

Nutrient Cycling in Forest Ecosystems: User Manual v.()

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Introduction

The Nutrient Cycling in Forested Ecosystems (NutsFor) model is a stand-level biogeochemical model which simulates the forest nutrient dynamics of 16 chemical species. These processes include hydrology, soil exchange site chemistry, mineral weathering, stand growth and uptake, and atmospheric deposition. This manual describes the most recent iteration of NutsFor (version), which further includes stand harvest, biomass residues, separate pools of soil water, and other small changes made to the original model described in van der Heijden et al, 2017. All changes from the original model are noted with an asterisk (“*”). As NutsFor is an active project of Gregory van der Heijden, model capabilities are open to change based on collaboration.

This user manual is intended to give relevant information about the model’s capabilities, useful tips regarding its usage, insight into the equations and theory which link model parameters, and information on how to effectively use NutsFor in an R-Studio based environment.

Model Start Up

Prior to running or implementing change to model parameters, the user should go through the input and output files for NutsFor using excel. NutsFor does not currently have a built-in method to visualize results, it is recommended that the user use excel macro commands or R to automatically read generated files (which will always output with the same structure) to visualize results. This is highly important in the calibration phase of model implementation.

The model is simple to run, simply double-click or other wise enact the NutsFor.exe file. The model will run and output results to its corresponding .csv files automatically. If the output files are moved from the NutsFor directory or removed, NutsFor will generate new csv files as long as the Output folder is still present in the NutsFor.exe

Table 1: Dry and Wet Deposition Files

Input	Units	Description
Ca, Mg, K, Na, NO ₃ , NH ₄ , SO ₄ , Cl, PO ₄ , DOC, H, Al, Si	$\mu\text{mol/L}$	Determines the amount of each species deposited into ecosystem by Dry Deposition

directory. A successful model run will be accommodated by a “Exporting Model Run Data” and “Model Run End-Press Return to Close”. Unsuccessful model runs (i.e., crashes) will result in either the NutsFor.exe closing on its own or on the former messages never appear in the NutsFor.exe terminal.

Input Files

There are 11 input files for NutsFor (.nut files). These files are csv files which can be opened through excel. A full list of the input parameters, separated by the file they appear in, is shown in the tables below. Below each table is a more extensive description of each variable and its effects on model outputs.

Deposition Files

Description of Parameters: Deposition Files

The dry deposition file is comparable to the Rain Concentration file. It simply delegates the deposition of chemical species without the deposition of water. The files start with An and Mois (Year and Month Columns), and then lists out chemical species from left to right.

Soil Files

Table 2: Soil Parameters File

Input Parameter	Units	Description
Soil Layer	N/A	Designates number of layers.
Soil Layer	N/A	Assigns layer number to each layer
Depth	cm	Tracks vertical depth of soil layer
Thickness	cm	Designates the individual thickness of each soil layer
Bulk Density	kg/m^3	N/A
Solid Density	kg/m^3	N/A
Stoniness	Percent	Determines the percent of soil particles greater than 2mm in diameter
Root Fraction	Fraction	Determines fraction of total tree root biomass in each layer
pKGibb	N/A	Gibbsite formation constant
pkAl precip	N/A	Al precipitation constant (unused in current version)
pCO ₂	Unknown	Partial Pressure of CO ₂
Area	m^2/m^3	Weatherable mineral area
Wilting Point	Percent	Soil moisture at which stand cannot extract water
Field Capacity	Percent	Soil moisture after excessive water is leached
Saturation	Percent	Soil moisture at which all pore space is filled with water
CEC	cmol_c/kg	Total cation exchange capacity
KH Cation	N/A	Gapon coefficients for each cation
Percent Mineral Area	Percent	Proportion of total mineral area that each individually defined mineral occupies
Uptake Fraction Per Layer (all nutrients)	Fraction (max 1)	Determines fraction of needed nutrient which stand uptakes from each
Nitrification (ks, knit)	ks: $\mu\text{mol/L}$, knit: Fraction	Nitrification constants that determines NO ₃ production
Microbial Turnover	Multiple of Microbial Pool	Determines fraction of SOM which turns over
Organic Matter Parameters	g Nutrient/kg soil)	Initial Amount of Nutrient Mineralized in the SOM pool.
Soil Solution Initial (Multiple Species)	$\mu\text{mol/L}$	Concentration of all chemical species at beginning of simulation
Soil Adsorbed Anions Initial	$\mu\text{mol}/\text{kg}$	Adsorbed Concentration of anions at the beginning of the simulation
CEC Initial	cmol_c/kg	Sorbed Concentration of Cations to the CEC at the beginning of the simulation

Description of Parameters: Soil Parameters

Soil Layers:

NutsFor allows any number of soil layers to be set in the model. Extra layers are added by typing in the new layer quantity into the Soil_Layer parameter, and adding the new layer to the Soil Parameter file by parameterizing the new layer as is done for layers before it. When a new layer is added, the spacing between the different tables in the soil parameters file is offset, the tables must be cut and pasted such that a single row of blank cells lies between the tables, otherwise NutsFor will not be able to read the tables. The total number of soil layers (Nb_Layers) must also be updated in the General Data File before running the model.

Depth and Thickness:

The depth of the soil layer represents the vertical distance of the soil layer from the surface of the soil, it is not used in any calculations. Soil layer thickness determines how thick each soil layer is, it is recommended that soil layers are set to less than or equal to 20cm thick. Overly thick soil layers may be liable to over-leaching of nutrients from the soil layers.

Bulk Density, Solid Density, and Stoniness:

Bulk density is defined as fine earth bulk density (particles less than 2mm in diameter). Solid density is not part of the calculations of NutsFor, and can be ignored. Stoniness is the percent of soil particles greater than 2mm in diameter, this parameter affects soil moisture and hydrology calculations and is important to calculate.

Root Fraction and Uptake Fraction per Layer:

Keeps trace of the root distribution of the stand between the soil layers, however it does not determine the uptake of nutrients per layer. The Uptake Fraction per layer parameter truly determines how the stand extracts nutrients from the soil layers, allowing for greater flexibility in determining tree uptake dynamics. Intra-annual uptake dynamics are changed through the Tree Parameter file.

pKGibb, pKAl_Precip, pCO2:

The pKGibb parameter is the -log of the reaction constant of gibbsite dissolution to free aluminum, similarly the pKAl_precip is the -log of the reaction constant of Al and its precipitated forms (i.e., the solubility product). The range of pKAl_precip (or Ksp of Al(OH)₃(s)) should be in the range of 32-35 depending on the pH of the soil layer, pKGibb ranges from 6-9. These aluminum parameters are important in determining pore water pH, as Al is the largest contributor of H⁺ compared to other acids in the model. pCO₂ is the partial pressure of carbon dioxide in the soil solution, it is a constant multiple of atmospheric CO₂ and is not dynamic with decomposition rates.

Mineral Area

This parameter designates the total weatherable mineral surface area of the soil. It is calculated from the equation: General Equation 1:

$$(8 * X.Clay) + (2.2 * X.Silt) + (0.03 * X.Sand)$$

Citation: (Sverdrup and Warfvinge 1993)

Note, that clays dominant in high area clays may be misrepresented by this equation (*Citation*)

A more detailed equation, which takes into consideration different sand and silt size particles;

General Equation 2:

$$() + () + ()$$

Citation:

The mineral area parameter is historically difficult to obtain empirically, clay mineralogy plays a large role in determining this parameter, and is seldom measured to its full capacity (SOURCE). The fraction of soil particles in each size class (X.Clay, X.Silt, and X.Sand) are to be calculated from the whole soil (including coarse fragment count), not just the fine particulate fraction. Since this parameter is difficult to calculate, it will be likely that simulated mineral weathering rates are lower than those observed or calculated for a given stand. In this case the mineral weathering rates must be calibrated by increasing (or decreasing, if weathering is too high) the mineral area parameter. Mineral weathering rates are linked to proton concentrations, lower pH stimulates mineral weathering. Mineral weathering thus consumes protons and can be included in the calibration of pH and alkalinity. Thus, another way of calibrating mineral weathering rates can be the calibration of proton concentrations.

Soil Moisture Parameters

1. Wilting Point

The percent soil moisture which corresponds to the wilting point; i.e., the pressure of water in the soil matrix is at -15kPa. Wilting point may have a different reference pressure depending on the texture of the soil.

2. Field Capacity

The percent soil moisture which corresponds to how much water the soil can hold after drainage of excess water. Typically this measurement is set to the reference pressure of -33kPa.

3. Saturation

The percent of soil moisture corresponding to all pore space in soil being filled with water. It can be set as the effective porosity of the soil.

CEC Parameters and CEC Initial

1. CEC

This parameter is the effective cation exchange capacity (ECEC) of each soil layer. This parameter is usually measured for every soil and soil layer for every depth increment, however there are multiple methods through which this can be accomplished (Citation, General technical manual). In general, ECEC can be calculated as:

General Equation #X.1

$$ECEC = 2[Ca^{+2}] + 2[Mg^{+2}] + [K^{+}] + [Na^{+}] + 3[Al^{+3}] + [NH_4^{+}]$$

2. Gapon Selectivity Coefficients (KH_Cation)

These coefficients determine the propensity of each cation to be replaced on the CEC with H+. High selectivity coefficients indicate that a cation has a high affinity for the CEC, and are thus liable to stay on the CEC rather than weather off due to the presence of other cations. Low coefficients will likely lead to high CEC weathering of cations, which may result in high soil solution pH. This is due to both the consumption of protons in the soil solution, which kick off low-affinity cations, as well as the increase in acid neutralizing capacity (ANC) that comes with increased base cation concentrations. This is because ANC is calculated as the sum of base cations minus the sum of acid anions. When ANC is near or above 0, soil solution pH will be difficult to constrain.

Gapon coefficients are to be calculated as:

General Equation #X.2

$$K_{H:Cation^{+n}} = (E_{Cation^{+n}}/[Cation^{+n}]) * ([H^{+}]/E_H)^n$$

Where;

$$E_H = [H^{+}]_{adsorbed}/ECEC$$

and

$$E_{Cation^{+n}} = [Cation^{+n}]_{adsorbed}/ECEC$$

Note that

$$n = Valence$$

All concentration units are in mmol/L. It should be noted that these values heavily rely on measured initial cation concentrations, and so they may be manipulated to get a better match between adsorbed and dissolved cations. Note that increasing the selectivity coefficient of one cation will change the relative selectivity of all cations. For instance, increasing Ca selectivity will lead to more Ca adsorption to the CEC, which will in turn kick off other cations, assuming the selectivity of the other cations remains the same.

3. CEC Initial

This parameter is not under the “CEC parameters” heading in the Soil Parameter file, rather it is located at the bottom of the Soil Parameter File (it is the last table, named CEC Initial). This parameter determines the total adsorbed supply of cations initially on the cation exchange complex.

4). AEC Parameters

Anion Exchange Capacity (AEC) is implemented in the model for 3 anions; Sulfate, Phosphate, and Chloride. Sulfate adsorption can be modeled using either a Langmuir or Freundlich adsorption isotherm. Chloride is modeled using the Langmuir model, Phosphate the Freundlich model. Sulfate adsorption isotherms can be selected in the General Data File (Input Table 4).

1. Soil Adsorbed Anions Parameters

Each anion has two AEC adsorption parameters associated with it, Parameter #1 and Parameter #2. These parameters will stand for different variables depending on the adsorption isotherm selected.

2. Soil Adsorbed Anions Initial

Table 3: Soil Temperature File

Input Parameter	Units	Description
Year	Year	Designates the year corresponding to layer and temperature data.
Month	Month	Sepecifies the month.
Layers (1-n)	Degrees Celsius	Specifies the average monthly temperature at each time point.

Description of Parameters: Soil Temperature File

The structure of this file is fairly straight forward, for each layer, month, and year of simulation, an average soil temperature is entered. The soil temperature value is used to calculate decomposition and chemical reaction kinetics. Numerous soil-temperature monitoring stations are active around the world [Cite Here.]

Table 4: OM Decomposition File

Input Parameter	Units	Description
Litter Concentration (N, Ca, Mg,K, S, P)	mmol Nutrient/mol C	Determines concentration of nutrient elements in the litter fraction of OM.
Litter C Pool	mmolC/m ²	Sets the litter carbon pool, and thus the amount of nutrients per unit area.
Layer frac (Fine, Coarse, Humus)	N/A	Designates the OM distribution between coarse litter (first column), fine litter (second column), and humus (third column)
Decomp rate	mmol/(m ² * mo)	Calibration decomposition factor shows up multiple times in the file for the 3 OM fractions (1-3) and for the mineral soil layers (1-n).
CO2FACT	N/A	Calibration factor that determines the proportion of decomposed carbon that effluxes as carbon dioxide.
Nutrient Factor (DOCFACT, N Fact, Ca Fact, Mg Fact, K Fact, S Fact, P Fact, NULL	mmol Nutrient/mol C Null	Calibration factors for both the 3 OM fractions (1-3) and the mineral soil fractions (1-n). Can be used to calibrate soil solution and liter flow ion fluxes, range from 0 to 1.

Description of Parameters: OM Decomposition

Litter Parameters

Litter parameters can be broken up into 3 sections:

1. Litter Concentration (N, Ca, Mg, K, S, P)
2. Litter Pool (Litter_C_Pool, Litter_Fraction)
3. Litter Nutrient Release Dynamics

I). Litter Concentration

This table sets the concentration of main nutrient cations in the litter layer relative to the amount of carbon in the litter.

II). Soil_Layer:

- 1). The coarse litter fragment of the litter layer (fresh litter included)
- 2). The fine litter fragment
- 3). The humus ("Very fine SOM") fraction

Decomp_Rate: The k of decomposition, determining how much carbon decomposes from litter pools.

Co2_Fact: Determines the fraction of decomposed carbon which is evolved as carbon dioxide

N_Fact, Ca_Fact, Mg_Fact, K_Fact, S_Fact, P_Fact: Determines release rate of corresponding nutrient relative to C release due to decomposition. These parameters can be tweaked to globally slow the mobilization of nutrients from the litter pool.

DOCFACT:

This factor determines the fraction of the decomposed C pool at each time step and for each litter pool which is released as DOC. Increasing this factor increases DOC and thus organic acid (R-) concentrations in the simulated soil. This tends to lower pH according to the set pKa of organic acids (See OA_pKa in Input table 4).

DOC_Decomp:

Determines the proportion of DOC evolved from decomposing litter that is itself decomposed. This parameter decreases OA (R-), however it does not link back to carbon dioxide release as carbon dioxide concentration is a fixed parameter (See, Input table 2, pCO2)

Table 5: General Data File

Input Parameter	Units	Description
Start Year	Year	Determines simulation start year.
End Year	Year	Determines simulation end year.
Nb Layers	N/A	Designates number of layers to be read
Nb Minerals	N/A	Designates the number of minerals
Mineral names	N/A	Lists out the minerals to be simulated
OA pka	N/A	Designates the pka of organic acid stages of dissolution
Aluminum	N/A	Designates Al pka
Phosphoric Acid	N/A	Designates phosphoric acid pka
DIC	N/A	Designates DIC pka
Organic acid size	Carbon/Charge	Determines how many C molecules are present for every negative charge on organic acids.
Nb Tree comp*	N/A	Determines the stand's species composition
Anion Adsorption isotherms	N/A	Determines adsorption isotherm used for anions (1=langmuir, 2=Freundlich)

General Files

Description of Parameters: General Data File

Simulation Length

Simulation length (the number of years which is simulated) is determined by the Start_Year and End_Year parameters. For example, a starting year of 2015 and an ending year of 2020 is 6 total years of simulation (starting in Jan of 2015 and ending in December of 2020). Note that deposition files and the soil temperature file must be extended by however long the simulation is run for (the program does NOT loop over these files).

Acid pka Numerous acids have their pKas (-log of their dissolution constant) set here. These parameters can be taken from online chemical databases, assuming an average room temperature (25 degrees celsius).

Organic Acid Size This parameters determines the number of carbons for every charged site on an organic acid; it is used to calculate the charge density of organic acids. Note that this is a global parameter, changing this number changes R- concentrations in all layers. Lowering this parameter leads to a higher charge density (and thus more acidic) soil solution, which tends to cause cations from the CEC to dissolve into solution.

A potential side effect of high cation concentrations due low charge density is suppressed weathering release of cations, as per equation X.X in Equations.

Description of Parameters: Mineral Data File

Dissolution Reaction Parameters The parameters which determine mineral dissolution dynamics are the equilibrium constants (pK values), the thermal dependencies (k values) and the reaction orders (n values). These are then combined in the following equation:

$$r_j = (k_{H^+} * [H^+]^{n_{H^+}} / f_{H^+}) + (k_{H_2O} / f_{H_2O}) + (k_{CO_2} * P_{CO_2}^{n_{CO_2}} / f_{CO_2}) + (k_R * [R^-]^{n_{R^-}} / f_{R^-})$$

where

$$r_j =$$

Weathering Rate

The equation calculates the summation of all chemical species (H+, H2O, CO2, and Organic Acid) has on mineral weathering rate. Each calculation has a restricting coefficient (

$$f_{species}$$

), which is a product inhibition coefficient discussed in the next sub-section.

Inhibition Reaction Parameters The inhibition coefficients are calculated dynamically based on the concentration of cations in soil solution layers. The theoretical reasoning of this parameter is straight forward: the higher the solution concentration of base cations, the lower favorability of the weathering reaction.

Table 6: Mineral Data File

Input Parameter	Units	Description
Mineral	N/A	Name of mineral.
pKH	N/A	Reaction constant of mineral with H+
pKH2O	N/A	Reaction constant of mineral with water.
pKCO2	N/A	Reaction constant of mineral with CO_2
pKr	N/A	Reaction constant of mineral with organic acid (R)
kH	N/A	Temperature dependence of mineral-H+ reaction.
kH2O	N/A	Temperature dependence of mineral water reaction.
kCO2	N/A	Temperature dependence of mineral CO_2 Reaction
kr	N/A	Temperature dependence of mineral Organic Acid reaction.
nH	N/A	Mineral dissolution H+ reaction order.
WAlH	N/A	Brake reaction order for Al (f_{H+})
WBCH	N/A	Brake reaction order for BC (f_{H+})
WAlH2O	N/A	Brake reaction order for Al (f_{H2O})
WBCH2O	N/A	Brake reaction order for BC (f_{H2O})
nCO2	N/A	Brake reaction order for CO_2 (f_{CO2})
nr	N/A	Brake reaction order for R (f_R)
$CAI * 10^{-6}$	$[Al] * 10^{-6}$	Limiting Al concentration
$CR * 10^{-6}$	$[R] * 10^{-6}$	Limiting BC concentration
$CBC * 10^{-6}$	$[BC] * 10^{-6}$	Limiting R- concentration
Ca, Mg, K, Na, Al, Si, PO4	Stoichiometric	Sets the stoichiometry of each mineral.
Ca.Iso, Mg.Iso, K.Iso Na.Iso, Al.Iso, Si.Iso, PO4.Iso	N/A	Unknown

These equations mean that as the base cation concentration of the soil solution increases, the weathering rate will become increasingly limited. The magnitude at which this occurs depends on the identity of the mineral and its defined parameters. An instance where this may become relevant is during calibration of free aluminum concentrations. Free aluminum will react with water in the model to release protons, which generally leads to enhanced mineral weathering as per Equation X. However, if aluminum concentrations are very high, the model will simulate a reduction in mineral weathering, cutting off the positive feedback between aluminum hydrolytic proton release and mineral weathering enhancement.

Note that the saturation constant (also known as the saturation concentration) sets the maximum solution concentration of each cation in water. The closer the simulated solution concentration is to the saturation constant, the higher the inhibition coefficient becomes and thus the slower the weathering.

New minerals can be added to the NutsFor mineral data file, a more extensive list of minerals is given in (“BGD - Reviews and Syntheses: Weathering of Silicate Minerals in Soils and Watersheds: Parameterization of the Weathering Kinetics Module in the PROFILE and ForSAFE Models,” n.d.). However, note that the exact parameters which control mineral weathering will depend on several real-world dependencies

Stoichiometry and Isometric Substitution

Tree and Stand Files

Table 7: Tree Parameters File

Input Parameter	Units	Description
Foliage.start	g/m^2	Starting biomass of foliage.
Foliage.End	g/m^2	Biomass of foliage at the end of simulation.
PET.winter.factor	Multiple	Multiplies by winter PET values to enhance or reduce PET.
PET.summer.factor	Multiple	Multiplies by summer PET values to enhance or reduce PET
interception	cm	Sets the volume of water which canopy can maximally intercept.
AET.Reduc	Multiple	Multiplies by calculated AET to reduce or enhance AET.
Leaching.alpha	N/A	Reaction order for foliar leaching reaction.
Absorption.alpha	N/A	Reaction order for foliar adsorption reaction.
Foliar.target.conc	$\mu\text{mol/g}$	Determines foliar concentration of nutrients.
Percent.variation, foliar	Fraction	Fraction of target concentration which foliage can reach before limitation.
Translocation.Percent	Fraction	Fraction of foliar nutrients that are translocated to stem during litterfall events.
Foliar.Exudation	N/A	NULL
Foliar.Leaching	N/A	NULL
Foliar.absorption	N/A	NULL
Wood.target.conc	$\mu\text{mol/g}$	Wood.target.conc
Wood.initial.conc	Percent.variation	Wood.initial.conc
Percent.variation, Wood	$\mu\text{mol/g}$	Percent.variation, Wood
Bark.target.conc	$\mu\text{mol/g}$	Bark.target.conc
Bark.initial.conc	Percent.variation	Bark.initial.conc
Percent.variation, Bark		Percent.variation, Bark
Branch.target.conc	$\mu\text{mol/g}$	Branch.target.conc
Branch.initial.conc	$\mu\text{mol/g}$	Branch.initial.conc
Percent.variation, Branch	Fraction	Percent.variation, Branch

Description of Parameters: Tree Parameter File

Table 8: Stand Harvesting File

Input Parameter	Units	Description
Year	Year	Designates the year of harvest event.
Month	Month	Designates the month of harvest event.
Stand.Frac	Fraction	Multiplies by stand biomass, determines what proportion of stand is removed.
Wood.Exp.frac	Fraction	Determines fraction of wood (bole) removed.
Bark.Exp.frac	Fraction	Determines fraction of bark removed
Branch.Exp.frac	Fraction	Determines fraction of branch removed.
Foliage.Exp.frac	Fraction	Determines the fraction of foliage removed.

Description of Parameters: Stand Harvesting File

Table 9: Tree Growth File

Input Parameter	Units	Description
Wood: Biomass.Start and Increment	g/m^2	Designates the starting bole biomass at start of simulation and yearly growth increment.
Bark: Biomass.Start and Increment	g/m^2	Designates the starting bark biomass at start of simulation and yearly growth increment.
Branch: Biomass.Start and Increment	g/m^2	Designates the starting branch biomass at start of simulation and yearly growth increment.
Fol.DW.min: Increment	g/m^2	Designates the minimum foliar biomass every year.
Fol.DW.max: Increment	g/m^2	Designates the maximum foliar biomass at every time step.

Description of Parameters: Tree Growth File

Output Files

There are 60 output files that NutsFor.exe generates, separated into 9 folders. All files are structured in a readable manner, with units *most* designated. All output files are .csv files separated by “;”, all can be read using R. Unlike for input parameter files, output files are largely self-explanatory, however some units are not noted, and some file structures are difficult to immediately read into programs such as R. This section will briefly describe file structures and folder contents, without the extensive descriptions offered for input files. It will also offer basic R studio-based approaches to reading and organizing the data for further analysis.

Output Folders

AEC

The first folder in the Output data directory is the AEC folder. AEC contains anion adsorption data (SO₄, PO₄, Cl) for each layer, and so the number of .csv files contained in this folder depends on the user-specified number of soil layers. Each file has a year and month column, and AEC data in units of $\mu\text{mol/kg}$ and kg/ha .

Biomass

The biomass folder contains the “Plant pool” and “Tree data” files. Plant pool contains (I don’t know). The Tree data file contains compartment nutrient content and biomass data for the stand. Nutrient contents are given in units of $\mu\text{mol/g}$ and kg/ha . Biomass or “dry weight” is given in kg/ha .

Budgets

The Budgets folder reports the “Above ground fluxes” and “Biological cycle” files. These files contain simplified yearly summary data on nutrient inputs and outputs, and can be used to calculate ecosystem nutrient budgets. The Above ground fluxes files contains deposition fluxes, throughfall flux, net foliar exchanges, litterflow flux, leaching flux, and weathering flux of each nutrient every annual time point. The Biological cycle file contains uptake, litterfall, and organic matter mineralization fluxes. All fluxes are in units of kg/ha/yr . NO₃, NH₄, SO₄, and PO₄ are in units of N, S and P (NH₄-N, NO₃-N, SO₄-S, and PO₄-P).

CEC

The CEC folder is identical to the AEC folder in basic structure, it holds a csv file for every soil layer specified. Each file contains cation adsorption data in both

$\mu\text{mol/kg}$ and kg/ha .

Hydrology

The hydrology folder has two datafiles, the “Hydrology Daily Output” and the “Hydrology Monthly Output” files. The monthly output file is smaller and more practical for use, although they contain the same data distributed over different time steps. The file begins by reporting the Year and month of each measurement, then reports the rainfall (RF), potential evapotranspiration (PET), the actual evapotranspiration (AET), the throughfall

Litter

Soil Solution

SOM

Weathering

Using R with NutsFor

This section assumes that the user has basic R studio skills, for more information on general R studio usage see the “Helpful Resources” section of this manual.

For layer-based output folders, such as AEC, CEC, weathering, and soil solution, it is most efficient to read all files from a single output directory into one R dataframe, and use an indexing function to define the individual layers. For instance, a code for reading CEC might look like:

```

#Requires this package for code to make sense (pipe operators)
library(dplyr)

#Generates a pattern within "files", locates folder
files <- list.files(path = "~/YourFilePath/Output data/CEC", pattern = "CEC", full.names = TRUE)

#Uses the defined "files", applies the read.csv2 function
#and generates an "id" column unique to each file.
CEC_All<- supply(files, read.csv2, simplify=FALSE, header=FALSE) %>%
  bind_rows(.id = "id")

#Designates an index value (1-n) that corresponds to each "id" value, named "group_id"
CEC_All$group_id <- CEC_All %>%
  group_by(id)%>%
  group_indices(id)

```

The above code essentially applies an identifying number for each soil layer in a large, aggregated dataset of all the soil layers, which makes it easier to apply graphing functions to the data as well as keep track of data in a single file. Graphing becomes particularly easy, for example the above CEC_All file generated above can be graphed using:

```

#Loads the ggplot2 package
library(ggplot2)

#Defines a graph for Ca, defines lines by group_id
CEC_Graph_Ca<-ggplot(CEC_All, aes(x=Date, y=Ca, group=group_id))

#Plots graph
CEC_Graph_Ca

```

It is likely that dataframes read into R will be in character format rather than numeric. This is because many of the NutsFor output files have 2 rows of character-containing values. Often, this leads to R not being able to read a descriptive header or graph the data correctly. Even if the character values are removed, the data will still be in character format and will not behave as a number in graphical or numerical analysis. To fix this, a simple code can be used:

```

#Specifies that only columns 2-16 are to be made numeric
CEC_All[c(2:16)]<-lapply(CEC_All[c(2:16)], as.numeric)

```

While R studio is a powerful for analyzing large datasets, it can also be used to generate manuscript-quality tables [Citation] and write dynamic reports or manuscripts [Citation]. Creating such reports can make the following stage of NutsFor usage, calibration, much easier.

Calibration

After starting parameters have been measured for the site or approximated from the literature, the calibration phase can begin. Calibration entails changing initial parameters within some acceptable range until model outputs match observed measurements. What determines the acceptable range of parameter variation depends on what is known about the site, as well as what is known about the standard error of the parameter itself.

I recommend planning out the process of calibration using workflows. By identifying which parameters are most likely to vary (and thus can be used to calibrate), a calibration workflow can be generated for every sub-module within the greater NutsFor module. The order which each sub-module is calibrated is very important, the sub-modules with the highest level of control over the outputs of the model should be calibrated first, those that are more precise and downstream of multi sub-modules last. Generally, the order I recommend is the same as described in (Munson et al. 1992), listed below. However, some processes can be calibrated before others, depending on their relative importance in determining model outputs on a site specific basis.

I also recommend using no more than 2 parameters to calibrate every 1 observed output. This is because the use of 3 or more parameters to calibrate a single output has an infinite amount of ways which the parameters can be

ordered or chosen (Sverdrup 1996). Thus, it is important to choose which parameters are allowed to vary for the site in question, and use *only* these parameters for calibration.

1). Hydrology

The calibration of the hydrological sub-module of NutsFor should always occur first, hydrology will affect seasonal decomposition patterns, soil solution concentrations, leaching fluxes, and weathering fluxes. It therefore has control over all other model outputs. To calibrate this system, the user should have some evaporation data for the region to confirm model output. Once the seasonality and magnitude of evaporation (in the model, the Actual Evapotranspiration output or AET) are confirmed against regional data, the hydrology calibration is complete. The user may also view soil moisture parameters over time, these values should be confirmed with collected data or known seasonal patterns. For instance, a soil with a drought season should have soil moisture parameters drop to near wilting point during such events.

Hydrological outputs are calculated from parameters entered in the Weather Data file, the Soil parameters file, and the Tree data file. The Weather Data file contains information on daily potential evapotranspiration and average air temperature, using the (which equation?) to calculate AET. The soil parameter file will contain soil moisture parameters specific to the site, these parameters will generally be held constant and shouldn't be used to calibrate hydrology.

To calibrate hydrology AET outputs, the user should either adjust the PET entered in the Weather Data file manually, or use the AET and PET factors in the Tree parameters file to generally calibrate winter and summer PET values. These parameters multiply by the Weather Data file PET or the calculated AET, a value of 1 indicates that the PET and AET is to be the same as entered and calculated, and so forth.

I found that spring time PET was often over estimated by the reference crop PET calculator that I used, so during my calibrations I chose to manually change PET values for each site I used. If possible, it is always more efficient to directly measured PET and AET for a specific site.

2). Throughfall & Deposition

Calibration of these inputs is rather simple, the user must observe whether or not depositional fluxes of key nutrient cations are correct given the inputs from the Rainfall concentrations, Tree parameters file, and Dry deposition file. The rainfall concentrations file will combine with the Weather data file to determine wet deposition flux, the dry deposition will determine nutrient flux from dry deposition, and the Tree parameters file have various parameters (described above) which dictate foliar leaching and adsorption parameters. All of these files will ultimately be used calculate net deposition of nutrients in the soil at every time step.

Generally, throughfall fluxes of K⁺ are significant, a source of data or direct measurement of throughfall should be used to calibrate K⁺ leaching fluxes as this process is important in determining K⁺ distribution in soil. Other nutrients, such as Ca and Mg, may experience little leaching or adsorption depending on the forest of interest [6].

Once throughfall concentrations and depositions fluxes match those observed or estimated, the calibration can be said to be complete.

3). Soil Organic Matter

Soil Organic matter should be calibrated using the OM decomposition file, there are numerous parameters which control SOM C stabilization. In general, unless data is available, SOM in mineral soil should not build up or decrease over the course of the simulation. The calibration of SOM is dictated by *Decomp_rate*, *C_Assim*, *DOC_Decom*, and *DOC_Assim*. The key to SOM calibration is to control DOC leaching and R- concentrations while keeping the SOM C content stable. *Decomp_rate* is the most sensitive parameter which determines SOM C dynamics, *C_Assim* and *DOC_Assim* dictate how much decomposed solid and dissolved carbon are assimilated into the SOM pool, and can be used to enhance or reduce SOM C buildup. *DOC_Decom* can be used to reduce DOC leaching.

4). Anion Calibration

Calibration of in-organic anions requires first that an adsorption isotherm is chosen for every anion (Sulfate, Chloride, and Phosphate) in the General Data file, and that a starting adsorption pool of each anion is entered in the Soil Parameters file (under the "Soil Adsorbed anions initial" header). The initial adsorbed pool of anions should either be directly measured or estimated from data in the literature. The parameters which can be used to calibrate anion concentrations are the half saturation constant (parameter 2, Langmuir isotherm) or the isotherm power "n" (parameter 2, Freundlich isotherm). Generally, increasing parameter 2 for the Langmuir isotherm leads to more

dynamic anion adsorption, often leading to high initial anion concentrations that equilibrate over time, whereas a smaller value leads to stronger adsorption and lower, although more stable, concentrations.

If S or P concentrations are too low in the observed layers, trending towards depletion of the dissolved and adsorbed pools, release rates of S and P in the OM decomposition file can be changed to increase S and P mineralization. If this calibration leads to unrealistic gain of S and P in the organic layer, the issue may have its roots in tree uptake per layer, with disproportionate tree uptake depleting the layer over others. In this case, the “Uptake Fraction per Layer” header within the Soil Parameters file can be edited.

Depending on the role of organic acids at the site, an initial calibration of the soil solution may yield an unrealistically high pH and high acid neutralizing capacity. Organic acids can make up a majority of soil anions in forest ecosystems (Johnson and Cole 1980), however these R- anions are distributed between constantly changing solid and dissolved phases. As NutsFor does not represent solid organic acids, dissolved organic acid can be used to calibrate ANC. The point of this calibration would be to ensure a rough charge balance in the soil solution, avoiding unrealistic chemical behavior derived from a high ANC. R- concentrations can be changed using the DOCFACT and DOC_Decom in each organic and soil layer in the OM decomposition file. Increasing the DOC_Fact will increase R- release, whereas increasing DOC_Decom will decrease R- concentrations. As these parameters are layer specific, calibrating R- in each layer may be tedious. In such a case, I recommend using the organic acid charge density parameter in the General Data file, called “Organic_acid_size”, to control R- concentrations. This option will *globally* (for all layers) change R- concentrations in the model, a benefit of using this parameter over the layer specific DOC_Fact and DOC_Decom factors is that changing the charge density won’t cause a change in DOC mobility in the model, which can help constrain DOC leaching. Lowering Organic_acid_size decreases the number of carbon per negative charge (increasing the charge density and thus also increasing R-), and increasing the parameter decreases the charge density, lowering R- concentrations.

It is important to calibrate these anions before moving on to cation calibration, all anions will have some control over CEC adsorption and thus cation concentrations.

5). Cation Calibration

6). Final Calibration

Hypothesis Testing

List of Equations

NutsFor Encoded Equations

General Equations

Helpful Resources

Learning R

Basic R Resources

Advanced R for Building Projects

Github Shoutout

Literature Cited

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Appendix

Appendix, maybe include screenshots of input interface?