

# A User Guide for the TRACE Model

Version 4.5.0, January 2009

William S. Currie, David Helmers and Willem W. Wessel

© W. S. Currie 2003 – 2009

Available at <http://www-personal.umich.edu/~wcurrie>

**Contents: TRACE User Guide**

**I. INTRODUCTION..... 4**

PURPOSE OF THIS USER GUIDE..... 4

BASIC MODEL OVERVIEW..... 4

USES AND APPLICATIONS OF TRACE ..... 5

**II. THE MECHANICS OF RUNNING THE TRACE MODEL ..... 7**

SOFTWARE NEEDED AND DIRECTIONS FOR DOWNLOAD ..... 7

DATA NEEDS FOR PARAMETERS AND INITIAL CONDITIONS..... 8

CONDUCTING SINGLE MODEL RUNS..... 9

*Input files for single-site runs* ..... 10

*Making interactive model changes at run time*..... 15

*Model output for single-site runs* ..... 18

*Commenting and logging model exercises to save* ..... 20

CONDUCTING MONTE-CARLO MODEL RUNS ..... 20

*Generation and storage of random factors*..... 21

*User action to initialize the random factors* ..... 21

*Set of parameters perturbed*..... 22

*Monte Carlo output files* ..... 23

CONDUCTING GIS MODEL RUNS ..... 24

*Input grids and files for GIS runs* ..... 24

*Output selections for GIS runs*..... 26

*Speed, memory, and optimizing efficiency in Visual Basic*..... 26

**III. GREATER DETAIL ON MODEL PROCESSES..... 28**

OVERVIEW OF MODEL POOLS ..... 28

*Units*..... 28

*Pool definitions* ..... 29

*Soil available N*..... 32

ISOTOPES AND POOL DILUTION ..... 32

DYNAMICS IN POOLS OF SOIL AVAILABLE N..... 33

FINE LITTER AND DECOMPOSITION ..... 35

*Validation tests of overall decay rates of fine litter* ..... 36

*Leaching fluxes of DOC, DON, POC, PON* ..... 36

*Net and gross N dynamics in fine litter*..... 38

WOODY DETRITAL POOLS ..... 39

*Parameters in the Scenario file*..... 39

*Inputs of woody litter to standing dead and downed pools*..... 40

*Decomposition, N dynamics, and humification of woody debris*..... 40

POOLS OF HUMIFIED MATTER (HOM, LSOM, HSOM)..... 41

*Humification as a decay process* ..... 41

*N dynamics in humified matter* ..... 42

PHOTOSYNTHESIS AND PLANT ALLOCATION OF C ..... 43

*The PlantC Pool*..... 44

PLANT UPTAKE AND INTERNAL CYCLING OF N ..... 44

*Internal source-sink model*..... 44

*N allocation to growing tissues*..... 45

## Purpose of this user guide

<i>N</i> concentration in foliar tissue.....	46
<i>N</i> concentration in woody and fine-root tissue .....	47
PARAMETERIZING THE TIMING OF THE FOLIAR MASS DYNAMICS .....	47
MICROBIAL REPRESENTATION .....	48
DETRITAL ENERGETICS .....	49
MORE DETAIL ON FORMATS FOR TEXT OUTPUT FILES.....	49
<i>Output of C:N in model pools and weighted C:N ratios of retention</i> .....	50
<i>Detrital-energetic fluxes</i> .....	50
<b>IV. METHODOLOGIES OF USING THE TRACE MODEL .....</b>	<b>52</b>
METHODOLOGICAL INTRODUCTION.....	52
TESTING OF TRACE FOR CONSISTENCY AND ERRORS.....	52
<i>Mass balance checks</i> .....	52
<i>Checks of the <sup>15</sup>N isotope calculations</i> .....	53
<i>The Echeck error-checking array</i> .....	53
MODEL PARAMETERIZATIONS AND CALIBRATIONS .....	54
A METHODOLOGY FOR TRACE APPLICATION: 12 STEPS .....	55
<i>Step 1: Assemble basic site information</i> .....	55
<i>Step 2: Create Parameter and Scenario files</i> .....	55
<i>Step 3: Parameterize litter quality and humus &amp; SOM turnover rates</i> .....	56
<i>Step 4: Test vegetation productivity</i> .....	57
<i>Step 5: Examine N mineralization and forest floor mass</i> .....	58
<i>Step 6: Parameterize or calibrate DOM and POM leaching fluxes</i> .....	59
<i>Step 7: Calibrate input rates of woody litter</i> .....	60
<i>Step 8: Examine forest floor C:N ratio</i> .....	61
<i>Step 9: Final ecosystem-level calibration of C and N cycling (independent of <sup>15</sup>N)</i> .....	62
<i>Step 10: Initial Model-data comparisons of <sup>15</sup>N recoveries</i> .....	63
<i>Step 11: Iterative model-data comparisons</i> .....	63
<i>Step 12: Modeling integrative quantities</i> .....	64
<b>V. MORE INFORMATION.....</b>	<b>66</b>
PUBLICATIONS.....	66
FAIR USE GUIDELINES AND CITING TRACE.....	67
CONTACT INFORMATION .....	68
ACKNOWLEDGMENTS .....	68
REFERENCES CITED .....	69

## I. Introduction

### Purpose of this user guide

This guide provides an overview of the basic principles of the TRACE model and suggestions for its use. Also included are step-by-step instructions for running the model, including explanations of input files and formats for the output of results. For those who may decide to use the TRACE model in scientific research, this guide also provides more detailed information concerning model processes and outlines some methodological considerations.

### Basic model overview

TRACE (Tracer Redistributions Among Compartments in Ecosystems) is a biogeochemical process model of C, N, and water fluxes in forest ecosystems. TRACE also predicts redistributions of  $^{15}\text{N}$  and  $^{14}\text{N}$  isotopes through time, by simulating  $^{15}\text{N}:^{14}\text{N}$  ratios of individual N pools and of N transferred between pools, incorporating principles of pool dilution and mass balance (Wessel and Tietema 1992, Nadelhoffer and Fry 1994). TRACE combines a complex soil process model (DocMod; Currie and Aber 1997) with the vegetation component of the PnET-CN model (Aber et al. 1997). TRACE was explicitly designed for use with large-scale  $^{15}\text{N}$ -labeled field studies, as it simulates the timing, atom%, and forms of  $^{15}\text{N}$  added to large plots. TRACE was developed as a tool to interpret processes controlling ecosystem-level redistributions of  $^{15}\text{N}$  in long-term, large-scale manipulations of pine and oak forests at the Harvard Forest, MA (Fig. 1; Aber et al. 1993, Magill et al. 2000). TRACE runs on a monthly timestep.

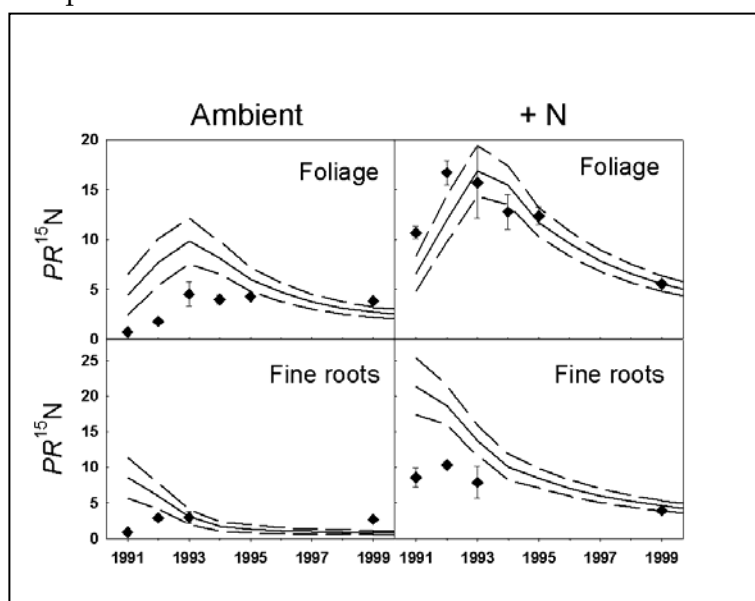
PnET-CN is an ecosystem-level model emphasizing links between vegetation physiology, biogeochemistry, and hydrology (Aber and Federer 1992, Aber et al. 1997, Ollinger et al. 2000). PnET models photosynthesis as a function of foliar N content, transpiration, vapor pressure deficit, stomatal conductance, and soil water availability. The model incorporates a multi-layered canopy model of phenology and photosynthesis, tested against gross carbon flux measurements at the Harvard Forest (Aber et al. 1996), together with allocation, respiration, and transpiration algorithms tested against both C and water balance data from the Harvard Forest and Hubbard Brook, NH.

In the development of TRACE, the vegetation and hydrology from PnET-CN became the starting point for submodels in TRACE. The TRACE model linked these with a more complex model of soil C and N interactions and plant-soil N cycling, developed a more detailed model of N mass balance in vegetation pools, and incorporated isotopic signatures to each pool and flux of N.

Soil pools in the TRACE model include separate layers for the forest floor (O horizon) and mineral soil. Fine litter enters detrital pools representing 'C classes' (acid-insoluble material, acid-soluble, and extractives; Ryan et al. 1990). Each carbon class loses dissolved organic C (DOC) via leaching and  $\text{CO}_2$  via respiration, while undergoing N dynamics. As litter decays, TRACE models the stabilization and humification of C and N in fine litter and coarse woody

debris in the forest floor and mineral soil. In litter, woody debris, and humified pools the model calculates gross N exchanges with pools of available N, necessary for simulating  $^{15}\text{N}$  redistributions. TRACE separates N into  $\text{NH}_4^+$ ,  $\text{NO}_3^-$  and organic N pools (including DON) within each soil horizon. Leaching of  $\text{NH}_4^+$ ,  $\text{NO}_3^-$  and DON are modeled as transfers from O horizon to mineral soil pools. The model explicitly includes gross N transformations including mineralization, nitrification, and gross detrital-microbial assimilation of  $\text{NH}_4^+$  and  $\text{NO}_3^-$ , again necessary for simulating  $^{15}\text{N}$  redistributions and atom%  $^{15}\text{N}$  values of plant-available  $\text{NH}_4^+$  and  $\text{NO}_3^-$  pools. These, in turn, determine the  $^{15}\text{N}:^{14}\text{N}$  ratios of N taken up by plants; soil processes link directly to plant production through water and N availability.

Plant uptake occurs in both horizons based on fine root distributions, plant demand, and competition with soil processes. These soil-plant links allow TRACE to predict both fine-scale changes in  $^{15}\text{N}$  distributions in soil and vegetation pools, together with plant-soil cycling of  $^{15}\text{N}$  in uptake and litterfall.



**Fig. 1.** Data-model comparisons of  $^{15}\text{N}$  tracer redistributions in a *Pinus resinosa* stand, Harvard Forest, MA. 'Ambient' refers to un-amended plots (30 × 30 m); '+N' refers to plots that received 5 g N  $\text{m}^{-2} \text{yr}^{-1}$  as  $\text{NH}_4\text{NO}_3$ .  $^{15}\text{NO}_3^-$  tracers were applied in 1991 and 1992 to forest floors. TRACE model predictions are shown as lines (means  $\pm$  1 SD from sets of Monte-Carlo simulations). Field results are indicated by symbols  $\pm$  1 SE. Model and field results are expressed as percent recovery of  $^{15}\text{N}$  tracers ( $PR^{15}\text{N}$ ) (Currie and Nadelhoffer, 1999; and unpublished data).

## Uses and applications of TRACE

The TRACE model was designed initially as a tool in interpreting temporal redistributions of  $^{15}\text{N}$  tracers observed in field studies. As a result, pools of N in TRACE are designed to be physically meaningful and directly comparable against field results where possible. This provides power in combined field and modeling studies, where direct model-data comparisons can be made (Fig. 1). The incorporation of  $^{14}\text{N}$  and  $^{15}\text{N}$  cycling allows the model to be used to compare against field results for both fine-scale processes (e.g. gross N dynamics in soil) and ecosystem-level N cycling (e.g. temporal changes of  $^{15}\text{N}$  in foliar litterfall) in the same field study. In addition, the use of  $^{15}\text{N}$  tracers allows direct analysis of the entry and retention of N in ecosystem pools that are otherwise difficult to assess changes in because of low signal-to-noise ratios (for example, pools of soil organic N). The use of a model in combination with such field data gives investigators a mathematical tool to help interpret  $^{15}\text{N}$  partitioning and temporal dynamics.

## Uses and applications of TRACE

Because TRACE has sophisticated production and decomposition submodels, it can be used to simulate or study organic matter budgets, C cycling and C/N interactions. The use of  $^{15}\text{N}$  tracers in field studies, combined with TRACE model-data comparisons for N pools and fluxes, C pools and fluxes, and C:N stoichiometries, together with  $^{15}\text{N}$  tracer redistributions provides a powerful set of techniques. But TRACE can be used to model interactions of C, N, and water in forest ecosystems even where  $^{15}\text{N}$  tracers are not used. In fact, this use of TRACE is an important first step before predicting or interpreting  $^{15}\text{N}$  tracer redistributions at a particular site.

The incorporation of mathematical algorithms simulating  $^{15}\text{N}$  tracer redistributions provides an additional bonus. It makes possible the technique of simulating temporal patterns of N cycling of N that entered the system through a particular mechanism in a particular year. For example, even in a forest system that received no  $^{15}\text{N}$  tracer, an investigator could use TRACE to simulate the short-term and long-term redistributions of N that entered the system in a particular year: for N that enters in 1990, for example, one could simulate where that “1990-N” is distributed in 2000, or 2010; one could simulate what the effect is of “1990-N” on forest C balance in 2000, or 2050, etc. One might repeat these model simulations for “1990-N” that entered as  $\text{NO}_3^-$ , or entered as  $\text{NH}_4^+$ , or entered via N fixation, etc.; alternatively, one might repeat these model simulations under different atmospheric  $\text{CO}_2$  concentrations, or different scenarios of temperature change. The mathematical algorithms in TRACE provide these abilities as a side benefit; in some cases, we have added additional bookkeeping code to augment these calculations (see *Modeling integrative quantities* below).

Equally important to understanding TRACE submodels and mechanics is thinking through the methodological issues that arise in using complex ecosystem models like TRACE. The utility of this model as a tool can be maximized if issues related to parameterization, setting of initial conditions, model calibration, and validation are approached carefully and methodically (see *Methodologies* below).

## II. The Mechanics of Running the TRACE Model

### Software needed and directions for download

The TRACE model software is available in two forms, both of which are bundled together in a single zip file that can be downloaded from the web site of W.S. Currie (see *Contact Information* below). Also, before downloading, please read the Fair Use Guidelines below). An executable-file version, [trace432.exe](#), can be run on any desktop or laptop computer using any version of Microsoft Windows®. No special software is needed, but you will need the model input files (which are bundled in the zip file in a default directory structure). The second form of TRACE available is the source code in Visual Basic. To read this code, to alter it, or to make use of debugging tools, you will need to have Visual Basic software on your computer (available in Microsoft Visual Studio® 6.0).

If you download TRACE from the web site (<http://sitemaker.umich.edu/currielab>), we recommend the following steps: (1) create a new directory on your computer 'c' drive named `c:\trace`, (2) download [trace432zipped.zip](#) into that directory, and (3) unzip this file. It will expand to produce a directory structure that includes the model and all of the associated input files in the default locations. This entire structure, when unzipped, will expand to about 25 Megabytes. (You can install the model on a different drive, but the default locations in the code will work most easily if you load the directory structure under `c:\trace`; if you prefer to use a different root location, it is recommended to use at least a similar directory structure). When running TRACE you will be able to browse for the input files in other locations, if you need to install the model in a different location. TRACE will now remember the last locations of the input and output files, and use them as defaults the next time you run the program. For this purpose it creates a small text file (`datafiles__.dat`).

If you have received TRACE on CD-ROM, nothing is compressed and it is not necessary to unzip any files. Simply drag the `trace\` directory, together with all of its subdirectories, to the `c:\` drive on your computer. This will create the directory `c:\trace` and preserve the subdirectory structure.

To run the executable file, in the directory `c:\trace\currentVBver\trace432code`, find the file [trace432.exe](#), and double-click on it to run TRACE. The first form that comes up will ask you to choose whether to conduct a single-site run, a Monte-Carlo run, or a GIS run (linked to a Geographic Information System for regional analysis). Detail on each of these types of model runs is provided here in the TRACE User Guide.

The Visual Basic source code also appears in the directory `c:\trace\currentVBver\trace432code`. The source code appears as a collection of about two dozen project, form, and module files. If you have Visual Basic installed on your machine, open [trace432.vbp](#) from within Visual Basic.

Sometimes Trace will not run properly because Windows® misses some .dll or other files. Therefore, these files have been provided in a separate subdirectory called "accessory Windows

## Data needs for parameters and initial conditions

files". Copying one or more of these files in their proper Windows directories will resolve these problems.

Other files that are included in the bundled zip file and on the CD-ROM are explained here in the TRACE User Guide. These include the parameter database file (TraceDataNeedsx.xls), files to assist in the creation of new input files for new sites (NewSite.xls), and others.

## Data needs for parameters and initial conditions

TRACE is a complex model with hundreds of parameters and initial conditions needed for state variables, although only a few dozen need to be altered to apply the model to a new site or region. We have constructed a database of parameters and other site-specific information, contained in the Excel file **TraceDataNeedsx.xls** (where  $x$  is the version number of this database). This database serves several purposes:

- Explains needed parameters, names in model code, units, and priorities
- Catalogues site-specific parameters
- Catalogues field-study results that are not model parameters, to compare against model results for testing and validation
- Logs comments, explanations, and literature citations for parameters and validation quantities
- Facilitates the needs of investigators at individual sites to collect and organize data needed to run TRACE
- Facilitates cross-site comparisons of model runs by standardizing parameter similarities and differences, together with the units and forms of validation data. Also facilitates comparison of TRACE cross-site analyses with other analyses of field data across the same sets of sites.

Data Priority Codes	
0	not required for model; does not currently use
1	low priority
2	intermediate priority
3	high priority
V1	useful for validation, low priority
V2	useful for validation, intermediate priority
V3	useful for validation, high priority

**Table 1.** Data Priority Codes used in TraceDataNeedsx.xls

Comments within TraceDataNeedsx.xls provide more information about the database, including an explanation of the 'data priority codes' listed in the database (Table 1). This code indicates how important it is to get *site-specific* data for a particular parameter or observable. The numerical value of this priority code reflects a combination of two things: how sensitive the model is to this parameter; and how well an existing value in the model is believed to suffice for other sites. If this model is very sensitive to the parameter, and the parameter is

## Conducting Single Model Runs

likely to vary significantly from site to site, then it will have a high priority code. Low priority does not mean that it is not needed -- or necessarily that the model is insensitive to it -- it means that it is not advisable to spend substantial effort working to get a site-specific value, relative to the effort that is advisable to spend on higher-priority parameters.

In using this database, we recommend:

- Use this Excel file conscientiously and methodically to enter validation data and citations, parameter changes and comments and citations. When it comes time to write up a manuscript, this serves as an invaluable resource.
- Take care not to add or delete rows or columns; all the rows and columns should line up across all of the different sites. This makes cross-site parameter comparisons quick and easy.
- If you make changes, save this Excel file as a new version, but not an integer increment (e.g. if it is version 9, save it as 9ab where 'ab' are your initials, but not as version 10); W. Currie will collate information at 'TRACE database central' and will save new integer-incremented versions of this database. Send your augmented file to W. Currie if you want to make your site information available for, or collaborate in, cross-site modeling activities.

## Conducting Single Model Runs

The TRACE model can be run in a single simulation for a specific forest site ('single model run', described here), in a Monte Carlo set (described below), or linked to a GIS for regional extrapolation (described below). When you start TRACE, the first form that appears offers this choice. The choice you make then guides you through the graphical user interface, allowing you to specify inputs, outputs, parameter changes, and so on. These choices are tailored for each run type. The most common use of TRACE is the single model run. The mechanics of conducting a single model run, or a set of them, are described in this section.

Data handling in TRACE is designed to facilitate simulations that are methodically structured for comparisons among field treatments, across sites, or among various future scenarios. All of the information used to conduct a single model run can be easily saved and logged together with the results. Extending this principle, multiple 'single' runs can be conducted, with all of the parameter and scenario information used for each run saved in text files together with the output.

For example, suppose one wanted to conduct TRACE simulations across a set of five forest sites along an N deposition gradient, carefully controlling and saving records of the similarities and differences in the model input parameters and scenarios used across the set of five model runs. One could construct five of each type of input file (Parameter, Scenario, and Climate files), label them A through E, comment them to indicate which site they were constructed for, and save them alongside output files containing model results (which can also be commented and labeled A through E). These input files used for particular model analyses should be retained as a permanent record. Later, if questions arise concerning the precise parameter information or scenarios used for the particular set of model runs, all of the information will be saved.

## Conducting Single Model Runs

The sections below outline the mechanics of the following:

1. Using our database for model parameters and validation data;
2. Using and constructing files for input data;
3. Making interactive model changes at run time;
4. Setting formats for ASCII output data and viewing plots on-screen;
5. Commenting and logging your model runs.

### Input files for single-site runs

#### *Parameter files*

Parameter files are named as Para\_\_\_\_.txt (for example ParaHFHW.txt for Harvard Forest Hardwoods). These are simple text files (i.e. plain text, same as ASCII text) that contain information about a site's initial parameter inputs. The file is structured as a list of two input items. The first item is a string representing the name of the parameter as used in TRACE, while the second item is the corresponding initial value of that parameter. The text file is comma delimited, and appears as follows:

```
K,                .58
AmaxA,           -46
AmaxB,           71.9
...
```

These parameters are location-sensitive by line: do not transpose or move lines in this file. Both the name of the parameter and its value are read into two separate arrays in *ParaInput()*: **ComVar\$()** stores the parameter name as a string and **VarValue()** stores the value. Each element of **VarValue()** is then assigned to each TRACE variable in the *ParaInput()* subroutine based on its position in the Para\_\_\_\_ file. Using the example above, the TRACE code appears as follows:

```
K = VarValue(1)
AmaxA = VarValue(2)
AmaxB = VarValue(3)
...
```

Also included in each parameter file, preceding the parameter values at the top of the file, are 2 lines of user comments. These two lines of comments can be used to store any relevant information about the file - site name, exercise number, or other notes. These two comment lines will appear on all ASCII output files. The two lines of comments must be included in each parameter file (even if only placeholders are used); otherwise TRACE will experience errors in reading in the parameters because they will be off by one line. (Note - do not use any commas in these comment lines; this will cause a mis-reading of the input file.)

The file '**ParaNewSite.txt**' is provided to help generate a new Para\_\_\_\_.txt file. All required parameters are listed in this file in the same order as they are read into TRACE, and two lines are provided at the top for user comments. Simply change the value of each parameter to

## Conducting Single Model Runs

match that of your site and save it as a new Para\_\_\_\_.txt file. We recommend a 3 or 4-letter code for each site  $x$  vegetation combination that you use for input files. For example, if your site is designated ABCD, name this file ParaABCD.txt. Existing input files are names as follows:

HFHW = Harvard Forest Hardwoods  
HFPN = Harvard Forest Pine  
BBWM = Bear Brooks Watershed, Maine (hardwoods portion)  
KLO = Klosterhede, Denmark  
ABER = Aber Forest, UK  
GARD = Gardsjon, Norway  
YSSL = Ysselsteyn, The Netherlands  
DUKE = Duke Experimental Forest FACE facility, North Carolina

### *Scenario files*

Scenario files, named as (Scen\_\_\_\_.txt) are also plain text files. These files provide model inputs that change through time – climate, harvest, N amendments, isotopic signatures of N amendments, etc. The fact that these are text files allows them to be constructed and saved. This provides a record of the model run, allows reproducibility, facilitates similar model runs across sites, and also allows several slightly different scenario files to be constructed, saved, and run one after another in a systematic way.

The Scen\_\_\_\_.txt files are generated initially as a series of Excel worksheets, differentiated by a combination of treatment type (ambient, low-N) and  $^{15}\text{N}$  form ( $\text{NH}_4^+$ ,  $\text{NO}_3^-$ ). Each of these spreadsheets is broken into 8 sections, grouped by sets of variables. They are: 1) Time Frame, 2) Harvest, 3) N Deposition and Inputs, 4)  $^{15}\text{N}$  additions and Fertilization amendments, 5) Throughfall, 6) Climate Change, 7) Agricultural Harvest, and 8) Soil Loss. Each of these sections is comprised of a set of variables that will be read into TRACE to run the model for a given site and scenario. For reference, the column header for each variable corresponds with the variable name in TRACE code. For information describing each scenario section and each variable in more detail, see the worksheet entitled “ScenarioInfo” in any of the provided **Scen\_\_\_\_.xls** files, or in the ‘**ScenNewSite.xls**’ file.

To construct a new series of Scen\_\_\_\_.txt files for a given site, see the Excel file ‘**ScenNewSite.xls**’, specifically the worksheet entitled “NewSiteInstruct”. Step-by-step instructions are provided as well as two empty worksheets for entering the new scenario values. Remember to include the 3 lines of comments at the top of the finished scenario .txt file.

Each worksheet is separated into two basic sections. The uppermost section (~top 30 rows) contains the base information that is used to generate the variable values (these are the ‘driving parameters’). When creating a new set of scenario files, you should begin by completing this section. Below this section is the actual scenario data, monthly values for each scenario-specific variable derived from the driving parameters. Two things to note: 1) the driving parameter section is separated from the values section by the color-coded scenario column headers; and 2) only the values section is actually copied and pasted (or saved) as a .txt file for reading by TRACE.

## Conducting Single Model Runs

For any given site there will be up to 4 separate scenario input files, based on differences in treatment and <sup>15</sup>N form. Once each treatment and <sup>15</sup>N form combination sheet is generated and verified for accuracy, the values section of the worksheet is saved as a .txt file (tab delimited) that will be read in to TRACE in the subroutine *ScenInputs()*. An example of one of these files would be ScenHFHWambNO3.txt. Notice the naming convention used: “Scen”+(site)+(treatment)+(<sup>15</sup>N form).txt.

At the top of each scenario file are 3 lines of comments. The first contains the site name, the second line displays the treatment type and the <sup>15</sup>N form, while the third line is provided for other comments such as exercise #, date, etc. Like the parameter files, this information must be included on every scenario .txt file as TRACE reads in these 3 lines of comments and displays them on the output printouts. If this information is missing, an error will occur in TRACE. (Note – do not use any commas in these comment lines; this will cause a mis-reading of the input file.) Each blank worksheet in the provided **Scen\_\_\_.xls** spreadsheets and the ‘**ScenNewSite.xls**’ contains three lines at the top for the user to enter this information before saving as a .txt file. Follow the instructions in “ScenarioInfo” in any of the Scen\_\_\_.xls files.

### *Note for former Trace 4.41 and lower users*

The format of the scenario files was changed in version 4.42. Those who have scenario files made for versions 4.41 and before need to update their files to make them work for version 4.42 and higher. There is a file ‘**FractionationScenMacro.xls**’ in the **scenfiles** directory, which contains a macro that can convert old scenario excel files into ones that can be used with the present version of TRACE. This excel file also contains all the necessary information how to perform this conversion. The change concerns the addition of several columns to the ‘N Deposition and inputs’ section.

### *Variables read in Scenario files*

Just like the Para\_\_\_.txt files, the order of variables listed in the Scen\_\_\_.txt file is important. TRACE reads in the scenario values directly into model variables in *ScenInputs()* in the following order:

Calyear, nYear, nMonth, BiomLossFrac, RemoveFrac, OMixFrac, WoodTurnover, FWDfrac, ninx, WetDepNH4Con, deltaWetDepNH4, WetDepNO3Con, deltaWetDepNO3, DryDepNH4, deltaDryDepNH4, DryDepNO3, deltaDryDepNO3, AONDepProp, deltaAONDep, ExtraNinput, deltaExtraNinput, NH4Amend, atomp15NH4, NO3Amend, atomp15NO3, NTracerAddLoc%, TFDOM, TFDON, DelTMax, DelTMin, DelPrec, DelPAR, Ca, O3, AgHarv%, AgRem, OSLossFrac, MSLossFrac

The following list provides additional information about the definitions and uses of the above-listed variables in the Scenario-generating Excel files and/or in TRACE code. This list of variables is significant. Unlike parameters read in from the Parameter files which are constant through a TRACE simulation, these variables or parameters in the Scen\_\_\_.txt files are read each month; thus the user-input values of these can change monthly through a TRACE simulation.

## Conducting Single Model Runs

### Time Frame variables

(Note that CalYear, nYear, nMonth are not used in TRACE code: simply used in Scenario input files for clarity when looking at those files, and read into TRACE but not used in the model.)

**CalYear :** actual Calendar Year in model run (starts at Baseyear%)  
**nYear :** current model run year (identical to iyear)  
**nMonth:** current model run month (identical to imonth)

### Harvest variables

**BiomLossFrac:** fraction of wood, canopy, and root mass lost from living pools during harvest  
**RemoveFrac:** fraction of wood mass cut (above + below ground), that is removed from site (the remainder is left on site as slash)  
**OMixFrac :** fraction of forest floor mixed down into mineral soil as a result of disturbance due to logging operations  
**WoodTurnover :** annual rate (as fraction) of living wood turnover (mortality) to standing dead wood  
**FWDfrac :** fraction of woody inputs to soil that is FWD (vs. CWD)

### Deposition and N input variables

**ninx :** percentage of present day background N deposition levels; ramps from some fraction, to 1.0, through time.  
**WetDepNH4Con:**  $\text{NH}_4^+$ -N in wet dep (mg N/L)  
**deltaWetDepNH4:** delta  $^{15}\text{N}$  in wet  $\text{NH}_4^+$  deposition  
**WetDepNO3Con:**  $\text{NO}_3^-$ -N in wet dep (mg N/L). These concentrations of  $\text{NH}_4^+$ -N and  $\text{NO}_3^-$ -N are multiplied by precipitation amounts, each month, to produce wet deposition inputs of inorganic N.  
**deltaWetDepNO3:** delta  $^{15}\text{N}$  in wet  $\text{NO}_3^-$  deposition  
**DryDepNH4:**  $\text{NH}_4^+$ -N in dry dep (g N/m<sup>2</sup> mo)  
**deltaDryDepNH4:** delta  $^{15}\text{N}$  in dry  $\text{NH}_4^+$  deposition  
**DryDepNO3:**  $\text{NO}_3^-$ -N in dry dep (g N/m<sup>2</sup> mo)  
**deltaDryDepNO3:** delta  $^{15}\text{N}$  in dry  $\text{NO}_3^-$  deposition  
**AONDepProp:** Atmospheric Organic N (AON) deposition: calculated as this decimal fraction multiplied by wet inorganic N deposition. For example, if wet inorganic N deposition = 4 g N m<sup>-2</sup> yr<sup>-1</sup> and AONDepProp = 0.5, then AON deposition = 2 g N m<sup>-2</sup> yr<sup>-1</sup>, or 1/3 of overall wet N deposition.  
**deltaAONDep:** delta  $^{15}\text{N}$  in AON deposition  
**ExtraNInput:** This is a means of adding explicit, extra inputs of N, on a monthly basis at a rate that can change over time, if needed to produce realistic N cycling but if the source(s) of such extra inputs are unknown. This 'extra' N input flux is added as half  $\text{NH}_4^+$ -N, half  $\text{NO}_3^-$ -N, at the atmospheric (background) isotopic ratio, to available pools of N in the O horizon.  
**deltaExtraNinput:** delta  $^{15}\text{N}$  in extra N input

### $^{15}\text{N}$ addition and fertilization variables

**NH4amend:**  $\text{NH}_4^+$ -N amendment in g N/m<sup>2</sup>/mo  
**atomp15NH4 :**  $^{15}\text{N}$ :Total N of  $\text{NH}_4^+$ -N amendment (atom %  $^{15}\text{N}$ )  
**NO3Amend:**  $\text{NO}_3^-$ -N amendment in g N/m<sup>2</sup>/mo

## Conducting Single Model Runs

**atomp15NO3 :** 15N:Total N of NO<sub>3</sub>-N amendment (atom % 15N)  
**NTracerAddLoc%:** Location of tracer application (0-4)  
0 = no N amendment or tracer  
1 = added to forest floor  
2 = added to moss layer  
3 = added to shrub layer  
4 = added to forest tree canopy  
(Note: at present, only 0 and 1 are operational; 2-4 are intended future model enhancements.)

### Throughfall variables

**TFDOM:** TF flux of DOM, dissolved organic matter (g mass/m<sup>2</sup> yr)  
**TFDON:** TF flux of DON, dissolved organic N (g N/m<sup>2</sup> yr)

### Climate Change variables

**DeITMax :** Absolute changes in max. and  
**DeITMin:** min. temperatures in degrees C  
**DelPrec:** Proportional changes in precipitation  
**DelPAR:** and solar radiation  
**Ca:** parts per million volume (ppmV) of CO<sub>2</sub> in atmosphere (normal value is assumed to be 350 ppmV)

## *Climate files*

The final required input file for single and Monte Carlo runs are climate files (named Clim\_\_\_\_.txt) Climate files are also plain text (ASCII) files that contain information about a site's monthly climatological inputs. The file has 12 separate records of data (one for each month), with each record being comprised of seven different climatological parameters. These seven parameters are read in monthly in *ScenInputs()* in ModInput as the following variables:

- **DOY** (day of year)
- **Tmin** (minimum temperature - °C)
- **Tmax** (maximum temperature - °C)
- **PAR** (photosynthetically active radiation- μmoles m<sup>-2</sup> s<sup>-1</sup>)
- **Prec** (precipitation - cm)
- **J1** (empty (junk) variable 1)
- **J2** (empty (junk) variable 2)

Special notes about **PAR**: Earlier versions of the TRACE user guide incorrectly listed the units; the correct units are listed above (consistent with Aber et al. 1996). In calculating values for PAR it is important to correct for the daylength on a monthly basis. The value of PAR needed by the model is the monthly average during daylight hours only, not the 24 hour average. (If PAR data are the average on a 24 hour base then they would be far too low.)

**J1** and **J2** are empty, place-holding variables that can be substituted for additional monthly climatological inputs; at present they are set to zero and are not used. Note that this format for

## Conducting Single Model Runs

the climate input file is the same format used for the PnET-CN model in the late 1990s (Aber et al. 1997); this allowed direct exchange of input files between the two models at that time. (However, this may no longer be the case, so check carefully before using an input file from PnET-CN for TRACE)

To construct a new climate file for a site, start with a blank .txt file. Enter the following 12 integers for the first column of data (DOY): 15, 46, 76, 107, 137, 168, 198, 229, 259, 290, 321, 351. For each of these DOY, enter the corresponding Tmin, Tmax, PAR, and Prec across all 12 rows, separating each value with a <TAB> or a <SPACE>. Enter "0" for both J1 and J2. A finished climate file should look as follows:

15	-3.9	6.1	130.23	9.8	0	0
46	-4.4	5.6	227.45	6.6	0	0
76	-2.4	7.6	340.44	7.5	0	0
107	0.8	10.8	495.78	5.1	0	0
137	5.9	15.9	634.40	5.5	0	0
168	8.4	18.4	620.37	5.2	0	0
198	10.5	20.5	583.55	7.0	0	0
229	10.0	20.0	533.05	9.9	0	0
259	6.8	16.8	422.38	11.7	0	0
290	3.6	13.6	272.03	11.6	0	0
321	0.0	10.0	184.40	10.4	0	0
351	-2.1	7.9	107.94	9.1	0	0

During a model run, the climate file is closed and then re-opened at the beginning of each year (except for year 1) so that input from the climate file starts with the first record in the file. The climate file is then accessed a total of 12 times over the course of a single year, reading in each record of the seven climatological parameters monthly as variables for use in TRACE.

It is possible to use a climatological sub-model in TRACE to generate a climate file within the New York – New England region (USA). This *climcalc* submodel was developed by Ollinger et al (1993) and it derives climate information, given latitude, longitude, and elevation, and is based on a statistical model of temperature and precipitation across the New York - New England region (it is not appropriate for use outside of this region).

To use *climcalc*, simply check the box entitled “No climate file; Generate one using Ollinger et al. model” on the InputSet form. This is the form that appears when the user clicks “Change Input files...” on the main form. When the “No climate file...” box is checked, *climcalc* generates a new climate file named ‘*tmpclim.dat*’ and stores it in \SiteInputs\climfiles. TRACE then uses this file for monthly climatological inputs, as described above.

## Making interactive model changes at run time

After the input files are read by TRACE, several types of changes can be made interactively at run time. These changes are made through the graphical user interface, the set of forms that the user steps through as the model run is constructed, just prior to starting the simulation.

### *Interactive parameter changes on the ParamChg form*

Selected parameters may be altered from their values in the Parameter input file (Para\_\_\_\_.txt) for a single model run, at run time, without changing the values stored in the Parameter input file. This is done through the *ParamChg* form, accessed by clicking 'Interactively change model parameters' on the main interface form.

The interactive parameter changes have two main uses. First, an investigator may want to explore the effects of changes to a single parameter or set of parameters, either to explore model behavior, or to perform parameter calibrations. This allows the user to quickly explore changes in a selected set of parameters without altering the Para\_\_\_\_.txt file. Second, this is a useful teaching tool. Dramatic differences can be obtained in model behavior with changes to a few key parameters, and this interactive form facilitates easy demonstration of this model behavior to students.

### *Month for which selected results are printed and plotted*

Many TRACE results are plotted or printed at the end of each year. But for some model results, it is more important to know the values at some point in the middle of each year. Foliar mass and the pool size of N in foliage, for example, would always be zero in a deciduous forest at the end of December, so these are more important to know in the middle of the growing season. Also, for direct comparison of simulated  $^{15}\text{N}$  tracer recoveries against field data, it is important to know model results in the summer or fall, when field samples are typically collected.

TRACE has a variable named '*Plotmo*' (Plot month), which refers to the month in which a selected set (Table 2) of model results will be plotted and printed in model results. The default value of *Plotmo* = 8. Thus, this set of results from August, rather than at year-end, will be plotted and printed. Values of  $PR^{15}\text{N}$  (percent recovery of  $^{15}\text{N}$  tracers) and  $\delta^{15}\text{N}$  are included in this set. All other model results (those not listed in Table 2) are plotted and printed at the end of December, including annual total fluxes – foliar litterfall, fine root production, wood production, N uptake, N mineralization, etc. These are summed over the year, printed, and plotted as annual values no matter what value of *Plotmo* is used. If, for a particular model run, values of all variables are needed at the end of December, this is easily accomplished by setting *Plotmo* = 12.

The value of *Plotmo* is set by the user at run-time. It is set from the Output Specifications form, which in turn is accessible from the main interface form by clicking 'Change Plots or File Printout.' This mid-year set of results controlled by *Plotmo* (Table 2) cannot be plotted or printed in more than one month. But an easy work-around is to complete identical runs of TRACE with different values for *Plotmo*. For example, if one needed to compare model simulations directly against field measures in which foliar  $^{15}\text{N}$  was measured in June, while litter  $^{15}\text{N}$  was measured in October, two identical runs of TRACE could be conducted, with *Plotmo* = 6 in the first and 10 in the second. In this case, the model runs would be identical, but results for different months would be plotted and printed. Users should be aware, however, that in the example given (foliar  $^{15}\text{N}$  measured in June, litter  $^{15}\text{N}$  in October), both the field study and the modeling simulation could double-count some  $^{15}\text{N}$  tracer, because  $^{15}\text{N}$  mass in foliage in June would appear in litterfall in October. This is important to take into account when field studies and data-model comparison studies are designed.

Variable name TRACE code	Explanation
ONH4, ONO3, MNH4, MNO3	Pool sizes: inorganic available N in O horizon (O) and mineral soil (M)
FolNTot	Pool size: Foliar N summed across cohorts
FolMassTot	Pool size: Foliar mass summed across cohorts
VascN	Pool size: Plant-internal, mobile N storage
RLpctNmeas	N concentration in fresh root litter
RootMassN	Pool size: N in living fine roots
RootMass	Pool size: Mass of living fine roots
WLpctNmeas	N concentration in fresh woody litter
Prvariablename	All results for $PR^{15}N$ , percent recovery of tracers. (Includes cumulative eluviation and bioturbation of tracer movements expressed as percent of tracer additions)
d15variablename	All results for $\delta^{15}N$ in model pools
WtdCNtracReten(x)	All calculations of weighted C:N ratios of $^{15}N$ tracer retention in aggregated model pools

**Table 2.** Variables stored in the month *Plotmo* for printing and plotting.

### *Model Structure Options*

Another set of run-time choices are included as ‘model structure options’, accessed from the main interface form just before running the simulation. Here, some simple choices can be made in how certain aspects of TRACE will be structured during a model run. Some of the choices are used for model testing and development. Other choices allow the model user to specify how some algorithms will be formulated for better model-data comparisons at a particular site. Some of these are changes to model algorithms, while others are changes to bookkeeping procedures used (e.g. whether  $^{15}N$  in dead fine roots is counted together with live fine roots, or in soil horizons). At present, some of these choices are not operational but are planned for a future version. Most of these options are explained here.

*Initial stabilization.* To avoid large initial fluctuations some seasonal and climate effects are not operative during the first 5 to 10 years of simulation. However, in case of short term runs or if such fluctuations are not expected, it is possible to switch off this initial stabilization and have the same relationships throughout the entire simulation.

*Nitrification.* (Future enhancement; a choice is not currently available). The user will be able to choose whether nitrification rates are controlled by parameters read in from the Parameter input file, or calculated internally based on the horizon C:N ratio. At present, only the first (default) option is available: net nitrification is calculated as a monthly difference in gross nitrification and gross  $NO_3^-$  assimilation; gross nitrification rates, in turn, are calculated as fractions of gross N mineralization rates in each horizon, input by the user as the parameters **OGNitFrac** and **MGNitFrac** in the Parameter input file. **OGNitFrac** can be changed interactively by the user through the *ParamChg* form.

## Conducting Single Model Runs

*N isotope fractionation / natural abundance.* (Future enhancement; a choice is not currently available.) At present, fractionation among  $^{14}\text{N}$  and  $^{15}\text{N}$  isotopes is not included in TRACE, nor are natural-abundance differences among model pools. In a future enhancement, these will be added. At present, it is assumed that field-applied  $^{15}\text{N}$  tracers are labelled strongly enough that fractionation and natural-abundance differences can be safely ignored when analyzing redistributions of  $^{15}\text{N}$  tracers.

*Location where  $^{15}\text{N}$  in dead roots is counted to compare against field studies.* Different field-study designs may sort dead roots into a separate detrital category, or include them with live roots, or include them with humus or LSOM in the horizon in which the roots occur. TRACE allows the user to select this choice, so that values of  $PR^{15}\text{N}$  in dead roots, live roots, HOM and LSOM pools can be correctly compared directly against field results.

*Effect of  $\text{CO}_2$  on stomatal conductance.* Elevated atmospheric  $\text{CO}_2$  can affect stomatal conductance and water use efficiency of photosynthesis in TRACE (adopted from PnET-CN, Ollinger et al. 2002). This effect can be turned on by the user at run time. Note that in order for this to have an effect, atmospheric  $\text{CO}_2$  concentration must also be altered in the Scenario input file.

*Effect of ozone on net photosynthesis.* Elevated tropospheric ozone ( $\text{O}_3$ ) can affect photosynthesis in TRACE (adopted from PnET-CN, Ollinger et al. 2002). This effect can be turned on by the user at run time. Note that in order for this to have an effect, tropospheric  $\text{O}_3$  concentration must also be altered in the Scenario input file.

*Effect of water stress in lowering canopy mass and thus foliar production.* In code adopted from PnET-CN (Aber et al. 1997), water stress (through the variable **avgDwater**) can reduce photosynthesis and foliar production two ways, directly and indirectly. In the direct effect, **avgDwater** scales back photosynthesis, (through the variable **CanopyGrossPsn**), given the current foliar mass. In the indirect effect, **avgDwater** also reduces the variable **EnvMaxFol**, which reduces the maximum canopy mass. This option allows the user to retain both effects (as in PnET-CN), or to disable the indirect (via **EnvMaxFol**) effect, while retaining the direct effect, if the indirect effect appears to cause problems in canopy mass at a particular site or under a particular set of conditions.

The chosen options are recorded in the header of the output file together with the header information from the input files.

## Model output for single-site runs

### *On-screen Graphics*

For single-site runs, on-screen plots are produced that display selected sets of model results over the course of the model run. The on-screen plot shows the annual trajectories of up to eight different model results. The user selects from pre-constructed combinations of results on a form (OutputSet) as TRACE is run. On each of the graphs, the X-axis is the year of the model

## Conducting Single Model Runs

run, while the Y axis is a percentage (0-100%) of the maximum graphed value for each model result. The on-screen graphic plots *relative percentages*, not actual values, because the range of values for different model results varies considerably. The legend of the plot details the maximum values for each parameter as a guide (under 'Max'). Each parameter is represented by a different colored line on the plot. This is simpler than it sounds. For example, if N mineralization is plotted alongside foliar litterfall, with 'Max' values of 20 g N m<sup>-2</sup> yr<sup>-1</sup> and 1000 g m<sup>-2</sup> yr<sup>-1</sup>, respectively, then the 25% line for each would represent values of 5 g N m<sup>-2</sup> yr<sup>-1</sup> for N mineralization and 250 g m<sup>-2</sup> yr<sup>-1</sup> for foliar litterfall.

The user may choose many different sets of model results to plot on-screen. Currently there are 12 different plot types to choose from (including the "no plot" option), with the default option being a plot of Nitrogen fluxes (with no isotope information). Most graphic options plot a line for each parameter starting in the specified site's base year (**Baseyear%**) through the model's termination year (**Baseyear% + Runyears%**). However, for the four graphic options that detail  $\delta^{15}\text{N}$  and  $PR^{15}\text{N}$  recoveries, the plotted temporal scale runs from 1985 to 2025.

### *ASCII printouts*

For each single-site run, the user can choose to print sets of model results, each year or each month, to an ASCII '.txt' file. This is the main format for saving model results and uploading to statistical or graphics software. Currently, there are 12 different sets of output parameters that the user can generate, and there is also a choice to have no output printout. Some of the options are lists of small groups of variables, while other options are larger lists of variables for direct uploading into a database. (Usually it will be necessary to open the .txt output file and remove comments or header lines, and re-save, prior to uploading directly into a database.) The current default ASCII printout file contains information on foliar litter, nitrogen mineralization, forest floor mass, and C:N.

Results for N isotopes can be plotted and printed two ways: in the widely used  $\delta^{15}\text{N}$  notation (in per mil), or as percent recovery of  $^{15}\text{N}$  tracers in ecosystem pools. The latter we designate as  $PR^{15}\text{N}$  and calculate as follows (Currie et al. 1999):

$$PR^{15}\text{N}(C_i, t) = \frac{N_{C_i}(t)(\text{atom}\%^{15}\text{N}_{C_i}(t) - \text{atom}\%^{15}\text{N}_b)}{A(t - t_0)(\text{atom}\%^{15}\text{N}_a - \text{atom}\%^{15}\text{N}_b)} \quad (1)$$

where  $N_{C_i}(t)$  is the amount of N [g/m<sup>2</sup>] in  $C_i$  at time  $t$ ,  $A(t-t_0)$  is the sum of N amendments [g/m<sup>2</sup>] to time  $t$ ,  $C_i$  is an ecosystem compartment, and the 'a' subscript denotes amendment, 'b' denotes background.

The user can specify the pathname for the ASCII output file to be saved; when running the model, location where to write the output .txt file. The current default filename is "TRACE1.txt" located in the directory -- C:\Trace\CurrentVBver\SiteOutput. (If running the program generates an error in trying to write to this file, check whether there is already a file by that same name that can not be over-written because it is write-protected.)

## **Commenting and logging model exercises to save**

In conducting model simulations for scientific research, it is important to use a systematic approach and to save copies of well-documented, clearly commented input and output files. This serves the same purpose in modeling as a laboratory or field notebook serves in field research. We have two main recommendations.

The first recommendation is to make use of the user comments (including run-time comments) features in TRACE. At the top of each ASCII output printout is a time stamp and a series of user comments. The automatically-generated 'time stamp' lists the version of TRACE, the type of run (single vs. Monte Carlo), and the date and time the model was run. The second set of comments are reproduced directly from the two comment lines at the top of the input Parameter file. These lines can be used to record any information deemed important inside the Parameter file. These comments could specify the site, forest type, a note about the assumed initial conditions, and so on. Similarly, the next three lines of comments in the ASCII output file are reproduced directly from the comment lines at the top of the Scenario input file. These comments might list the level of N amendment, the simulated forest harvests, the scenario of atmospheric CO<sub>2</sub> concentrations or temperatures, and so on. The next and final set comments that appear at the top of each ASCII output file are run-time comments, up to three lines of comments entered by the user during the model run. These could be used to describe any aspects of the particular run, including its number in a series of analyses, or a changed value for a parameter, for example. The form to enter these comments (the *frmUserCom* form) can be accessed from the Main interface, in the same section where the user specifies the Output conditions (click 'Add User Comments').

Our second recommendation is to adopt a simple and clear method to save and log model runs. Our method is described briefly here. Each time we run TRACE, whether for testing or for results to publish, we call it an "Exercise" and save two things: (1) a "log file" as a Microsoft Word® document, with a brief, free-form notation describing the reasons and specifics for the model run, how it fits into current research goals, what we concluded from the results, etc.; and (2) a separate directory, with a name similar to the log file, containing all other relevant files (input files, model results output, and sometimes spreadsheet analyses of model results, or graphs, and so on, related to the particular Exercise). In our system, all of the MS-Word "log files" are saved together in one location so they can be searched using the sophisticated 'Find' tools in the MS-Word 'Open file' dialogue. The names of each of our log files is similar to the directory name containing all of the saved files from the model run so they are easily matched. The Exercise names are also sequential and contain the date. All of the model results are thus saved in an unchanging archive that can be off-loaded to CDs or backed up. At the same time, the MS-Word 'log files' can easily be searched as a group for words or phrases when we need to go back and locate a particular Exercise.

## **Conducting Monte-Carlo Model Runs**

The basic idea behind Monte-Carlo model runs is to perform multiple runs (50, for example) for a single site with randomly and independently perturbed values for model parameters and other site parameters. We thus explore model behavior under random combinations of altered

parameter values or initial conditions. This feature could be used in sensitivity analyses, uncertainty analyses, or tests of model robustness. These simulations are somewhat more involved than single model runs, and they produce a large amount of formatted output that the investigator must upload into a separate database or statistical package for analysis.

### **Generation and storage of random factors**

Monte-Carlo runs involve one additional input file, a 'Monte' file, which stores groups of random number sets. These are generated through the Monte-Carlo user interface when setting up a TRACE simulation; they are stored so they may be re-used in subsequent simulations. For example, when we conduct a Monte-Carlo uncertainty analysis for the 8-factorial field experiment of <sup>15</sup>N labeling at the Harvard Forest, MA, we use the same file of random numbers for all 8 combinations of forest stand, N treatment, and <sup>15</sup>N form. This allows for a consistent analysis of model uncertainties across the 8 factors of the field experiment, and we can be confident that differences in the Monte Carlo results are due to differences in the modeled treatments, not different random numbers.

The Monte input files are structured as follows. The first row contains the number of "groups" of random numbers, which equals the number of single runs to be performed in the Monte-Carlo set (5, 10, 50, etc.). This value is read in as **nsets**. Each subsequent row (line) contains a sequence of 63 numbers, the randomization factors, used to randomize parameters in a single model run in the Monte-Carlo set. The number of lines (model runs) equals the number of **nsets**. In all Monte files and all Monte-Carlo runs, the first group of these factors, the first line, has values all equal to 1, thus producing a 'nominal' simulation in which all parameter values are unchanged. In each subsequent row of the Monte file, and thus each subsequent model run in the Monte-Carlo set, the factors are stochastic. They are generated using the **Randomize** function in Visual Basic (using the computer clock as a random seed).

Each of the random factors is generated with a normal distribution, expectation (mean) value of 1, and standard deviation of 10% (i.e. 0.1). The tails are cut at plus or minus 50% (5 sd's), resulting in a range of 0.5 to 1.5 for the stochastic factors.

In TRACE, during each model run in the Monte-Carlo set, the row (line) of 63 random factors is read in from the Monte file and stored in an array named **monte()**. Before the simulation begins, the 63 parameters subject to Monte-Carlo analysis are then multiplied by the factors in the **monte()** array.

### **User action to initialize the random factors**

The Monte Carlo form in the TRACE user interface allows the user to either generate a new monte file, or to load an existing monte file to complete a set of Monte Carlo simulations. To generate a new Monte file, simply enter the number of sets, select a file name and location, and click "Generate & Load". This creates a new monte file and loads it into TRACE. To load an existing Monte file, just select the file using the dialog under "Load Existing File" and click 'Load'. The status bar at the bottom of the form will tell you the size and condition

(NEW/EXISTING file) of the current monte file that is loaded into TRACE. Click 'OK' to finish specifying the monte file.

## Set of parameters perturbed

This list included all parameters in the model that are not internally calculated, are not well-known constants or empirical coefficients, and are not initial conditions or climatic data. (Exceptions are parameters describing initial litter chemistry, which do vary stochastically). Parameter randomizations are carried out in the subroutine **MonteCarlo**. This code is copied below, showing the complete set of parameters currently perturbed using the set of random factors in the **monte()** array:

```
'Gross / Net Photosynthesis variables

k = k * monte(1)
HalfSat = HalfSat * monte(2)
BaseFolRespFrac = BaseFolRespFrac * monte(3)
RespQ10 = RespQ10 * monte(4)

'Vegetation variables

SLWMax = SLWMax * monte(5)
GDDFolStart = GDDFolStart * monte(6)
GDDFolEnd = GDDFolEnd * monte(7)
GDDWoodStart = GDDWoodStart * monte(8)
GDDWoodEnd = GDDWoodEnd * monte(9)
FolRelGrowMax = FolRelGrowMax * monte(10)
WoodTurnover = WoodTurnover * monte(11)
RootTurnoverA = RootTurnoverA * monte(12)
RootAllocA = RootAllocA * monte(13)
RootAllocB = RootAllocB * monte(14)
GRespFrac = GRespFrac * monte(15)
WoodMRespB = WoodMRespB * monte(16)
RootMRespFrac = RootMRespFrac * monte(17)
PlantCReserveFrac = PlantCReserveFrac * monte(18)
MinWoodFolRatio = MinWoodFolRatio * monte(19)
MaxNStore = MaxNStore * monte(20)

'Water Balance Variables

WHC = WHC * monte(21)
PrecIntFrac = PrecIntFrac * monte(22)
FastFlowFrac = FastFlowFrac * monte(23)
f = f * monte(24)

'Litter chemistry

FpctACI = FpctACI * monte(25)
FpctACS = FpctACS * monte(26)
FpctTEX = 100 - FpctACI - FpctACS
FLPctN = FLPctN * monte(27)
RpctACI = RpctACI * monte(28)
RpctACS = RpctACS * monte(29)
```

## Conducting Monte-Carlo Model Runs

```
RpctTEX = 100 - RpctACI - RpctACS
RLPctN = RLPctN * monte(30)
WLPctN = WLPctN * monte(31)

'Decomposition variables

WoodLitTrans = WoodLitTrans * monte(32)
WoodLitCLoss = WoodLitCLoss * monte(33)
Kho = Kho * monte(34)
Kblt = Kblt * monte(35)
Klct = Klct * monte(36)
Kwt = Kwt * monte(37)
Kcwt = Kcwt * monte(38)
kwoodyO = kwoodyO * monte(39)
kwoodyM = kwoodyM * monte(40)
CNwdw = CNwdw * monte(41)
SOMdec = SOMdec * monte(42)
omega = omega * monte(43)
Bioturb = Bioturb * monte(44)
ANpref = ANpref * monte(45)
OGNitFrac = OGNitFrac * monte(46)
MGNitFrac = MGNitFrac * monte(47)
BODdecayRat = BODdecayRat * monte(48)
ACIleach = ACIleach * monte(49)
ACSleach = ACSleach * monte(50)
TEXleach = TEXleach * monte(51)
MpctN = MpctN * monte(52)
MeACI = MeACI * monte(53)
MeACS = MeACS * monte(54)
MeTEX = MeTEX * monte(55)
MeBL = MeBL * monte(56)

FWDfrac = FWDfrac * monte(57)
AGWoodFrac = AGWoodFrac * monte(58)
DOMsorbFrac = DOMsorbFrac * monte(59)
DONsorbFrac = DONsorbFrac * monte(60)
MnitLeach = MnitLeach * monte(61)
NfixRat = NfixRat * monte(62)
NRTp = NRTp * monte(63)
```

### **Monte Carlo output files**

Monte Carlo output files are very similar to the single-site output text files. Output is printed to a single file ([trace1.txt](#)), and the comments section at the top of the output file is structured identically to that of a single-site run output. However, multiple sets of model output are printed below the header. Simulations in the Monte-Carlo set are printed sequentially in the output file. Thus, if the user constructed a monte file of size 5 and chose 'Forest Floor N Dynamics' as the printout type, then there will be five different sets of model output results for 'Forest Floor N Dynamics' listed sequentially in the output file. These can be easily separated by eye, using the 'year' in the output file. There is one choice of ASCII output file that is specifically designed for Monte Carlo runs; it contains an integer index for the number of the run in the set (i.e. 1 to 50 for a set of 50 runs) in the leftmost column. Any ASCII output file can be used in a Monte Carlo set, however; TRACE will simply produce multiple single-run outputs

## Conducting GIS Model Runs

appended one after the next. Statistics for mean and variance, within the Monte-Carlo set, for each model result in each year, then need to be calculated in a separate statistical package.

Notes:

1. Some of these single runs within the Monte-Carlo set may be incomplete if certain disallowed errors result from the random combinations of parameters (*see* Echeck error-checking below).
2. No on-screen graphics will be printed if the user chooses to perform a Monte Carlo run.

## Conducting GIS Model Runs

TRACE can be linked to a GIS (Geographic Information System) and applied, cell by cell in a grid, across a heterogeneous landscape or region. Extrapolating TRACE across a region allows us to model C and N pools and fluxes across gradients in elevation, forest type, soil water holding capacity,  $\text{NH}_4^+$  deposition,  $\text{NO}_3^-$  deposition, monthly precipitation, monthly temperature, or land use and disturbance history.

At the time of this writing (August 2005 and version 4.3.2), **this feature of the model is still in development**. All of the data layers necessary to run TRACE in a GIS are not yet assembled, and all of the code is not yet finalized; it is a work in progress. We anticipate other research groups and collaborators to be able to run TRACE easily in single-site mode and Monte Carlo mode, but we do not expect others to be able to make use of the GIS mode quite yet. This section of the User Guide is provided only for purposes of information.

The GIS main interface form in the TRACE user interface guides the user through the setup of a regional, GIS-linked simulation. A GIS run is completed by running TRACE for each individual cell in a GIS grid. The output GIS grid's spatial extent and resolution will be the same as the input grid's extent and resolution. All input grids must be constructed with the same spatial extent, cell size, and projection. In the case of the 13 states of the northeast US, for a cell size of 1 km<sup>2</sup> there are 1,694,880 cells. In our research, all input grids for this region were projected using the Albers-Equal Area projection.

### Input grids and files for GIS runs

For direct input into TRACE, all input GIS grids must first be converted to text (.txt) files. Most commercial GIS software platforms provide this functionality, but we recommend using ESRI Arc/INFO, as the input routine is designed to match the structure of the Arc GRID text files. All Arc GRID text files have six lines of comments (headers) at the top of the file that document the number of columns, the number of rows, x and y coordinates of the lower left corner, the cell size, and the NODATA value. Using the NE US example, a sample comments section would appear as follows –

```
ncols,          1177
nrows,         1440
xllcorner,     1088685
yllcorner,     1576155
```

## Conducting GIS Model Runs

```
cellsize,          1000  
NODATA_value,    -9999
```

These 6 lines of comments are read into TRACE as six strings and six integer values. The six integer values are used as a guide for allocating arrays (ncols, nrows), checking for NODATA values, and for general error-checking (making sure all input grids have the same spatial extent and resolution). It is vital that all input GIS grid files contain these 6 lines of comments and that they are the same for all of them. If you use a different platform other than Arc/INFO to convert your GIS grids, you must enter these six lines of comments into the grid .txt files. One last thing of note: Arc/INFO does not place a 'comma' between the string description and its integer value for each comment. However, this comma is needed for Visual Basic to differentiate between the string and the integer value when inputting the text file. Therefore, once the user converts the Arc GRID to a text file, they must go into the text file and physically enter all six commas before using it in TRACE.

Once all the input .txt files are created, the user can select each file using the *GISInput* form. The user can directly select the elevation, forest type, soil WHC, NH<sub>4</sub><sup>+</sup> dep., and NO<sub>3</sub><sup>-</sup> dep. text files on this form. Because of the large number of text files representing monthly precipitation, minimum temperature, and maximum temperature, the user cannot specify each .txt file directly on this form. Instead the user must specify the **directory** containing all 12 monthly prec., min. temp., and max. temp. text files. For this to work properly, all .txt files in the directory must have the following naming convention:

<Region><parameter>\_month.txt.

An example would be NEprec\_jan.txt.

The monthly abbreviation must be one of the following: jan, feb, mar, apr, may, jun, jul, aug, sep, oct, nov, or dec. The name of the directory containing the 12 text files must be identical to the <Region><parameter> portion of the text file name. Using the above example, the file NEprec\_jan.txt would be located in the NEprec directory. If the directory and text file name prefixes do not match, TRACE will be unable to successfully read in the input grid values.

Once the text files are selected and finalized, they are read into 2-dimensional arrays (nrows, ncols) for use in TRACE. Elevation values are read into **dem()**, forest type values are read into **forest()**, soil WHC is read into **soilWHC()**, NH<sub>4</sub><sup>+</sup> deposition are read into **nh4GIS()**, and NO<sub>3</sub><sup>-</sup> deposition are read into **no3GIS()**. Monthly prec., min. temp. and max. temp are stored in 3-dimensional arrays, where the 3<sup>rd</sup> dimension represents month (1 to 12). These arrays are **precGIS()**, **tminGIS()**, and **tmaxGIS()**. Individual array elements, such as precGIS(75, 474, 12), are then assigned to individual parameters (such as Prec) for each model run per cell.

Just like single-runs and Monte-Carlo runs, GIS runs require input of a parameter and scenario file. However, these files are different for GIS runs. Both the parameter and scenario files will have six sets of parameters. These six sets of parameters correspond to six different forest types: northern and southern deciduous, coniferous, and mixed forests. These files have the naming convention **Para\_GIS.txt** and **Scen\_GIS.txt**.

## Conducting GIS Model Runs

Once all grid, parameter, and scenario inputs are finalized, TRACE will execute for each cell that meets the following selection criteria (based on the grid values):

- Each input grid must have a value for that cell (no NODATA values)
- Must be a “forested” cell (fortype > 0)
- Soil water holding capacity must be > 0

If any of these criteria are false, then a NODATA value is printed to the output grid for that cell. If all the criteria are true, then TRACE completes its run and outputs the chosen parameter(s) to the output file(s).

### **Output selections for GIS runs**

The user can choose from six different model results to print to output grids for up to six different years using the GIS user interface. For example, one might print key results for C and N cycling and pool sizes in the years 1990, 2000, 2010, and 2050. A matrix on the user interface form allows the user to choose any combination of listed model results and year(s) of interest. Enter the year(s) in the appropriate spaces on the form and click the check box under each year for the desired model results to output. (Only the model results listed can be output to GIS grids; if you have Visual Basic on your computer, then the source code can be easily altered to accommodate additional model outputs.) The GIS main interface form will show the output selections.

### **Speed, memory, and optimizing efficiency in Visual Basic**

Depending on the size and resolution of your input grids, a GIS run can run for a long time and require substantial memory for input and output grids. With a reasonably fast desktop computer in early 2003, and with a substantial amount of attention given to speed and memory optimization, a single TRACE run takes roughly 1 second to complete per grid cell. An output grid of 1 million cells would take an estimated 27 hours to complete (assuming each cell meets all 3 of the criteria for run completion). A grid with non-forest cells will take a proportionally shorter time to complete.

Since each grid is read into a multi-dimensional array, a great deal of memory is used to store the input grid values. Arrays of any data type require 20 bytes of memory plus 4 bytes for each array dimension plus the number of bytes occupied by the data itself. Elevation and forest type can be constructed to contain integer data types, which require 2 bytes per data element. For the NE US (Maine to VA, west to PA) at 1 km resolution, there are 1,694,880 elements meaning the elevation and forest type arrays require 3.4 MB of memory each. The soil WHC and N Deposition data layers may be constructed as single data type (single-precision real number), which require 4 bytes per data element. In our example, each of these arrays requires 6.8 MB of memory. The precipitation and temperature arrays are also single data type, but are 3-dimensional, so they require more memory than the WHC and N dep. arrays. In our example, the precipitation and minimum and maximum temperature arrays each require 81.4 MB.

## Conducting GIS Model Runs

Combining all of the files mentioned, for this example, these GIS data layers for model inputs for a single run require 271 Megabytes of memory.

Also, since the output grids are printed from 2-dimensional output arrays, you need to add another 6.8 MB (2-D, Single) for each output grid that you specify. Thus, to perform a GIS run in our example and to produce only 10 output grids of model results for a single year, it would require about another 136 MB of memory for the arrays.

Some steps can be taken to optimize speed and efficiency. One possible step is to construct all GIS inputs as integer data type (e.g. for a water holding capacity of 10.2 cm, construct the GIS data layer as integer and store it as 102 mm), and convert values to the single (single-precision real number) data type in TRACE, with the units needed internally for model algorithms (i.e. cm, in the example given). Try to work with integers where possible. In GIS applications, try to *avoid* using the variant data type, because this ties up system resources unnecessarily and slows the model run significantly.

Additional steps to optimize system resources involve the structural design of the source code in Visual Basic. When calling functions or subroutines, always pass parameters by value (ByVal), not by reference (default), if the value does not change. Another way to speed up performance is to limit sequential file I/O (input-output) during the model run. This can be accomplished by reading all of the input data necessary, for each grid cell, into arrays at the start of a model run instead of reading input data inside the monthly do-loops through the simulation. Similarly, where practical, store model results in arrays that can be printed once the model run is complete, rather than inside the monthly do-loops through the simulation.

Finally, if you have Visual Basic (VB) software on your computer, you can take advantage of some VB-provided optimization options that can be switched on and off. These options are accessed from the Project→ Properties menu. Click on 'Advanced Optimizations...' under 'Compile'. These should be used carefully, because although they significantly speed up model runs, they may alter model results (round-off errors may be significantly increased, for example). If using these VB-provided optimizations is necessary to achieve reasonable time spans for model runs, we recommend thorough testing by comparing representative model runs with and without the optimizations.

### III. Greater Detail on Model Processes

## Overview of model pools

TRACE was designed primarily as a tool for (1) the interpretation of patterns of  $^{15}\text{N}$  redistributions among ecosystem pools in field studies, together with (2) detailed analysis of C balance and C/N interactions. As a result, pools of C and N in TRACE were designed to be physically meaningful and directly comparable against field data where possible (Fig. 2). To make these comparisons, field data must first be scaled up to an areal basis, usually conceived as representing the size of a large-scale experimental plot containing enough trees to be representative areally of the particular forest stand. Pools of organic matter and N in TRACE are lumped-parameter pools expressed on an areal basis.

### Units

All pools of vegetation biomass, soil detritus, and soil organic matter in TRACE are defined as ash-free organic matter mass in the units **g OM / m<sup>2</sup>**. Thus, plant biomass as litter can be transferred directly to litter and soil pools with no ash correction in the model. In the literature, soil pools are often expressed as ash-free organic matter, but in contrast, vegetation biomass pools are typically expressed as dry weight, ash-included. Thus, care must be used in comparing model pools of plant biomass, or fluxes of biomass and litter production, with published numbers from field studies. Model numbers should be slightly lower because they are expressed as ash-free.

Carbon pools in TRACE are related to biomass pools through a simple scalar that is constant throughout the model: *CfracBiomass*, defined as the C mass per unit ash-free organic-matter mass. The value for *CfracBiomass* is currently set at 0.52 in TRACE.

All pools of N in TRACE are in the units **g N / m<sup>2</sup>**. Hydrologic pools, including soil water and snowpack, are in units of **cm water**. Pools of energy stored in organic matter are in units of **kilocalories** (kcal); 1 kcal = 10<sup>3</sup> gram calories. Detrital energetic pools are parameterized through laboratory-determined values of tissue energy content in **kcal/g**.

Because TRACE runs on a monthly timestep, fluxes of organic matter, C, and N that are within the monthly-timestep loop are in the units of **g OM m<sup>-2</sup> mo<sup>-1</sup>**, **g C m<sup>-2</sup> mo<sup>-1</sup>**, or **g N m<sup>-2</sup> mo<sup>-1</sup>** (where mo refers to month). For bookkeeping purposes and for plotting and printing model results, many of these fluxes are summed on an annual basis and reported as **g OM m<sup>-2</sup> yr<sup>-1</sup>**, **g C m<sup>-2</sup> yr<sup>-1</sup>**, or **g N m<sup>-2</sup> yr<sup>-1</sup>**. Hydrologic fluxes are in units of **cm / mo** or **cm / yr**. Energetic fluxes related to heterotrophic activity are in fluxes of **kcal / mo** or **kcal / yr**. In many cases, ASCII output files of model results contain headers that list units. In addition, the parameter and validation-results database, [TraceDataNeedsx.xls](#), lists units. Finally, if you have Visual Basic and can view the source code, many lines of source code have comments that list units.

## Overview of model pools

Description of model pool	OM pool name	N pool name
Foliage in each cohort	FolMass(i)	FolN(i,j)
Fine roots ( $\leq 2$ mm)	RootMass	RootMassN(j)
Plant-internal, mobile, C and N storage for source-sink physiology	PlantC, RootC	VascN(j)
Living wood (branches, boles, and woody roots)	WoodMass	WoodMassN(j)
Standing dead wood (Standing woody debris)	SWD	SWDN(j)
Downed fine woody debris ( $< 10$ cm. diam) in O horizon	OFWD	OFWDN(j)
Downed coarse woody debris ( $\geq 10$ cm. diam.) in O horizon	OCWD	OCWDN(j)
Downed fine woody debris in mineral soil	BFWD	BFWDN(j)
Acid insoluble material in fine litter in O horizon	ACI	ACIN(j)
Acid soluble material in fine litter in O horizon	ACS	ACSN(j)
Total extractives in fine litter in O horizon	TEX	TEXN(j)
Fine litter in mineral soil	BL	BLN(j)
Humified matter in O horizon	HOM	HON(j)
Light-fraction of humified matter in mineral soil	LSOM	LSON(j)
Heavy-fraction of humified matter in mineral soil	HSOM	HSON(j)

**Table 3.** Pools of organic matter and N in TRACE

Listed are names of pools as they appear in the model code. Units for these pools are g OM / m<sup>2</sup> or g N / m<sup>2</sup> (OM = ash free organic matter); exceptions are PlantC and RootC, which are in g C / m<sup>2</sup>. The subscript (i) refers to foliar cohorts; the subscript (j) refers to <sup>14</sup>N and <sup>15</sup>N isotopes.

### Pool definitions

This section provides definitions of each pool of organic matter and N in TRACE. Subsequent sections describe model processes.

**Foliage.** Foliar mass is a lumped-parameter representation of canopy mass in TRACE, as in PnET-CN, although a difference in TRACE is that the foliage is separated into two cohorts or age classes. Cohort (1) includes current-year foliage, while cohort (2) includes foliage from all prior years. In coniferous vegetation, foliar litterfall takes place from cohort (2). This model structure was designed to allow comparison against <sup>15</sup>N recoveries in field studies in which investigators analyze <sup>15</sup>N in current-year vs. prior-year foliage. (A future model enhancement is planned to increase these foliar cohorts to 6, for 6 separate years, to accommodate the design of some European field studies.)

**Roots.** ‘Roots’ pools in TRACE are conceived as living fine roots, i.e. living roots in  $< 2$ mm in diameter. Larger roots are conceived as being woody, and considered part of the pool of living

## Overview of model pools

wood. When fine roots die, their tissue is input to pools of fine litter in the soil O horizon (forest floor) and M horizon (mineral soil). See 'Fine litter and decomposition' below.

**Plant-internal N storage.** In TRACE, there is a pool of plant-internal, mobile N storage (**VascN**) that is a central pool in the model. N uptake enters this pool, as does resorbed N from senescing foliage; allocations of N to growing tissues are made from this pool. Greater detail is provided below.

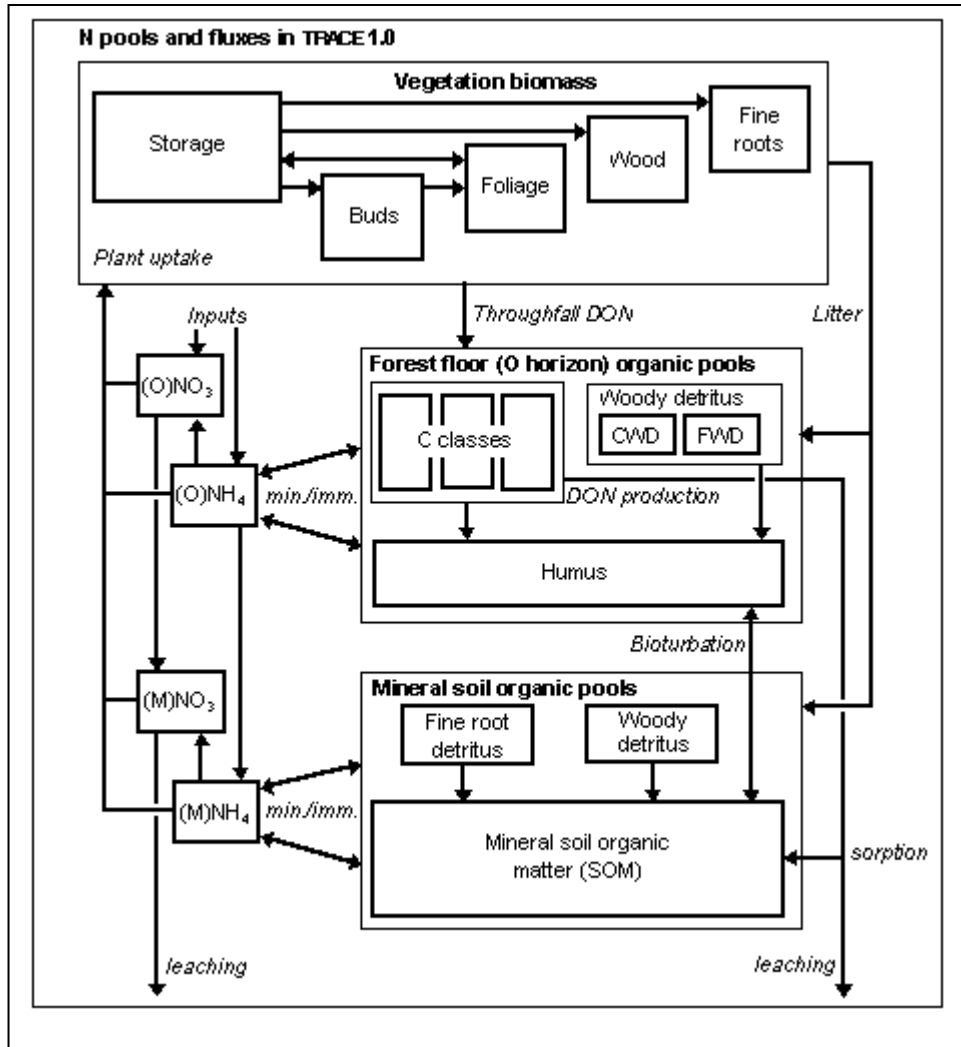
**Plant-internal C storage.** Plant physiology represented in TRACE, building on the structure of PnET-CN (Aber et al. 1997), includes a plant-internal source-sink model for C and N. The pool **PlantC** includes photosynthate, produced through photosynthesis, stored and mobile within the vegetation. Allocation to new growth of foliage, wood, and roots results in debits to this pool. A similar pool, **RootC**, is a temporary holding pool for C that has been transferred there for fine root production (and debited from **PlantC**), but not yet used for root production. Two other variables are important in controlling C allocation to growth: **BudCJan** and **WoodCJan** (renamed, but similar in function to the variables BudC and WoodC in PnET-CN). These latter two variables are not true pools; their values are set once per year, at the end of December in the subroutine **AllocateYr**, and carried forward as information to limit the overall, annual C allocations from **PlantC** to foliar production and wood production the following year. The pools **PlantC** and **RootC**, together with the variables **BudCJan** and **WoodCJan**, are in the units **g C/m<sup>2</sup>**, which differ from the units of biomass pools in vegetation and soil.

**Living wood.** This pool, **WoodMass** (Table 3) is a single pool of organic matter mass in TRACE, comprising twigs, branches, boles (stems), and belowground material, including large roots and roots > 2 mm in size.

**Woody debris, or dead wood.** There are four pools of this material in TRACE. **SWD**, Standing woody debris, includes snags (standing dead trees) as well as attached dead wood (dead branches on living trees) and suspended dead wood (woody debris broken from trees but suspended in the canopy or above the forest floor). Downed woody debris on the forest floor surface and in the O horizon is composed of two pools: **OFWD**, O-horizon fine woody debris, defined as material 0.5 cm diam. or greater and less than 10 cm diam.; and **OCWD**, O-horizon coarse woody debris, material 10 cm or greater in diameter (Harmon et al. 1996, Currie and Nadelhoffer 2002). Finally, **BFWD** comprises "buried" fine woody debris (0.5 to < 10 cm diameter) in the mineral soil, primarily conceived of as large dead roots. There is no corresponding pool of "buried" coarse woody debris. Large logs and stumps embedded in the upper mineral soil are conceived as part of **OCWD**.

**Fine litter.** Unhumified fine litter (conceived as being derived from foliage, fine roots, reproductive parts, and woody tissues < 0.5 cm diameter) is composed of four pools: In the O horizon, three "Carbon-class" pools; and in the mineral soil, one fine-litter pool that is not broken into C classes. The C-class pools in the O horizon are defined according to the wet-chemistry method of "proximate analysis" (Ryan et al 1990). The **TEX** pool contains material in the 'total extractives' fraction; the **ACS** pool contains the 'acid-soluble' fraction, and the **ACI** pool contains 'acid-insoluble' fraction. See the descriptions below of the processes of decomposition, leaching, N dynamics, and humification as related to these fractions. In the mineral soil, **BL** for 'buried litter' contains the unhumified fine litter, comprising fine root litter in mineral soil together with any foliar litter modeled as being mixed downward into the

## Overview of model pools



**Figure 2.** Schematic of the hierarchical structure of pools and fluxes of nitrogen in TRACE 4.1. Plant uptake of N, detrital N dynamics, and N transformations are calculated separately in each soil layer. Pools of KCl-extractable N are separated by soil layer: (O) = O horizon, (M) = mineral soil. DON = dissolved organic nitrogen. CWD, FWD = coarse and fine woody detritus. Min./imm. = Mineralization and assimilation. Inputs = NO<sub>3</sub><sup>-</sup> and NH<sub>4</sub><sup>+</sup> in atmospheric deposition, fertilizer, and isotopic tracer additions. For clarity, not all fluxes are shown in detail.

mineral soil during forest harvest (Yanai et al. 2004). As described below (Microbial representation), bacteria and fungi associated with these litter fractions are also, by conception, included in each of these pools. These fine-litter pools are operationally defined and directly comparable against laboratory measurements to determine how much OM, C, N, or <sup>15</sup>N is present in each pool.

**Humified matter.** There are three pools of humified matter in TRACE, **HOM** in the O horizon, **LSOM** and **HSOM** in the mineral soil. These abbreviations mean the following:

- **HOM** = Humified O-horizon Material, or Humified Organic Matter (O-horizon only)

## Isotopes and pool dilution

- **LSOM** = Light-fraction Soil Organic Matter (Mineral soil horizon)
- **HSOM** = Heavy-fraction Soil Organic Matter (Mineral soil horizon)

By definition, in TRACE, transfer of detritus from fine-litter (foliage and roots) to these pools takes place when there is 20% of the initial mass remaining. These are conceived as containing partially humified and/or stabilized detritus, Phase II material according to the Phase I - Phase II separation of decay rates (Aber et al. 1990). The distinction between the physical locations of the **HOM** vs. **LSOM + HSOM** pools follows the definition of organic vs. mineral soil horizons: The O horizon, a surface organic horizon, contains 40% organic matter by mass or 20% organic C by mass. It is also important to note that the physical conceptions of the **HOM**, **LSOM**, and **HSOM** pools exclude both living roots and unhumified root litter. Laboratory analyses to compare directly against **HOM**, **LSOM**, and **HSOM** pools would need to exclude living and dead roots. However, because field studies are designed a variety of ways in terms of how fine roots are treated, TRACE allows percent recovery of  $^{15}\text{N}$  in dead fine roots to be counted separately in its own pool, or counted together with live fine roots, or counted together with the soil horizon in which the dead roots are found (see *Model structure options* below).

### Soil available N

There are four pools of plant-available N in soil, i.e. soil pools of N from which plant uptake can draw. Plant-available N is explicit in TRACE because plant uptake is mechanistic (depending on plant demand, ambient temperature, microbial competition for forms of inorganic N, and sizes of soil-available pools), and isotopic ratios of N taken up by plants reflects isotopic ratios and sizes of plant-available pools in soil. In the current version of TRACE, plant uptake draws from pools of inorganic N in each soil horizon (i.e. no uptake of organic soil N occurs), conceived as being closely related to KCl-extractable pools of inorganic N in soils. The four pools are  $\text{ONH}_4$  ( $\text{NH}_4^+$  in the O horizon),  $\text{ONO}_3$  ( $\text{NO}_3^-$  in the O horizon),  $\text{MNH}_4$  ( $\text{NH}_4^+$  in the mineral soil), and  $\text{MNO}_3$  ( $\text{NO}_3^-$  in mineral soil).

## Isotopes and pool dilution

In the source code, each N pool is constructed as a 1-dimensional array with 2 values. The first value is  $^{14}\text{N}$  mass ( $\text{g } ^{14}\text{N} / \text{m}^2$ ), the second value  $^{15}\text{N}$  mass ( $\text{g } ^{15}\text{N} / \text{m}^2$ ). For example, in the model code, for the ACIN pool (acid insoluble material in fine litter in the O horizon), ACIN(1) stores the amount of  $^{14}\text{N}$  in this pool and ACIN(2) stores the amount of  $^{15}\text{N}$  in this pool. The ratio of  $^{14}\text{N} / ^{15}\text{N}$  in this pool is equal to ACIN(1) / ACIN(2). The total amount of N in this pool is ACIN(1) + ACIN(2). The atom% $^{15}\text{N}$  in this pool is  $100 * \text{ACIN}(2) / (\text{ACIN}(1) + \text{ACIN}(2))$ .

When a flux of N occurs between a source and a target pool, the flux carries the isotopic ratio of the source pool. This leaves the isotopic ratio of the source pool unchanged, while it alters the isotopic ratio of the target pool, depending on the size of the flux, the size of the target pool, the isotopic ratio of the flux, and the isotopic ratio of the target pool. This phenomenon, known as *pool dilution*, is a central principle in the use of  $^{15}\text{N}$  tracers. Algorithms in TRACE carry out these calculations for all N transfers and fluxes in the model.

## Dynamics in pools of soil available N

As outlined above, TRACE includes pools of soil-available N as  $\text{NH}_4^+$ -N and  $\text{NO}_3^-$ -N separately, and in the forest floor vs. mineral soil separately. A central feature of the TRACE model comprises the dynamics in these pools and their N isotopic ratios. Quantities of N and  $^{15}\text{N} / ^{14}\text{N}$  ratios in these pools are determined by inputs of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  together with their isotopic ratios, outputs of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  due to microbial uptake, plant uptake, and leaching, and gross N transformations. A high level of detail is necessary to model these quantities because fine-scale (soil core) studies have shown temporal patterns in  $^{15}\text{N}$  in soil-available pools to be very sensitive to gross N dynamics in soils.

TRACE models gross fluxes of mineralization (ammonification), nitrification, microbial-detrital  $\text{NH}_4^+$  assimilation, and microbial-detrital  $\text{NO}_3^-$  assimilation (Currie et al. 1999). The gross assimilation fluxes are called 'microbial-detrital' because these are modeled as gross assimilation fluxes into combined microbial-detrital pools (see Microbial representation below), which may arise through a combination of microbial uptake and abiotic reactions in detritus. Net mineralization and nitrification fluxes are not modeled directly in TRACE; they are calculated on a monthly basis as a difference in gross fluxes, and summed over the months of year in a 'bookkeeping' manner to produce annual values of net N transformations in soil.

In TRACE, assimilation demand of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  by microbial-detrital pools out-competes plant demand for N simply by occurring prior to plant uptake on a monthly basis. Plant uptake of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  then takes place prior to leaching of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  from each soil horizon. Within each month, within each soil horizon, events related to the gross N dynamics in soil-available pools of N occur in this order:

1.  $\text{NH}_4^+$ -N and  $\text{NO}_3^-$ -N in atmospheric deposition (and/or experimental N amendments) are added to soil-available pools.
2.  $\text{NH}_4^+$  is mineralized as a gross flux from woody debris pools (if the C:N ratios are below the 'critical' threshold in these pools).
3.  $\text{NH}_4^+$  is mineralized as a gross flux from humified matter (HOM or SOM; see *Pools of humified matter* for further details). This results in a large, gross flux of N to the  $\text{NH}_4^+$  pool, which then mixes isotopically with the N already in the  $\text{NH}_4^+$  pool, prior to assimilation in other detrital pools. (This dilutes the  $^{15}\text{N}$  in the  $\text{NH}_4^+$  pool when the latter is strongly labeled; in later years after  $^{15}\text{N}$  labeling, when the  $\text{NH}_4^+$  pool is less strongly labeled, this large flux of N from the humus, if it is enriched, acts as to continually enrich the  $\text{NH}_4^+$  pool in  $^{15}\text{N}$ .)
4. Fine litter pools undergo gross assimilation of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  based on modeled microbial demand and a microbial 'preference' for  $\text{NH}_4^+$  vs.  $\text{NO}_3^-$  (see *Microbial representation* for an explanation of these processes).

## Dynamics in pools of soil available N

5. In each of the fine litter pools, the *net* monthly N dynamics are then achieved (see *Fine litter and decomposition* below) through either additional gross N assimilation or gross N mineralization. When gross mineralization fluxes occur from highly  $^{15}\text{N}$ -labelled litter, strong  $^{15}\text{N}$  labels enter the soil-available  $\text{NH}_4^+$  pool here.
6. Soil-available  $\text{NH}_4^+$  and  $\text{NO}_3^-$  are then *re-immobilized* in pools of humified matter, as gross assimilation fluxes, offsetting the gross mineralization that occurred in step (3) to the extent necessary to achieve the correct *net*, monthly, N mineralization from humified matter. The extent of these re-immobilization fluxes in each soil horizon depend on the pool sizes of humified matter in each horizon, the C:N ratios of humified matter, and the ratio of gross:net N mineralization from humified matter (in turn governed by the parameter  $\omega$ ; Currie et al. 1999). If soil-available  $\text{NH}_4^+$  or  $\text{NO}_3^-$  pools are strongly  $^{15}\text{N}$ -labelled, this gross assimilation flux into humified matter acts to transfer large quantities of  $^{15}\text{N}$  label to humified matter (consistent with field observations at the Harvard Forest).
7. In the above steps, each time a flux of gross N mineralization takes place (whether from woody debris, fine litter, or humified matter), a flux of gross nitrification takes place. This is meant to model competition of nitrifiers against heterotrophic  $\text{NH}_4^+$  assimilators; any time N is mineralized to  $\text{NH}_4^+$ , a fraction of it is nitrified to  $\text{NO}_3^-$ . The relationship between gross ammonification and gross nitrification in each soil horizon is governed simply by two user-input parameters, **OGNitFrac** and **MGNitFrac** (for the O horizon and M horizon [mineral soil], respectively). In the O horizon, for example, every time there is a gross  $\text{NH}_4^+$  mineralization flux, it is multiplied by **OGNitFrac** to determine the corresponding gross nitrification flux to  $\text{NO}_3^-$ . The gross nitrification flux then takes place before any other processes are able to draw on the soil-available N pools.
8. Finally, in each horizon, after all gross N dynamics related to detrital pools are complete, plant uptake and leaching processes compete for the remaining soil-available N in the  $\text{NH}_4^+$  and  $\text{NO}_3^-$  pools. Plant uptake of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  occurs first, on a monthly basis, then leaching of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  from each horizon takes place, calculated as a proportion of the remaining N in each pool after plant uptake.

In each of the above steps, whenever a pool of soil-available N (or any other pool of N) receives a flux of N into it, isotopic ratios in the pool are recalculated before any other flux takes place. This incorporates the principles of pool dilution in all model processes.

These fine-scale processes, acting at the ecosystem level together with plant-soil feedbacks in litter quality and N cycling, emerge to create a representation of the set of processes governing N limitation or N saturation at a particular site (Aber et al. 1989, 1998). Leaching losses of N occur when soil-available N pools grow or are replenished at rates exceeding microbial and plant demand.

In addition to the processes described above, diffusion of N isotopes occurs between soil horizons. This has no effect on N concentrations or the form of N as  $\text{NH}_4^+$  or  $\text{NO}_3^-$ . Its only effect concerns the  $^{15}\text{N}:^{14}\text{N}$  ratios in each pool of soil available N. At the end of each monthly

time step,  $^{15}\text{N}:^{14}\text{N}$  ratios are set equal between  $\text{ONH}_4$  and  $\text{MNH}_4$  pools, and equal between the  $\text{ONO}_3$  and  $\text{MNO}_3$  pools. This represents complete diffusion of isotopes between horizons. It is calculated in a manner fully tested to preserve mass balance in  $^{15}\text{N}$  and  $^{14}\text{N}$  within each form of N ( $\text{NH}_4^+$  and  $\text{NO}_3^-$ ) separately.

## Fine litter and decomposition<sup>1</sup>

The detailed dynamics of litter decomposition are a strength of TRACE. Decomposition dynamics derive from DOCMOD (Currie and Aber 1997), a model of litter decomposition, humification, and production of dissolved organic C and N in the forest floor. Decomposition of foliar and fine root litter follows two phases in the model: short-term decay of fresh litter with stabilization of decomposition intermediates (henceforth “phase I”), followed by the much slower process (“phase II”) of humus turnover (Berg 1986; Melillo et al. 1989; Aber et al. 1990; Nadelhoffer et al. 1995; Coleman and Crossley 1996; Gholz et al. 2000). In TRACE, mass is lost in phase I through C mineralization and leaching until 20% of the original litter mass remains. The rate of decay in this phase is determined by climate (as represented by actual evapotranspiration) and litter quality (Meentemeyer 1978; Berg et al. 1993). Litter quality controls decay rates through the mixture of operationally-defined classes of carbon known as proximate C fractions (henceforth “C classes”), representing extractives, acid-soluble, and acid-insoluble material (McClaugherty et al. 1985; Ryan et al. 1990; Aber et al. 1990; Preston et al. 1997; Moorhead et al. 1999). In TRACE many of the pools, parameters, and other variables that refer to these C classes make use of the shorthand **ACI** for acid-insoluble, **ACS** for acid-soluble, and **TEX** for total extractives.

The chemistry of foliar and fine root litter are specified as model inputs in the Parameter input file (**FpctACI**, **FpctACS**, and **FpctTEX** for foliage; **RpctACI**, **RpctACS**, and **RpctTEX** for roots). Ash-free mass from foliar and fine-root litter merge together in TRACE into three pools corresponding to the three C classes. Throughfall DOC is included as a carbon input to the forest floor, entering the **TEX** pool, because it comprises relatively labile material (Qualls and Haines 1992).

Each carbon class undergoes first-order (single-exponential) decay. The decay constant  $k$  for each carbon class is calculated from the current value of the lignocellulose index (LCI), where  $\text{LCI} = \text{lignin} / (\text{lignin} + \text{holocellulose})$  (Melillo et al. 1989). Rates of decay of material in each carbon class is thus a function of the LCI of the overall fine litter in the O horizon (Aber et al. 1990). Equations for  $k$  values derive from dynamics in carbon classes in decomposing litter from three locations: Blackhawk Island, WI; the Harvard Forest, MA; and Hubbard Brook, NH (Aber et al. 1990). Loss of **TEX** material dominates mass losses in the early stages, while the rate of **ACS** loss is important throughout decay and **ACI** decay controls the later stages (Berg and Staaf 1980, McClaugherty 1983; McClaugherty and Berg 1987). Examples exist in the literature in which litter N content either correlates or does not correlate with decay rates; TRACE adopts the null hypothesis that N content does not affect rates of decay.

---

<sup>1</sup> Much of the material in this section is taken from Currie and Aber (1997), *Ecology* 78:1844-1860.

Climatic controls on decay rates are included as a function of **AET** (actual evapotranspiration), a convenient climatic surrogate because it combines temperature and moisture information. We derived an **AET** effect from data published by Berg et al. (1993) for pine needle litter studied in 17 sites in Central Europe and North America. We normalized the **AET** effect to Blackhawk Island, Wisconsin, the site from which our litter decay constants derive (Aber et al. 1984, Aber et al. 1990).

Some mismatch exists between the model and field methods for litter pools. The process model separates fine detritus into Phase I and Phase II decay, in which litter is passed to humus when 20% of initial mass remains (Aber et al. 1990, Currie and Aber 1997). In the field study, in contrast, a separation is made based on physical horizon, not on the degree of humification of the material. TRACE is likely to over-predict the N pool size and <sup>15</sup>N recovery in the Oi pool because it views all foliar litter in the Oi until 20% of initial mass remains; whereas some of this material is probably included in the Oe sub-horizon in typical field studies.

### **Validation tests of overall decay rates of fine litter**

Because decay of fine litter in TRACE is calculated through regressions based on proximate carbon chemistry, it is useful to test the overall rates of litter decay against observed values for a particular site as a check on the model. For this purpose, a subroutine **Kweighted** is called to calculate the variable **KweightAnn** (in the units yr<sup>-1</sup>.) This is calculated as a single first-order decay constant for fine litter in the O horizon overall; proportions of foliar vs. fine-root litter inputs for each C class are used in the weighting calculation. **KweightAnn** is not used in the model. Its only purpose is to allow comparison against field measurements as a check on the model. It can be printed with the 'Forest floor mass' set of results.

The litter decay algorithms in TRACE, deriving from the DOCMOD model, were tested in a model intercomparison and blind test as part of the LIDET study (Long-Term Ecological Research Intersite Decomposition Experiment Team). Models were tested against one another and in blind predictions of litter decomposition at four sites with widely varying climates and soils: the Harvard Forest; Luquillo Experimental Forest, Puerto Rico; Arctic Tundra, AK, USA; and Jornada Field Station, AZ, USA (Moorhead et al. 1999).

### **Leaching fluxes of DOC, DON, POC, PON**

A strength of TRACE is that it contains production of DOC and DON (dissolved organic C and N) in the forest floor, leaching fluxes from the forest floor, sorption of DOC and DON in mineral soil, and export of non-sorbed portions from the solum. These fluxes are important controls on long-term C and N dynamics in the forest floor and mineral soil. They also play a role in <sup>15</sup>N movement to mineral soil in TRACE. In constructing DOCMOD (and in incorporating it as a submodel in TRACE), our goal was to synthesize current understanding of qualities and quantities of leachate from forest floors in a process model of decomposition that included leaching, and to represent patterns in leaching relative to other processes controlling C and N storage and fluxes across a heterogeneous landscape (Currie and Aber 1997). Here, we briefly describe controls on DOC leaching, then explain DON production and movement.

At the foundation of virtually all decomposition models is a single or multiple empirical constant,  $k$  in the expression  $e^{-kt}$ , indicating the rate of detrital mass loss over time (Olson 1963). Leaching and CO<sub>2</sub> mineralization are two separate mechanisms of mass loss (Gosz et al. 1973, Berg and Staaf 1980, Schlesinger and Hasey 1981, McClaugherty 1983, Cronan 1985, Yavitt and Fahey 1986). However, because of the difficulty of distinguishing between these mechanisms in the field, mass loss in litter decay studies has typically been measured as a single process (e.g. Aber et al. 1984, Fahey et al. 1988).

Within each carbon class, TRACE partitions C loss into fluxes of DOC and CO<sub>2</sub>-C. (Because detrital pools are organic matter, OM, the leaching fluxes are calculated as fluxes of DOM, dissolved organic matter. This is translated to DOC in the model using the constant **CfracBiomass**.) We calibrated the partitioning parameters based on fluxes of litterfall, chemistry of litter, and fluxes of DOC in Oa leachate from the Harvard Forest, MA (Currie et al. 1996, Currie and Aber 1997). We performed separate calibrations for a mixed hardwood stand and a red pine stand because the hardwoods and conifers showed markedly different DOC leaching fluxes. These partitioning parameters, which control the relative contributions to DOC leaching vs. CO<sub>2</sub> mineralization from each C class, are now included in the TRACE Parameter input files as **ACIleach**, **ACSleach**, and **TEXleach**.

TRACE adds an additional calibration parameter, **OLscalar** (for O-horizon leaching calibration). This is a scalar that is used to adjust the relative partitioning of O-horizon mass-loss to DOC up or down for other sites, based on field data from the site. The proportions of DOC leaching that derive from each C class remain constant (if the partitioning parameters **ACIleach**, **ACSleach**, and **TEXleach** are left unchanged, which is our recommendation.)

Fluxes of DON production and leaching in TRACE arise simply and directly from the DOM production and leaching model. In each timestep, and from each C class, the DOM production and loss carries with it the N concentration in the C class at that time; the summation of these contributions across C classes composes the flux of DON production. This isotopic signature of this DON production also results from the relative contributions of DON from each C class, together with the N isotopic signatures in each C class at the time. As a result this embodies a mechanistic model of DON production and its <sup>15</sup>N signature.

TRACE version 4.20 and later versions include leaching fluxes of **POC** (particulate organic C) and **PON** (particulate organic N). These are conceived as leaching fluxes from the O horizon to the mineral soil, analogous to DOC and DON leaching fluxes, but containing particle sizes greater than those passing through DOC filters. Further explanation of why these fluxes were added is given in Currie et al. (For. Ecol. Manage. *In review*). Source pools for POC and PON eluviation from the O horizon are analogous to those for DOC and DON. Fluxes of POC and PON eluviation are calculated through a simple scalar **OPscalar** (input as a user-changeable parameter) multiplied by DOC and DON eluviation fluxes.

The user can track this movement of <sup>15</sup>N in leaching of DON and PON from the forest floor, as well as the leaching of <sup>15</sup>NH<sub>4</sub><sup>+</sup> and <sup>15</sup>NO<sub>3</sub><sup>-</sup> from the forest floor, by using the bookkeeping variables **Cum15DPONeluv** (which tracks DON + PON eluviation), **Cum15NH4eluv**, and

**Cum15NO3eluv**. Named for ‘cumulative’, these variables are *not* re-initialized to zero at the start of each year, but continue to accumulate through the model run.

If you work with the model code, you will note that DOM and POM (dissolved and particulate organic matter) leaching and eluviation are tracked, since detrital pools in the model are pools of OM; DOM and POM are multiplied by the parameter *CfracBiomass* wherever they need to be converted to C units for user output of results. After eluviation from the O horizon, a fraction of DOM flux (controlled by the parameter *DOMsorbfrac*) together with the entire POM flux, enter the LSOM pool (light-fraction soil organic matter) in mineral soil. Similarly, a fraction of the DON flux (controlled by the same parameter, *DOMsorbfrac*) together with the entire PON flux enter the LSON pool in mineral soil.

### Net and gross N dynamics in fine litter

As outlined above, there are four pools of fine litter (nonhumified foliar and fine-root litter) in TRACE: Three C-class pools in the O horizon, and one combined fine-litter pool in the mineral soil horizon. Each of these pools has N dynamics that include gross assimilation of  $\text{NO}_3^-$  and  $\text{NH}_4^+$ , gross mineralization of  $\text{NH}_4^+$ , and net N mineralization equal to the difference from the gross assimilation and mineralization fluxes. The model of N dynamics in these litter pools is not difficult to understand, but in terms of the model code this is among the most complex fine-scale processes in TRACE. Briefly, for each of these pools TRACE calculates the net N dynamics based on the C:N ratio in the pool, then TRACE calculates the gross N assimilation in each pool based on a traditional model of microbial growth, and finally TRACE calculates the gross N mineralization needed to balance the other two calculations. Assimilation and mineralization fluxes are modeled as exchanges of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  with the soil-available pools in the O horizon and mineral soil, carrying the isotopic signatures of the appropriate source pool in each time step.

In fine litter pools, the *net* monthly N dynamics are calculated based on annual-time-scale ‘attractors’ governing the C:N ratios in each of these pools (Currie et al. 1999). Ratios of C:N above or below the attractor value result in net immobilization or mineralization of N, respectively, at rates based on field studies (Aber et al. 1984, Currie et al. 1999, Schlesinger and Lichter 2001). These attractor C:N values are used for each C class separately in the O horizon, and for fine-litter as a whole in the mineral soil. Annual net mineralization or immobilization of N in each litter pool is distributed among months based on monthly distribution of AET (actual evapotranspiration). When gross immobilization into a litter pool is positive, then flux of each N isotope is controlled by the isotopic signatures in the appropriate pools of soil-available N: **ONH4** and **ONO3** in the O horizon, for example. When mineralization occurs, then the flux of each N isotope is controlled by distribution of isotopes in litter N pool associated with that fine-litter pool.

Although TRACE contains no explicit pool of microbes (see *Microbial representation* below), a traditional conceptual model of microbial growth is used to calculate gross N assimilation in each fine-litter pool. For these calculations, N concentration in microbial tissue is used as a parameter (**MpctN**), together with microbial C-use efficiencies on acid-insoluble, acid-soluble,

## Woody detrital pools

and total-extractives substrates in the O horizon (**MeACI**, **MeACS**, and **MeTEX**, respectively) and on whole litter in the mineral soil (**MeBL** for 'buried litter').

A strength of this sub-model is that it predicts  $^{15}\text{N}$  dynamics in each C class independently; this could serve as a means for assessment of model processes, if field data become available regarding temporal patterns in  $^{15}\text{N}$  tracer recoveries in each of the C-classes. This should be possible, since the C classes are operationally defined, based on laboratory methods. In addition, since DON leaching from the O horizon in TRACE is produced from decomposition in the C classes, the  $^{15}\text{N}$  signatures on the DON in TRACE are determined by the  $^{15}\text{N}$  dynamics in the C classes, and could also be tested if field data on temporal patterns in  $\text{DO}^{15}\text{N}$  become available.

## Woody detrital pools

### Parameters in the Scenario file

Several parameters that control the production of woody litter appear in the Scenario input file, allowing these to be given values that change on a monthly basis throughout the model run, simulating changes in the age structure of the forest, self-thinning (stem exclusion) in the forest through certain years, and/or multiple forest harvests of varying forms and intensities. These parameters in the Scenario file are as follows (see comments in NewSite.xls for further information):

Parameters meant to be nonzero in each month, throughout the model run:

**WoodTurnover:** Monthly turnover (mortality) of living wood mass to standing dead  
**FWDfrac:** Fraction of woody litter inputs to soil that is FWD (fine woody debris < 10 cm. diam) as opposed to CWD (coarse woody debris).

Parameters meant to be nonzero only in months when forest harvest occurs:

**BiomLossFrac:** Fraction of living wood biomass (including belowground woody tissues, large roots) that is lost from living pool during harvest  
**RemoveFrac:** Fraction of wood biomass cut, that is removed from site  
**OMixFrac:** Fraction of forest floor mixed down into mineral soil as a result of disturbance due to logging operations

During each harvest simulated, the parameter **BiomLossFrac** is used to calculate losses from the pool of living wood, **WoodMass**; these losses include both wood removed from the site together with wood transferred to the standing dead pool, **SWD**, during harvest operations. The wood physically removed from the site during harvest is equal to **WoodMass**\* **BiomLossFrac** \* **RemoveFrac**. The pool **WoodMass** includes belowground wood, including live woody roots, so the parameter **RemoveFrac** should be set so that it accounts for woody roots not removed.

## Inputs of woody litter to standing dead and downed pools

Inputs of woody litter derive from turnover (mortality) of living wood plus wood left on the site during forest harvests.

For those users familiar with PnET-CN, there are important differences in the way PnET-CN and TRACE deal with dead wood. In PnET-CN, there is living wood (WoodMass), it turns over, and through the WoodLitM (and N) fluxes it moves to DeadWoodM (and N). Then it undergoes some decay and loss of C, and eventually is 'transferred' to humus pool HOM. In other words, there is one big pool, DeadWood, that includes standing dead, downed CWD, and downed FWD. In the augmentation of this code from PnET-CN to TRACE (replacing the single pool of woody debris with the 4 pools in TRACE), many of the pool names and flux names were changed or meanings were changed.

In TRACE these are how the pool and flux names are used:

**WoodMass** and **WoodMassN**: Living wood, a pool.

**WoodtoSWDM** and **WoodtoSWDN**: Transfer fluxes from living wood to standing dead wood.

**WoodtoDWDM** and **WoodtoDWDN**: Transfer fluxes from living wood (as slash during harvest) and/or from standing dead wood, to downed woody debris pools. (Later, in the subroutine **Separate**, this flux is separated into inputs to **OFWD**, **OCWD**, **BFWD**).

**WoodTurnover** (a user input parameter in the Scenario input file) is rate of transfer of living wood mass to standing dead (annually, or in the units year<sup>-1</sup>). This parameter governs the transfer of living wood to standing dead wood via mortality, and can be adjusted to reflect periods of self-thinning, insect disturbance, etc.

**WoodLitTrans** (a user input parameter in the Parameter input file) governs the flux **WoodMassLoss** (through C respiration, and through falling to downed pools). In PnET-CN (there named WoodLitLossRate) refers to mass loss from all DeadWood but in TRACE, **WoodLitTrans** refers to just the mass loss from standing dead wood, **SWD**. This parameter, **WoodLitTrans**, governs the relative differences in pool sizes between standing dead and downed woody debris in TRACE.

**WoodLitCloss** (a user input parameter in the Parameter input file) governs the decay of standing dead wood; i.e. the difference between **WoodMassLoss** and **WoodtoDWDM**. **WoodLitCloss** is rate of *mass* loss (not C loss) due to respiration of all DeadWood in PnET-CN, but respiration in just standing dead wood in TRACE. The corresponding C flux is calculated as **WoodDecResp**. **WoodMassLoss** is the flux of standing dead wood mass lost each month (from both decomposition of standing dead, and production of woody litterfall).

## Decomposition, N dynamics, and humification of woody debris

First-order decay constants (in the units month<sup>-1</sup>) for woody debris are **kwoodyO** and **kwoodyM**, for the O horizon and mineral soil horizon, respectively. These parameters are set

## Pools of humified matter (HOM, LSOM, HSOM)

by the user in the Parameter input file. Typically, woody debris is modeled as decaying more slowly than fine litter, and more slowly in the O horizon than in the M horizon.

In TRACE, nitrogen dynamics work the same way in each of the **OFWD**, **OCWD**, and **BFWD** pools (see *Pool definitions* above). In each of these pools, nitrogen enters with woody litter mass, and concentrates in these pools, as mass is lost through decay, until the C:N ratio of the entire pool reaches the critical C:N ratio for woody debris, **CNwdw** (which is set in the Parameter input file). If this critical woody C:N ratio is reached, excess N undergoes net mineralization as necessary, during decay, to maintain the C:N ratio at or above the value of **CNwdw**. (Under most circumstances, net N mineralization from these pools is small in the model).

Even though the C:N ratio of woody debris pools may be above the critical C:N ratio, and no net N mineralization may occur, TRACE includes an independently-calculated gross exchange of N between pools of woody debris and soil-available N pools each month. Thus, <sup>15</sup>N isotopes in soil-available N pools can be immobilized in woody debris pools even if they are not undergoing net N mineralization. This gross N exchange is small, however, as verified in field studies of 8-yr recoveries of <sup>15</sup>N in fine woody debris at the Harvard Forest (Currie et al. 2002).

A portion of FWD in each horizon, as it undergoes decay, is considered humified. A portion is transferred to pools of humified matter in each horizon (**HOM** and **LSOM**). This portion is equal to 5% of the initial mass of material entering the pools of downed woody debris. In the O horizon, coarse woody debris does not have a transfer rate to humus, but it does have a rate of fragmentation to fine woody debris. In other words, some portion of **OCWD** fragments to **OFWD**, and a portion of that will be decayed to humus over time.

## Pools of humified matter (HOM, LSOM, HSOM)

Pools of humified matter are conceptually defined as pools containing material in 'Phase II' of decay (see *Fine litter and decomposition* above), representing a partially stabilized state with a much slower rate of C mineralization. These pools are named **HOM** (humified organic matter) in the forest floor and **LSOM** + **HSOM** (light-fraction soil organic matter and heavy-fraction soil organic matter) in mineral soil. The corresponding N pools are **HON**, **LSON** and **HSON**. These are important pools in TRACE because they store and cycle much C and N and their N dynamics are key in controlling ecosystem-level redistributions of <sup>15</sup>N over short-term (**HON** and **LSON**) and longer-term (all three pools) timescales. TRACE N dynamics and <sup>15</sup>N redistributions are very sensitive to the decay rates and gross N dynamics, in these pools. At the same time, the turnover rates and initial sizes of these pools for model runs (in the early 20<sup>th</sup> century, for example) are difficult to parameterize with confidence.

## Humification as a decay process

Humification in TRACE is conceived as a convergence of material that may have had differing initial characteristics (Melillo et al. 1982; Zech and Kögel-Knabner 1994; Coleman and Crossley 1996). Humification occurs in TRACE as transfers of 20% of the initial mass of fine litter to **HOM** in the O horizon and **LSOM** in mineral soil. TRACE does not include litter cohorts; thus, when

## Pools of humified matter (HOM, LSOM, HSOM)

material is passed to humus, it carries the N concentration(s) of the overall source pool(s) together with their overall isotopic ratios. In the O horizon, transfers of mass and N to humus occur from the **ACI** and **ACS** pools (in mineral soil, from the BL pool). Using the **ACI** and **ACS** pools as the source means that the mass ratio of lignin:cellulose in well-decayed litter is approximately 1:1 (Berg 1986).

Well-decayed woody debris ultimately enters the same pools of humified matter as fine litter in TRACE, although a lesser portion of woody litter is ultimately humified. Organic matter mass and N are transferred from the fine woody debris pools at rates lower than those of fine litter. Organic matter and N in coarse woody debris undergoes fragmentation to fine woody debris, but is not directly transferred to humus; the portion of it that does become FWD will have a portion transferred to humus ultimately. The rate constant (**kwt**) that controls humification of FWD in TRACE can be changed by the user. Its default value was parameterized so that 5% of the organic-matter mass in woody litter inputs (CWD + FWD) to the O horizon will ultimately be transferred to humus in the O horizon, given the distribution of CWD and FWD inputs and the rate of fragmentation of CWD to FWD parameterized for stands at the Harvard Forest. This same rate, controlled by **kwt**, is applied to calculate transfers of well-decayed woody debris in the mineral soil horizon to **LSOM**.

In the current version of TRACE outlined here (TRACE 4.20), all humified litter in mineral soil, together with DOM and POM illuviation in mineral soil, enter the **LSOM** pool. The **HSOM** pool receives no inputs at all in the present version. **HSOM** does turn over very slowly and release mineralized C and N very slowly, but receives no inputs; it is conceived as being very old material that was present at the start of the model run.

## N dynamics in humified matter

In their gross and net N dynamics, O-horizon humus (**HOM**, **HON**) and light-fraction mineral-soil humified matter (**LSOM**, **LSON**) operate in a completely analogous fashion. N dynamics in the O-horizon humus, **HON**, will be described immediately below, but this description also applies to **LSON**. (N dynamics in **HSOM**, in contrast, are very simple: **HSOM** undergoes very slow turnover and release of N to the **MNH4** pools, and that is all.)

The **HON** pool gains  $^{15}\text{N}$  based on the  $^{15}\text{N}$  content of fine-litter pools during humification. Humus loses  $^{15}\text{N}$  based on its own  $^{15}\text{N}$  content, during humus decay. There is another major process that controls  $^{15}\text{N}$  dynamics in humus, though it has no effect on net N dynamics in humus: the gross assimilation and release of N in each timestep. Gross N mineralization and assimilation fluxes can be much larger than net N dynamics.

Within each monthly timestep, humus first undergoes gross mineralization of  $\text{NH}_4^+$ . This flux is based on the rate of mass loss (decomposition) of the humified matter, the N concentration in the humified matter, and the value of **omega**, a parameter that directly relates gross  $\text{NH}_4^+$  mineralization to mass turnover of humified matter (Currie et al. 1999). For our TRACE modeling to date for the Harvard Forest, we have used **omega** = 5; the rate of gross  $\text{NH}_4^+$  mineralization from humus is thus 5 times the rate that would be produced by the mass turnover multiplied by the N concentration in the pool. The parameter **omega** is closely related

to the ratio of gross:net mineralization, but not exactly equal to it (see Currie et al. 1999 for detailed equations). Next, the  $^{14}\text{NH}_4^+$  and  $^{15}\text{NH}_4^+$  mineralized mix with the pools of soil-available  $^{14}\text{NH}_4^+$  and  $^{15}\text{NH}_4^+$  in O horizon. Then after gross N immobilization in fine litter, humus undergoes 're-immobilization' of N, controlled by an attractor C:N ratio for humified matter. Gross fluxes of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  assimilation take place (Currie et al. 1999); the preference of  $\text{NH}_4^+$  over  $\text{NO}_3^-$  assimilation in humus pools is controlled by the parameter **ANpref**.

Unlike the microbially-modeled immobilization process in fine litter pools,  $\text{NH}_4^+$  and  $\text{NO}_3^-$  assimilation in humus pools are considered as assimilation into combined microbial-detrital material. The gross assimilation fluxes are controlled by the value of **omega**, which is decoupled from C mineralization rates or the availability of C to soil microbes. The gross N assimilation in humus in TRACE can thus be viewed as an unspecified combination of microbially-mediated, enzymatic, and abiotic processes (Aber et al. 1998) decoupled from soil C availability. In an early inverse-modeling analysis with TRACE at the Harvard Forest, we determined that this model structure was needed in order to account for the rapid (1-2 yr) incorporation of  $^{15}\text{N}$  tracers into humus in the O horizon (Currie et al. 1999). Fine-scale work at the Harvard Forest subsequently verified that high gross rates of inorganic N assimilation did take place in both the oak and pine forest soils at this site (Berntson and Aber 2000).

## Photosynthesis and plant allocation of C

Photosynthesis and plant allocation of C in TRACE are largely unchanged from the PnET-CN model (Aber et al. 1997, Ollinger et al. 2002). To incorporate  $\text{CO}_2$  - nitrogen interactions on aboveground processes, TRACE includes a recently-developed algorithm based on the work of Ollinger et al. (2002). Photosynthetic rates are driven by foliar N concentrations and atmospheric  $\text{CO}_2$  levels, using a Michaelis-Menten equation fit to normalized  $A-C_i$  curves (photosynthesis in relation to internal leaf  $\text{CO}_2$  concentrations) that can be measured for particular forest sites. This approach expresses the magnitude of  $\text{CO}_2$ -saturated photosynthetic rates as a function of leaf N concentrations. The equation has the form  $R_{C_i} = k (C_i - C_o) / (C_i + 2C_o)$ , where  $R_{C_i}$  is the proportional difference in photosynthesis between ambient and elevated atmospheric  $\text{CO}_2$ ,  $C_i$  is the internal leaf  $\text{CO}_2$  concentration that occurs at a given ambient  $\text{CO}_2$  concentration,  $C_o$  is the internal  $\text{CO}_2$  half saturation concentration and  $k$  is an empirically-derived constant. In the program the ambient  $\text{CO}_2$  concentration is assumed to be 350 ppmV.

Coniferous canopies have a different architecture from deciduous ones with clumped arrangements of foliage. This makes it possible for the light to penetrate further into coniferous canopies at similar LAI levels as deciduous ones. Therefore, a correction factor, **LAIadj**, was introduced to reduce the effect of the LAI upon the light extinction. This parameter can be set in the parameter input file. Presently for coniferous canopies this parameter was set to 1.5 (for deciduous canopies it should be 1.0).

Maximum rates of photosynthesis are controlled by the internal model-internal variable **Amax**, which is dependent on foliar nitrogen concentration together with three parameters set by the user in the parameter file: **AmaxA**, **AmaxB**, and **AmaxFrac**:

## Plant uptake and internal cycling of N

$$\begin{aligned} \text{Amax} &= (\text{AmaxA} + \text{AmaxB} * \text{FolNCon}) * \text{DelAmax} \\ \text{Amax} &= \text{Amax} * \text{AmaxFrac} \end{aligned}$$

Where the units on **Amax** are  $\text{nmol CO}_2 (\text{g foliage})^{-1} \text{s}^{-1}$ , **FolNCon** is a model-calculated internal variable that represents concentration of N in foliage ( $\text{g N} / \text{g OM}$ ), and **DelAmax** is a model-internal variable that allows **Amax** to increase under elevated  $\text{CO}_2$  (Ollinger et al. 2002). The values of **AmaxA** and **AmaxB** should not be altered unless you have site-specific measurements of the relationship between Foliar N and photosynthesis and you work closely with the above equations, together with other parts of the model code, to calculate better values of these parameters for your site. The parameter **AmaxFrac** should always lie between 0 and 1. It represents the daily-averaged maximum rate of gross photosynthesis as a fraction of the instantaneously-measured maximum rate. (The nominal value used for the Harvard Forest oak forest is 0.75). This is not a variable normally changed by the user. At the same time, **AmaxFrac** does provide a simple scalar that could be used to calibrate gross photosynthesis up or down, while leaving all of the processes and relationships among foliar N, temperature, water availability, light availability,  $\text{CO}_2$ , and gross photosynthesis intact.

### The PlantC Pool

The **PlantC** pool is not a sum total of C in vegetation; rather, it is a single pool, the central plant-internal storage pool for photosynthate. **PlantC** is credited a C flux each month from net photosynthesis. Then **PlantC** is debited for foliar growth, foliar respiration, wood production, wood growth respiration, maintenance respiration for living wood, and root allocation (which includes both root production and respiration.) **PlantC** is a pool [ $\text{g C}/\text{m}^2$ ] that is continually updated.

In TRACE, production of foliage, wood, and roots can be limited if not enough N is available in the plant-internal N pool, **VascN**, to provide the requisite N for allocation to the new tissue. The operation of **VascN** is described below.

## Plant uptake and internal cycling of N

### Internal source-sink model

The main internal storage pool of N in TRACE is the **VascN** pool (named conceptually for N storage that is accessible by the vascular system, i.e. mobile inside the vegetation). Carbon and nitrogen inside the vegetation are modeled conceptually using a physiological source-sink framework. Sources to the **VascN** pool include N taken up from the soil by plant roots (taken up as  $\text{NH}_4^+$  and  $\text{NO}_3^-$  separately, from the O horizon and mineral soil separately) and N that is resorbed from senescing foliage. (There is no explicit resorption from senescing wood tissue or root tissue in TRACE.) Sinks from **VascN** include allocation of N to growing foliar, fine-root, and woody tissues. The maximum amount of N that can be stored in the **VascN** pool (as a lumped-parameter pool, in the units of  $\text{g N}/\text{m}^2$ ), is set by the user in the parameter **MaxNStore**, in the Parameter input file.

The **VascN** pool is modeled as being a single homogeneous, well-mixed pool throughout the plant. Thus, isotopic signatures of N fluxes that are taken up from soil horizons, together with isotopic signatures of N resorbed from senescing foliage, mix together with the isotopic signatures of N already stored in the VascN pool in each timestep. N allocated to growing tissues from the VascN pool then carries the isotopic signature produced by mass-balance and pool dilution in the single VascN pool.

For the purposes of comparing tissue N concentrations and tissue  $PR^{15}N$  recoveries in field data against model, the VascN pool must be given a physical location. TRACE models the pool as being distributed between living wood and living fine roots using the parameter **VascNWprop**, which is a user input parameter (see *N concentration in woody and fine-root tissue*, below). In the source code, where  $\delta^{15}N$  values and  $PR^{15}N$  values in vegetation pools are calculated in the subroutine **MidYrPlot** (in the month *Plotmo*) for plotting and printing, N and  $^{15}N$  in the VascN pool is distributed among the pools of living wood and fine roots. Care must be taken in altering any of these calculations, as the code that brings this about can appear confusing. Care must also be taken in interpreting printouts, and in summing  $PR^{15}N$  values across pools. Where  $PR^{15}N$  in roots and woody tissues are printed, they include the appropriate amounts from the **VascN** pool based on its physical location. Sometimes  $PR^{15}N$  or  $\delta^{15}N$  in the VascN pool itself is printed alongside; this is simply to provide more information for model interpretations. To calculate total ecosystem  $PR^{15}N$ , the  $PR^{15}N$  in **VascN** should not be summed with  $PR^{15}N$  in living wood and fine roots, because it is already included.

## N allocation to growing tissues

Allocation of N to growing tissues works in a simple and straightforward manner. First, C allocation to growing tissues is calculated based on plant internal C storage and other factors (see *Photosynthesis and plant allocation of C*, above). Then, based on the requisite N concentration in the foliar, root, or wood tissue to be produced, the tissue is produced and the needed N flux is transferred to the new tissue (carrying the isotopic signature of the VascN pool at that point in time). If insufficient N is available in the VascN pool for the tissue construction at that time, then the tissue production is scaled back proportionally. In other words, N availability in the plant-internal VascN pool can limit tissue production. Each month, tissues are produced in the order foliage first, roots next, and wood last.

**BudN** is a variable that controls the N allocation to growing foliage. As in PnET-CN, **BudN** is not a pool. It is a year-end parameter that has the units of g N / m<sup>2</sup>, but used only as an intermediary to calculate value of **FolNCon** for the next year. In TRACE, as in PnET-CN, BudN is simply a means of transferring information (about the concentration of N that should be allocated in new foliage, **FolNCon**) from the end of one year to the time of leaf-out in the next year. Thus, the amount of N represented by **BudN** is not debited from the **VascN** pool until foliar mass is actually produced in the spring, during leaf-out; growing foliage thus gains the isotopic signature of the VascN pool at that time, which in turn may carry some isotopic signature from soil-available pools in the spring, during leaf-out. At the Harvard Forest, recovery of  $^{15}N$  in foliage during the first year of  $^{15}N$  labeling showed this to be realistic (Currie and Nadelhoffer 1999).

As N availability increases in the environment, relative to plant N demand, plant availability will increase inside the plant. This is measured in absolute terms as **VascN** storage or, in relative terms, as the ratio of **VascN** to **MaxNStore**. N concentrations in all tissues will rise as the size of the **VascN** pool rises. For woody tissue and root tissue, N concentrations (as **WLpctNmeas** and **RLpctNmeas**; see more information below) will rise as a direct result of the rise in **VascN**. This will occur in a manner quantitatively consistent with the overall mass in these tissues, the proportion of **VascN** physically associated with each tissue type, and the 'minimum' N concentration in these tissues (parameterized as **WLpctN** and **RLpctN**).

## **N concentration in foliar tissue**

In TRACE, concentration of N in green foliage (**FolNCon**) is usually higher than that in foliar litter (minimum value **FLPctN**), because of resorption (retranslocation) of N from senescing foliar tissue back to the plant-internal storage pool. Resorption is controlled by the parameter **FolNRetrans** and by the amount of N that can be stored in the tree (as **VascN**). If retranslocation means that **VascN** will exceed its maximum value (**MaxNStore**) retranslocation is reduced in size and litter N content will be higher. In TRACE, **FolNRetrans** and **FLPctN** are parameters set by the user, and are used to initialize foliar N concentrations as follows:

$$\text{FolNCon} = (\text{FLPctN} / (1 - \text{FolNRetrans})) * 100$$

However, the value of **FolNCon** can vary over time, through the model run. It can rise above the above baseline value as N availability increases. In TRACE, the best way to represent this change in N availability was found to be the overall flux of gross N mineralization in the whole soil. This is a sensitive (but not too sensitive) index of the overall N availability, and model testing showed that it provided a useful way to model the rise in foliar N concentration in experimental N amendments in field plots. The model calculates the variable **Nratio**, which is used to increase **FolNCon**. **Nratio** varies between 1 and  $(1 + \text{FolNConRange})$  as follows:

```

NRatio = GrossNMinLastYr / BaseGrossNmin
If NRatio > (1 + FolNConRange) Then
  NRatio = 1 + FolNConRange
ElseIf NRatio < 1 Then
  NRatio = 1
End If

```

Whether **FolNCon** is really increased by **Nratio** also depends upon the amount of available N in the tree, **VascN**. If this is insufficient, **FolNCon** will not increase as much.

(Note that this is very different from the way **Nratio** is calculated in PnET-CN, and that in TRACE, **Nratio** is used only to alter foliar N concentration, not root or wood N tissue N concentration. The latter two, in TRACE, are calculated directly from plant-internal N storage in **VascN**, together with the biomass values of wood and root tissues, as described below).

The threshold parameter **BaseGrossNmin** is read in from the Parameter files as a site parameter. This can be estimated, for a site, from the estimated value of gross:net N mineralization for the site, and from an estimate of the threshold in net N mineralization at

## Parameterizing the timing of the foliar mass dynamics

which foliar N concentration begins to rise above its baseline value (its baseline value being determined by **FLPctN** and **FolNRetrans**, as outlined above).

### **N concentration in woody and fine-root tissue**

There are four variables that represent these concentrations of N: **WLpctN**, **RLpctN**, **WLpctNmeas**, and **RLpctNmeas**. The first two are user-set parameters that represent the minimum N concentration in woody and fine-root tissues – the values that occur when plant-internal N storage (**VascN**) is zero. These will be less than the measured concentration, because measured value will include some amount of storage or movable N. The latter two variables, **WLpctNmeas**, and **RLpctNmeas**, are variable through the model run as the value of **VascN** varies.

The amount of N stored in **VascN** (maximum controlled by **MaxNStore**, a user parameter), is physically distributed between living wood and living fine roots in TRACE. The proportions are controlled by the user parameter **VascNWprop** (VascN Wood Proportion), which can vary from zero to 1. The remainder of **VascN** is physically located in living roots. When the values of **WLpctNmeas** and **RLpctNmeas** are printed out, and also when the values of  $PR^{15}N$  in living wood and roots are calculated, TRACE makes the following calculation. The model takes the total amount of N in the VascN pool, partitions it physically between living wood and roots, and uses the mass in living wood and roots pools to calculate the contribution to N concentration (and  $^{15}N$ ) in these pools, and adds these amounts to the non-mobile N in wood and root tissue (controlled by **WLpctN** and **RLpctN**). The result (1) is an algorithm that allows N concentration in wood and roots to rise realistically and mechanistically as plant N storage rises, and (2) values of **WLpctNmeas**, **RLpctNmeas**, and  $PR^{15}N$  in woody tissues and roots that can be compared directly against field study results.

## Parameterizing the timing of the foliar mass dynamics

The timing of the foliar mass growth in the spring is determined by the temperature and the foliar growing degree day parameters, **GDDFolMin** and **GDDFolMax**. The moment of leaf shedding is determined by the parameter **SenescStart**, and the actual conditions in the canopy. **SenescStart** just indicates the earliest possible moment in the year foliage can be shed. Only that part of the foliage will be shed, however, that cannot perform net photosynthesis. Otherwise it will not be shed before the last month of the year. The parameter **FolReten** determines which fraction of the foliage will be shed in a year. In case of a deciduous forest its value should be one. In case of coniferous forests with foliage that lasts more than a year, it must be larger than one. The unit of **FolReten** is year, but it does not stand for the average age of the foliage. If its value is 3 it means that one third of the foliage is shed each year. Under steady state conditions a similar amount of foliage will be produced each year. The average age of such foliage will be smaller than 3 as the foliage starts growing some time after January 1<sup>st</sup> and will be shed before the end of the third calendar year. The exact timing of growth and shedding is not determined by **FolReten**, but by the parameters described earlier. **FolReten** need not be a whole number. If the value is 2.5, half of the foliage will be shed in its second year and the other half in its third

year. As TRACE does not keep track of all the foliar cohorts this is done implicitly by shedding the correct fraction.

A special characteristic of TRACE is, that for coniferous forests, with a **FolReten** larger than 1, it does not allow any of the current year foliage to be shed. The consequence of this is that it is impossible to have foliage that is shed partly within one year and partly in its second year. Even if **FolReten** is diminished from 2 to 1.5, still the foliage will be shed in the second year. So it makes no sense to choose a value between 1 and 2 for **FolReten**. In fact it has strong disadvantages, as under special conditions such a value can result in strong oscillations of the yearly foliar production.

## Microbial representation

Pools of detritus in TRACE are designed as combined detrital-microbial pools. Microbial biomass is thus included not as a separate set of pools, but as a portion within each detrital pool of organic matter and N. The reason for this structure was the principle, in model design and development, that pools should be comparable against field data where possible. In the initial, large-scale  $^{15}\text{N}$  tracer studies conducted at the Harvard Forest, investigators measured  $^{15}\text{N}$  recoveries in detrital pools as combined detrital-microbial material.

This aspect of TRACE model structure has strengths and weaknesses. A weakness is that a combined microbial-detrital pool of N (**ACIN**, for example, the N contained in the acid-insoluble fraction of fine litter) is modeled as a homogeneous, well-mixed pool. We know that this is a coarse approximation, because in reality the N isotopes in the microbial matter in this **ACIN** pool probably does not have the same isotopic signature or turnover time as the detrital material in this pool. At the same time, however, a strength of this model structure is that the sink strength of the **ACIN** pool for N assimilation can be parameterized without an explicit, detailed treatment of microbial uptake processes vs. chemical or abiotic processes of N incorporation into this material. These detailed processes are a subject of current debate, and difficult to parameterize in a way that would reflect consensus in the field. The pool structure in TRACE represents what is typically measured in large-scale  $^{15}\text{N}$  tracer studies (microbial-detrital material combined in soil samples), without postulating values for a large number of additional, detailed-process parameters that are topics of current debate.

Even though TRACE does not include explicit pools of microbial biomass, microbial principles are included in several mechanistic processes. Microbial representation is included in these processes through algorithm formulations and through certain parameters. For example, microbial C-use efficiency on **ACI**, **ACS**, and **TEX** materials (C classes of fine litter) are parameters. These enter into the calculations of the gross rates of N assimilation in these fine-litter pools of combined microbial-detrital material. In the case of these fine litter pools, N assimilation is modeled as microbially-driven alone, with no chemical or 'abiotic' component, and with a traditional view of microbial N uptake, microbial production, and microbial C-use efficiency (Currie et al. 1999).

Another important parameter that represents microbial activity is **ANpref**, short for 'Ammonium - Nitrate Preference'. This parameter is used to calculate microbial-assimilation transfers of  $\text{NH}_4^+$  and  $\text{NO}_3^-$  from source pools, based on a total N demand in a target pool

containing microbes, together with a microbial preference for  $\text{NH}_4^+$  over  $\text{NO}_3^-$ . The variable **ANDemand** (in the source code) is Assimilation N demand. **ANPref** (supplied by the user in the Parameter input file) is ratio of preference for  $\text{NH}_4^+$  to  $\text{NO}_3^-$ . A value of 2 means that preference is to assimilate  $\text{NH}_4^+$  at a 2:1 molar N ratio over  $\text{NO}_3^-$ , i.e. 66.6%  $\text{NH}_4^+$  and 33.3%  $\text{NO}_3^-$ . If source pools are unlimited, **ANDemand** is met and **ANPref** determines the uptake of each form of N. If demand for either  $\text{NH}_4^+$  or  $\text{NO}_3^-$  exceeds the amounts available in the source pool, then the alternate form of N, if available, will be used to make up the N demand.

## Detrital energetics

Theoretically, because energy flow is fundamental to the function of decomposer organisms and ecosystems, energetics could provide complimentary fundamental constraints on soil C dynamics. Often, however, C is considered as a surrogate for energy in studies of detrital decay and C turnover in soil. Bomb calorimetry has long been used to measure stored energy in organic matter, but in detritus not all of the energy is bioavailable. The incorporation of detrital energetics in TRACE was used in an approach to quantify the flux of bioavailable energy dissipated by resident heterotrophic communities in soil organic horizons *in situ* (Currie 2003). This approach made use of the principle of energy balance together with the biogeochemical processes in the TRACE model.

Pools and fluxes of energy, in **kcal/m<sup>2</sup>**, **kcal m<sup>-2</sup> mo<sup>-1</sup>**, and **kcal m<sup>-2</sup> yr<sup>-1</sup>**, were added to pools of fine litter, woody debris, and humus in TRACE, based on a calorimetry study of field samples from the Harvard Forest mixed oak and red pine stands. At present, these only include fluxes related to energy storage and dissipation in soils, detritus, and the forest floor (i.e. living vegetation is not presently included in the energetic analyses in TRACE). The model was used to calculate rates of bioavailable energy dissipation by the heterotrophic communities *in situ*, and compare these with fluxes of C stabilization and mineralization (Currie 2003). Caloric values of fresh foliar litter and fine roots were used to parameterize the appropriate energy inputs in litter production. Caloric values of older categories of foliar litter and of well-decayed Oea material were used to set the average energy contents of material in phase I and phase II decay, respectively. Energy fluxes included those associated with leaching losses of **DOM** and **POM** from the forest floor, transfers of material from the phase I fine litter and woody debris pools (**OFWD** and **OCWD** pools) to phase II decay, and energy dissipation associated with mass loss through oxidation of organic constituents. In phase I decay, energy dissipation was calculated as the net effect of two processes, the loss of stored energy due to mass loss and the change in energy content (kcal/g) of a proportion of the material as it was humified.

## More detail on formats for text output files

In many cases, the quantities printed in text output files may be a bit difficult to understand at first. Many of the headers include short codes and abbreviations: O for soil organic horizon, M for mineral soil horizon; 'nitr' for nitrification, 'gr' for gross, etc. Thus the header for gross nitrification in the mineral soil may be 'M gr nitr'.

In other cases, model results are stored in arrays, and the headers may simply contain numbers in the array. Examples are the NFA array (for N flux analysis), the EFA array (for Energy flux

analysis), and the **MidYrPoolCN** array, for storing C:N ratios in model pools in the month *Plotmo* for later printing. In many of these cases the quantities represented in the arrays are too complex to describe in a simple word or simple abbreviation. Tables below provide some elaboration on these quantities stored in arrays for printing. In other cases, you need to look at the printout statement in the model code, and possibly the assignment statements in the model code (the parts of the code where the array variables are assigned values).

## Output of C:N in model pools and weighted C:N ratios of retention

When the results format for the ASCII text file is chosen as 'Weighted C:N ratios of <sup>15</sup>N retention', the printout format includes values of  $PR^{15}N$  for many model pools, values of C:N ratio (in the month *Plotmo*) for many model pools (**MidYrPoolCN**), and the weighted C:N ratios of <sup>15</sup>N tracer retention (**WtdCNtracReten**, also in the month *Plotmo*; for more information about these, see *Modeling integrative quantities*, below). The latter two sets of results are printed as indices, defined as follows:

Pool CN(1) = foliar cohort 1  
Pool CN(2) = foliar cohort 2  
Pool CN(3) = fine roots  
Pool CN(4) = living wood  
Pool CN(5) = SWD  
Pool CN(6) = (not currently used)  
Pool CN(7) = OFWD  
Pool CN(8) = OCWD  
Pool CN(9) = BFWD  
Pool CN(10) = ACI  
Pool CN(11) = ACS  
Pool CN(12) = TEX  
Pool CN(13) = BL  
Pool CN(14) = HOM  
Pool CN(15) = LSOM + HSOM

WtdCNtracReten(1) = Foliage + fine roots (including portion of VascN in living roots)  
WtdCNtracReten(2) = Living wood, standing dead wood, + downed woody debris  
(together with portion of VascN in living wood)  
WtdCNtracReten(3) =  $O_i + O_e + O_a$  humus, excluding woody debris  
WtdCNtracReten(4) = Mineral LSOM + HSOM + buried litter in mineral soil  
WtdCNtracReten(5) = Overall weighted C:N ratio of <sup>15</sup>N tracer retention

## Detrital-energetic fluxes

Energy fluxes calculated by the model, as described above, can be plotted on screen and printed to a text output file. Energy fluxes are stored in TRACE in a data array named **EFA(n)**, for "Energy Flux Analysis", in the units **kcal m<sup>-2</sup> yr<sup>-1</sup>**. Fluxes stored in this array are defined and calculated as follows, where the number refers to the index (n) in the data array:

## More detail on formats for text output files

- 1: Input in foliar litter in forest floor
- 2: Input in fine root litter in forest floor
- 3: Contained in DOM + POM leached from forest floor
- 4: Dissipated due to mass loss from mineralization in C classes, plus due to change in energy content of mass in place in C classes (i.e. from fresh litter to older litter, and older litter to commingled).
- 5: Dissipated due to mass loss from mineralization in FWD and CWD.
- 6: Contained in material passed from woody debris to humus in forest floor
- 7: Contained in material passed from C classes to humus in forest floor
- 8: Dissipated in humus in forest floor due to mass loss from mineralization
- 9: Dissipated in humus in forest floor due to change in energy content of mass in place.
- 10: Input to forest floor in DOM in throughfall
- 11: Input to forest floor in FWD and CWD litter inputs.

## IV. Methodologies of Using the TRACE Model

### Methodological introduction

The methods that we use to undertake ecosystem modeling as a scientific endeavor are a subject of experimentation, development, and current debate. Field studies, laboratory analyses, and statistical analyses all have more well-defined methodologies than does the process modeling of ecosystem biogeochemistry. Partly this is because ecosystem modeling is relatively new (only a few decades old) compared with field work, laboratory work, and statistics. In this sense the radiative growth of multiple competing methodologies is a positive advance for modeling. At the same time, unfortunately, the lack of a meaningful and informed dialogue between model developers, model users, and others concerning modeling methodology limits the advance of ecosystem science. Promoting an open dialogue about modeling methodology and techniques of applying and using the TRACE model (rather than simply covering the structure and mechanics of the model) is the purpose of this section.

### Testing of TRACE for consistency and errors

This section deals not with testing of the model against field data, for scientific purposes, but with testing and debugging of the model code to ensure that it is working properly. The TRACE model code incorporates several mechanisms for testing model consistency, model performance, and for trapping errors.

### Mass balance checks

In single-site runs, the user can easily check for C mass balance and N mass balance. There are two variables named **Cmassbal** and **Nmassbal**; these are graphed in two of the graphical outputs. These should show up as flat lines across the graphical output screens. They are set up this way because a slight deviation from a straight line would be easy to see. This is how they work, using N mass balance as an example (the C mass balance check is analogous): At the start of the model run, and at the end of each year, all of the N pools are summed (for <sup>14</sup>N mass and <sup>15</sup>N mass separately) and stored in the variables **Ecosystem14N** and **Ecosystem15N**, respectively. Then, as the model runs, any N that enters or leaves the ecosystem (through deposition inputs, N fixation inputs, leaching losses, harvest removals, etc.) is tracked using the bookkeeping variable **CumNinout**. Through a run, this variable tracks the cumulative inputs minus outputs (inputs being positive). At the end of each year, the error-checking term **NmassBal** is calculated as follows.

$$\text{NMassBal} = \text{Ecosystem14N} + \text{Ecosystem15N} - \text{CumNinout}$$

Under normal operation, graphing **NmassBal** results in a straight line. If you have Visual Basic and you make changes to the TRACE source code, we suggest you test for C mass balance and N mass balance after each change, by simply looking at these graphically. If you introduce a

mass-balance error, often it is easy to guess the source of the error by looking at the shape of the **CmassBal** graph or **NmassBal** graph and comparing it with the dynamics in C and N pools and fluxes.

## Checks of the <sup>15</sup>N isotope calculations

TRACE performs three types of automated tests on the <sup>14</sup>N/<sup>15</sup>N isotope calculations. The first is a repeated set of tests, distributed throughout much of the model code, for round-off errors. All isotope-related variables and calculations in the current version of TRACE are carried out in double-precision. Even so, because isotopic ratios are significant to four decimal places and because some calculations (gross N dynamics in soil-available NH<sub>4</sub><sup>+</sup> and NO<sub>3</sub><sup>-</sup> pools, for example) are conducted repeatedly, round-off errors can arise. TRACE contains a subroutine **ROEcheck** (Round-Off Error check) that is called repeatedly to find and correct some of these when they occur in ways that would affect model results in the significant digits.

The second type of automated test is accomplished by running TRACE without any <sup>15</sup>N tracer additions and checking that the simulated values of δ<sup>15</sup>N and PR<sup>15</sup>N remain close to zero. Since all model pools contain “background” non-zero values of atom%<sup>15</sup>N (= 0.3663) at the start of the model run, and since all of the <sup>14</sup>N and <sup>15</sup>N calculations are performed continually even in the absence of tracer additions, this provides one test of the consistency of the model algorithms: in the absence of <sup>15</sup>N tracers, in model pools the atom%<sup>15</sup>N values should remain at background and the values of δ<sup>15</sup>N should be calculated as zero. Performing this test may show that round-off errors creep into the 4<sup>th</sup> or 5<sup>th</sup> significant digit in the isotope results (i.e. δ<sup>15</sup>N values up to ± 0.03‰). This is normal.

The third automated test is conducted by plotting PR<sup>15</sup>N (percent recovery of <sup>15</sup>N tracers) on the screen and viewing the overall PR<sup>15</sup>N sum. This is set up as a model check because all individual values of PR<sup>15</sup>N in model pools are calculated first, then summed to plot for this purpose. The sum of PR<sup>15</sup>N should begin at 100% immediately after tracer addition, then begin a slow decrease as <sup>15</sup>N is lost from the ecosystem over time. (Note: if one prints out PR<sup>15</sup>N values in all model pools, including **VascN**, and sums them, the sum would be greater than 100% because **VascN** would be double-counted. For our pre-programmed calculation of PR<sup>15</sup>N values, the <sup>15</sup>N in **VascN** is already distributed physically between roots and living wood – see *Plant Uptake and Internal Cycling of N*.)

## The *Echeck* error-checking array

When running the model in Monte Carlo mode, numerous (e.g. 50) model runs may be executed sequentially, with randomly varying perturbations made systematically to a large set of model parameters (see *Conducting Monte-Carlo model runs*). Infrequently, this can produce a strange combination of parameters far outside their normal domains, causing disallowed model behavior. TRACE contains code to check for the occurrence of disallowed behavior and record any errors in the **Echeck** array. At many points in the model code, **Echeck** checks are made for the following types of errors:

## Model parameterizations and calibrations

- Values of  $^{14}\text{N}$  or  $^{15}\text{N} < 0$  in the **VascN** pool
- Values of  $^{14}\text{N}$  or  $^{15}\text{N} < 0$  in the pools of soil available N (**ONO3, ONH4, MNO3, MNH4**)
- Violations of N mass balance in the mineralization / immobilization algorithms in litter C class pools (**ACIN, ACSN, TEXN**)
- Violations of N mass balance in any gross transfer of  $^{14}\text{N}$  or  $^{15}\text{N}$  among model pools
- Foliar mass or foliar  $^{14}\text{N}$  or  $^{15}\text{N} < 0$  in any foliar cohort
- Foliar mass or foliar N  $> 0$  at year-end in a deciduous forest
- Foliar mass or foliar N  $> 0$  in the 2<sup>nd</sup> or higher cohort at any time in a deciduous forest

The error-counter is an array **Echeck(iset)**, where **iset** is the counter of the Monte Carlo set (e.g. 1 to 50, or just 1 for a single run of the model). The value of **Echeck** is initialized to zero, and incremented to 1 if any of these violations is detected. The single model run is then stopped, but the Monte Carlo set is allowed to continue, by terminating the current single run and skipping to the next single run in the set. For example, if a Monte Carlo set of 50 runs is performed, and the random combination of parameter values in run #21 causes violations, TRACE will complete runs 1 through 20 and 22 through 50. The output will show that in run #21 **Echeck** was  $> 0$  and that run #21 was stopped.

The **Echeck** error-checking code is operational in all model runs, whether single-site, Monte-Carlo, or GIS. Under normal model use, it is unlikely that any parameter set in a single-site run or a GIS run will cause the type of violation detected by *Echeck*. But if one is detected, a single-site run will terminate. (If you have Visual Basic software, you can find exactly where the error occurred by running the source code in debugging mode, with a flag set to indicate the line where the value of **Echeck** becomes  $> 0$ .)

In GIS mode, if an **Echeck** violation is detected, the model run for that grid cell will be stopped and TRACE will move on to the next grid cell. A value of -9999 will be recorded for that cell in each output grid. Because **Echeck** is a convenient way to stop the run and move on to the next cell, it also serves a second purpose in GIS runs: for a particular cell in the grid, after input data are read from each data layer, if the land use type is non-forest then **Echeck** is incremented and the model moves on to the next cell in the grid.

## Model parameterizations and calibrations

Parameterizations begin by filling in the [TraceDataNeeds.xls](#) spreadsheet as well as possible for a new site, making use of the *data priority codes* described above. It is important to record citations for data entered into this database. At the same time, data used for model assessment are recorded (with citations) in the same database. These will be used as checks and tests against model results.

Some parameters clearly involve no calibration – litter quality, LAI, and so on. Some other parameters involve varying degrees of calibration. Conceptually we separate the activity of parameter calibration into two categories. The first includes parameters that involve some degree of calibration to get certain fine-scale processes functioning properly in the model. For example, because we need the decomposition algorithm to pass a portion (20%) of the initial mass of fine litter to humus, we calibrated the parameter **klct** (named for “ligno-cellulose

## A methodology for TRACE application: 12 steps

transfer”) so that this transfer takes place at the proper rate. There are many similar parameters in TRACE that have been calibrated for fine-scale processes without assessing whole-system behavior. In some sense, these can be viewed as numerical or algorithmic parameterizations.

The second category of calibrations involves the adjustment of parameter values while assessing integrated model behavior or system-level C and N pools and fluxes. If this type of calibration is omitted completely, then the C and N pools and fluxes are likely to be unrealistic for the site. This would limit our ability to test  $^{15}\text{N}$  redistributions, to make predictions, or to simulate integrative quantities of interest such as the effects of elevated N deposition on forest C balance. On the other hand, too much of this type of calibration could produce a model that simply reproduces all of the data used to calibrate it with no possibility of being wrong. This is a potential methodological pitfall in that it could result in an approach that is not falsifiable. Our approach has been to complete just enough of this system-level type of calibration to make the model a useful tool to interpret or assess field-study results, but no more. We have found the most instructive and useful sets of simulations to be those in which disagreements occur between model results and field results.

## A methodology for TRACE application: 12 steps

Based on our experience applying TRACE at the Harvard Forest, we have developed a suggested methodology to use in applying TRACE in other field studies to interpret redistributions of  $^{15}\text{N}$  tracers. This methodology can be described as a series of steps. It begins with parameterization, then proceeds to calibrations, with a final, small set of parameters being calibrated to produce desirable coarse aspects of whole-system C and N cycling (but independent of  $^{15}\text{N}$ ). Then the  $^{15}\text{N}$  redistributions are predicted and model-data comparisons are made. Finally, the methodology includes the use of iterative model-data comparisons or inverse modeling, followed by the simulation of integrative quantities of interest.

### **Step 1: Assemble basic site information**

Construct the climate input file that includes precipitation, solar insolation, and monthly minimum and maximum temperatures for the site as described above.

In the database [TraceDataNeedsx.xls](#), create a new worksheet page based by copying the page from a previous site (the one that is most similar). Referring to the *data priority codes* described above, begin filling in basic information about present-day pool sizes, fluxes, and other parameters. Decide on the year in which model runs will begin (e.g. 1900 if the land was forested then), and work out a means of estimating the soil and vegetation C and N pool sizes in that year. Keep careful notes and citations in the [TraceDataNeedsx.xls](#) database.

### **Step 2: Create Parameter and Scenario files**

Copy an existing Parameter file from another site (or the blank parameter file intended for this purpose), and begin filling in the information for the new site from the database [TraceDataNeedsx.xls](#). For many parameters, it is best to use default, unchanging values already

in TRACE. For many others, changes can improve the model if site-specific values are available, but it is acceptable to use values from other sites or estimates from the literature. For still others, it is important to put some effort into obtaining site-specific values. Use the *data priority codes* (explained above) to help make this determination.

In cross-site analyses, one of the methodological decisions to be made concerns how many parameters should be set differently, vs. held constant, across sites. The more parameters that are standardized across sites (if standardization is reasonable), the easier it will be to interpret differences in model results among sites.

Scenario input files contain information about N deposition, land use and disturbance history, experimental treatments such as N amendments, and detailed specifics about the timing, amount, and atom% of the  $^{15}\text{N}$  label that was applied (see *Conducting Single Model Runs*, above, for more information). Using the file [NewSite.xls](#) as a template, construct the Excel file for the site, fill in the necessary information, and use it to generate the Scenario (Scen\_\_\_\_.txt) input file.

At this early stage of parameterization, pay particular attention to parameters related to vegetation physiology and phenology (foliar retention time, specific leaf weight, growing-degree days, etc.).

### **Step 3: Parameterize litter quality and humus & SOM turnover rates**

A. Find data for litter chemistry (foliar and fine roots) for the site, or use values from similar species at a similar site.

B. Estimate **k<sub>ho</sub>**, the turnover rate of humus in the forest floor (under hypothetical steady-state conditions), in the units ( $\text{month}^{-1}$ ). If a measurement is available for the site, you may use it, although a direct measurement is unlikely to be available. A first approximation can be estimated simply and easily in the file [Kho estimator.xls](#), which is provided alongside the file [TraceDataNeeds.xls](#) in the TRACE package.

Alternatively, estimate **k<sub>ho</sub>** by hand, as follows (this is the same method used in the file [Kho estimator.xls](#)). Estimate hypothetical steady-state values of foliar and fine-root litter production and woody litter production. Multiply the steady-state foliar litter production plus half the fine-root litter production (assuming about half enters the forest floor) by 0.2, thus assuming 20% of this mass enters the humus pool in the forest floor (O horizon). Multiply the woody litter production by 0.05, thus assuming 5% of this material eventually enters the O-horizon humus pool in the hypothetical steady-state. Together, these comprise the inputs to the humus pool. Next, estimate the size of the humus pool in the O horizon in this hypothetical steady-state. (Use a value from a representative stand, 60 years old or more if second-growth, on similar soil, with similar species, and similar climate. Note that this is humus mass, not the mass of the entire O horizon. Depending on your site, you might exclude the O<sub>i</sub>, or O<sub>i</sub> and O<sub>e</sub> in the estimate of humus mass. Recall that in TRACE, entry into the humus pool is defined as the stage at which 20% of initial mass remains.) Divide the steady-state humus mass by the inputs to the humus pool: this yields the residence time in the pool in years; the inverse of this residence time is the first-order decay constant for O-horizon humus in the units ( $\text{years}^{-1}$ ).

Divide this by 12 to calculate, **k<sub>ho</sub>**, the first-order decay constant in (month<sup>-1</sup>) needed in TRACE. Enter this coarse estimate in the parameter file.

C. Next, estimate **SOMdec**, the ratio of the mass loss rate of humified matter in mineral soil to that of humified matter in the O horizon. This ratio, **SOMdec**, controls turnover of the **LSOM** pool in TRACE. (Note that it is not a ratio of *k* constants, it is a ratio of mass loss rates, i.e. a ratio of values of  $[1 - e^{-k}]$  for the **LSOM : HOM** pools). Measures of relative turnover rates from laboratory studies can be used for initial attempts to parameterize this ratio, but unfortunately it will probably be necessary to calibrate this ratio for TRACE to produce realistic C and N pools and fluxes over time for the site.

### **Step 4: Test vegetation productivity**

By now, all of the files needed to run TRACE for a new site should be constructed, many of the key parameters should be estimated or finalized, and climate and scenario-file information should be complete. The TraceDataNeedsx.xls database should also list present-day pool sizes and fluxes for comparison against model results.

Run TRACE for the new site, and examine foliar and wood production in the present-day. These should appear reasonable before proceeding. Foliar production is a central flux in the model and highly indicative of model behavior, because it is sensitive to many model processes and, at the same time, drives many ecosystem-level cycles through plant-soil feedbacks. If photosynthesis is proceeding correctly, but foliar N production is held too low for any reason, then wood production will be too high as a result, because foliar and wood production draw on the same **PlantC** pool of photosynthate.

Some adjustment parameters that may be useful at this stage:

**WoodMRespB:** This parameter directly controls maintenance respiration of living wood. Maintenance respiration of living wood also rises with living wood biomass in TRACE. The higher the amount of wood maintenance respiration, the lower the value of **PlantC** as a storage pool, resulting in lower production of all tissues. Values increasing from 0.07 to about 0.25 may cause wood production to drop without adversely affecting foliar or root production; above 0.25, **PlantC** may fall low enough to begin reducing foliar and fine root production.

**MinWoodFolRatio:** This is a check to disallow wood production dropping too low relative to foliar production. This parameter provides an easy way to adjust the relationship between foliar production and wood production, if the overall photosynthesis is right. Raise or lower the value of **MinWoodFolRatio** to raise or lower wood production relative to foliar production. Values ranging from 0.75 to 1.5 are reasonable, and possibly outside this range, depending on the site. Beware, however, that this variable can cause problems. For example, if **PlantCReserveFrac** is set too high, too close to 1.0, then wood production will be severely reduced, and this **MinWoodFolRatio** will kick in, and severely reduce foliar and fine root production too. If the model exhibits behavior in which foliar production declines steadily to zero over a few decades, or root production drops to nearly zero, the problem could be that the

value of **MinWoodFolRatio** is too high for the amount of photosynthesis that is occurring. Either **MinWoodFolRatio** needs to be lowered, or overall photosynthesis needs to be raised.

**PlantCReserveFrac:** This parameter determines the part of **PlantC** that will be reserved in **Sub AllocateYr**, and will not be allocated to wood or foliar production for the next year. See the model source code for its exact definition. Nominal value is 0.75. If **PlantCReserveFrac** is set too low, the model may exhibit periodic rises and falls (decadal scale, for example) in foliar production or overall NPP. A higher value of **PlantCReserveFrac** acts as a capacitor; it lets the model damp out shorter-term variability in production so they do not lead to longer-term rises and falls.

**FolRelGrowMax:** This is somewhat complex, but basically it relates to the relative amount that canopy mass can increase from one year to the next. This is a sensitive variable if it is outside of the needed range, because it sets up a feedback in the canopy -- ultimately the canopy mass will stabilize, but the value at which it stabilizes is strongly controlled by this parameter because of feedbacks in canopy mass and **avgPCBM** (average positive C balance mass in each layer of the canopy), mediated by water and light availabilities. A higher value of **FolRelGrowMax** causes canopy mass to reach a higher attractor value (if there is enough N and water available), and this in turn raises root production, and these effects lower the **PlantC** pool, which lowers wood production. In addition, the higher foliar litter production brings more N into the shorter-term soil cycling, raising N mineralization.

**AmaxFrac:** This is a site-specific parameter (in the Parameter input file) that represents whole-day photosynthesis as a fraction of instantaneously-measured values of photosynthesis from field data. Its nominal value is 0.75 and its alteration should be avoided. At the same time, if all other elements relating to vegetation production and phenology have been checked, and overall production is simply too high or too low, **AmaxFrac** provides a convenient calibration scalar for overall photosynthesis. This parameter can be increased or decreased to scale overall production to match field-measured NPP, without affecting any of the interacting processes that the model captures in its algorithms: effects of N availability and foliar N on photosynthesis; effects of elevated CO<sub>2</sub> on photosynthesis; effects of changing temperature or precipitation on photosynthesis and NPP.

## **Step 5: Examine N mineralization and forest floor mass**

The flux of annual, net N mineralization is another central flux in the model, both driving, and driven by, foliar production and foliar-litter N concentration, in a strong system-level feedback. Modeled fluxes of annual, net N mineralization do not always agree well with field measurements using the buried-bag technique. Some disagreement is acceptable (because in reality the vegetation may be drawing on a pool of available N that is not measured in the buried-bag technique, or this field technique may produce artifacts that result in over-estimation of N availability). At the same time, if modeled N mineralization is too low, vegetation production will be too low, because TRACE algorithms embody a strong N limitation for N-poor sites.

At this stage of model parameterization, forest floor mass should also lie in the approximately realistic range, but need not be precisely right. Forest-floor mass is less important than foliar production. If foliar and wood production are not in the approximately right range in the simulations, then re-examine the values for N inputs (present-day and historical), tissue N content, humus turnover rate, and vegetation parameters related to phenology and growth. If the forest floor mass is high, experiment with increasing the decay rate of humus; this could increase N mineralization and plant production. Once vegetation production does appear reasonable, proceed to the next step.

If TRACE still can not produce reasonable values for foliar production and wood production, it may be due to one of two problems. The first possible problem may be that the vegetation phenology is not working properly for the new site, so photosynthesis or water stress are not realistic in the model. In this case, unfortunately, fairly involved testing and debugging may be required. The second possible problem is that N inputs, together with N releases from existing soil organic pools in the early years of the simulation, may not be sufficient to produce realistic N cycling at the site. If this is the case, extra N inputs can be artificially and explicitly added using the **ExtraNinputs** variable in the Scenario input file. This is to be avoided if possible, because it limits the interpretation of model results. (See *Scenario files*, above, for more explanation; also see Step 8 below).

## **Step 6: Parameterize or calibrate DOM and POM leaching fluxes**

Leaching of DOM and POM (dissolved organic matter) from the forest floor is a significant set of processes in TRACE because this moves mass, C (as DOC and POC, dissolved and particulate organic C) and N (as DON and PON, dissolved and particulate organic N) out of the forest floor. This loss of organic-matter mass from the O horizon for DOM alone may amount to roughly 3-7% of the mass flux of foliar plus fine root litter inputs each year, and thus plays a role in the relationship between litter production, humification, humus turnover rate, and forest floor mass.

At this stage, given foliar production working reasonably well, rates of DOM leaching should be parameterized to match measured rates at the site, or if unmeasured, parameterized to reasonable estimates from comparable sites. The leaching rates are controlled by the parameters **ACIleach**, **ACSleach**, and **TEXleach**, which control DOM leaching relative to CO<sub>2</sub> mineralization as mass-loss processes in each of the C-class pools (Currie and Aber 1997). We recommend that you begin with the 3 parameter values from the Harvard Forest oak stand (if your vegetation is deciduous) or pine stand (if your vegetation is coniferous), then keep the relative proportions of the three parameters constant, as you scale the three up or down as a group, to produce reasonable fluxes of DOC losses from the O horizon at the site. An additional parameter, **OLscalar**, can be used to scale the O-horizon DOM (and thus DOC) leaching fluxes higher or lower, while preserving the relationships between **ACIleach**, **ACSleach**, and **TEXleach** for the forest type. **OLscalar** is a parameter in the Parameter input file, and can be changed interactively on the Parameter change form. Note that increasing the value of **OLscalar** is likely to decrease the value of forest floor (O horizon) mass, and alter the value of the forest floor (O horizon) ratio of C:N.

Once rates of DOM leaching have been parameterized, the value of **OPscalar** can be altered, to alter the rates of POM leaching from the forest floor. This parameter controls the relationship between DOM and POM leaching fluxes, and thus the amount of POM leaching once DOM leaching is set. The relationship between DOM and POM leaching is probably best left at its default value, or left as is for the forest type, unless it is necessary to increase or decrease the movement of C and N out of the forest floor to obtain realistic relationships among litter inputs, O horizon N mineralization, DOC leaching, and patterns of O horizon mass accumulation over time.

### **Step 7: Calibrate input rates of woody litter**

First, double-check that production of living wood through time is approximately right for the site. Second, ensure that any major harvests or disturbances such as fires, hurricanes, major mortality caused by insect defoliations, etc. are represented correctly in the Scenario input file, and show up as major drivers in the dynamics of woody debris pools when these pools are graphed. Third, assemble reasonable values, from relevant field studies, for pool sizes of living wood, standing dead wood, and downed woody debris for your site. These may be difficult to assemble as site-specific values, but it is important to have reasonable numbers to check against model results. Try to assemble values from a similar forest with a similar stand age and similar history if possible. In the case of downed woody debris, pool sizes will reflect not only the history of the current stand, but also the history of the previous forest stand at the site (Harmon et al. 1986, Currie and Nadelhoffer 2002). Assemble these values as best you can, using the TraceDataNeedsx.xls file to organize them.

Next, make your best estimates for the biomass pool sizes of woody pools, living and dead, in the initial year of the model run. For example, if the initial year of the model run will be 1901 (Baseyear% = 1900 in TRACE), and the forest dates to 1870, then estimate pool sizes for the 30-year old forest at the end of 1900. Again, for downed woody debris, the history of the land prior to that will have to be considered – whether it was in agriculture, or dated to a disturbance in 1870 that resulted in a large pool of downed woody debris. Estimate initialization-year pool sizes for WoodMass (living wood), SWD (standing dead wood), OFWD, OCWD, and BFWD. TraceDataNeedsx.xls contains spaces for recording most of these values and notes regarding how they were estimated. Enter all of these initial conditions in the Parameter file.

Now run TRACE and graph the woody biomass pools. Look at the relationship between living wood (WoodMass) and standing dead wood (SWD). Adjust the mortality of living wood to get a better relationship between these two if necessary. This is governed by the parameter **WoodTurnover**, which is read in from the Scenario input file, and can thus vary through the simulation. For example, if the forest was likely to have gone through a self-thinning phase from 1940 to 1970, the value of **WoodTurnover** could be increased for those three decades. While adjusting the value of this parameter, also keep a close eye on the sizes of woody debris pools in the present day because it is important that these be reproduced fairly well for the site. Still, it is most important to get the size of the living wood pool approximately right through time and in the present day; adjust the values of WoodTurnover through time to achieve that goal.

If the pool of living wood biomass now looks good, but pools of SWD, OCWD, and OFWD are either too high, too low, or have the wrong proportions, these can be altered by adjusting three parameters as follows. (1) The rates that SWD decays, via heterotrophic respiration and CO<sub>2</sub> mineralization prior to woody litterfall, will control both the size of the SWD pool and the rate of transfers (woody litterfall) to OCWD and OFWD. The decay of SWD is controlled by the parameter **WoodLitCloss** in the Parameter file. (2) The value of **WoodLitTrans**, also in the Parameter file, can be adjusted to control the rate of transfer of SWD to downed woody debris pools, and thus the proportions between standing dead and downed woody debris. (3) The parameter **FWDfrac**, in the Scenario file, will control the separation between FWD (< 10 cm diam.) and CWD (≥ 10 cm diam.) in woody litter inputs to the forest floor. This is in the Scenario file because it may be realistic to change the proportion of FWD vs. CWD inputs through time.

In summary, it is possible to reproduce good relationships through time, and in the present day, among pool sizes of living wood, standing dead wood, and downed woody debris in TRACE. Key starting points are (1) realistic rates of wood production, and (2) realistic estimates of pool sizes through time from relevant field data. The parameters described here can then be adjusted to achieve the required pool sizes and transfers. If little is known regarding pool sizes of woody debris at the site, default values from other site parameterizations may be used. Be aware that the pool sizes of standing dead and downed woody debris, however, contains potentially a large storage reservoir of C that is dynamic over the decadal and century time scale, and is likely to reflect the idiosyncrasies of the site history (Currie and Nadelhoffer 2002).

### **Step 8: Examine forest floor C:N ratio**

The mass ratio of C:N in the forest floor is a key indicator of ecosystem C and N cycling in forests (Gundersen et al. 1998, Currie 1999). This is reflected in the modeled ecosystem structure and function in TRACE; key model processes such as gross and net N mineralization and nitrification are sensitive to this ratio. As a result, it is important for the O-horizon C:N ratio to be modeled fairly realistically in TRACE.

If the C:N ratio is unrealistic in model simulations, several parameters or conditions can be re-examined. These include N inputs (present-day or historical), N concentrations in plant tissues, rates of woody litter inputs or woody litter pool sizes, humus and SOM decay rates, leaching rates of DOM from the forest floor, bioturbation (the partial mixing of O-horizon humus and mineral LSOM that takes place each month), and estimated pool sizes of C and N in the initial year of the model run (e.g. in the year 1900). This assumes foliar and fine root litter production are already modeled reasonably well for the site; if not, those should be examined. Because so many other modeled quantities impact the forest floor C:N ratio, testing and parameterization of the other quantities should be undertaken first. These other quantities should be re-examined, if the forest-floor C:N ratio is unrealistic, before proceeding to the next step.

In some cases, it is possible that all of the N inputs may be parameterized based on values in the literature, concentrations of N in litterfall tissues may be realistic in the model, and the land use history and initial conditions may be specified according to one's best understanding, yet still the forest floor is too N-poor and/or the forest-floor C:N ratio is too high. If this is the case,

forest N mineralization, foliar production, and wood production are likely to be too low, and this will have ramifications for many aspects of system functioning in TRACE. For this reason there is an additional N input flux, **ExtraNinput**, that can be included in the Scenario file as a monthly flux ( $\text{g N m}^{-2} \text{mo}^{-1}$ ) that can vary over time. This is meant to supply an explicit means of increasing N inputs when necessary to obtain realistic N cycling at the site, but when the source(s) for such input is unknown (see Scenario section for more details). Normally, the value of **ExtraNinput** should be zero, but it can be increased if necessary if all else fails to get the forest floor C:N ratio to approach a reasonable value. Obviously, if this feature is used to include inputs of N through unknown mechanisms, this should be stated in the description of modeling methods in a manuscript, and this strongly impacts the interpretations and conclusions that can be drawn from the modeling study or model-data comparisons.

### **Step 9: Final ecosystem-level calibration of C and N cycling (independent of $^{15}\text{N}$ )**

For this step, we have chosen a few final calibration parameters with the following characteristics: (a) they are known to show high sensitivity in C and N pools and fluxes; (b) they effect ecosystem-level processes in an integrated way; and (b) they are difficult to measure with precision in the field. If such a parameter can not be determined in the field to within 10%, and at the same time a 10% deviation causes very different model predictions in several integrated processes, then it lends justification to the calibration step. But in order to avoid progression toward non-falsifiability in the simulations, this final set should comprise only a small set of parameters that are chosen carefully. For the Harvard Forest oak and pine stands, Currie et al. (2004) used the following set of parameters:

<b>kho</b>	Decay constant for O-horizon humus (HOM)
<b>LSOMdec</b>	Ratio of rate of mineral LSOM decay to rate of HOM decay
<b>HSOMdec</b>	Ratio of rate of mineral HSOM decay to rate of LSOM decay
<b>OLscalar</b>	Scaling parameter to adjust rate of DOM leaching loss from O horizon
<b>OPscalar</b>	Scaling parameter to adjust rate of POM leaching loss from O horizon

We alter these parameters in order to achieve reasonable simulation of a pre-determined set of model results (**target variables**). For the target variables, we use a larger set of model results that are (a) physically meaningful, (b) indicative of whole-system behavior, and (c1) reasonable to infer from the literature or (c2) reasonable to compare against other models or our conceptual understanding of forest biogeochemistry. We adjust the above system-level calibration parameters to achieve reasonable overall results in this set of **target variables**:

- Annual net N mineralization (relative changes, not absolute numbers)
- Flux of foliar litterfall
- NPP of wood
- DOC leaching from the forest floor
- Total forest floor mass
- C:N ratio in the forest floor
- Foliar N concentration, root N concentration, wood N concentration

We do the full set of above parameterizations and calibrations *without examining  $^{15}\text{N}$  partitioning or redistributions in the model*. For each of the target variables listed above, the main goal is to ensure that coarse patterns over time, or differences among forest types or experimental treatments are captured with some realism. It is not necessary to calibrate the model to produce the precise values measured in field studies. This is particularly true in the case of net N mineralization, in which field results from the buried-bag technique are quite often outside of the range that causes other aspects of N cycling to be realistic in the model.

### **Step 10: Initial Model-data comparisons of $^{15}\text{N}$ recoveries**

TRACE is designed to allow, where feasible, direct model-data comparisons of the partitioning and temporal redistribution of  $^{15}\text{N}$  tracers in large-scale field studies. Model simulations or predictions can be compared with field data to analyze areas of agreement and disagreement, looking at patterns across forest types, field treatments, and isotope forms. Monte Carlo runs can be incorporated as a means of quantifying uncertainties in simulated values of  $PR^{15}\text{N}$  in soil and vegetation pools.

Once our parameterizations and system-level calibrations of coarse-scale C and N cycling are complete, we run TRACE to simulate or predict  $^{15}\text{N}$  recoveries in vegetation and soil pools on an annual timestep. We then make direct comparisons among model predictions and field results for  $^{15}\text{N}$  recoveries (typically scaled up from tissue and soil-core measurements, and converted to values of  $PR^{15}\text{N}$ , in an Excel spreadsheet). If there are multiple forest types, N-amendment treatments,  $\text{CO}_2$ -fumigation treatments, or multiple isotope forms used at a site, it is best to make model-data comparisons across the entire suite simultaneously. At the Harvard Forest, for example, we made model-data comparisons across the 8-factorial study (Nadelhoffer et al. 1999, Currie and Nadelhoffer 1999).

Patterns of agreement and disagreement among model results and field-study results can be analyzed at this stage. One of the goals at this stage is to use the model to help interpret the field-study results, and to use the comparisons to learn more, regarding system N-cycling behavior and C/N interactions, than investigators learned from the field study alone.

### **Step 11: Iterative model-data comparisons**

In the initial use of TRACE to help interpret initial (2-yr) field recoveries of  $^{15}\text{N}$  tracers at the Harvard Forest, Massachusetts, we conducted a set of iterative model-data comparisons in which three sets of model predictions were compared against soil and vegetation partitioning of  $^{15}\text{N}$  tracers (Currie et al. 1999). In that study, we proceeded by the following set of steps, which we believe could be effectively used by other researchers in some situations.

First, a comprehensive set of model-data comparisons of  $PR^{15}\text{N}$  was conducted, with areas of agreement and disagreement carefully interpreted. The next step was to search the literature to find likely areas where the model might be altered and re-tested. Next, a simple, clear, and independently justified change (or small set of changes) was made to the model structure or to a key parameter. Finally, the model was run again, and another set of model-data comparisons of

$PR^{15}N$  analyzed and interpreted. We called this 'iterative model-data comparisons'; it could also be termed a form of 'inverse modeling'.

If a substantial improvement in the patterns of model-data comparisons results, then several things may be accomplished through this process: (1) Insight may be gained into the ecosystem ecology and biogeochemistry of the system through the use of inverse modeling; and (2) the model may be improved in a way that can allow more robust subsequent extrapolations or simulations of integrative quantities of interest. (3) In addition, the changes can be tested at other sites or with future data from the same site.

In order to make the types of changes to the model structure that are required for the type of inverse modeling described here, it is probably necessary to work with the source code in Visual Basic.

## **Step 12: Modeling integrative quantities**

We refer to 'integrative quantities' as quantities that we are interested in analyzing, predicting, or extrapolating, that are not feasible to measure, but nonetheless important to estimate. These include quantities such as the weighted C:N ratio of N retention in a forest, or marginal C storage per unit marginal N deposition in forests, or the residence time of C stored through elevated N deposition.

Models such as TRACE can provide estimates of such integrative quantities. If the model results are not testable, then the simulations are not falsifiable, and thus have limited claim to be considered traditional scientific hypotheses. At the same time, indirect estimates or best-available calculations of certain quantities are useful to science and to society.

A strength of our methodology is that it allows direct testing of  $^{15}N$  redistributions in a manner that is falsifiable, and which provides us with the ability to gauge our confidence in the N cycling and C/N interactions in the model. After the model has been tested, or after an inverse-modeling analysis has been used to improve the model across treatments or sites, we propose that it is fruitful and useful to apply the model to simulate integrative quantities. Indeed, ecosystem models that are testable at multiple levels of organization (fine-scale to ecosystem-scale) may be our most well-advised means of estimating integrative quantities that are not measurable or testable. Some examples follow.

### ***Weighted C:N ratios of N retention***

A set of integrative quantities that it may be useful to print include the weighted C:N ratios of N retention. These model results essentially allow the user to follow the overall, weighted C:N ratio of all of the pools retaining the  $^{15}N$  tracer over time. For example, if the  $^{15}N$  tracer is retained initially in pools with a narrow C:N ratio (e.g. humus in the O horizon), the weighted C:N ratio of retention would initially be narrow; if, over time, the  $^{15}N$  tracer moves into pools with wide C:N ratios (such as living wood and dead wood), the weighted C:N ratio of retention of the  $^{15}N$  tracer will then grow over time. This is a useful and interesting index of the potential (upper-limit) effect of N deposition, in the year of the tracer addition, on changes in ecosystem

C balance through time. The calculation is made possible by the algorithms in TRACE that model the  $^{15}\text{N}$  tracer redistributions and recoveries.

Calculation of the weighted C:N ratio of N retention is done in the month *Plotmo*, and makes use of the following:

- (a) C:N ratio of each pool, in this month. These are stored in the array **MidYrPoolCN(n)**;
- (b)  $PR^{15}\text{N}$  in each pool, in this month (all calculated above);
- (c) Weighted C:N ratios of  $^{15}\text{N}$  retention for various combination pools, meaning  $PR^{15}\text{N}$  of each pool used to weight the C:N ratios of those pools. These weighted C:N ratios of combined pools can be printed together with  $PR^{15}\text{N}$  of the same combined pools. The results of these calculations are stored in **WtdCNtracReten(n)**,  $n = 1$  to 4;
- (d) An overall weighted C:N ratio of  $^{15}\text{N}$  retention, calculated as in (c) for combined pools, where the combined pool here is the whole ecosystem. Stored in **WtdCNtracReten(5)**.

Notes:

**VascN** is assumed stored as amino acids, C:N mass ratio = 2.8:1

Available N, i.e. **NH<sub>4</sub>** and **NO<sub>3</sub>** pools, figured in combined pools as C:N = 0.

## *N flux analysis*

The theory behind the calculations of  $PR^{15}\text{N}$ , percent recovery of  $^{15}\text{N}$  tracers, is defined for recovery of  $^{15}\text{N}$  in ecosystem pools at a point in time. However, it may shed light on N fluxes in the system if N fluxes are expressed in the  $PR^{15}\text{N}$  notation (Currie and Nadelhoffer 1999). In essence, each annual redistribution *flux* of the  $^{15}\text{N}$  tracer that was added in a particular year or years, is quantified in subsequent years. In other words, if the  $^{15}\text{N}$  tracer was applied in 1991, we can analyze what portion of this tracer was taken up by plants in 1992, then in 1993, etc. These should be interpreted carefully. To the extent that  $^{15}\text{N}$  is recycled within an annual period, for example, the sum of  $PR^{15}\text{N}$  fluxes will sum to greater than 100%.

In TRACE, fluxes of N expressed as  $PR^{15}\text{N}$  are stored in the array **NFA(n)**, for "N Flux Analysis." These are defined and calculated as follows, where the numbers refer to the index (n) in this data array:

- 1: Plant uptake from O horizon
- 2: Plant uptake from M horizon
- 3: humification flux from all detrital pools in O horizon
- 4: humification flux from all detrital pools in M horizon
- 5: foliar litter N flux to O horizon
- 6: fine root litter N flux to O horizon
- 7: fine root litter N flux to M horizon
- 8: Net N flux annually from avail. N pools into nonwoody litter in O -- i.e. net assimilation in nonwoody in O.
- 9: Net N flux annually from avail. N pools into humus in O; i.e. net result of direct assimilation minus mineralization in O horizon humified organic matter.

10: Net N flux annually from avail. N pools into LSON + HSON; i.e. net result of direct assimilation minus mineralization in combined mineral soil pools of humified organic matter.

## V. More Information

Further information about TRACE is available from the web page of W. S. Currie (<http://sitemaker.umich.edu/currielab>). Further information is also available on the model, its submodels, and its applications in the following publications in the open scientific literature. (Many of these publications can also be downloaded as .pdf files from the web page).

## Publications

The following is an annotated list of TRACE publications, briefly describing the model use in each paper:

Currie, W. S., K. J. Nadelhoffer and J. D. Aber. 1999. Soil detrital processes controlling the movement of  $^{15}\text{N}$  tracers to forest vegetation. *Ecol. Appl.* 9, 87-102.

*This was the first use of TRACE in the literature and is often cited for basic reference to the model. This paper provides detailed equations regarding gross and net soil N dynamics in the model, and focused on 1-2 yr plant-soil partitioning of  $^{15}\text{N}$  following field application of tracers. Field sites were Harvard Forest mixed oak and red pine stands, under ambient and N-amended conditions.*

Currie, W. S. and K. N. Nadelhoffer. 1999. Dynamic redistribution of isotopically labelled cohorts of nitrogen inputs in two temperate forests. *Ecosystems* 2, 4-18.

*Examined time series in  $^{15}\text{N}$  tracer redistributions over the 4-yr time scale at the Harvard Forest.*

Currie, W. S. and J. D. Aber. 1997. Modeling leaching as a decomposition process in humid, montane forests. *Ecology* 78, 1844-1860.

*Developed the DocMod model (Dissolved Organic Carbon Model), which linked fine litter decay, humification, and leaching of DOC and DON (dissolved organic N) for deciduous and coniferous forests across a heterogeneous landscape. The decomposition submodel in trace was developed from DocMod principles.*

Moorhead, D. L., W. S. Currie, E. B. Rastetter, W. J. Parton and M. E. Harmon. 1999. Climate and litter quality controls on decomposition: an analysis of modeling approaches. *Global Biogeochemical Cycles* 13, 575-589.

*A blind model-data comparison and cross-model comparison involving four decomposition models (one of which was DocMod), in which predictions were tested against 2-yr time courses of litter decay in four biomes (temperate forest, arctic tundra, tropical forest, and desert) from the LIDET study (LTER Intersite Decomposition Experiment Team).*

## Fair use guidelines and citing TRACE

Yanai, R. D., W. S. Currie and C. L. Goodale. 2003. Soil carbon dynamics following forest harvest: an ecosystem paradigm reconsidered. *Ecosystems* 6:197-212.

*A precursor to TRACE, a linked version of PnET and DocMod, was used to study processes of decomposition, production, and logging disturbance-induced soil mixing as contributing to patterns of organic-matter dynamics in the forest floors of New Hampshire through the 20<sup>th</sup> century.*

Currie, W. S. 2003. Relationships between C turnover and bioavailable energy fluxes in two temperate forest soils. *Global Change Biology* 9:919-929.

*Energy pools and fluxes were added to pools of fine litter, woody debris, and humus in TRACE, based on a calorimetry study of field samples from the Harvard Forest mixed oak and red pine stands. The model was then used to calculate rates of bioavailable energy dissipation by the heterotrophic communities in situ, and compare these with fluxes of C stabilization and mineralization.*

Currie, W. S., K. J. Nadelhoffer and J. D. Aber. 2004. Redistributions of <sup>15</sup>N highlight turnover and replenishment of mineral soil organic N as a long-term control on forest C balance. *Forest Ecology and Management* 196:109-127

*Included in a special issue on C and N studies at the Harvard Forest, this paper compares earlier TRACE predictions for 8-yr time series in <sup>15</sup>N redistributions with field data. TRACE is then used in an inverse-modeling analysis to explore changes to the structure of the soil C/N interactions that could better account for the time series observed across the 8-factorial field experiment. The final version is then used to forecast rates of ecosystem C storage and differences in ecosystem C storage between ambient and N-amended treatments.*

## Fair use guidelines and citing TRACE

Because TRACE has been supported by public funds in its development and applications, the model, including its algorithms and source code, are available to researchers and to the public. TRACE remains the intellectual property of W. S. Currie and others who have participated in its development. Many elements of the model code have derived from previous work or collaborative work by other scientists (including K. Nadelhoffer, J. Aber, A. Federer, C. Driscoll, S. Ollinger, and others), and remain the intellectual property of those individuals.

With proper citation and acknowledgment, the TRACE model may be used as a tool for scientific research or in other natural-resource applications. You should cite the publications in the open scientific literature that describe TRACE (Currie et al. 1999 *Ecol. Appl.* 9:87-102, Currie and Nadelhoffer 1999 *Ecosystems* 2:4-18, etc.). In your Acknowledgments section you should also acknowledge that you received a copy of the model.

If equations, algorithms, or any other short pieces of model code from TRACE are used, the source should be cited as the publications describing TRACE in the open scientific literature. If

## Contact information

the particular code elements derive from other models, especially PnET-CN, the appropriate literature describing the PnET-CN model should be cited.

If you would like to adapt or incorporate longer sections of code from TRACE into a separate model, you must likewise cite the open literature describing TRACE. In addition, you should contact W. S. Currie about possible participation in the adaptation process and to inquire whether intellectual ownership may belong to other collaborators.

You may not use TRACE or any part of the model algorithms or code for profit.

## Contact information

William S. Currie  
School of Natural Resources & Environment  
University of Michigan  
Dana Building, 440 Church Street  
Ann Arbor, MI 48109-1041

USA

Phone: 734-647-2453

Email: [wcurrie@umich.edu](mailto:wcurrie@umich.edu)

## Acknowledgments

The development and application of the TRACE model has received support from:

- The National Science Foundation Ecosystems Studies Program
- The USDA National Research Initiative Competitive Grants Program
- The USDA Forest Service NERC Cooperative
- The European Union, through the CENTER project

Many scientific collaborators have given their expertise to the development and use of this model or of elements incorporated into this model. These include John Aber, Christine Goodale, Per Gundersen, Knute Nadelhoffer, and Scott Ollinger. Many others, through testing or discussion of model characteristics, have contributed to improvements of the model. In particular, these include Gary Lovett, Steve Perakis, Patrick Schleppei, and Albert Tietema.

## References cited

- Aber, J. D. and C. A. Federer. 1992. A generalized, lumped-parameter model of photosynthesis, evapotranspiration and net primary production in temperate and boreal forest ecosystems. *Oecologia* 92, 463-474.
- Aber, J. D., C. A. McLaugherty and J. M. Melillo. 1984. Litter Decomposition in Wisconsin Forests - Mass Loss, Organic-chemical constituents and Nitrogen. School of Natural Resc. College of Agricultural and Life Sciences, U of Wisconsin - Madison.
- Aber, J. D., J. M. Melillo and C. A. McLaugherty. 1990. Predicting long-term patterns of mass loss, nitrogen dynamics, and soil organic matter formation from initial fine litter chemistry in temperate forest ecosystems. *Can. J. Bot.* 68, 2201-2208.
- Aber, J. D., A. Magill, R. Boone, J. M. Melillo, P. Steudler and R. Bowden. 1993. Plant and soil responses to three years of chronic nitrogen additions at the Harvard Forest, Massachusetts. *Ecol. Appl.* 3, 156-166.
- Aber, J. D., P. B. Reich and M. L. Goulden. 1996. Extrapolating leaf CO<sub>2</sub> exchange to the canopy: A generalized model of forest photosynthesis compared with measurements by eddy correlation. *Oecologia* 106, 257-265.
- Aber, J. D., S. V. Ollinger and C. T. Driscoll. 1997. Modeling nitrogen saturation in forest ecosystems in response to land use and nitrogen deposition. *Ecol. Modelling* 101, 61-78.
- Aber, J. D., W. H. McDowell, K. J. Nadelhoffer, A. Magill, G. Bernston, M. Kamakea, S. G. McNulty, W. Currie, L. Rustad and I. Fernandez. 1998. Nitrogen saturation in temperate forest ecosystems: hypotheses revisited. *Biosci.* 48, 921-934.
- Berg, B. 1986. Nutrient release from litter and humus in coniferous forest soils -- a mini review. *Scand. J. For. Res.* 1, 359-369.
- Berg, B. and H. Staaf. 1980. Decomposition rate and chemical changes of Scots pine needle litter. II. Influence of chemical composition. *Ecol. Bull.* 32, 373-390.
- Berg, B., M. P. Berg, P. Bottner, E. Box, A. Breymeyer, R. Calvo de Anta, M. Couteaux, A. Escudero, A. Gallardo, W. Krantz, M. Madeira, E. Mälkönen, C. McLaugherty, V. Meentemeyer, F. Munoz, P. Piussi, J. Remacle and A. Virzo de Santo. 1993. Litter mass loss rates in pine forests of Europe and Eastern United States: some relationships with climate and litter quality. *Biogeochemistry* 20, 127-159.
- Berntson, G. M. and J. D. Aber. 2000. Fast nitrate immobilization in N saturated temperate forest soils. *Soil Biol. Biochem.* 32, 151-156.

## References cited

- Coleman, D. C. and D. A. J. Crossley. 1996. *Fundamentals of Soil Ecology*. San Diego: Academic Press. 205 pp.
- Cronan, C. S. 1985. Comparative effects of precipitation acidity in three forest soils: Carbon cycling responses. *Plant Soil* 88, 101-112.
- Currie, W. S. 1999. The responsive C and N biogeochemistry of the temperate forest floor. *TREE* 14, 316-320.
- Currie, W. S. 2003. Relationships between carbon turnover and bioavailable energy fluxes in two temperate forest soils. *Global Change Biology* 9:919-929.
- Currie, W. S. and J. D. Aber. 1997. Modeling leaching as a decomposition process in humid, montane forests. *Ecology* 78, 1844-1860.
- Currie, W. S. and K. J. Nadelhoffer. 2002. The imprint of land use history: Patterns of carbon and nitrogen in downed woody debris at the Harvard Forest. *Ecosystems* 5, 446-460.
- Currie, W. S. and K. N. Nadelhoffer. 1999. Dynamic redistribution of isotopically labelled cohorts of nitrogen inputs in two temperate forests. *Ecosystems* 2, 4-18.
- Currie, W. S., K. J. Nadelhoffer and J. D. Aber. 1999. Soil detrital processes controlling the movement of <sup>15</sup>N tracers to forest vegetation. *Ecol. Appl.* 9, 87-102.
- Currie, W. S., K. J. Nadelhoffer and B. Colman. 2002. Long-term movement of <sup>15</sup>N tracers into fine woody debris under chronically elevated N inputs. *Plant Soil* 238, 313-323.
- Fahey, T. J., J. W. Hughes, M. Pu and M. A. Arthur. 1988. Root decomposition and nutrient flux following whole-tree harvest of northern hardwood forest. *Forest Sci.* 34, 744-768.
- Gholz, H. L., D. A. Wedin, S. M. Smitherman, M. E. Harmon and W. J. Parton. 2000. Long-term dynamics of pine and hardwood litter in contrasting environments: toward a global model of decomposition. *Global Change Biology* 6, 751-765.
- Gosz, J. R., G. E. Likens and F. H. Bormann. 1973. Nutrient release from decomposing leaf and branch litter in the Hubbard Brook Forest, New Hampshire. *Ecol. Mon.* 43, 173-191.
- Gundersen, P., B. A. Emmett, O. J. Kjönaas, C. J. Koopmans and A. Tietema. 1998. Impacts of nitrogen deposition on nitrogen cycling: a synthesis. *For. Ecol. Manage.* 101, 37-55.
- Harmon, M. E., J. F. Franklin, F. J. Swanson, P. Sollins, S. V. Gregory, J. D. Lattin, N. H. Anderson, S. P. Cline, N. G. Aumen, J. R. Sedell, G. W. Lienkaemper, K. J. Cromack and K. W. Cummins. 1986. Ecology of coarse woody debris in temperate ecosystems. *Adv. Ecol. Res.* 15, 133-302.
- Magill, A. H., J. D. Aber, J. J. Hendricks, R. D. Bowden, J. M. Melillo and P. A. Steudler. 1997. Biogeochemical response of forest ecosystems to simulated chronic nitrogen deposition. *Ecol. Appl.* 7, 402-415.

## References cited

- Magill, A. H., J. D. Aber, G. M. Berntson, W. H. McDowell, K. J. Nadelhoffer, J. M. Melillo and P. Steudler. 2000. Long-term nitrogen additions and nitrogen saturation in two temperate forests. *Ecosystems* 3, 238-253.
- McClaugherty, C. A. 1983. Soluble polyphenols and carbohydrates in throughfall and leaf litter decomposition. *Acta Oecologia / Oecol. Gener.* 4(4), 375-385.
- McClaugherty, C. and B. Berg. 1987. Cellulose, lignin and nitrogen concentrations as rate regulating factors in late stages of forest litter decomposition. *Pedobiologia* 30, 101-112.
- McClaugherty, C. A., J. Pastor, J. D. Aber and J. M. Melillo. 1985. Forest litter decomposition in relation to soil nitrogen dynamics and litter quality. *Ecology* 66, 266-275.
- Meentemeyer, V. 1978. Macroclimate and lignin control of litter decomposition rates. *Ecology* 59, 465-472.
- Melillo, J. M., J. D. Aber and J. F. Muratore. 1982. Nitrogen and lignin control of hardwood leaf litter decomposition dynamics. *Ecology* 63, 621-626.
- Melillo, J. M., J. D. Aber, A. E. Linkins, A. Ricca, B. Fry and K. J. Nadelhoffer. 1989. Carbon and nitrogen dynamics along the decay continuum: plant litter to soil organic matter. *Plant Soil* 115, 189-198.
- Moorhead, D. L., W. S. Currie, E. B. Rastetter, W. J. Parton and M. E. Harmon. 1999. Climate and litter quality controls on decomposition: an analysis of modeling approaches. *Global Biogeochemical Cycles* 13, 575-589.
- Nadelhoffer, K. J., A. F. Bouwman, M. Delaney, J. M. Melillo, W. Schäfer, M. C. Scholes, R. J. Scholes, C. Sonntag, W. G. Sunda, E. Veldkamp and E. B. Welch. 1995. Group Report: Effects of climate change and human perturbations on interactions between nonliving organic matter and nutrients. In: Zepp, R. G. and C. Sonntag (Eds.) *Role of Nonliving Organic Matter in the Earth's Carbon Cycle*. New York: John Wiley & Sons Ltd. 227-256.
- Nadelhoffer, K. J., M. Downs and B. Fry. 1999. Sinks for <sup>15</sup>N-enriched additions to an oak forest and a red pine plantation. *Ecol. Appl.* 9, 72-86.
- Ollinger, S. V., J. D. Aber, G. M. Lovett, S. E. Millham and R. G. Lathrop. 1993. A spatial model of atmospheric deposition for the northeastern U.S. *Ecol. Appl.* 3, 459-472.
- Ollinger, S. V., J. D. Aber, P. B. Reich and R. J. Freuder. 2002. Interactive effects of nitrogen deposition, tropospheric ozone, elevated CO<sub>2</sub>, and land use history on the carbon dynamics of Northern Hardwood forests. *Global Change Biology* 8, 545-562.
- Olson, J. S. 1963. Energy storage and the balance of producers and decomposers in ecological systems. *Ecology* 44, 322-331.

## References cited

- Preston, C. M., J. A. Trofymow, B. G. Sayer and J. Niu. 1997.  $^{13}\text{C}$  nuclear magnetic resonance spectroscopy with cross-polarization and magic-angle spinning investigation of the proximate-analysis fractions used to assess litter quality in decomposition studies. *Can. J. Bot.* 75, 1601-1613.
- Ryan, M. G., J. M. Melillo and A. Ricca. 1990. A comparison of methods for determining proximate carbon fractions of forest litter. *Can. J. For. Res.* 20, 166-171.
- Schlesinger, W. H. and M. M. Hasey. 1981. Decomposition of chaparral shrub foliage: losses of organic and inorganic constituents from deciduous and evergreen leaves. *Ecology* 62, 762-774.
- Schlesinger, W. H. and J. Lichter. 2001. Limited carbon storage in soil and litter of experimental forest plots under increased atmospheric  $\text{CO}_2$ . *Nature* 411, 466-469.
- Yanai, R. D., W. S. Currie, and C. L. Goodale. 2003. Soil carbon dynamics after forest harvest: an ecosystem paradigm reconsidered. *Ecosystems* 6:197-212.
- Yavitt, J. B. and T. Fahey. 1986. Litter decay and leaching from the forest floor in *Pinus contorta* (Lodgepole pine) ecosystems. *J. Ecol.* 74, 525-545.
- Zech, W. and I. Kögel-Knabner. 1994. Patterns and regulation of organic matter transformation in soils: litter decomposition and humification. In: Schulze, E.-D. (Ed.) *Flux Control in Biological Systems*. San Diego: Academic Press. 303-334.