How to use the NESIS software

The source code and a compiled version (NESIS.EXE) of the software have been provided. The compiled version of NESIS runs in Windows™ 2000 or XP. It requires two input files: a specification file and a file of data generated by the parent model. The software generates one output file in Microsoft EXCEL format. Samples of the two input files are provided. Because NESIS uses Microsoft EXCEL to create the output file Microsoft EXCEL must be installed on computer used to run NESIS.

Data file: The file containing data from the parent model must be a comma-delimited file in a column format. The first line of the file must have the names of the variables in each column. The second line of the file can contain any ancillary information about the variables like the associated units. This information is not used, but the line must be in the file. The remaining lines list the data in chronological order.

Data for the stocks and fluxes can appear in any column except column 1, which is reserved for time. The units for time in column 1 must be consistent with the time units used to express the flux rates. The file can also contain columns of data not used in the isotope simulation (e.g., you might have both C and N data in the same file, but can use only one at a time in the NESIS). Most of the data in the columns will be derived directly from the parent model. However, additional columns are likely to be needed to specify the isotopic signature of any flux into the system. Add these columns wherever it is most convenient. The signature of all incoming fluxes must be specified for each time step and can change through time.

We recommend that you build your data file in EXCEL and then save it as a comma-delimited text file with a "`.out`" suffix. The `NESIS` uses the "`.out`" suffix as its default for the data file.

Specification file: The specification file contains all the information needed by the software to calculate the isotope dynamics from the output of the parent model. The software expects a text file with a "`.spe`" suffix. The file will have a format similar to this:

23	number of columns in data file
0.0036765	standard isotope ratio for N
6	number of stocks
4 0	leaves (stock 1)
5 0	wood (stock 2)
6 0	roots (stock 3)
7 0	organic soil (stock 4)
8 0	mineral soil (stock 5)
9 0	available N (stock 6)
12	number of fluxes originating within the system
6 1 10 0	uptake to leaves (from stock 6 to stock 1)
1 4 11 0	leaf litter (from stock 1 to stock 4)
6 2 12 0	uptake to wood (from stock 6 to stock 2)
2 4 13 0	wood litter (from stock 2 to stock 4)
6 3 14 0	uptake to roots (from stock 6 to stock 3)

3 4 15 0 root litter (from stock 3 to stock 4)

4 6 16 0 N mineralization organic soil (from stock 4 to stock 6)

6 4 17 0 N immobilization organic soil (from stock 6 to stock 4)

5 6 18 0 N mineralization mineral soil (from stock 5 to stock 6)

4 5 19 0 organic soil to mineral soil flux (from stock 4 to stock 5)

5 5 20 0 DON loss (from stock 5 to outside of system)

6 6 21 0 DIN loss (from stock 6 to outside of system)

2 number of input fluxes to the system

6 2 22 N deposition (to stock 6)

4 3 23 N fixation (to stock 4)

Only the numbers to the left are important. Any comments you wish to add can be added on the right but must be preceded by at least one blank space or tab. Numbers should be separated by a space and all the expected numbers must be specified.

The first line of the file specifies the total number of columns in the data file. This includes both used and unused columns and the first column for time. For the example, there are 23 columns in the data file.

The second line specifies the ratio of the heavy to light isotope in the standard for the element you are simulating. For ^{13}C:^{12}C, this value is 0.0112372; for ^{15}N:^{14}N it is 0.0036765. The example is for N, so the N isotope ratio is specified.

The third line specifies the number of stocks of the element that are being simulated (***n***). There are six stocks in the example.

The next ***n*** lines specify the column and initial δ value for each stock, one stock per line. The stocks will be automatically numbered from 1 to ***n*** in the order they are listed. For the example, the data for stock 3 are listed in column 6 of the data file and the initial δ value for stock 3 is 0.

The next line specifies the number of simulated fluxes that originate from any of the simulated stocks (***m***). This includes fluxes from one stock to another and fluxes leaving the system from a stock. There are 12 fluxes in the example.

The next ***m*** lines specify the stock from which the flux originates, the stock to which the flux flows, the column in the data file where the flux rate is specified, and the isotopic discrimination associated with that flux. For fluxes that leave the system, the first two numbers on the line should both specify the stock from which the flux originates. Note that in the specification of these fluxes, the stock numbers, *not* the column numbers of those stocks, are used. The stocks are numbered by the `NESIS` in the order they are listed in the specification file. Thus, in the example above, stock 1 is found in column 4, stock 2 is found in column 5, etc.. For example, the fourth flux is from stock 2 to 4, its magnitude is found in data file column 13, and it has a fractionation of 0 associated with it.

The next line specifies the number of fluxes into the system originating from outside the system (***p***). There are two input fluxes in the example.

The next ***p*** lines specify the stock to which the flux flows, the column in the data file that specifies the flux rate, and the column in the data file that specifies the δ value for that flux. For example, the first input flux is into stock 6, the flux rate is listed in column 2, and the flux δ value is listed in column 22.

Running the simulator: Once the data and specification files have been created, the simulator is easily run. Double click on the NESIS.exe file in your windows explorer and a window will open with three edit boxes into which you can type the names and path for the three required files: a specification file, a data file, and a file for the NESIS results. Alternatively, if you click on the labels to the left of each edit box, a browse window will open that will allow point-and-click access to the appropriate files. The default suffixes used by the browse windows are ".spe", ".out", and ".xls" for the specification, data, and results file, respectively. Similar point-and-click access is also available through the "Files" option on the main menu.

Once the three files have been specified, the "RUN" button on the bottom of the window will become active. Click it and the button will become inactive again until the simulation is finished. Output can be viewed directly from within NESIS by clicking the "Output" option on the main menu. In the pull-down menu that appears, you can select either graphic output by selecting the "Chart" option or tabular output by selecting the "Table" option. All the variables from the data file will be listed along with the δ values for all the stocks and fluxes for which isotopic signatures were calculated in the simulator. The δ data will be labeled with a "del " followed by the name of the stock or flux as it was specified in the data file. To plot a graph, simply highlight the variables you want to plot and press the "update plot" button. The data can also be examined from outside the software in EXCEL. The output file you specified will open directly in EXCEL.