Frequently Asked Questions

General

What is NOM?

NOM is Natural Organic Matter, operationally defined as the non-living organic molecules found in the environment. Although living matter is composed largely of well-defined molecules (proteins, nucleic acids, lipids, sugars, cellulose... etc.), NOM is composed largely (>80%) of molecules of unknown structure. In spite of this, NOM has been extensively studied because it is ecologically and geochemically important and because it influences pollutant fate and transport in the environment.

What is the NOM Stochastic Synthesis Project?

The NOM Stochastic Synthesis Project is an NSF-funded effort to produce a computer model which simulates the environmental transformation of biomolecules into NOM and ultimately into new organisms or CO_2. The model should simulate chemical, photochemical and biochemical transformations, transport through soils, water and sediments, and feedback between organic matter and the microbial community. The model is founded on the representation of molecules as individual agents which interact in a random manner. The term stochastic synthesis thus refers to the manner in which NOM molecules are created from biomolecules. The NSF project (ITR/AP DEB 0113570) is funded by the Information Technology Research initiative and the Division of Environmental Biology, with principal investigators at the University of New Mexico (Steve Cabaniss), Notre Dame University (Greg Madey, Patricia Maurice), Kent State University (Laura Leff) and the University of North Carolina (Robert Wetzel) and collaborative support from the United States Geological Survey (Jerry Leenheer, Bob Wershaw).

What is the program AlphaStep?

AlphaStep is a Windows-based program which simulates the transformation of biological molecules into NOM and the eventual consumption/destruction of that NOM. AlphaStep simulates a variety of chemical and biological transformations in a well-mixed reactor, but does not model transport.

The program allows the user to control the input molecules (number and structure) and a variety of chemical (pH, dissolved oxygen), physical (light intensity, temperature) and biological (enzyme activities, microbial consumption) parameters. The program simulates transformations for a specified time period, and then allows the user to examine changes in aggregate parameters (elemental composition, molecular weight, percent aromaticity) of the entire mixture of molecules with time. The user may also examine the properties of individual molecules at the end of the simulation.

AlphaStep is limited to simple well-mixed systems, and so will not provide accurate simulations of the entire process of NOM evolution. However, it provides model results to be compared with simple experiments, and provides a basis for the reaction algorithms to be used in a more complete model incorporating transport and biological feedback loops.

How do I download the program AlphaStep?

David....?

How do I learn how to use AlphaStep?

When you unzip the file containing the current version of AlphaStep, you will also obtain the user's guide in pdf format, AlphaUser.pdf. Print and read this guide, and work through the tutorial before attempting your own simulations. Although AlphaStep contains some context-sensitive help, it is really not enough to allow you to use the program without the user guide.

How do I learn how AlphaStep works?

From a scientific perspective, the details of the simulation are given in a series of 'white papers' available as .pdf downloads from this site. The white papers are zipped together in a single downloadable file, and include

Definition — a statement of the problem- a framework for discussing what types of information, molecules, reactions, properties, etc. must be considered for a successful simulation

DataStruct — a description of the data structure being used to represent each molecule.

StartingNOM* — a brief description of the types of input molecules available, including their elemental and functional group compositions in Delphi format

ParameterList* — a list of the user-settable chemical, physical and biological parameters which control reaction rates in AlphaStep

ReactionList* — a list of the various chemical and biological transformations which can occur in AlphaStep, including the exact changes to each molecule and a short justification (with references, in some cases) of the kinetic parameters used to determine apparent rate constants

ProbabilityCalc — a discussion of how the apparent rate constants are calculated and how these constants are treated as probabilities in the stochastic reaction algorithm.

PropertyEst* — explains how various molecular properties- both individual and aggregate- are calculated within the program

The *-ed documents are highly recommended for anyone using the program. The DataStruct and ProbabilityCalc documents may be of interest to programmers trying to understand/modify the program code. The Definition document is a big-picture overview of the modeling problem.

From a programming perspective, the AlphaStep source code can be obtained from Steve Cabaniss (cabaniss@unm.edu). AlphaStep is coded in Borland Delphi version 6, and contains no proprietary source code. Although the GUI uses Borland and Steema VCL units w/o source code, all the actual simulation source code is available for your inspection.

Program Problems

AlphaStep.exe won't run on my computer.

AlphaStep has been tested on computers running Windows XP. If you have a different version of Windows or another operating system, you may be unable to run the program.

AlphaStep gives different results for replicate runs.

There are two possible problems here- the inherent randomness of a stochastic algorithm and the 'carry-over' of results from one simulation to another.

'Carry-over'- The AlphaStep program keeps all molecules in memory at the end of a simulation. If you simply press the 'Simulate' button after running a simulation, the new simulation will use the output of the last simulation as input. Of course the results will be quite different ! To avoid this and run a true replicate calculation, press the 'Create' button after the first simulation to place the designated set of input molecules into the simulation.

Inherent randomness- Since AlphaStep uses a stochastic algorithm, each run can have a different set of reactions even though all the inputs and reaction parameters are the same. In general, we expect that if the number of molecules is large, these differences will 'average out' over time and produce very similar aggregate properties even if the individual molecules have rather different structures. To obtain a true 'replicate' with exactly the same set of reactions, you must have a) identical input molecules, b) identical reaction parameters, and c) the same set of pseudo-random numbers. Use the 'Random Seed' field under 'Simulation Control' to ensure that the latter condition is met.