

# The NutsFor User Manual

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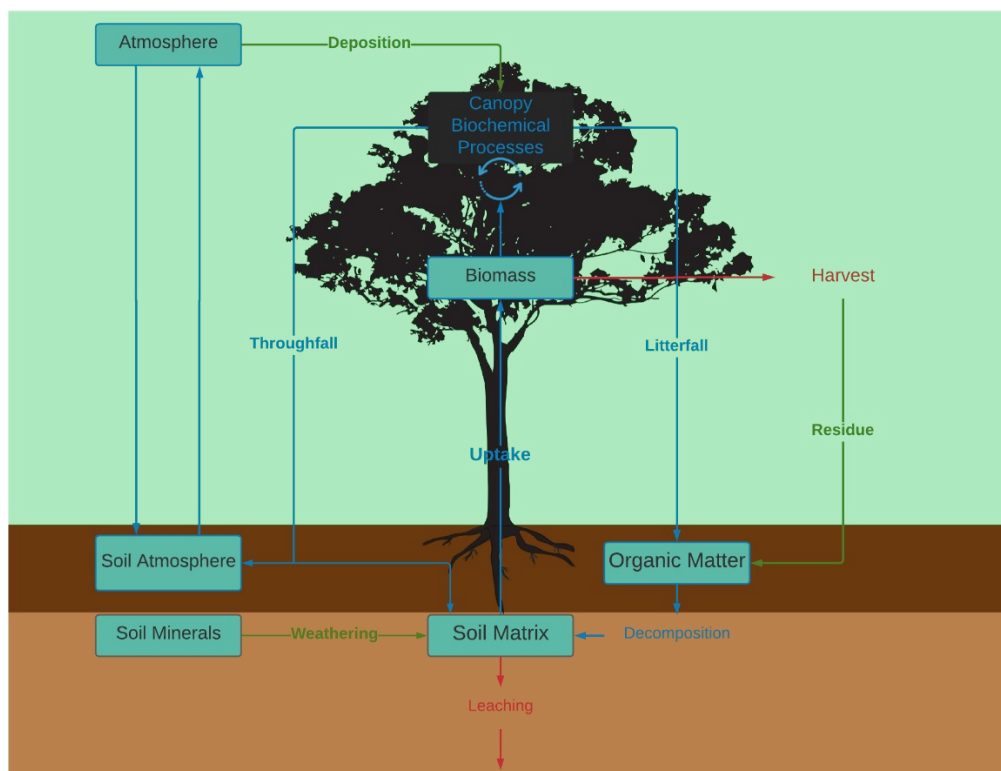
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# 1. Introduction

The Nutrient Cycling in Forested Ecosystems (NutsFor) model is a stand-level biogeochemical model that simulates the forest nutrient dynamics of 16 chemical species (Ca, Mg, K, Na, Al,  $\text{NO}_3$ ,  $\text{NH}_4$ ,  $\text{PO}_4$ ,  $\text{SO}_4$ , Si,  $\text{R}^-$ , H,  $\text{CO}_2$ , Cl, DOC, ANC, DON, DOP). It was developed to study a broad range of forest types at the Breuil-Chenue experimental site in Burgundy, France (van der Heijden et al. 2017). NutsFor is based on aspects of the Nutrient Cycling Model (NuCM) (Munson et al. 1992), and the ForSAFE model (Wallman et al. 2005). NutsFor integrates several biogeochemical processes, including hydrology, soil exchange chemistry, mineral weathering, stand growth and uptake, and atmospheric deposition. This manual describes the most recent iteration of NutsFor (version 07\_20\_21), which further includes stand harvest, biomass residues, the ability to limit plant access to cation nutrients in solid phases, SOM-N, P, and S availability to trees, and DON/DOP production in soil.



**Figure 1:** Pool and Flux Diagram for NutsFor. Blue text represents internal cycling processes, green input fluxes, and red output fluxes. Blue boxes show nutrient pools.

As NutsFor is an active project of Gregory van der Heijden, model capabilities are open to change based on collaboration, removals noted from the original 2017 model are noted with an asterisk (“\*”). 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 that link model parameters, and some information on how to effectively use NutsFor in parallel to R-Studio. Below is a table of NutsFor’s capabilities compared to other contemporaneous and historically used models, to help guide model use choices.

**Table 1:** Common Biogeochemical Forest Growth Models Compared to NutsFor

Model Names	Forest Management	Base Cations	Mineral Weathering	N Cycle	Soil Layers	Organic-Al reactions
NutsFor	X	X	X	X	X	
Pnet-BGC	X	X	X	X	*X*	X
NuCM		X	X	X	X	X
ForSAFE	X		X	X	X	
CENTURY	X					
3-PG	X					

\*Some versions contain this attribute\*

## 2. 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 (these files will always output with the same structure) to visualize results. This is important in the calibration phase of model implementation and should be done prior to attempting to test model parameters for every file and output.

The model is simple to run, simply double-click or otherwise enact the NutsFor.exe file. The model will run and output results to its corresponding .csv files automatically. If the output files are removed from the NutsFor directory, NutsFor will generate new csv files as long as the Output folder is still present in the NutsFor.exe 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 in the former messages never appearing in the NutsFor.exe terminal, instead the model will appear to stop part way through its run.

**Helpful Note:** It is always good to have a “base case” or other operational dataset for NutsFor. The starting parameters should be changed slowly from one site to another, as to help identify potential crash-inducing parameters.

### 3. Input Files

There are 11 input files for NutsFor (.nut files). These files are csv files that can be opened through a spreadsheet program. 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.

**Helpful Note:** All .nut files are semicolon (“;”) separated. If the user wants to edit these files in a spreadsheet program, they must specifically designate the kind of separation to be used when opening the file. This is because NutsFor is European in origin, and European column separation is designated by “;”, while decimals are designated with “.”. If the comma separation is used, all data will appear in a single column. To fix this, highlight the entire column containing incorrectly formatted data, and change the column separation by going to Excel/LibreOffice Top Menu → Data → Text to Columns → Select “Semicolon”. This also affects how NutsFor data is read by R, and is further discussed in the R section.

#### 3.1 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 (Table 2).

The second deposition file is the Weather Data file. This data file is set in a daily time step, requiring rainfall (mm), potential evapotranspiration (mm), and average temperature. Rainfall volume is multiplied by rainfall concentration from the rainfall concentration file to yield total wet deposition (Table 3).

**Helpful Note:** In the event that site-specific data cannot be measured, PET can be approximated using several online evapotranspiration calculators, such as the Food and Agriculture Organization of the United Nations free online software:  
<https://www.fao.org/land-water/databases-and-software/eto-calculator/en/>

**Table 2:** Dry Deposition and Rainfall Concentration Files

Input	Units	Description
Ca, Mg, K, Na, NO <sub>3</sub> , NH <sub>4</sub> ,	μmol/L	Determines the amount of each species deposited

**Table 2:** Dry Deposition and Rainfall Concentration Files

Input	Units	Description
SO4, Cl, PO4, DOC, H, Al, Si		into ecosystem by Dry Deposition

**Table 3:** Weather Data File

Input	Units	Description
Year	Year	Designates the year of rainfall event.
DOY	Day	Designates the day of the year rainfall occurs.
RF	mm	Designated volume of rainfall.
PET	mm	Designates the potential evapotranspiration.
Tave	Degrees Celsius	Designates the average air temperature every time step.

## 3.2 Soil Parameter File

### 3.2.1 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.

### **3.2.2 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 20 cm thick. Overly thick soil layers may be liable to over-leaching of nutrients from the soil layers.

### **3.2.3 Bulk Density, Solid Density, and Stoniness:**

Bulk density is defined as fine earth bulk density (particles less than 2 mm 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 2 mm in diameter, this parameter affects soil moisture and hydrology calculations and is important to calculate.

### **3.2.4 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.

### **3.2.4 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). These aluminum parameters are important in determining pore water pH, as Al is the largest contributor of H<sup>+</sup> compared to other acids in the model. pCO<sub>2</sub> is the partial pressure of carbon dioxide in the soil solution, it is a constantly held value and is not dynamic with decomposition rates.

### **3.2.5 Mineral Area**

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

General Equation 1:

$$(8 * X.Clay) + (2.2 * X.Silt) + (0.3 * X.Sand)$$

Citation:(H. Sverdrup and Warfvinge 1993).

Where X.Clay is the fraction of particles in the soil that are clay sized,

X.Silt the fraction of particles that are silt sized, and



X. Sand is the fraction of particles that are silt sized.

Note, that clayey soils may be misrepresented by this equation, different clays have variable specific mineral areas (Hodson, Simon, and Wilson, 1997; Macht et al., 2011). A more detailed equation, that takes into consideration different sand and silt size particles is given below.

General Equation 2:

$$(8 * X . Clay) + (2.2 * X . Silt) + (0.3 * X . FineSand) + (0.05 * X . CoarseSand)$$

Citation: (Harald Sverdrup 1996).

The mineral area parameter is historically difficult to obtain empirically, as clay mineralogy plays a large role in determining this parameter and is seldom described fully. 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. The above approximations of weatherable mineral area do not include the mineral surface area contributed by amorphous minerals such as Al and Fe sesquioxide. General Equation 2 tends to “breakdown” when soils are high in clay (>20%) (Hodson, Langan, and Meriau 1998). In cases where a soil is high in clay, calculated mineral areas must be calibrated to achieve desired weathering rates. It is likely that the Sverdrup 1993 simple surface area equation will underestimate mineral area in high clay soils than overestimate.

Since this parameter is difficult to implement for many soils, 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, as protons stimulate mineral weathering. Mineral weathering thus consumes protons and is included in the calibration of pH and alkalinity.

### **3.2.6 *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.

### **3.2.7 *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 in soil moisture databases.

### 3.2.8 Saturation

The percent of soil moisture corresponding to all pore space in soil being filled with water. Effective porosity can be measured to obtain this parameter, although a field measurement would better encapsulate aggregate and SOM effects on this parameter.

**Helpful Note:** NutsFor does not use soil water parameters to drive tree growth limitation. Growth limitation occurs only due to nutrient deficiencies and user-defined access/uptake parameters.

### 3.2.9 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, there are multiple methods through which this can be accomplished (Carter and Gregorich, 2007). In general, ECEC can be calculated as:

Equation 1:

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

### 3.2.10 Gapon Selectivity Coefficients (KH\_Cation)

These coefficients determine the propensity of each cation to be replaced on the CEC with H<sup>+</sup>. 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.

Gapon coefficients are calculated as:

Equation 2:

$$K_{H:Cation^{+n}} = \left( \frac{E_{Cation^{+n}}}{[Cation^{+n}]} \right) * \left( \frac{[H^+]}{E_H} \right)$$

Where;

$$E_H = \frac{([H^+]_{adsorbed})}{ECEC}$$

and

$$E_{Cation^{+n}} = \frac{([Cation^{+n}]_{adsorbed})}{ECEC}$$

Note that

$$n = \text{Valence}$$

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.

### ***3.2.11 CEC Initial***

These parameters are located at the bottom of the Soil Parameter File (it the last table, named CEC Initial). CEC Initial determines the total adsorbed supply of cations initially on the cation exchange complex.

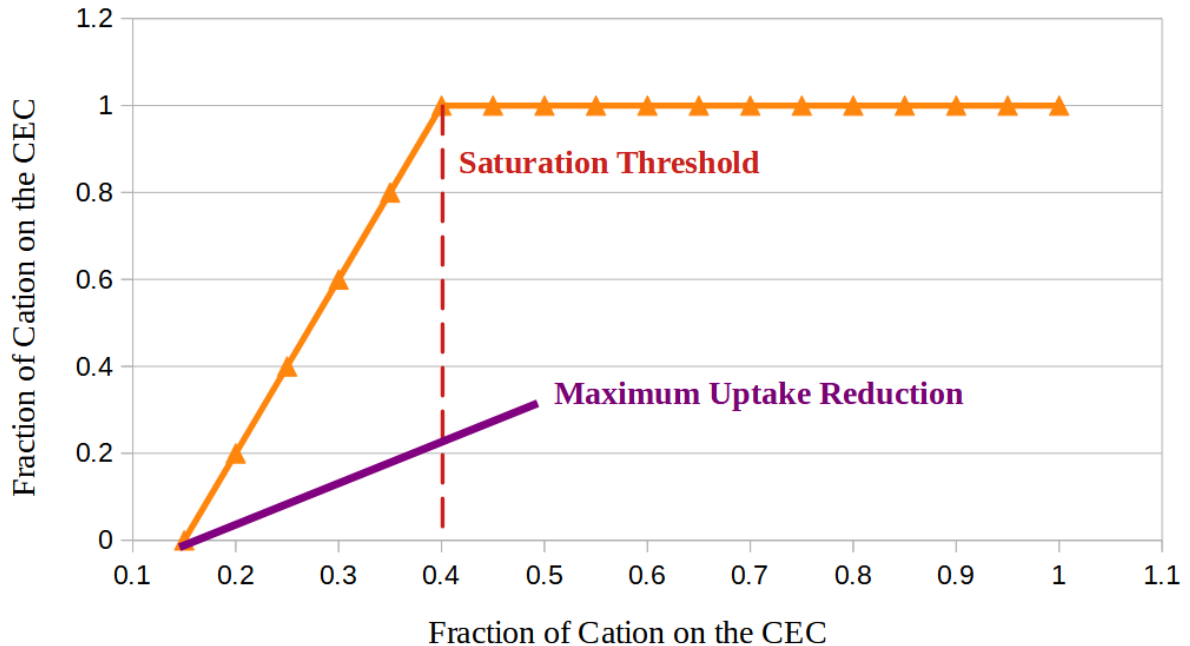
### ***3.2.12 Organic Matter Parameters and Organic Uptake Parameters***

The organic matter parameters allow for the user to set the amount of nutrients (N, P, S, Ca, Mg, and K) that are fixed in the SOM of each layer. The release of these nutrients is determined by the release factors and SOM decomposition rates set in the OM decomposition file. As of NutsFor v. 03\_04\_2021, SOM N, P and S can be directly accessed by the stand. This is set through the Organic Uptake parameters; these parameters represent the fraction of the soil layer's SOM nutrient pool that can be accessed by the stand at any timestep. This change was implemented because the previous version of NutsFor showed P limitation, in soils where P-limitation was considered unrealistic. These parameters are meant to represent the process of fungal nutrient acquisition from SOM, such as that observed by ectomycorrhizal fungi with P and N, which is thought to facilitate tree N and P uptake (Näsholm, Kielland, and Ganeteg, 2009; Plassard and Dell, 2010).

### ***3.2.13 Sat\_Thresh and Max\_Reduc***

These parameters are newly implemented, they are meant to limit tree access to the exchangeable pool. They tell the model to limit access to the exchangeable pool at any given time.

The function reducing plant uptake is a “threshold model”. Above a user-defined threshold (Sat\_Thresh), uptake is not reduced. Below this threshold plant uptake is gradually and linearly reduced until Max\_Reduc is reached (Figure 2).



**Figure 2:** Graphical representation of Sat\_Thresh (red), Max\_Reduc (blue). When the CEC fraction reaches Sat\_Thresh (.4), tree uptake of exchangeable cations is linearly reduced to the Max\_Reduc value (0.15). When Max\_Reduc is reached, uptake of the specified cation is turned off.

Sat\_Thresh sets the fraction of the exchangeable pool (the fraction of the CEC which a base cation occupies per soil layer) that the CEC reaches before cation uptake is slowed. Max\_Reduc sets the lowest CEC concentration fraction that the exchangeable cation can have on the exchangeable pool (i.e., a totally closed off pool from tree uptake). Sat\_Thresh and Max\_Reduc are used to calculate a linear function that limits the potential uptake of a given cation (Ca, K, or Mg) in a soil layer. If the potential uptake of a cation cannot be met in one layer, it is transferred to the next layer. In practice, these parameters are very “strong”, meaning that small changes in their values tend to force base cation limitations, even in base-rich soils.

### 3.2. 14 Soil Adsorbed Anions 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. Note

that anion adsorption is non-competitive, pH insensitive, and is disconnected from metal-oxide complexes.

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

### ***3.2.15 Soil Adsorbed Anions Initial***

The initial adsorbed anion pool must be specified in the model. This value is in  $\mu\text{mol/kg}$ . This parameter can be estimated for each anion using specific extraction methods

**Table 4: Soil Parameters File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
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 <sup>3</sup>	N/A
Solid Density	kg/m <sup>3</sup>	N/A
Stoniness	Percent	Determines the percent of soil particles greater than 2 mm in diameter
Root Fraction	Fraction	Determines fraction of root distribution in each layer
pKGibb	N/A	Gibbsite formation constant
pkAl precip	N/A	Al precipitation constant (unused in current version)

**Table 4: Soil Parameters File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
pCO <sub>2</sub>	Unknown	Partial Pressure of CO <sub>2</sub>
Area	m <sup>2</sup> /m <sup>3</sup>	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 <sub>c</sub> /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	Determines fraction of needed nutrient which stand uptakes from each
Nitrification (ks, knit)	Ks: μmol/L, knit: Fraction	Nitrification constants that determine NO <sub>3</sub> 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)	μmol/L	Concentration of all chemical species at beginning of simulation
Soil Adsorbed Anions Initial	μmol/kg	Adsorbed Concentration of anions at the beginning of the simulation
CEC Initial	cmol <sub>c</sub> /kg	Sorbed Concentration of Cations to the CEC at the beginning of the simulation
Organic Uptake Fraction (N, P, S)	Fraction	Allows trees to access nutrient directly from SOM. Represents the fraction of the soil N, P, or S pool in

**Table 4: Soil Parameters File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
		layer N that trees can access.
Sat_Thresh (Ca, Mg, K)	Fraction	Sets the fraction of exchangeable pool at which a nutrient base cation is no longer 100% available to the stand.
Max_Reduc (Ca, Mg, K)	Fraction	Sets the fraction of exchangeable pool a nutrient base cation occupies, at which point the stand can not longer access it.

### **3.3 Soil Temperature File**

The structure of this file is 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 further defined in the OM decomposition file.

**Table 5: Soil Temperature File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
Year	Year	Designates the year corresponding to layer and temperature data.
Month	Month	Specifies the month.
Layers (1-n)	°C	Specifies the average monthly temperature at each time point for each layer.

### **3.4 OM Decomposition File**

#### ***3.4.1 Litter Parameters***

The litter nutrient concentration, C pool, and decomposition rate parameters are used to calculate the litter decomposition of carbon at every time and the nutrient release rate (also known as the mineralization rate). Nutrient release also uses the release factor parameter specified by the user.

Litter decomposition follows the equation:

Equation 3:

$$DecompC(t, n) = k_n * Pool_C(t, n) * f(T) * 10^3$$

Where  $DecompC$  is the decomposition rate of C at time step  $t$  for litter layer  $n$  ( $mmol \cdot m^{-2} \cdot mont h^{-1}$ ),

$k_n$  is the user specified decomposition rate or "Decomp rate" ( $mmolC * mont h^{-1}$ ),

$Pool_C$  is the carbon pool at time step  $t$  for litter layer  $n$  ( $mol * mol l^{-2}$ ), and

the temperature limiting factor  $f(T)$  is given by:

Equation 4:

$$f(T) = e^{\left(\frac{T_{ave} - T_{ref}}{m}\right)}$$

Where  $T_{ave}$  is the average air temperature from the weather data file (or soil layer in Soil Temperature File),

$T_{ref}$  is the optimal temperature of decomposition, and

$m$  is a function parameter.

Equation 5:

$$R_\sigma = DecompC(t, n) * [\sigma]_{Litter}(t, n) * ReleaseFact(\sigma, n) * 10^{-3}$$

Where  $R_\sigma$  is the flux of nutrient  $\sigma$  ( $mmol \cdot m^{-2} \cdot mol l^{-1}$ ),

$[\sigma]$  is the concentration of nutrient  $\sigma$  at time  $t$  for litter layer  $n$  ( $mol \cdot m^{-2} \cdot mol l^{-1} C$ ), and

$ReleaseFact(\sigma, n)$  is the user-specified nutrient release factor for each litter layer  $n$ .

The release factor parameter designates the mol of nutrient  $\sigma$  which releases for every mol C, setting this value to 1 indicates a stoichiometrically proportional release between C and



the nutrient  $\sigma$ . Below one indicates a slower release rate and net retention relative to C. As NutsFor does not simulate litter CEC base cation stabilization nor litter-layer organic complexation, the release rates of base cations may require reduction if litter nutrient buildup is net-negative over a short, simulated time frame, where it should be constant or building. Release rates of all nutrients will depend on the species of tree, with broadleaf litter tending to lose nutrients faster than coniferous needle litter (Dijkstra 2003; Bockheim, Jepsen, and Heisey 2011). The  $Al^{+3}$  will tend to increase in litter as it forms organo-metallic complexes with negatively charged sites of decomposed litter (Rustad 1994). However, NutsFor does not simulate organic-Al chemical interactions, so Al mobility will likely be overestimated. Since the short-term behaviors of nutrient release and retention in litter can vary significantly (Rustad 1994), the user should look to broader nutrient build-up trends over decadal time scales to confirm model outputs. The user should also observe seasonal trends in litter decomposition and nutrient release fluxes to help confirm model parameters.

**Table 6: OM Decomposition File**

Input Parameter	Units	Description
Litter Concentration (N, Ca, Mg,K, S, P)	mol Nutrient/mol C	Determines concentration of nutrient elements in the litter fraction of OM.
Litter C Pool	mmol C/m <sup>2</sup>	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 <sup>2</sup> *mo <sup>-1</sup> ))	Calibration decomposition factor shows up multiple times in the file for the 3 litter 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 (DOCFAC, N Fact, Ca Fact, Mg Fact, K Fact, S Fact, P Fact	mol Nutrient/mol C	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.

**Table 6: OM Decomposition File**

Input Parameter	Units	Description
DONFact, DOPFact	Fraction	Sets the fraction of released (decomposed) N and P that is DON and DOP.

### 3.5 General Data File

#### 3.5.1 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).

#### 3.5.2 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°C).

#### 3.5.3 Organic Acid Size

This parameter 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.

**Table 7: General Data File**

Input Parameter	Units	Description
Start Year	Year	Determines simulation start year.

**Table 7: General Data File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
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)

### **3.6 Mineral Data File**

The NutsFor weathering sub-module is derived from the PROFILE mineral weathering model (H. Sverdrup and Warfvinge 1993). PROFILE is based on transition state theory, which dictates how the mineral weathering reaction equations are formulated. The mineral parameters in the Mineral data file were empirically derived from research in Swedish and European soils, assuming congruent weathering of mineral components (Sverdrup and Warfvinge. 1993). PROFILE uses five weathering reactions:

- 1). H<sup>+</sup> and Al
- 2). H<sub>2</sub>O and Al
- 3). OH<sup>-</sup> and Al
- 4). CO<sub>2</sub>
- 5). Organic acids

Citation: (Hodson, Langan, and Wilson 1997).

Note that the mineral data file of NutsFor does not contain the OH<sup>-</sup> reaction parameters.

In general, NutsFor mineral weathering will be controlled by weatherable mineral area, soil moisture, and the release of weathering agents H<sup>+</sup>, R<sup>-</sup>, and H<sub>2</sub>O. This section introduces how the parameters contained in the Mineral data file of NutsFor are used to calculate mineral weathering rates.

### 3.6.1 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:

Equation 6:

$$r_j = \left( \frac{k_{H^+} * [H^+]^{n_{H^+}}}{f_{H^+}} \right) + \left( \frac{k_{H_2O}}{f_{H_2O}} \right) + \left( \frac{k_{CO_2} * P_{CO_2}^{n_{CO_2}}}{f_{CO_2}} \right) + \left( \frac{k_R * [R^-]^n}{f_{R^-}} \right)$$

where  $r_j$  is the Weathering Rate of mineral  $j$ ,

$k_{species}$  is the rate coefficient of each species for each mineral,

and  $n_{species}$  is the reaction order (or weathering dependence) of each species.

The reaction rate coefficient  $k_{species}$  of a specific reaction is calculated by the equation:

Equation 7:

$$k = 10^{-(pK + (E_A / R * \ln(10)) * (1/T) - 8.56 * 10^{-3})}$$

Where  $pK$  is the rate coefficient of the reaction at the temperature  $T=280^\circ K$ , expressed as  $-\log_{10}(K)$ ,

$E_A$  is the Arrhenius activation energy ( $J * kmol^{-1}$ ),

$R$  is the universal gas constant ( $J * kmol^{-1} * K^{-1}$ ), and

$T$  is the absolute temperature ( $^\circ K$ ).

The equation calculates the summation of all chemical species ( $H^+$ ,  $H_2O$ ,  $CO_2$ , and Organic Acid) has on mineral weathering rate  $r_j$ . Each calculation also has a restricting coefficient ( $f_{species}$ ), that is a product inhibition coefficient discussed in the next section.

### 3.6.2 Inhibition Reaction Parameters

The inhibition coefficients are calculated dynamically based on the concentration of cations in soil solution layers. The higher the solution concentration of base cations, the lower favorability of the weathering reaction due to the generation of less active surface complexes over the course of weathering (Palandri and Kharaka, 2004). The equation which calculates the product inhibition factor rate  $f_{species}$  for each weathering agent is:

Equation 8:

$$f_{H^+} = \left(1 + \frac{[Al]}{C_{Al}}\right)^{W_{AlH^+}} * \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BCH^+}}$$

Equation 9:

$$f_{H_2O} = \left(1 + \frac{[Al]}{C_{Al}}\right)^{W_{AlH_2O}} * \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BCH_2O}}$$

Equation 10:

$$f_{CO_2} = \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BCCO_2}}$$

Equation 11:

$$f_{R-} = \left(1 + \frac{[R]}{C_R}\right)^{W_{R_H}} + f_{CO_2} = \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BC_{H_2O}}}$$

Where the  $C_{Al}$ ,  $C_{BC}$ , and  $C_R$  are saturation concentration parameters, and the  $W_{BC_H}$ ,  $W_{BC_{H_2O}}$ , and  $W_{Al_H}$  are reaction orders.

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. However, if free 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 (Sverdrup et al. 2019). However, the PROFILE model has recently been updated, and now contains saturation concentration and inhibition coefficients for silica and hydroxide. These updates are not currently in the NutsFor model.

### 3.6.3 Weathering Flux

With the calculation of the mineral weathering rate  $r_j$  for each mineral  $j$  over the simulated timestep, the total weathering flux  $W_M$  can be calculated as

Equation 12:

$$W_M = \sum_{j=1}^{mineral} \left( \frac{r_j * A_w * X_j * \Theta * z}{Norm} \right)$$

Where  $r_j$  is the specific mineral weathering rate,  
 $A_w$  is the user-specified exposed mineral area surfaces ( $m^{-2}/m^{-3}$ ),  
 $X_j$  is the user-specified fraction exposed mineral area which mineral  $j$  occupies,  
 $\Theta$  is the soil moisture saturation,  
 $z$  is the soil layer thickness (m),  
and  $Norm$  is the number of base cation charges released per mol of weathered mineral  $j$  ( $mol_c \cdot mol^{-1}$ ).

Equation 13:

$$\Theta = \frac{(\theta * \rho_{solid})}{(\rho_{solid} - \rho_{soil} + \theta * \rho_{water})}$$

Where  $\theta$  is the soil volumetric water content ( $m^3 * m^{-3}$ ),  
 $\rho_{solid}$  is the solid density of soil ( $kg \cdot m^{-3}$ ),  
 $\rho_{soil}$  is the bulk density of soil ( $kg \cdot m^{-3}$ ), and  
 $\rho_{water}$  is the density of water ( $kg \cdot m^{-3}$ ).

**Table 8: Mineral Data File Parameters**

Input Parameter	Units	Description
Mineral	N/A	Name of mineral.
pKH	N/A	Reaction constant of mineral with H <sup>+</sup>
pKH2O	N/A	Reaction constant of mineral with water.
pKCO2	N/A	Reaction constant of mineral with CO2
pKr	N/A	Reaction constant of mineral with organic acid (R)
kH	N/A	Temperature dependence of mineral-H <sup>+</sup> reaction.
kH2O	N/A	Temperature dependence of mineral water reaction.
kCO2	N/A	Temperature dependence of mineral CO2 Reaction
kr	N/A	Temperature dependence of mineral Organic Acid reaction.
nH	N/A	Mineral dissolution H <sup>+</sup> reaction order.

**Table 8: Mineral Data File Parameters**

Input Parameter	Units	Description
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 CO2 ( $f_{CO2}$ )
nr	N/A	Brake reaction order for R ( $f_R$ )
CAI*10 <sup>-6</sup>	[Al]*10 <sup>-6</sup>	Limiting Al concentration
CR*10 <sup>-6</sup>	[R]*10 <sup>-6</sup>	Limiting BC concentration
CBC*10 <sup>-6</sup>	[BC]*10 <sup>-6</sup>	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

### 3.7 Tree Parameters File

#### 3.7.1 Tree Nutrient Content

The biomass of the tree is split into 4 compartments, the non-bark bole (heartwood and sapwood), the bark, the foliage, and the branches. Each compartment has target nutrient concentration ( $\mu\text{mol/g}$ ) for each major nutrient. There is a percent variation parameter for each nutrient for each biomass compartment, this parameter allows the user to model the threshold of tree nutrient uptake before growth limitation is initiated. For instance, a percent variation of .8 for foliar N would mean that the stand would be able to grow at its full potential with 80% or more of its N demand being met by uptake.

Initial nutrient concentrations can be set separately from target nutrient concentrations, this allows for the simulation of nutrient deficient or stands with luxurious nutrient uptake at the beginning of the simulation.



### 3.7.2 Foliar Exchange Reactions

The tree parameter file holds several parameters which will drive foliar leaching, adsorption, exudation, and nutrient translocation processes over the course of the simulated stand.

#### 3.7.2.1 Foliar Leaching

Foliar leaching parameters describe the intensity at which nutrient leaching occurs from the foliage. Leaching is known to be a significant determinant of base cation cycling in forests and other plant communities but is particularly important for K cycling (Tukey 1970; Sollins et al. 1980). It is important to include this process even if little is known about throughfall chemistry at the site of interest. The magnitude of leaching is known to depend on the pH of the throughfall solution, the concentration of elements in the foliage, the volume of rainfall which is intercepted by the canopy, and the available leaf surface area through which leaching occurs.

Foliar leaching follows the equation:

Equation 14:

$$FolLeach(t, \sigma) = L_{\sigma} * [\sigma]_{Leaf}(t) * DW_{Leaf}(t) * [H^+]^{\alpha}$$

Where the  $L_{\sigma}$  is the specific leaching rate coefficient of ionic nutrient  $\sigma$  ( $mont\ h^{-1}$ ), and

$[\sigma]_{Leaf}(t)$  is the concentration of ionic nutrient  $\sigma$  at time  $(t)$  in the foliage ( $\mu mol * g^{-1}$ ), and

$[H]^{+\alpha}$  is the hydrogen concentration of throughfall to the power of leaching rate dependence  $\alpha$  ( $\mu mol/L$ , unitless).

#### 3.7.2.2 Foliar Absorption

Foliar adsorption is the process through which throughfall nutrients are absorbed into the leaf, acting as a kind of foliar nutrient uptake.

Equation 15:

$$FolAbs(t, \sigma) = A_{\sigma} * [\sigma]_{TF}(t) * TF(t) * [\sigma]_{TF}(t)^{\beta}$$

Where foliar adsorption for nutrient  $\sigma$  at time  $(t)$  ( $FolAbs(t, \sigma)$ ) ( $\mu mol * m^{-2} * mont\ h^{-1}$ ),

$A_{\sigma}$  is the specific adsorption constant ( $mont\ h^{-1}$ ),

$[\sigma]_{TF}(t)$  is the throughfall concentration of nutrients at time  $(t)$  ( $\mu\text{mol} \cdot \text{L}^{-1}$ ),

$TF(t)$  is the throughfall flux at time  $(t)$  (mm or  $\text{L} \cdot \text{m}^{-2}$ ), and

$\beta$  is the rate dependence of adsorption (unitless).

### 3.7.2.3 Foliar Exudation

Some nutrients are exuded from leaf surfaces over time and can be picked up by intercepted water to be deposited onto the soil.

Equation 16:

$$FolEx(t, \sigma) = \gamma_{\sigma} \cdot [\sigma]_{Leaf}(t) \cdot DW_{Leaf}(t)$$

Where foliar exudation ( $FolEx(t, \sigma)$ ) at time step  $(t)$  for nutrient  $\sigma$ ,

$\{\gamma_{\sigma}\}$  is the effective leaf turnover rate of ionic species  $\sigma$  ( $\text{month}^{-1}$ ),

$[\sigma]$  is the concentration of ionic nutrient  $\sigma$  in the foliage ( $\mu\text{mol} \cdot \text{m}^{-2}$ ), and

$DW_{Leaf}(t)$  is the dry weight of the leaf at time step  $(t)$  ( $\text{g} \cdot \text{m}^{-2}$ ).

### 3.7.2.4 Translocation (redistribution)

Translocation allows for the model to store a fraction of the stand's nutrients during litterfall events. This reduces the uptake demand of the foliar biomass compartment. The equation which calculates translocation in NutsFor is as follows:

Equation 17:

$$T_{\sigma}(t) = [\sigma]_{Leaf}(t) \cdot DW_{Litterfall}(t) \cdot TransFact(\sigma)$$

Where  $T_{\sigma}(t)$  is the translocation of nutrient  $\sigma$  at time  $(t)$ ,

$[\sigma]_{Leaf}(t)$  is the concentration of nutrient  $\sigma$  in the foliage at time  $(t)$ ,

$DW_{Litterfall}(t)$  is the dry weight of litterfall at time  $(t)$ , and

$TransFact(\sigma)$  is the user-specified fraction of foliar nutrient translocated during each litterfall event.

### ***3.7.3 Litterfall Parameters***

At the very bottom of the Tree parameters file are the litterfall parameters. There is a row of months underneath the heading “Evergreen litterfall distribution throughout the month”, where the monthly fraction of litterfall is set. For each month of the year, the fraction of total annual (set in the tree growth file) litterfall that is shed each month is set. The monthly fractions must add to 1.

Directly below this row are three rows designating the litterfall dynamics of the model. The model was updated to include flexibility in determining how litterfall responds to nutrient depletion. The first of these parameters is the LF\_Reduction\_Model parameter. If a value of 0 is entered, litterfall is calculated from the Tree growth file as the difference between annual maximum and minimum foliar biomass, and is insensitive to nutrient limitation and thus canopy dynamics.

When a value of 1 is entered for LF\_Reduction\_Model, litterfall is reduced by the same proportion as foliar biomass as calculated by the model in response to nutrient limitation. The LF\_Reduction\_Threshold parameter sets the fraction of canopy biomass that the canopy must reach before litterfall reduction is calculated. A value of 1 indicates that litterfall reduction occurs as soon as foliar biomass is reduced below 100% of its potential, and a value of 0 would indicate that the model is to never reduce foliar biomass.

When LF\_Reduction\_Model is set to 2, the model uses a user-defined fraction to calculate litterfall. This fraction is a constant multiple of the dynamic foliar biomass, designated in the final row LF\_Fixed\_Proportion. Hence, the canopy biomass at any time point is used to calculate litterfall by multiplying the current foliar biomass by the LF\_Fixed\_Proportion parameter.

### ***3.7.4 Hydrology Parameters***

The PET winter and PET summer factors are calibration factors which can be used to modify PET parameters in the Weather Data file. They serve as constant multiples over the summer and winter PET entries. The user should consider that springtime PET must be manually calibrated, requiring that the hydrology file is opened and edited for precise changes to PET.

### ***3.7.5 Uptake Distribution Throughout the Year***

NutsFor does not simulate water limitation, instead seasonal growth limitation must be explicitly set by the user. This is achieved with the “Uptake Distribution” parameters, which set the fraction of required nutrient that is to be accrued by the stand each month, the sum of all fractions for each nutrient should add to 1. If the monthly fraction of nutrient uptake is set to 0, growth does not occur for that month, allowing for the mimicry of water limitation in certain months.

### ***3.7.6 Foliar Growing Season***

The growing season of the foliage is determined by the Foliage\_Start and Foliage\_End parameters. These parameters represent the day of year in which foliar growth starts and ends (1 is Jan 1, 365 is Dec 31). NutsFor does not have leap years, so these parameters will always be in the 1-365 range.

**Helpful Note:** Depending on what kind of forest (Deciduous or evergreen), Foliage\_Start and Foliage\_End may be of varying importance. Evergreen forests will not have such distinct growth periods, as they are always growing “maintenance” biomass throughout the year, whereas deciduous forests lose all foliage biomass for the winter. For evergreen forests, I suggest setting Foliage\_Start to 1 and Foliage\_End to 365, such that the forest always has the potential to maintain biomass.

**Table 9: 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 that 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, Foliage	Fraction	Fraction of target concentration that tissue can reach before limitation.
Translocation_Percent	Fraction	Fraction of foliar nutrients that are translocated to stem

**Table 9: Tree Parameters File**

Input Parameter	Units	Description
		during litterfall events.
Foliar_Exudation	N/A	Specifies foliar exudation term.
Foliar_Leaching	N/A	Specifies foliar leaching term.
Foliar_absorption	N/A	Specifies foliar absorption term.
Wood_target_conc	μmol/g	Specifies the target stoichiometry for each nutrient in the bole tissue.
Wood_initial_conc	μmol/g	Sets the initial concentration in tissue for each nutrient.
Percent.variation, Wood	Fraction	Fraction of target concentration that tissue can reach before limitation.
Bark.target.conc	μmol/g	Specifies the target stoichiometry for each nutrient in the bark tissue.
Bark.initial.conc	μmol/g	Sets the initial concentration in tissue for each nutrient.
Percent.variation, Bark	Fraction	Fraction of target concentration that tissue can reach before limitation.
Branch.target.conc	μmol/g	Specifies the target stoichiometry for each nutrient in the branch tissue.
Branch.initial.conc	μmol/g	Sets the initial concentration in tissue for each nutrient.
Percent.variation, Branch	Fraction	Fraction of target concentration that tissue can reach before limitation.
Litter	Fraction /mo	Designates the monthly fraction of litterfall (set in the tree growth file) that is distributed each month. Should all sum to 1.
LF_Reucdtion_Model	N/A	Designates the LF reduction model of choice (0 = no LF reduction, 1 = LF reduction is proportional to biomass reduction, 2 = LF is a fixed proportion of foliar biomass)

**Table 9: Tree Parameters File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
LF_Reduction_Threshold	N/A	For LF_Reduction_Model = 1, when foliar growth is reduced below this threshold, litterfall also is reduced. Ranges from 0 (no LF reduction) to 1 (LF reduction as soon as growth limitation occurs)
LF_Fixed_Proportion	Fraction	Sets a multiplicative fraction of simulated foliar biomass that is designated as litterfall.
Uptake Distribution	Fraction	Sets the fraction of required nutrient to be taken up each month.

### **3.8 Stand Harvesting File**

The Stand Harvesting file is used to dictate when and what intensity of harvest events over the course of a stand. The Year and Month sections designates which year and month a harvest event is to occur. The stand fraction parameter tells the model what fraction of the total stand is harvested (ranges from 0 to 1). If the stand fraction parameter is set below 1, this indicates a partial harvest or a thinning event. The compartment biomass export fractions dictate what fraction of the harvested stand is taken off site, these parameters can be used to test a range of residue removal conditions on the stand.

Biomass removal is calculated following the equation:

Equation 18:

$$\text{Harvested Fraction} = \text{Stand.Frac} \cdot \text{Export.Frac}$$

**Table 10: Stand Harvesting File**

<b>Input Parameter</b>	<b>Units</b>	<b>Description</b>
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.

### **3.9 Tree Growth File**

The tree growth file contains a growth increment ( $\text{g}\cdot\text{m}^{-2}\cdot\text{yr}^{-1}$ ) column for every biomass compartment except for foliage. Foliage instead has a maximum biomass and a minimum biomass column, that allows the user to set the maximum possible foliar biomass and the minimum foliar biomass, such as that achieved in spring and winter. The user should set these parameters using data on tree growth specific to their stand or ecosystem of interest. If relevant, the user can specify the number of trees that compose the stand (in the tree parameters file, removed in the current version). However, the growth increment of the total stand per year should be a lumped average growth increment of all the trees within the stand.

The user must include growth increment data post-harvest manually. Say, for instance, that a harvest event is to occur in the year 2025, reducing the tree biomass of the stand to 0 kg/ha. The user must have a growth rate entered for 2026 and beyond which aligns with the

growth rate of a newly planted stand. The user may also choose to simulate “empty” or 0 growth years incident with gap years between harvest and replanting phases of site usage.

When simulating stands, the user should take extra care to include growth and nutrient cycling processes uniquely present in every kind of ecosystem. For instance, as forests reach old growth stages, mortality tends to increase, and biomass stabilizes for some tree species (DeBell and Franklin 1987; Bible 2001). Highly productive forests may have high tree mortality, contributing significantly to nutrient turnover and thus productivity (Malhi et al. 2004). The user can attempt to simulate the nutrient inputs from mortality by utilizing the stand harvesting file, removing and leaving behind some portion of the stand biomass that matches with known mortality inputs.

**Helpful Note:** The Foliage\_Start and Foliage\_End parameters in the Tree parameters file have similar names to the Biomass\_Start parameters in the Tree growth file. However, the Foliage\_Start and Foliage\_End parameters refer to the DOY in which foliar growth begins and ends (i.e., the growth season), rather than a starting biomass.

**Table 11: 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.

## 4. Output Files and Folders

There are 60 output files that NutsFor.exe generates, separated into 9 folders. All files are structured in a readable manner, with *most* units designated. All output files are .csv files separated by a semicolon (“;”), all can be read using R. Unlike for input parameter files, output



files are largely self-explanatory, however some units and definitions 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.

## 4.1 AEC

The first folder in the Output data directory is the AEC folder. AEC contains anion adsorption data ( $\text{SO}_4$ ,  $\text{PO}_4$ ,  $\text{Cl}$ ) 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  $\text{kg/ha}$ .

## 4.2 Biomass

The biomass folder contains the “Plant pool” and “Tree data” files. Plant pool contains information describing nutrient limitation. The “PP” output represents the “plant pool” (not to be confused with the file’s name) that temporarily stores resorbed foliar nutrients and nutrients acquired from the soil, before allocating these nutrients to the different biomass tissues. The size of this plant pool is limited. When a nutrient limitation occurs, the plant pool size is reduced or “capped” in turn, according to the limiting nutrient. The model therefore does not allow for “PU” (potential uptake) that exceeds the plant pool size, so it reduces PU accordingly. After completing this calculation step, the model can calculate the output designated “AU” (actual uptake), corresponding to the amount of nutrient added to the stand biomass during a time step. This means that PU is relative to the limiting nutrient(s) of the stand, in addition to the set growth increment of the stand. PU is calculated based on biomass increment designated in the “Tree growth” input file. First, the PU is calculated for ligneous tissue by taking the sum of each ligneous compartment, multiplied by the target concentration. Then, foliar PU is calculated on a monthly basis. Foliar PU depends on the potential foliage growth (depending on annual min and max values set by the user and on the month of the year: foliar growth being set to occur during spring). Additionally, after a harvest, PU is reduced so that it corresponds to the remaining standing biomass. Limiting nutrients can be identified by observing the difference between PU and AU, this calculation reveals the deficit between what the current stand needs to acquire according to its biomass, and what is acquired.

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  $\text{kg/ha}$ . Biomass or “dry weight” is given in  $\text{kg/ha}$ . Note that root biomass is not present in this display, as root biomass is not simulated by NutsFor.

## 4.3 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, litter flow 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  $\text{kg}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ .  $\text{NO}_3$ ,  $\text{NH}_4$ ,  $\text{SO}_4$ , and  $\text{PO}_4$  are in units of N, S and P ( $\text{NH}_4\text{-N}$ ,  $\text{NO}_3\text{-N}$ ,  $\text{SO}_4\text{-S}$ , and  $\text{PO}_4\text{-P}$ ).

#### 4.4 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  $\text{kg/ha}$ . In general, most soil base cation content will be stored in these layers (in addition to the litter pool).

#### 4.5 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.

#### 4.6 Litter

The litter output folder the “Litter pool and decomp” file, the “Litter\_kg\_ha” file, and the “litterfall” file. The litter pool and decomp file hold nutrient data specific to the O-horizon layers. It contains nutrient pool data on the harvest residue litter pool, the coarse litter pool (L1), the fine litter pool (L2), and the humic (or very fine) litter pool (L3). The file gives data for each pool separately and combined for faster analysis. For each layer, decomp% outputs are given. These values show what percent of O-horizon nutrients has decomposed. The nutrient pool is represented in units of  $\text{mmol}\cdot\text{m}^{-2}$ . The next file in the directory is the Litter\_kg\_ha file. This data file contains the same litter nutrient pool data as the Litter pool and decomp file, but in a more recognizable  $\text{kg}\cdot\text{ha}^{-1}$  unit. The final output file in the Litter directory is the litterfall file. This file contains information on litterfall distribution throughout the time frame simulated. Litterfall dry weight ( $\text{g}\cdot\text{m}^{-2}$ ) and nutrient concentrations ( $\mu\text{mol}\cdot\text{g}^{-1}$ ) are given in this file.

#### 4.7 Soil Solution

The soil solution output folder will contain a throughfall concentration file, a litter flow concentration file, and both a soil solution and leaching layer concentration file for each soil

layer specified. All files display concentration in units of ( $\mu\text{mol}\cdot\text{L}^{-1}$ ), except for the leaching layer files, which gives leaching fluxes in units of ( $\text{kg}\cdot\text{ha}^{-1}$ ). All data is output on a monthly time step.

## 4.8 SOM

The SOM output folder contains a SOM data file for each soil layer specified. The file reports nutrient content in the SOM mineral pool in terms of total storage of nutrient every month ( $\text{mol}\cdot\text{month}^{-1}$ ) and the gain of nutrients every month ( $\text{mmol}\cdot\text{m}^{-2}\cdot\text{month}^{-1}$ ). This file should be used to calibrate SOM outputs in the model.

## 4.9 Weathering

The weathering output folder reports the weathering of every layer for every chemical species defined in the mineral pool. The “Weathering Annual” file contains average annual weathering data over the total length of the simulation, whereas the layer-specific weathering files contain weathering data on a monthly time step. Both files report in units of  $\text{kg}\cdot\text{ha}^{-1}$ .

## 4.10 Using R with NutsFor

The described output files tend to be long, containing years of simulated data among several files. As mentioned previously, the user should come up with some system to read the NutsFor csv files and visualize the outputs along some time scale. R code should be written in a structured manner following best-coding practices to avoid data-mix up or other errors. The simplest two things that a user can do to avoid mistakes is to clear the R studio working directory of objects before each piece of code is run, and to set a working directory such that saved images are automatically deposited to designated folders.

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 data frame and use an indexing function to define the individual layers. For instance, a code for reading CEC might look like:

```
#Clears R studio environment
```

```
rm(list = ls())
```

```
#Sets working directory
```

```
setwd("~/Your_Directory_Path/Folder")
```

```
#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<- apply(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 locally
```

```
CEC_Graph_Ca
```

```
#Saves a png of the graph to the working directory
```

```
png('CEC_Ca.png', height=480, width=600)
plot(CEC_Graph_Ca)
dev.off()
```

It is likely that data frames 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 single line of code can be used before a graph is designated:

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

**Helpful Note:** While R studio is a powerful for analyzing large datasets, it can also be used to generate manuscript-quality tables and write dynamic reports or manuscripts. Creating such reports can make model calibration much easier.

## 5. Calibration

After starting parameters have been measured for the site or approximated from the literature, and once a reliable method of monitoring NutsFor outputs is constructed, 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 variation at the site.

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 continuous parameters to calibrate a single output has an infinite number of ways which the parameters can be ordered (Harald Sverdrup 1996). Thus, it is important to choose which parameters can vary for the site in question and use *only* these parameters for calibration.

Finally, the user should accept or reject model calibration based on a quantitative, goodness of fit criteria, such as percent differences between predicted and observed leaching rates.

## **5. 1 Hydrology**

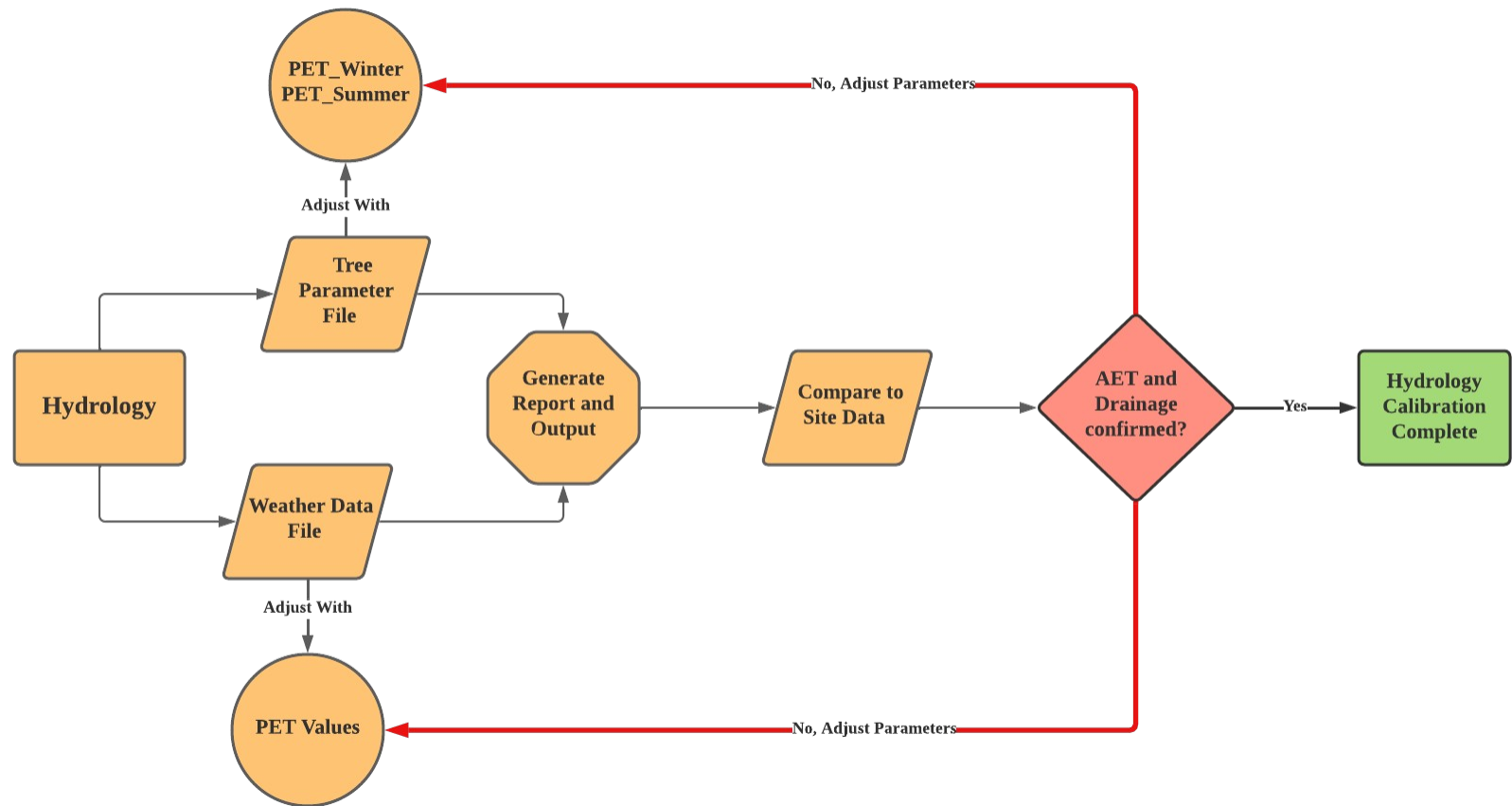
The calibration of the hydrological sub-module of NutsFor should always occur first, hydrology will affect seasonal decomposition patterns, soil solution concentrations, leaching fluxes, and weathering fluxes. It therefore has control over all other model outputs. The NutsFor hydrology sub-module is an integration of the WATFor hydrological model, developed for the same site (Breuil, France) as NutsFor (Legout et al. 2016).

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 periods.

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. The soil parameter file will contain soil moisture parameters specific to the site, these parameters will generally be held constant and should not 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 springtime PET was often overestimated 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 measure PET and AET for a specific site than to rely on estimates.



**Figure 3:** Hydrological Calibration Workflow. Hydrology can be calibrated using PET and AET factor adjustment parameters located in the tree parameters file. The weather data file can also be edited for more precise adjustment.

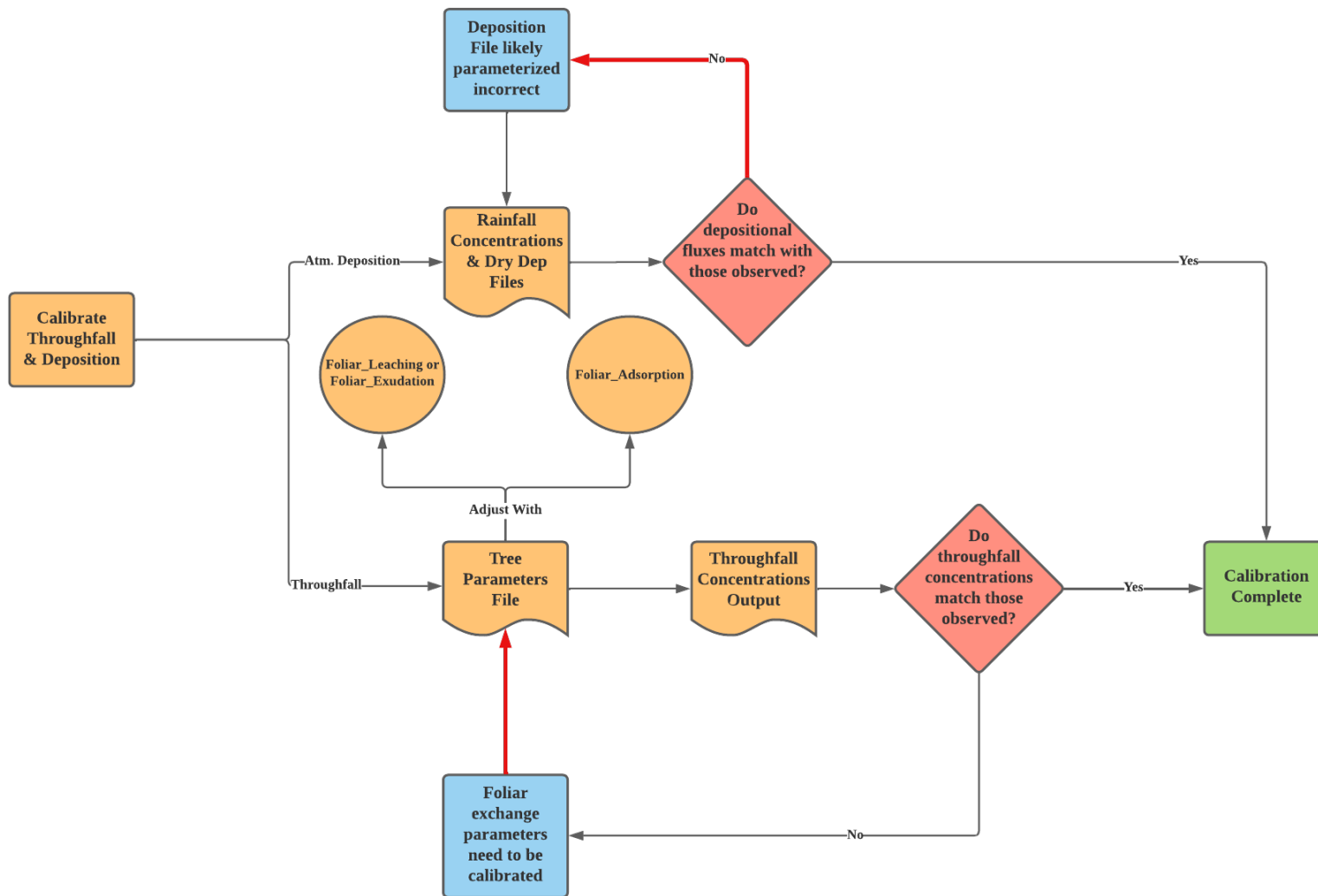
## 5.2 Throughfall & Deposition

Calibration of these inputs is rather simple, the user must observe whether deposition 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 these files will ultimately be used calculate gross 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. Some species of tree can absorb N, P, and S through their foliage cycles (Johnson and Lindberg, 1992).

Once throughfall concentrations and depositions fluxes match those observed or estimated, the calibration can be said to be complete. If little is known about a depositional input, an effort should be made to estimate or measure its contribution.

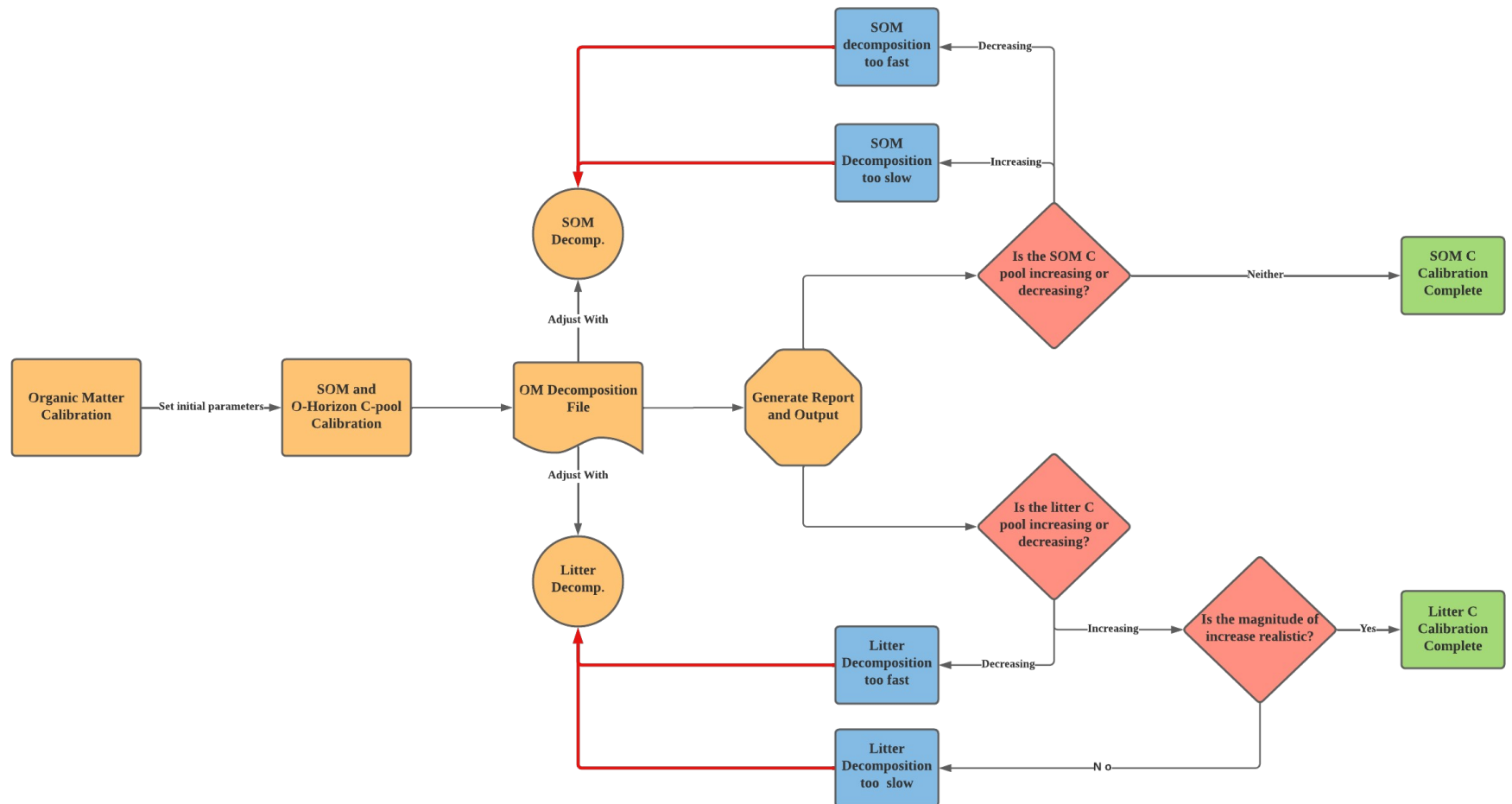




**Figure 4:** Throughfall deposition calibration workflow. Foliar adsorption, leaching, and exudation parameters can be adjusted to calibrate this parameter. These parameters are all in the tree parameter's file, output is observed in the Above ground fluxes output file in the Budgets file.

### 5.3 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, particularly over short time frames. The calibration of SOM is dictated by `Decomp_rate`, `C_Assim`, `DOC-Decomp`, 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-Decomp` can be used to reduce DOC leaching.



**Figure 5:** Soil organic matter calibration workflow. All SOM adjustment can be achieved in the OM decomposition file. Output can be observed by graphing the files in the SOM output folder.

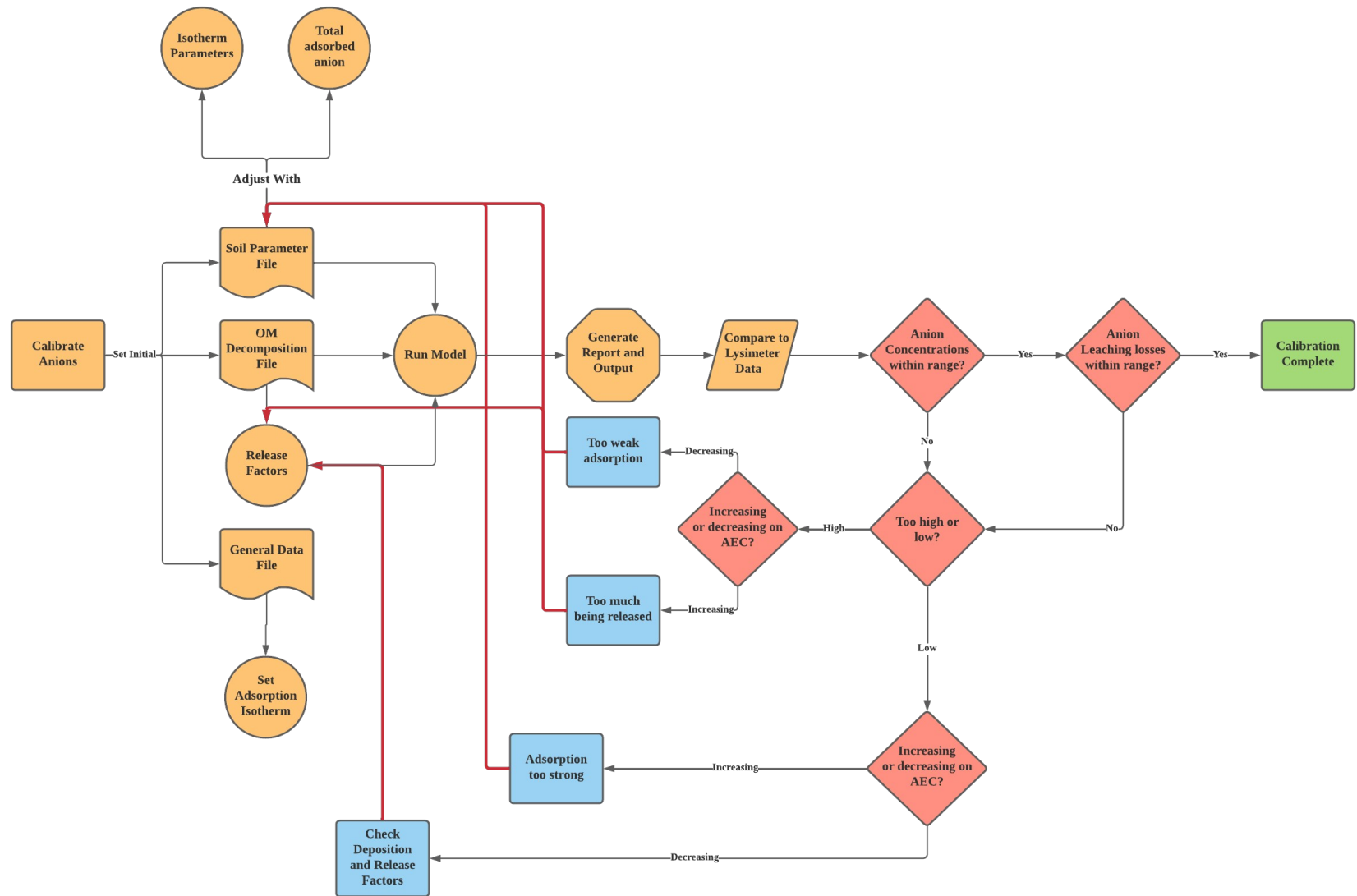
## 5.4 Anion Calibration

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 most soil anions in forest ecosystems (Dale W. Johnson and Cole 1980), however these R<sup>-</sup> 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<sup>-</sup> 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<sup>-</sup> release, whereas increasing DOC\_Decom will decrease R<sup>-</sup> concentrations. As these parameters are layer specific, calibrating R<sup>-</sup> 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<sup>-</sup> concentrations. This option will *globally* (for all layers) change R<sup>-</sup> 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 will not cause a change in DOC mobility in the model, which can help with the constraint of DOC leaching. Lowering Organic\_acid\_size decreases the number of carbons per negative charge (increasing the charge density and thus also increasing R<sup>-</sup>), and increasing the parameter decreases the charge density, lowering R<sup>-</sup> concentrations.

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



**Figure 6:** Anion calibration workflow. Anion soil solution adjustment is achieved by adjusting sulfate, phosphate, and chloride adsorption. Sulfate and phosphate concentrations may minorly be adjusted through SOM release.

## 5.5 Cation Calibration

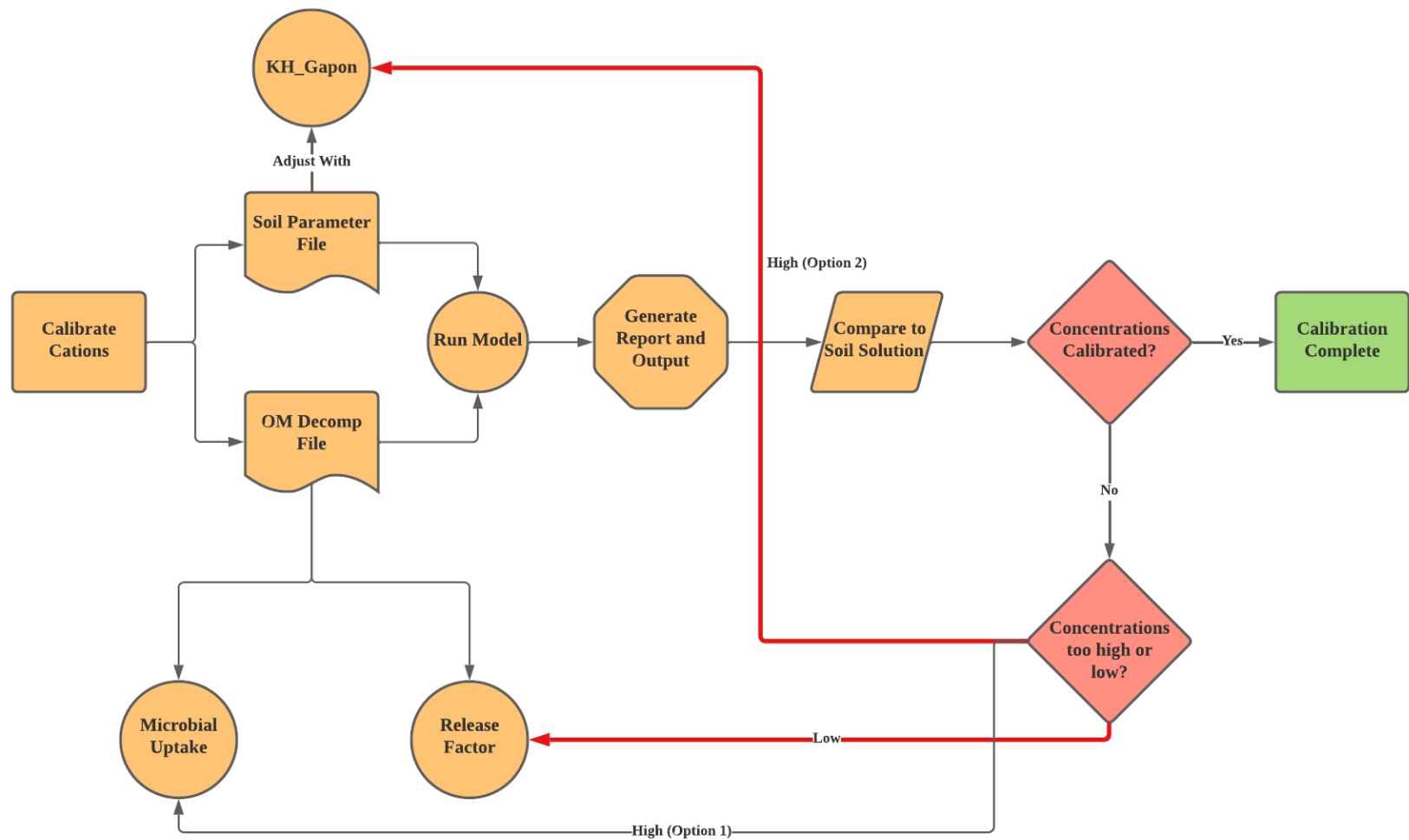
Cation concentrations should be calibrated last as every other sub-model can affect cation release through mineral weathering or acidification of the exchange complex. This calibration requires knowledge of cation concentrations in the soil solution, such as those measured by lysimeters, in order to complete calibration. The point of this calibration would be to match simulated cation concentrations to those observed. Another point of constraint on cation concentrations would be leaching fluxes, which can also be calculated from lysimeter measurements.

Generally, the cations on the exchange complex should not rapidly change-although decadal responses in CEC chemistry are not unreasonable (Johnson 1992). Gapon selectivity coefficients calculated for each cation will generally exert the greatest control on cation mobility and concentrations in the soil solution. However, I do not suggest using these Gapon coefficients for calibration of cation concentrations. Changing the value of the coefficient for, as example, Ca, will change the relative strength of adsorption for all cations.

If concentrations are generally too low, the issue may be with hydrological calibration, in which hydrological calibration is not leading to enough evaporation. If hydrology calibration is acceptable, the issue may be with the release rate of nutrient cations from litter and SOM pools. Initially, the release factors of Ca, Mg, and K in the OM decomposition file should be set to 1 and reduced if cation concentrations exceed those desired for calibration, assuming hydrology calibration has been accepted. If the cation concentrations are generally too high, the issue may be with an unbalanced anion calibration, too much mineral weathering, or too weak CEC adsorption. Pin-pointing the source of error in this case requires that the user has a way to visualize these changes in the model graphically, as noted in the previous section.

The user should be able to directly tell if an over-abundance of anions is responsible for high Ca concentrations as anion concentrations will also be too high, pH and ANC may be too low. In this scenario anion concentrations should be re-calibrated.

Ideally, an approximation of mineral weathering fluxes should be made, however it can be difficult to achieve such a calculation. In such a case, mineral area can be calibrated until silica concentrations match those observed. The model does not simulate the uptake or secondary mineral formation of silica, only mineral weathering and hydrology enact control on silica concentrations. Silica can thus be used as a kind of tracer on the calibration of both hydrology and weathering release rates of cations but will certainly underestimate weathering.



**Figure 7:** Cation calibration workflow. Cation calibration is achieved by adjusting Gapon selectivity coefficients, after accounting for every other ecosystem process. Microbial uptake may be implemented if the microbial pool is a large sink of cation nutrients. Cation monthly soil solution concentrations and leaching fluxes can be viewed in the Soil solution output folder.

## 5.6 Final Calibration

After the above calibration steps has been completed along the time frame of calibration (i.e., the years where soil solution or other confirmation data is available), the user should run the model past the period in which confirmational data is available. This ensures that the longer-term behavior of the site is reasonable with respect to the expected behavior of the site. I suggest running the model for an additional 10 years, and observing how cation exchange, soil solution concentrations, and anion adsorption change over this time.

For instance, cations and anions on the exchange complex may steadily deplete over this time period, however a steep decline is unrealistic over such a short time frame (Richter et al. 1994). Cation concentrations should be stable within this time frame, although if the stand is modeled to grow quickly, the concentrations might gradually reduce over time.

The “goodness of fit” of modeled parameters (or some other model comparison) should be calculated, this statistic allows the user to determine whether the model “adequately” simulates observed trends over time. A good example of this for a similar process-based model, Pnet-BGC, can be found in Gbondo-Tugbawa et al. 2001. In this study, the normal mean error (NME) and normal mean absolute error (NMAE) are calculated for volume-weighted-mean soil solution concentrations. Additionally, there are several other quantifications of error and fit that can be used (Janssen and Heuberger, 1995).

## 5.7 Alternative Calibration

Depending on the site in question, another sub-system of the model may need to be addressed through calibration. For example, forest soils with extremely high N content will likely have mineral weathering and nutrient cycling of base cations dominated by nitrogen transformation and cycling (Perakis et al. 2006). To calibrate the model to be representative of a high N site, the N-cycle sub-system of NutsFor must be individually calibrated. Since the N-cycle is dependent on multiple other sub-modules and sub-systems within NutsFor, this kind of calibration necessitates that a hierarchical order is established among the model’s sub-systems. This ensures that “over-calibration” does not occur, and that the calibration of sub-systems does not perturb that of others.

For the above stated order of calibration, N-cycle calibration could be placed directly after SOM calibration, with anion calibration following. This is because SOM stabilization and release rates will dictate N release, and nitrification rates will affect anion concentrations, the N-cycle calibration can therefore be placed in between these steps.

Another kind of alternative calibration, where the user lacks knowledge about a major aspect of model constraint, can be to calibrate the model based on higher-level observed ecosystem behaviors. This kind of calibration would typically occur when, for instance, lysimeter data is unavailable but past weathering, deposition, and tree data are. With the known past behavior of the site, the user can calibrate the model’s parameters until all the constraining outputs matches observed measurements. According to this sort of method, the user would have to accept whatever soil solution concentrations and leaching fluxes the model calculates.



However, an initial estimate of soil solution concentrations is required to set the Gapon selectivity coefficients for the model.

## 6. Hypothesis Testing

After the final calibration of a base site, hypothesis testing may begin. This process may undertake many forms. For example, the user may test how changes in atmospheric deposition, soil temperature, harvest scenarios, and growth scenarios affect simulation outputs over whatever time frame desired. Since NutsFor has a Stand Harvesting specific file, which allows for harvest residues to be left over, many hypotheses pertaining to harvest intensity may be tested. If the user wishes to simulate long term nutrient cycling behavior (under any set of conditions), the Weather data, soil temperature, rain fall concentration, and tree growth files must be lengthened such that input data is present for every time point to be simulated.

If the user wishes to exact change on the simulated system over the simulated time period, parameterization can be used accordingly. For instance, the program does not currently include N-fixation or fertilization specific processes. If these processes occur in the stand, they can be broadly simulated by “dosing” the atmospheric deposition file with regular increments of N (or other fertilizer nutrients) as needed by the user. The user may also include fertilizers as minerals in the Mineral Data file, adjusting mineral reaction parameters to replicate the release rate of the fertilizer. An example of this can be found in Johnson, Swank, and Vose 1995, where the potential nutrient additions of forest soil liming were observed for the Hubbard Brook Forest (WS-6) using the related NuCM. The user would need to estimate the average release rate of the fertilizer prior to dosing the rain concentration file or adding a fertilizer mineral.

## 7. Sensitivity Analysis

The purpose of conducting sensitivity analysis on process-based models is to exam the influence of parameter uncertainty on model outputs, the relative strength of a parameter in determining model outputs or as a way of testing alternative scenarios within naturally occurring parameter bounds (Pianosi et al., 2016). Sensitivity analysis takes the range of numbers in a standard deviation for a given measurement, separates them into discrete increments, and runs the model with each increment as a parameter value. For large numerical models like NutsFor, sensitivity analysis is best (most easily) done by setting a minimum and maximum around the parameter of interest (e.g. a multiple of  $\pm 20\%$  from the original parameter value), holding all other parameters constant. This is also known as a one-at-a-time local sensitivity analysis (Hamby, 1994). To accomplish this in the current framework of NutsFor, a new NutsFor directory should be made for every sensitivity parameter and increment. If sensitivity analysis is examined for the same response variables at different sensitivity scales (e.g., the parameters are in different units), or different sensitivity increments, a coefficient called a "relative sensitivity coefficient" should be calculated. This coefficient allows for direct comparisons to be made between the different analyses through a sensitivity index number. The higher the number, the

more sensitive the model output is to the parameter tested. There are several sensitivity analyses schemes that can be used, large ecosystem models like NutsFor tend to be complex, and so simpler options may be more appealing, at the detriment of understanding the full range of interactions in the model (Saltelli and Annoni, 2010). In the case where the entire breadth of parameter interactions wants to be observed, a global sensitivity analysis can be conducted (Xu et al., 2004).

General Equation 3:

$$SI = \left| \frac{\delta Output}{\delta Input} \right|$$

This equation is represented as the finite difference:

$$SI = \left| \frac{R_p - R_b}{P_p - P_b} \right|$$

The equation can be extended to represent a relative sensitivity coefficient (also called the percent difference sensitivity index):

General Equation 4:

$$SI = \left| \frac{\left( \frac{R_p - R_b}{R_b} \right)}{\left( \frac{P_p - P_b}{P_p} \right)} \right|$$

**Helpful Note:** Note that these methods are meant to analyze parameters one at a time, and do not represent interactive parameter effects. Interacting parameter effects require more robust sensitivity analysis schemes, such as the elementary effects analysis (Saltelli et al., 2010). In short, this method, while simple, is better suited for scenario testing than it is for a genuine consensus on model sensitivity to a given parameter.

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## Appendix

Please contact [KavehSiah@gmail.com](mailto:KavehSiah@gmail.com) with any questions pertaining to this manual.

Contact Gregory van der Heijden ([gregory.van-der-heijden@inrae.fr](mailto:gregory.van-der-heijden@inrae.fr)) for collaboration and modeling questions.

All vector art images made from: <a href="https://www.vecteezy.com/free-vector/tree-silhouette">Tree Silhouette Vectors by Vecteezy</a>, user tonyjack5p, and <a href="https://www.vecteezy.com/free-vector/pine-tree">Pine Tree Vectors by Vecteezy</a>, user krustovin.

## List of Equations

## ***NutsFor Equations***

### *Chemical Equations*

#### Equation 1:

$$ECEC = 2[C a^{+2}] + 2[M g^{+2}] + [K^{+}] + [N a^{+}] + 3[A l^{+3}] + [N H_4^{+}]$$

#### Equation 2:

$$K_{H:Cation^{+n}} = \left( \frac{E_{Cation^{+n}}}{[Cation^{+n}]} \right) * \left( \frac{[H^{+}]}{E_H} \right)$$

Where;

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

and

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

Note that

$$n = \text{Valence}$$

### *Litter*

#### Equation 3:

$$DecompC(t, n) = k_n * Pool_C(t, n) * f(T) * 10^3$$

Where *DecompC* is the decomposition rate of C at time step *t* for litter layer *n* ( $mmol \cdot m^{-2} \cdot month^{-1}$ ),

$k_n$  is the user specified decomposition rate or "Decomp rate" ( $mmolC \cdot month^{-1}$ ),

$Pool_C$  is the carbon pool at time step *t* for litter layer *n* ( $mol \cdot mol^{-2}$ ), and

the temperature limiting factor  $f(T)$  is given by:

#### Equation 4:

$$f(T) = e^{\left(\frac{T_{ave} - T_{ref}}{m}\right)}$$

Where  $T_{ave}$  is the average air temperature from the weather data file,

$T_{ref}$  is the optimal temperature of decomposition, and

$m$  is a function parameter.

Equation 5:

$$R_{\sigma} = DecompC(t, n) * [\sigma]_{Litter}(t, n) * ReleaseFact(\sigma, n) * 10^{-3}$$

Where  $R_{\sigma}$  is the flux of nutrient  $\sigma$  ( $mmol \cdot m^{-2} \cdot mol^{-1}$ ),

$[\sigma]$  is the concentration of nutrient  $\sigma$  at time  $t$  for litter layer  $n$  ( $mmol \cdot m^{-2} \cdot mol^{-1} C$ ), and

$ReleaseFact(\sigma, n)$  is the user-specified nutrient release factor for each litter layer  $n$ .

*Weathering*

Equation 6:

$$r_j = \left( \frac{k_{H^+} * [H^+]^{n_{H^+}}}{f_{H^+}} \right) + \left( \frac{k_{H_2O}}{f_{H_2O}} \right) + \left( \frac{k_{CO_2} * P_{CO_2}^{n_{CO_2}}}{f_{CO_2}} \right) + \left( \frac{k_R * [R^-]^{n_R}}{f_{R^-}} \right)$$

where  $r_j$  is the Weathering Rate of mineral  $j$ ,

$k_{species}$  is the rate coefficient of each species for each mineral,

and  $n_{species}$  is the reaction order (or weathering dependence) of each species.

The reaction rate coefficient  $k_{species}$  of a specific reaction is calculated by the equation:

Equation 7:

$$k = 10^{-\left(pK + (E_A / R * \ln(10)) * (1/T) - 8.56 * 10^{-3}\right)}$$

Where  $pK$  is the rate coefficient of the reaction at the temperature  $T=280^\circ K$ , expressed as  $-log_{10}(K)$ ,

$E_A$  is the Arrhenius activation energy ( $J \cdot kmol^{-1}$ ),

$R$  is the universal gas constant ( $J \cdot kmol^{-1} \cdot K^{-1}$ ), and

$T$  is the absolute temperature ( $^{\circ}K$ ).

Equation 8:

$$f_{H^+} = \left(1 + \frac{[Al]}{C_{Al}}\right)^{W_{AlH}} * \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BC_H}}$$

Equation 9:

$$f_{H_2O} = \left(1 + \frac{[Al]}{C_{Al}}\right)^{W_{Al_{H_2O}}} * \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BC_{H_2O}}}$$

Equation 10:

$$f_{CO_2} = \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BC_H}}$$

Equation 11:

$$f_{R^-} = \left(1 + \frac{[R]}{C_R}\right)^{W_{R_H}} + f_{CO_2} = \left(1 + \frac{[BC^{+2}]}{C_{BC}}\right)^{W_{BC_{H_2O}}}$$

Where the  $C_{Al}$ ,  $C_{BC}$ , and  $C_R$  are saturation concentration parameters,

and the  $W_{BC_H}$ ,  $W_{BC_{H_2O}}$ , and  $W_{Al_H}$  are reaction orders.

Equation 12:

$$W_M = \sum_{j=1}^{mineral} \left( \frac{r_j * A_W * X_j * \Theta * z}{Norm} \right)$$



Where  $r_j$  is the specific mineral weathering rate,

$A_w$  is the user-specified exposed mineral area surfaces ( $m^{-2} \cdot m^{-3}$ ),

$X_j$  is the user-specified fraction exposed mineral area which mineral  $j$  occupies,

$\Theta$  is the soil moisture saturation,

$z$  is the soil layer thickness (m),

and  $Norm$  is the number of base cation charges released per mol of weathered mineral  $j$  ( $mol_c \cdot mol^{-1}$ ).

Equation 13:

$$\Theta = \frac{(\theta * \rho_{solid})}{(\rho_{solid} - \rho_{soil} + \theta * \rho_{water})}$$

Where  $\theta$  is the soil volumetric water content ( $m^3 \cdot m^{-3}$ ),

$\rho_{solid}$  is the solid density of soil ( $kg \cdot m^{-3}$ ),

$\rho_{soil}$  is the bulk density of soil ( $kg \cdot m^{-3}$ ), and

$\rho_{water}$  is the density of water ( $kg \cdot m^{-3}$ ).

Equation 14:

$$FolLeach(t, \sigma) = L_{\sigma} * [\sigma]_{Leaf}(t) * DW_{Leaf}(t) * [H^+]^{\alpha}$$

Where the  $L_{\sigma}$  is the specific leaching rate coefficient of ionic nutrient  $\sigma$  ( $mont h^{-1}$ ), and

$[\sigma]_{Leaf}(t)$  is the concentration of ionic nutrient  $\sigma$  at time ( $t$ ) in the foliage ( $\mu mol * g^{-1}$ ), and

$[H^+]^{\alpha}$  is the hydrogen concentration of throughfall to the power of leaching rate dependence  $\alpha$  ( $\mu mol/L$ , unitless).

Equation 15:

$$FolAbs(t, \sigma) = A_{\sigma} * [\sigma]_{TF}(t) * TF(t) * [\sigma]_{TF}(t)^{\beta}$$

Where foliar absorption for nutrient  $\sigma$  at time ( $t$ ) ( $FolAbs(t, \sigma)$ ) ( $\mu mol * m^{-2} * mont h^{-1}$ ),

$A_{\sigma}$  is the specific absorption constant ( $mont h^{-1}$ ),

$[\sigma]_{TF}(t)$  is the throughfall concentration of nutrients at time  $(t)$  ( $\mu\text{mol} * L^{-1}$ ),  
 $TF(t)$  is the throughfall flux at time  $(t)$  (mm or  $L * m^{-2}$ ), and  
 $\beta$  is the rate dependence of adsorption (unitless).

Equation 16:

$$FolEx(t, \sigma) = \gamma_{\sigma} * [\sigma]_{Leaf}(t) * DW_{Leaf}(t)$$

Where foliar exudation ( $FolEx(t, \sigma)$ ) at time step  $(t)$  for nutrient  $\sigma$ ,  
 $\{\gamma_{\sigma}\}$  is the effective leaf turnover rate of ionic species  $\sigma$  ( $\text{month}^{-1}$ ),  
 $[\sigma]$  is the concentration of ionic nutrient  $\sigma$  in the foliage ( $\mu\text{mol} * m^{-2}$ ), and  
 $DW_{Leaf}(t)$  is the dry weight of the leaf at time step  $(t)$  ( $g * m^{-2}$ ).

Equation 17:

$$T_{\sigma}(t) = [\sigma]_{Leaf}(t) * DW_{Litterfall}(t) * TransFact(\sigma)$$

Where  $T_{\sigma}(t)$  is the translocation of nutrient  $\sigma$  at time  $(t)$ ,  
 $[\sigma]_{Leaf}(t)$  is the concentration of nutrient  $\sigma$  in the foliage at time  $(t)$ ,  
 $DW_{Litterfall}(t)$  is the dry weight of litterfall at time  $(t)$ , and  
 $TransFact(\sigma)$  is the user-specified fraction of foliar nutrient translocated during each litterfall event.

**Other Equations**

General Equation 1: Mineral Area 1

$$(8 * X_{Clay}) + (2.2 * X_{Silt}) + (0.3 * X_{Sand})$$

Where  $X_{Clay}$  is the fraction of particles in the soil that are clay sized,  
 $X_{Silt}$  the fraction of particles that are silt sized, and  
 $X_{Sand}$  is the fraction of particles that are sand sized.

General Equation 2: Mineral Area 2

$$(8 * X_{Clay}) + (2.2 * X_{Silt}) + (0.3 * X_{FineSand}) + (0.05 * X_{CoarseSand})$$

### General Equation 3: Sensitivity Index

$$SI = \left| \frac{\delta Output}{\delta Input} \right|$$

Or:

$$SI = \left| \frac{R_p - R_b}{P_p - P_b} \right|$$

### General Equation 4: Relative Sensitivity Index

$$SI = \left| \frac{\left( \frac{R_p - R_b}{R_b} \right)}{\left( \frac{P_p - R_p}{P_p} \right)} \right|$$

## **Github**

For a working example of a NutsFor analysis system:

[https://github.com/Coffee-Powered-Scientist/NutsFor\\_OR2](https://github.com/Coffee-Powered-Scientist/NutsFor_OR2)

Note that this repository will be depreciated as of December 25, 2022.

## **R Resources**

Install R: <https://www.r-project.org/>

Install R Studio: <https://www.rstudio.com/products/rstudio/download/>

R Markdown: The Definitive Guide: <https://bookdown.org/yihui/rmarkdown/>

Basics of ggplot2 for Beginners: <https://rpubs.com/arvindpdmn/ggplot2-basics>

Overview of dplyr: <https://dplyr.tidyverse.org/>