

Cabaniss, S.E., Univ. New Mexico, Albuquerque, USA cabaniss@unm.edu
Madey, G.R., Univ. Notre Dame, South Bend, USA gmadey@cse.nd.edu
Maurice, P.A., Univ. Notre Dame, South Bend, USA pmaurice@nd.edu
Leff, L.G., Kent State Univ., Kent, OH lleff@kent.edu

STOCHASTIC SIMULATION OF NOM FORMATION AND TRANSFORMATION IN SURFACE WATERS

The AlphaStep program simulates reactions of organic molecules in natural waters and sediments using a stochastic, agent-based algorithm. Molecules are defined by composition and reactivity, and react individually as a function of biogeochemical parameters, including temperature, light intensity, and enzyme activity. The composition of precursor molecules (proteins, tannins, lignin, etc.) and stoichiometries of reactions (hydrolyses, oxidation, etc.) are specified, but the composition of product molecules is not constrained- the program may produce known products (e.g., small peptides, acids) or molecules of unanticipated composition such as might be found in natural organic matter (NOM). Surface water simulations starting with biopolymer precursors produce molecular assemblages with elemental composition, molecular weight, acidity and polarity similar to NOM in 4-12 months. In the absence of sunlight and/or oxygen AlphaStep produces molecules which are larger and more aromatic on average. Exposure of “freshwater” NOM to sunlight for prolonged periods produces assemblages with properties more typical of marine NOM. Algorithms from this batch reaction program are being incorporated into a spatially-aware simulator available on the web at <http://tobit.cse.nd.edu:7777/nom/>

SS11 SS19 CS38 Modeling Approaches
Oral
Cabaniss, S.E.