcmpc} \quad 35$$

$$\text{UGRTC} = \text{CONF} * \text{PRODC} * \text{ROOTC} * \text{rtcmpc} \quad 36$$

where

PRODC = annual vegetation growth

BOLEC = trunk fraction of trunk and root

ROOTC = root fraction of trunk and root

Finally the potential demand for NH_4 (UPDNC) and SO_4 are calculated by simply adding up the whole tree's demand e.g.:

$$\text{UPDNC} = \text{ULIFC} + \text{UGTRC} + \text{UGRTC} \quad 37$$

The actual uptake is described in 5 different FORTRAN programs spread over 20 pages of programming. A description of all the equations would take too long and therefore a description of the main points and the subroutine's purpose is more useful.

The main subroutine is UPTAKE, which calls the following programs; TBACK, ROOT (which calls NUPTKE and NTAKE), LFUPTAKE, TRUPTAKE, EXCESS and CUPTAKE.

UPTAKE.FOR itself is called by PROSOC.FOR, the main soil simulation program. It begins by checking that there are roots in the actual layer or in terms of input parameters, that $etwght$, the root distribution factor for layer L is greater than 10⁻⁸. If it is not, the program returns to PROSOC. If roots are present, the leaf's, trunk's, and root's demand and translocation uptake are zeroed for the new month and ion. If the conditions for deciduous translocation are met, TBACK is called, which uptakes nutrients from translocation reserves.

NuCM first uptakes nutrients to satisfy the potential leaf demand and then, if nutrients are still available to satisfy the potential trunk and root demand.

ROOT is called for leaf uptake. The amount of nutrient uptake satisfied by absorption for NH_4 (ABN) and SO_4 is calculated. The demand for N (DN) is calculated:

$$DN = DEMAND(MNH4) * disun(MNH4,L) - ABN + DEFICIT(MNH4) \quad 38$$

where

DEMAND = UPDN (potential uptake/demand for NH_4)

DEFICIT = amount of NH_4 missing to satisfy potential uptake from last timestep

NUPTKE is called by ROOT. Its purpose is to compute the potential amount of N to be taken up by the tree depending on the amount available in the soil. The amount of NH_4 and NO_3 that can be withdrawn from solution is calculated. If demand is greater, NH_4 can be withdrawn from CEC. If demand is still not met, N is limiting and the minimum limit for uptake (parameter input) is checked and the program returns to ROOT. Here the uptake of all other nutrients except N are calculated. Their demand, and satisfaction by absorption (SO_4), translocation (only deciduous trees), from soil solution and CEC is calculated. If a nutrient should become totally depleted, the simulation stops and an error message is generated telling time, which layer and which nutrient is deficient. Otherwise the shortage/excess of nutrient is calculated and the actual amount removed from solution allowing for limitations. The nutrients are now subtracted from the soil solution and CEC and placed ready in a flux for biomass distribution. The alkalinity of the soil is adjusted.

NTAKE is now called. Its purpose is to compute the actual amount of N to be taken up by the tree, having considered possible limiting nutrients. The program returns to UPTAKE, where assuming no nutrient limitation, ROOT is called for trunk and root uptake. Here the demand by the trunk/root (DTRUNK) is defined as:

$$DTRUNK(I,M) = DTRUNK(I,M) + (UGTR(I,M) + UGRT(I,M)) * disun(I,L) \quad 39$$

The same sequence of processes occurs. In addition now that the whole tree's potential has been calculated against what is available in the soil, excess nutrient in solution can be calculated. Finally the program returns to UPTAKE, where the next set of processes occur if there are no roots in layer L or one has reached the lowest layer.

LFUPTAKE is called, which adds leaf nutrient to appropriate leaf biostorage variables.

TRUPTAKE is called, which adds nutrient uptake to root and trunk biomasses.

If excess ions in solution, EXCESS is called. Its purpose is to compute luxury uptake to an upper limit designated by the user as a parameter input.

CUPTAKE is then called, which uptakes C to total tree system from atmospheric CO_2 . This C uptake can be limited by deficiency of other nutrients but it is assumed that CO_2 is always plentiful.

Finally the new biomass is summed and the growth of the stand for the timestep is simulated.

Litterfall, litter decay and (de)nitrification

Various parameters involved in calculating litterfall are defined and zeroed in the subroutine INITL.FOR. However the subroutine DECAY.FOR called by PROSOC.FOR calculates litterfall and its consequences on weight of the topsoil, litter decay and biomass storage. Firstly the mass of the different groupings (coarse litter(WGTL), fine litter (DWGTF), humus (DWGTH) and minerals) of the organic layer are established e.g.

$$WGTL = xlit * dnsity(1) * thick(1) * scarea(1) \quad 40$$

Then the litterfall during the timestep is established (FALLC):

$$FALLC = lfc * scarea * timstp * pconf \quad 41$$

and the total monthly litterfall (DWGTL) is the sum of the three areas.
This newly fallen litter is added to the weight of the coarse litter:

$$WGTL = WGTL + DWGTL \quad 42$$

The 3 components of litter, WGTL, DWGTF and DWGTH are decayed following rate expressions with first order dependency on the mass of the reactant, e.g. the fraction of coarse litter broken into fine litter is shown in equations 43-45.

$$DWGTF = WGTL * LBFAC \quad 43$$

where

$$LBFAC = 1 - e^{-LBR * TIMSTP} \quad 44$$

$$LBR = lbrate * 1.05^{(soltmp - 12)} \quad 45$$

The new total weight of fine litter (WGTF) in this timestep is calculated:

$$WGTF = WGTF + DWGTF \quad 46$$

The new weights of humus and solutes are calculated in a similar way. However NuCM makes the fine litter decay rate to humus (FBR) dependent on the C:N ratio in the fine litter (FCtoN) compared to a parameter input microbial C:N ratio (mcton). If (mcton)/(FCtoN) is less than or equal to 1, then the rate is reduced:

$$FBR = FBR * [(mcton)/(FCtoN)] \quad 47$$

This gain in litter weight for the top soil layer must be subtracted from the leaf or needle biomass.

Apart from coarse litter C content, the coarse litter ion contents are adjusted for the fraction of immediately leachable ions in newly fallen litter (frlch(1)). The amounts of these ions and their contribution to solute dryweight is also calculated.
The alkalinity of biomass and litter is adjusted.

For NH_4 to SiO_2 (not NO_3 or organic acid)

Now the individual ion contents of the decay fractions are calculated. Coarse litter (CMPLIT) is broken into fine litter (CMPFIN) and the alkalinity of the litter fractions is adjusted.

$$\text{BRK} = \text{CMPLIT(I)} * \text{LBFRAC} \quad \mathbf{48}$$

$$\text{CMPFIN(I)} = \text{CMPFIN(I)} + \text{BRK} \quad \mathbf{49}$$

$$\text{CMPLIT(I)} = \text{CMPLIT(I)} - \text{BRK} \quad \mathbf{50}$$

Fine litter is decomposed into humic materials and dissolved ions in a similar manner. Because S and N can be mineralised when fine litter decomposes to humus (frlch(2)), this fraction is subtracted for NH_4 and SO_4 going to humus and added to the solutes. The humus C, NH_4 and SO_4 content is now decomposed to fulvic acid. If one follows the calculation sequence for N, the mass of N that is being oxidised from the humus in a timestep (HBFRAC is similar to LBFRAC but for humus to fulvic acid).:

$$\text{OXDN} = \text{CMPHUM(MNH4)} * \text{HBFRAC} \quad \mathbf{51}$$

The resulting N mass left in humus:

$$\text{CMPHUM(MNH4)} = \text{CMPHUM(MNH4)} - \text{OXDN} \quad \mathbf{52}$$

The ratio of N (RN) being oxidised divided by the amount of N in organic acid can govern the production of fulvic acid. This is the minimum of the ratios of N or C or S multiplied by the fraction of S and N that is incorporated into organic acid during humus decay.

$$\text{RN} = \text{OXDN} / \text{oa1n} \quad \mathbf{53}$$

$$\text{FA} = \text{DMIN1(RN,RC,RS)} * \text{frlch(3)} \quad \mathbf{54}$$

The amount of N being oxidised minus that being incorporated in fulvic acid:

$$\text{OXDN} = \text{OXDN} - \text{FA} * \text{oa1n} \quad \mathbf{55}$$

The new amount of NH_4 in solution.

$$\text{solion(MNH4,1)} = \text{solion(MNH4,1)} + \text{OXDN} \quad \mathbf{56}$$

The new amount of organic acid in solution is calculated,

$$\text{solion(MOACD,1)} = \text{solion(MOACD,1)} + \text{FA} \quad \mathbf{57}$$

and a new adsorbed H^+ on CEC is calculated:

$$\text{adscat(MH,1)} = (\text{adscat(MH,1)} + (\text{DWGTH} - \text{DWGTSH} - \text{DWGTS})) / 100 * \text{cec(1)} \quad \mathbf{58}$$

where

DWGTH = weight of humus from fine litter decay during this timestep

DWGTSH = weight of solutes (SO₄ & NH₄) decayed from humus during this timestep

DWGTS = weight of fulvic acid produced from humus decay during this timestep

The fluxes of C, NH₄, SO₄, alkalinity, C and organic acid are calculated for humus to fulvic acid and solutes.

The density of the litter and organic layers must then be adjusted:

$$\text{WGTL} = \text{WGTL} - \text{DWGTF} - \text{DWGTSL} \quad 59$$

The new weight of litter equals the original weight minus that broken down to fine litter and solutes.

$$\text{WGTF} = \text{WGTF} - \text{DWGTH} \quad 60$$

The new weight of fine litter equals the original weight minus that decaying to humus.

$$\text{WGTH} = \text{WGTH} - \text{DWGTS} - \text{DWGTSH} \quad 61$$

The new weight of humus equals the original weight minus that decaying to fulvic acid (DWGTS) and that going to solutes (DWGTSH).

$$\text{WEIGHT}(1) = \text{WGTL} + \text{WGTF} + \text{WGTH} + \text{WGTM} + \text{WGTI} \quad 62$$

where

WGTM = weight of minerals

WGTI = weight unaccounted for (inorganic components) (only calculated if the fractions of minerals, coarse litter(xlit), fine litter (fines) and humus (humus) add up to less than 0.99)

The new fractions xlit, fines, humus and minerals (slcomp) are now calculated.

$$\text{xlit} = \text{WGTL} / \text{WEIGHT}(1) \quad 63$$

$$\text{slcomp}(\text{NM}, 1) = \text{slcomp}(\text{NM}, 1) * \text{WGT0} / \text{WEIGHT}(1) \quad 64$$

where

WGT0 = weight of layer 1 before this time step

Finally a new density is calculated.

The contribution of non-structural ions in litter to soil solution is calculated. If there is water (DEPTH) infiltrating layer 1 then the amount of ion washed out is equal to the fraction of available ions in litter for leaching multiplied by this exponential expression, which increases with increased water volume:

$$\text{WSHLIT} = \text{LITION}(I) * (1 - \text{DEXP}(-0.05 * \text{DEPTH})) \quad 65$$

The remaining available ions for leaching in litter:

$$\text{LITION(I)} = \text{LITION(I)} - \text{WSHLIT} \quad 66$$

The new solution ions:

$$\text{solion(I)} = \text{solion(I)} + \text{WSHLIT} \quad 67$$

The alkalinity of the washed out ions, LITION and SOLION and fluxes are then calculated.

The decay of organic acids to inorganic carbon, NH_4 , H and SO_4 occurs in all layers of the soil. This is programd as a **zero-order reaction** (equation 68), **even though the manual implies it is first-order.**

$$\text{ABFRAC} = \text{orate} * (1.05^{(\text{soltmp(L)} - 23)}) * \text{TIMSTP} \quad 68$$

The oxidation of organic acid is calculated,

$$\text{OAOXD} = \text{solion(MOACD, L)} * \text{ABFRAC} \quad 69$$

and this amount multiplied by the content of the element in organic acid is added to the solution for C, alkalinity, NH_4 , SO_4 and subtracted for organic acid. The fluxes are also calculated.

Nitrification is carried out by calling the subroutine, NITRFY.FOR.

Equation 70 integrates the rate of nitrification during the timestep and has its maximum rate at 20°C.

$$\text{VMAX} = \text{ckvnh4} * (1.1^{(\text{soltmp} - 20)}) * \text{TIMSTP} \quad 70$$

The Michaelis-Menton reaction rate occurs only at $\text{pH} \geq 2$:

$$\text{V} = \text{VMAX} * \text{NH4CNC} / (\text{RKS NH4} + \text{NH4CNC}) \quad 71$$

where

$$\text{NH4CNC} = [\text{NH}_4]$$

RKS NH4 = half saturation constant, $[\text{NH}_4]$ where the rate of conversion is half the maximum = 0.1 (in BLOCKDAT.FOR)

Equation 72 calculates the mass of NH_4 oxidised.

$$\text{OXNH4} = \text{V} * \text{VOL} \quad 72$$

OXNH4 is then minimised to either the above statement or the mass of NH_4 in solution and on CEC (OXMAX). OXSOL (the oxidised NH_4 in solution) is minimised to OXNH4 or the mass of NH_4 in solution. The new reduced adsorbed quantity of NH_4 is calculated and increased adsorbed H are calculated.

The new masses of NH_4 , NO_3 and alkalinity are calculated e.g.

$$\text{ION}(\text{MNO}_3) = \text{ION}(\text{MNO}_3) + \text{OXNH}_4 \quad 73$$

Denitrification can also take place if $\text{fdnit} > 0$, a parameter input for denitrification rate.

$$\text{RDENIT} = \text{fdnit} * 1.07^{(\text{soltmp} - 15)} \quad 74$$

$$\text{DCNO}_3 = \text{RDENIT} * \text{CNCNO}_3 * \text{TIMSTP} / 86400 \quad 75$$

This concentration of denitrified NO_3 (DCNO_3), is subtracted from the original $[\text{NO}_3]$. The new masses of NO_3 and alkalinity are calculated. The subroutine ends and returns to `DECAY.FOR`. A new nitrify flux is calculated and the solution masses of NH_4 , NO_3 and alkalinity are adjusted.

Respiration

This is calculated by the subroutine `RESPIR.FOR` called by `PROSOC.FOR`. Respiration for coniferous roots, $\text{mg C cm}^{-2} \text{ s}^{-1}$, is calculated as follows:

$$\text{RESPC} = \text{respem} + \text{udistc} * \text{respccg} * \text{FAC} \quad 76$$

where

$\text{FAC} = \text{timestep factor}$

Total respiration (RESPT) is calculated:

$$\text{RESPT} = ((\text{RESPD} * \text{pcdecd}) + (\text{RESPC} * \text{pcconf}) + (\text{RESPO} * \text{pcopen})) * \text{scarea}(\text{L}) * \text{TIMSTP} * \text{etwght}(\text{L}) \quad 77$$

The new $[\text{C}]$ is calculated.

$$\text{solion}(\text{MTIC}, \text{L}) = \text{solion}(\text{MTIC}, \text{L}) + \text{RESPT} \quad 78$$

The flux of C in exudation is reduced by RESPT while the flux of C fixed is increased by RESPT .

Mineral weathering

The concentration of H^+ in solution is calculated first $[\text{H}]$.

Then for each mineral, K, in each layer the weathering of K (DELTA P) is integrated over the timestep:

$$\text{DELTA P} = \text{ckmnr1}(\text{K}, \text{L}) * \text{TIMSTP} * \text{slcomp}(\text{K}, \text{L}) * [\text{H}]^{\text{wexp}(\text{K})} \quad 79$$

Obviously DELTA P cannot be greater than SLCOMP and maximum $\text{DELTA P} = \text{SLCOMP}$. DELTA P is subtracted from SLCOMP to find the new % weight of primary minerals.

Equation 80 calculates the number of moles of mineral actually weathered.

$$\text{DELTA E} = \text{DELTA P} * \text{WEIGHT}(\text{L}) / \text{mnmwt}(\text{K}) \quad 80$$

Equation 81 calculates the mmol_c of I (ion) weathered for each mineral,

$$\text{SOL} = \text{DELTA}E * \text{mnwth}(I,K)$$

81

and equation 82 the resulting ion concentration.

$$\text{solion}(I,L) = \text{solion} + \text{SOL}$$

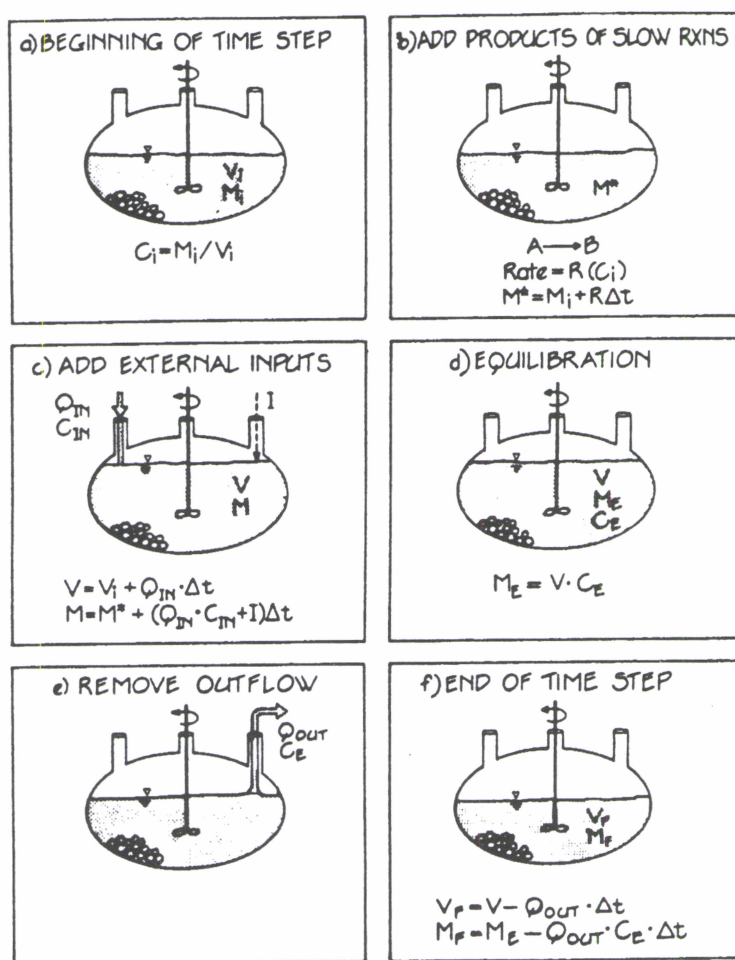
82

Finally the flux from weathering is calculated.

Chemical Equilibrium

NuCM like ILWAS is based on the batch reactor analogy for a stirred reactor compartment over a timestep (Gherini et al, 1986), figure 5.

Figure 5. Batch reactor analogy for stirred reactor compartment over a time step (after Gherini et al., 1986).



where

C = concentration

M = mass

V = volume

i and F denotes initial and final

Q = flow

Decay and weathering reactions are examples of b) slow reactions. The flux of water and species from layer 1 to 2 are examples of QIN and CIN, and the dry deposition, exudation are examples of I in c). Equilibration, d), will now be described which involves equilibrium reactions between the new solutes, the adsorbed phase and minerals. This includes cation exchange reactions, anion adsorption, gibbsite dissolution and aluminium and organic acid dissociation reactions, which will be presented in a similar way as in the original manual.

Cation Exchange

Seven cations: Ca, Mg, Na, K, NH₄, H and Al are included in the cation exchange reactions in NuCM, which uses a Gapon formulation. The exchange of each ion is calculated in relation to calcium concentration. The general form of the Gapon selectivity equation is:

$$K_{Ca-A} = (Ca^{2+})^{1/2} / (A^{y+})^{1/y} \cdot (E_A/E_{Ca}) \quad 83$$

where

(A^{y+}) = the concentration of the metal cation of charge y

E = the fraction of charge occupied by a particular cation on the exchange complex

The Gapon selectivity coefficient is not a parameter input but calculated from the adscat(I) and solion(I) inputs.

Given the 7 cations which are exchanged, each of which exists in 2 phases, there are 14 equations which must be solved to characterise cation exchange. Six of these are exchange expressions, Ca-Mg, Ca-K, Ca-Na, Ca-Al, Ca-H and Ca-NH₄.

Conservation of mass, as shown in equation 84 provides another 7 equations:

$$\text{adscat(I)} + \text{solion(I)} = \text{TOTION(I)} \quad 84$$

The 14th equation comes from the condition of electroneutrality:

$$\text{adscat(Ca)} + \text{adscat(Mg)} + \text{adscat(K)} + \text{adscat(Na)} + \text{adscat(Al)} + \text{adscat(H)} + \text{adscat(NH}_4) = \text{cec} \quad 85$$

Anion Adsorption

Three anions: SO₄, PO₄ and organic acids are considered non-competitively adsorbed in NuCM. SO₄ adsorption is simulated using the Langmuir adsorption isotherm (Johnson et al. 1993):

$$\text{adscat(SO}_4) = (\text{emax} * \text{b} * \text{solion(SO}_4)) / (1 + (\text{b}) * \text{solion(SO}_4)) \quad 86$$

where

b = constant = K(H⁺)² and so makes SO₄ adsorption pH dependent.

$$K = X_{H_2SO_4} / [(X_s) * (H)^2 * (SO_4)] \quad 87$$

which describes the reaction:



where

$X_{\text{H}_2\text{SO}_4}$ = number of sites onto which SO_4^{2-} is adsorbed = $\text{adscat}(\text{SO}_4)$ in equation 88

X_s = unfilled SO_4^{2-} sites

$e_{\text{max}} = X_{\text{H}_2\text{SO}_4} + X_s$

The adsorption of organic acid (OA) and phosphate is strong in soils and is represented in NuCM by pH dependent linear isotherms, the sorption coefficient, K being calculated from inputs $\text{adscat}(\text{I})$ and $\text{solion}(\text{I})$.

$$\text{adscat}(\text{OA}) = \text{KOA} * \text{solion}(\text{OA}) \quad 88$$

$$\text{adscat}(\text{PO}_4) = \text{KPO4} * \text{solion}(\text{PO}_4) \quad 89$$

Aluminium Dissolution

As pH decreases, the concentration of metals including Al tend to increase. In low pH systems, below the bicarbonate buffering range, aluminium hydroxide species and organic acids are the principle pH buffering groups.

Depending on the model options selected, Al^{3+} can be in equilibrium with $\text{Al}(\text{OH})_3$:



At 20°C, the equation is:

$$k_{\text{so}} = [\text{Al}^{3+}]/[\text{H}^+]^3 \quad 90$$

If the dissolution of Al is rate limited, [Al] will not build up in solution to its equilibrium level. Under such conditions, the dissolution of aluminium is represented by the following mass cation limited rate expression:

$$-d[\text{Al}(\text{OH})_{3(s)}]/dt = w_{\text{exp}} ([\text{Al}_e] - [\text{Al}]) \quad 91$$

where

$[\text{Al}_e]$ = the concentration of Al^{3+} for a solution in equilibrium with $\text{Al}(\text{OH})_3$ at the pH of the soil solution

$[\text{Al}]$ = actual Al^{3+} concentration = $\text{solion}(\text{Al})$ input initially

The model user can decide whether to have no equilibrium, rate limited or equilibrium processes deciding Al dissolution in each layer, parameter naloh3 .

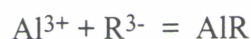
Al^{3+} can hydrolyse to form a series of aluminium hydroxides e.g.



$$k_{\text{al1}} = ([\text{Al}(\text{OH})^{2+}][\text{H}^+])/[\text{Al}^{3+}] \quad 92$$

Similar expressions are used to represent the formulation of $\text{Al}(\text{OH})^{2+}$ and $\text{Al}(\text{OH})^{4-}$.

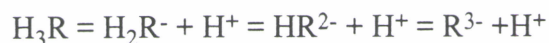
Organic complexation of aluminium is assumed to occur only with the fully dissociated organic acid



$$k_{ar1} = [\text{AlR}] / ([\text{Al}^{3+}] [\text{R}^{3-}])$$

93

The organic ligand R^{3-} is also in equilibrium with less dissociated forms of organic acid:



Three pKa values are parameter inputs and are used as shown in equation 94:

$$k_{r3} = [\text{H}_2\text{R}^-] / ([\text{R}^{3-}] [\text{H}^+])$$

94

The actual program coding for soil equilibration is written in C language and because of this, I have problems following the processes in detail. The original manual states that the solution technique is based on MINEQL (Westall et al., 1976) and is then extended to include the kinetic behaviour of aluminium in organic soil horizons. Because the equilibrium processes are described over several files, which are called throughout the program, I will now present the subroutines called by the main routine of the NuCM chemistry model, CLDMAIN.FOR. When equilibrium routines are called (in bold), I will describe the processes as far as my understanding permits.

Program Description

CLDMAIN.FOR

CALL READ reads and checks system data.

CALL OPEN opens input/output files, opens and reads a file name's "files.lis", which lists the input and output files and their unit numbers.

CALL INTERP interprets the user river segment numbers, initialises variables and output the system data.

Timestep calculation, depends on user input of day, week, month, year.

CALL HEADUP puts information on screen.

CALL HEADX stops calculation if a certain condition is met and show this on screen.

CALL **INITCHEM**

INITCHEM.C

This is a very important subroutine as it defines the matrixes used in all the equilibrium calculations. From reading about the Steadyql model (Westall et al., 1991), a newer version of mineql, I could recognise some of the starting matrixes. I have therefore chosen to include a passage describing the formulation of a general equilibrium problem in steadyql matrixes and the solution to the problem. The problem definition has three parts: mass action equations (fast processes), flux equations (slow processes) and mole-balance equations (conservation of matter and charge). I recognise the mass action equation in INITCHEM.C and can present the species and components used in NuCM in the a_{ij} matrix (table 9). If one looks how H^+ as a

component is related to the different species, one can see that SO_4 , H_2PO_4 and H_2ORG anion adsorption is pH dependent.

The general form of the mass action equation is:

$$C_i = K_i \prod_{\text{all components } j} x_j^{a_{ij}} \quad 95$$

where

C_i = concentration of species i (38*1)

K_i = conditional formation constant of species i (38*1)

x_j = concentration of component j (17*1)

a_{ij} = stoichiometric coefficient of component j in species i (38*17)

The numbers in parentheses refer to the dimensions of the matrixes used in NuCM.

It is more convenient and computationally more efficient to work with equation 95 re-expressed in logarithmic terms.

$$\log C_i = \log K_i + \sum_{\text{all components } j} (a_{ij} \log X_j)$$

The k matrix is set up by calling the subroutine **INITK.C**.

The chemical equilibrium problem is solved iteratively as follows.

- 1) Initial estimates of the free concentrations of the components at steady state are made.
- 2) From these initial estimates, the corresponding concentrations of all the species are computed from the mass action equation.
- 3) From the concentrations of the species, the fluxes are calculated.
- 4) The concentrations of the species and fluxes are then substituted into the flux- and mole-balance equations. The sums of the terms on the left-hand side of the equation are referred to as the difference functions for the components.
- 5) If all the difference functions are sufficiently close to zero, the Newton-Raphson method is used to calculate improved values of the free concentration of components. The process is repeated with the improved values until the convergence criterion is satisfied.

INITCHEM.C is used to set up 8 different sets of components in addition to the base set shown in matrix a_{ij} . These are used later by other C programs to solve the equilibrium problem.

CALL INITL Initialises parameters and vectors.

Table 9. Matrix a_{ij}

species components ==>

	H	H2ORG	Al	H2CO3	Ca	Mg	Na	K	NH4	SO4	H2PO4	Ca0.5Xc	Xs	Xa	NO3	Cl	SiO2
H	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2CO3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
HCO3	-1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
CO3	-2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Al	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AlOH	-1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AlOH2	-2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AlOH4	-4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H3ORG	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2ORG	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HORG	-1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ORG	-2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AlORG	-2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ca	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Mg	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Na	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
K	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
NH4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
SO4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
H2PO4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
Ca0.5Xc	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Mg0.5Xc	0	0	0	0	-0.5	0.5	0	0	0	0	0	1	0	0	0	0	0
NaXc	0	0	0	0	-0.5	0	1	0	0	0	0	1	0	0	0	0	0
KXc	0	0	0	0	-0.5	0	0	1	0	0	0	1	0	0	0	0	0
NH4Xc	0	0	0	0	-0.5	0	0	0	1	0	0	1	0	0	0	0	0
HXc	1	0	0	0	-0.5	0	0	0	0	0	0	1	0	0	0	0	0
Al0.33Xc	0	0	0.33	0	-0.5	0	0	0	0	0	0	1	0	0	0	0	0
Xs	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
H2SO4Xs	2	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0
Xa	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
H3PO4Xa	1	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0
H3ORGXa	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
CO2(g)	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
ALH-3(s)	-3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
Cl	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
H4SiO4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

INITL.FOR

Many of the instructions throughout INITL.FOR are to zero parameters or convert m to cm, m^2 to cm^2 , days, months, years to seconds and kg to g. The subroutine MGMEQ.FOR is frequently called, which converts units from mg to mmolc. These are the internal working units for NuCM. The following list of instructions includes only those I find interesting and omits the above mentioned conversion instructions.

$$1. \text{CONVRT}(\text{MOACD}) = ((\text{DOC in mg l}^{-1})/12)*\text{OA1C}$$

96

This is used to convert the DOC input in mg l^{-1} to $\text{mmol}_c \text{l}^{-1}$ throughout the program. If one looks at the HELP screen (HS70) attached to the input of DOC (menu screen (S70), it says; " The strong organic acid ligand (SOAL) is calculated form DOC as follows: $\text{SOAL} = 5 * \text{DOC}$ (i.e., charge density of strong organics = $5 \mu\text{mol}_c \text{mg}^{-1} \text{DOC}$)" This is **wrong**. The manual is also **wrong** as it writes on p.2-31, "An organic acid analogue is simulated by the model. Charge density of acid is fixed at $15 \mu\text{mol}_c \text{mg}^{-1} \text{DOC}$ ".

2. Initialise variables for both understory and overstory, which includes calculating max/min LAI, initialising interception storage and converting canopy % to decimal fraction.

3. The sum of annual litterfall for the 3 areas is calculated and converted into useful units.

4. The leaf, trunk and root compositions for the 3 areas are converted from mg g^{-1} to $\text{mmol}_c\text{g}^{-1}$ and the alkalinity of each pool is computed by calling the INTBIO subroutine. This in turn calls MGMEQ.FOR and IONBAL.FOR. The IONBAL subroutine calculates the alkalinity (MALK) or ANC (NuCM uses both names) as:

$$\text{MALK} = \text{sum cations} - \text{sum anions} \quad (\text{all units in } \text{mmol}_c) \quad 97$$

where

$$\text{sum cations} = \text{MNH}_4 + \text{MAL} + \text{MCA} + \text{MMG} + \text{MK} + \text{MNA}$$

$$\text{sum anions} = \text{MSO}_4 + \text{MNO}_3 + \text{MCL} + \text{MPO}_4 + \text{MOACD}$$

5. The amount of standing biomass (trunk), root biomass and biomass associated with leaf in the catchment are calculated for each area. It is important to note that the parameter input as **standing biomass, Stand/d/c/o is not the sum of leaf and bole biomass above ground but only the bole biomass**. The biomass associated with leaf (BIOSTC) in mmol_c is calculated from the leaf area index as follows:

$$\text{BIOSTC} = \text{laic}(\text{BMNTH}) * \text{scarea}(1) * \text{constc} * \text{lfcmpc}(\text{I}) * \text{pconf} \quad 98$$

where BMNTH denotes in the beginning month of simulation

6. The snow quality is initialised for all areas in the catchment, if one begins the simulation with snow on the ground. This includes calling MGMEQ, IONBAL to calculate ALK and calculating ALT and OACD. C6 is set equal to $1.00\text{E}-4$ and pHSILLEN.C is called.

pHSILLEN is described as a program for simple pH calculations. The following arguments are listed and those with an asterisk are given a value before it is called:

NAL = number for gibbsite rate*

XCO2 = number to multiply atmospheric CO_2 concentration with*

IT = temperature*

C6 = initial guess for H^+ concentration*

ALK = alkalinity concentration*

ALT = total Aluminium concentration*

TIC = CO_3 concentration

OAAL = organic aluminium concentration

CO2 = H_2CO_3 concentration

The purpose of this subroutine is to return a concentration of H^+ , CO_3 and organic Al. I find the C program too complex to describe any further.

7. The alkalinity is balanced in the minerals (cations - anions).

8. Initialise litter and organic matter composition.

The weight of layer1 is calculated. For all components: The sum of all litterfall from both stories and all areas is calculated; The fraction of weight of coarse litter, fine litter and humus is calculated; For humus, C, NH_4 , SO_4 and ALK are defined separately.

Then the weight, the volume of water in $\text{dm}^3 \text{l}^{-1}$, the CEC and the decimal fraction weight of mineral are calculated. The CEC(CCE) for layer 1 is defined as:

$$\text{CCE} = \text{cec} * (1 - \text{xlit} - \text{fines})$$

99

This means NuCM is only considering the humus and minerals present (if any) in the organic layer to contribute to the cation exchange surface. The consequence will be faster cation depletion from an initially smaller pool. This is not clear from the manual or menu/HELP screens. One would generally expect the CEC measured in the laboratory for the organic layer to refer to at least the humus and fine litter, if not the whole LFH layer.

9. Adsorbed ions are converted from % or $\text{mmol}_c 100\text{g}^{-1}$ to mmol_c and solution ions from $\text{mmol}_c \text{l}^{-1}$ to mmol_c . IONBAL.FOR is called to calculate MALK.

10. The soil temperature is converted into an integer and an upper (40 °C) and lower (1°C) limit is enforced. INITSOIL.C, which has the arguments, layer and soil temperature is called. Its purpose is to initialise the equilibrium calculations.

11. MEGMEQ and IONBAL are called to calculate ALK. Values are also given to ALT, OACD, TIC, C6 and IT before pHSILLEN is called. Its purpose is to calculate the H^+ and organic Al concentration.

12. Return to CLDMAIN.FOR

CALL PQUAL

CALL WPLOT both calls are to set up result plots and summaries

The simulation then begins. The beginning date is calculated.

DO 600 LOOP =1, NLOOPS sets the program to reloop at line 600, if user has indicated entire data set to be simulated more than once.

DO 580 I = 1, NTOTAL sets the program to reloop at line 580. This line is setting the total number of time steps, the chemistry model is to calculate, e.g if simulation length is one year and one has chosen day, week or month, NTOTAL = 365, 52 or 12 respectively.

CALL STATUP

CALL HEADX

CALL READH2O reads in the hydrological data from file SITENAME.H2O for the present timestep

The daily meteorological data is then read in and changed to average of correct timestep. The chemistry model is only interested in converting the maximum and minimum temperature and wind speed.

The SITENAME.AIR file is read in, rain, air and cloud quality data. Cloud water for the month is converted to per week or per day, depending on timestep. The following sequence of instructions occurs for rain and cloud quality. For air quality, pH and unit conversion are omitted:

The pH is converted to H^+ in $\text{mmol}_c \text{l}^{-1}$; Units are converted, if necessary; The deposition factors are applied; IONBAL is called.

Monthly soil temperatures are read in.

CALL CATCHM described as the chemistry for the land catchment.

CATCHM.FOR

1. Various fluxes and reaction variables are zeroed.

2. The uptake demand for the month is calculated.

CALL GROW This subroutine computes stand productivity and the corresponding increase in the canopy. Also, atm. CO₂ is interpolated from the input co2atm v. time graph.. These increments and CO₂ adjustments are made after a full year of simulation, rather than at beginning of calendar year.

CALL CALUPD This subroutine computes potential uptake in one timestep for each constituent for leaf, bole and root separately.

3. The canopy processes are computed.

CALL LEAF (described in CLDLEAF.FOR)

a. Computes nitrification on canopy

b. Assigns terrestrial gas deposition velocity

c. Accumulates dry and wet deposited matter

d. CALL pHSILLEN (all arguments except OAAL and CO2 are given a value)

e. Adds all contributions to canopy storage

f. CALL EXUD calculates exudation and adsorption of gases and ions

g. CALL TLEACH calculates leaching of gases and ions, CALL pHSILLEN(all arguments except TIC, OAAL and CO2 are given a value. C6 is calculated from ALK).

h. Calculates washoff of quality constituents and net accumulation on leaf surface.

i. Sums all components of throughfall and compute total wet deposition

j. CALL pHSILLEN (all arguments except OAAL and CO2 are given a value. C6 is calculated from ALK) to determine pH in throughfall.

4. CALL SNQUAL computes snow quality

a. Adds constituents in throughfall and snowfall to snoion

b. Adds dry deposition

c. Computes nitrification in snowpack

d. CALL pHSILLEN (all arguments except OAAL and CO2 are given a value) to calculate snowpack pH.

e. Computes quantity of snowmelt and remaining snowpack.

5. Different water volumes (litres) needed in PROSOC are calculated .

water reaching upper surface

TWATER = runoff + throughfall + snowmelt **100**

volumetric moisture content

SH2O =theta(L) * thick(L) * scarea(L)*1/1000 **101**

lateral flow

DH2OF = FLOW(L)/1000 **102**

infiltration and percolation

DH2OI =INFIL(L) * scarea(L+1) * 1/1000 **103**

CALL PROSOC (L,SH2O,DH2OI,DH2OF,TWATER,OLDMO)

PROSOC.FOR

This subroutine computes translocation and all soil processes.

- a. Adds dry deposition to detention storage and computes quality of detention storage, overland flow and solution percolating into layer 1.
- b. Mixes incoming and existing solutions.
- c. CALL TRANSL, translocation subroutine, which removes nutrients from leaves during senescence and before abscission
- d. Computes extent of first order reactions for all active layers
CALL DECAY (CALL NITRIFY) determines OM decomposition and (de)nitrification
CALL WEATHR determines mineral weathering
CALL UPTAKE determines nutrient uptake
CALL RESPIR computes transport of CO₂ by vapour flow and diffusion
- e. Computed multiphase equilibrium for layer L
CALL SOILEQL This is the most thorough soil equilibrium calculation.
- f. Subtracts outgoing constituents
- g return to CATCHM.FOR (from PROSOC)

Return to CLDMAIN.FOR (from CATCHM)

If channel equation is on, CALL RIVERS

Set up output files for plotting (MPSWZT = 0)

CALL PQUAL(IITIME)

CALL WPLOT(IITIME)

580 CONTINUE This statement is the end of the DO loop, "DO 580 I = 1,NTOTAL" and therefore a new day, week, month or year will be used as the next time step, and so on until the total number of steps is used up (NTOTAL).

600 CONTINUE This is the end of the DO loop, "DO 600 I = 1,NLOOPS"

A few error statements

END The end of the program.

Chemistry Simulation Results

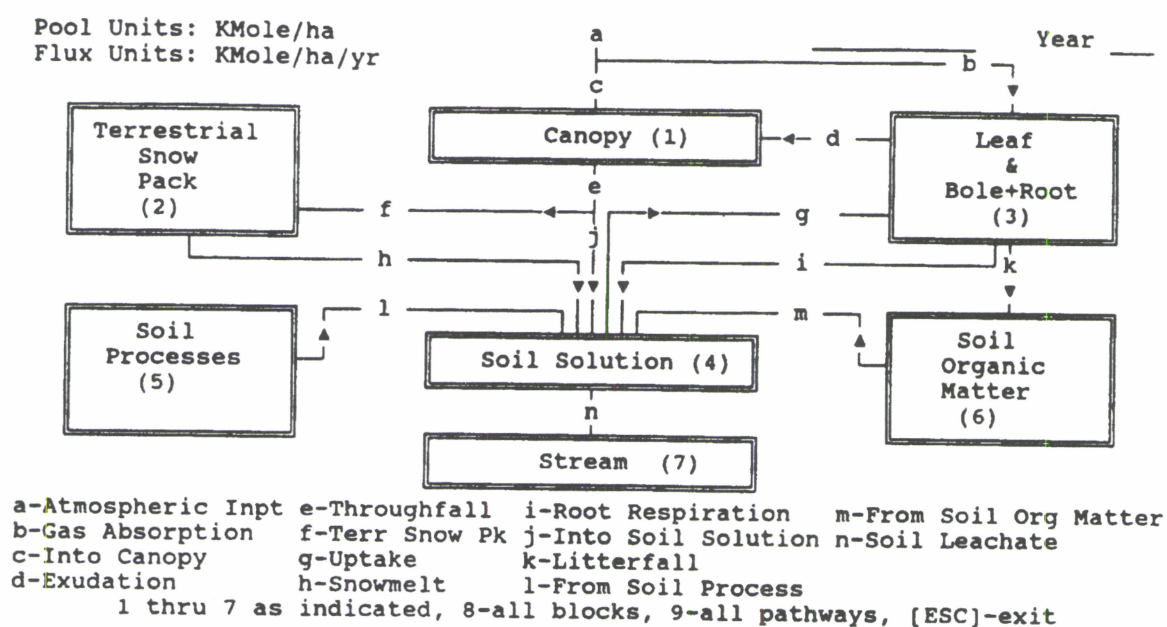
The first menu to appear after choosing to see the results of the chemistry simulation is shown in table 10.

Table 10. Chemistry output options

1	Pool and flux diagrams
2	Sorbed concentrations vs. Time plot
3	Solution concentration vs. Time plot for throughfall, soil layers or stream outflow
4	Litter pool C:N vs. Time plot
5	Plant growth vs. Time Plot
6	Store output data to ASCII file for subsequent analysis
7	Save input data to ASCII file for reference or next session
8	Cycle diagram
9	Observed and simulated vs. Time plot

I have personally found options 2, 3, 6 and 8 the most useful. The plots are good for a first look but for more detailed study the ASCII files of options 2 and 3 are necessary. The pool and flux diagram is really a simpler form of the cycle diagram but I am more certain of the definition of pools and fluxes in the cycle diagram and so I prefer this, even if it is more complex. One must select the substances one is interested in; NO_3 , NH_4 , PO_4 , Ca, K, Mg, SO_4 , Cl, Na, SiO_2 , pH, ANC, total monomeric Al, organic monomeric Al, DIC and DOC and the year (fluxes are calculated $\text{KMole ha}^{-1}\text{year}^{-1}$). Then figure 6 appears on the screen. By choosing the letters and numbers shown at the bottom of the figure, one can see the fluxes and pools indicated. 8 and 9 are summaries over the pools and fluxes for the component selected.

Figure 6. Cycle results diagram for NuCM chemistry simulation



Final Comments

I have deliberately avoided writing about calibration. The original manual gives fairly detailed guidelines on how to calibrate both the hydrological and chemical model. I have followed the suggested order of calibration as far as possible and cannot at this point suggest any better order of procedures.

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