Simulation of natural organic matter adsorption to soils: A preliminary report

Indiana Biocomplexity Symposium, Notre Dame, IN, April 2003

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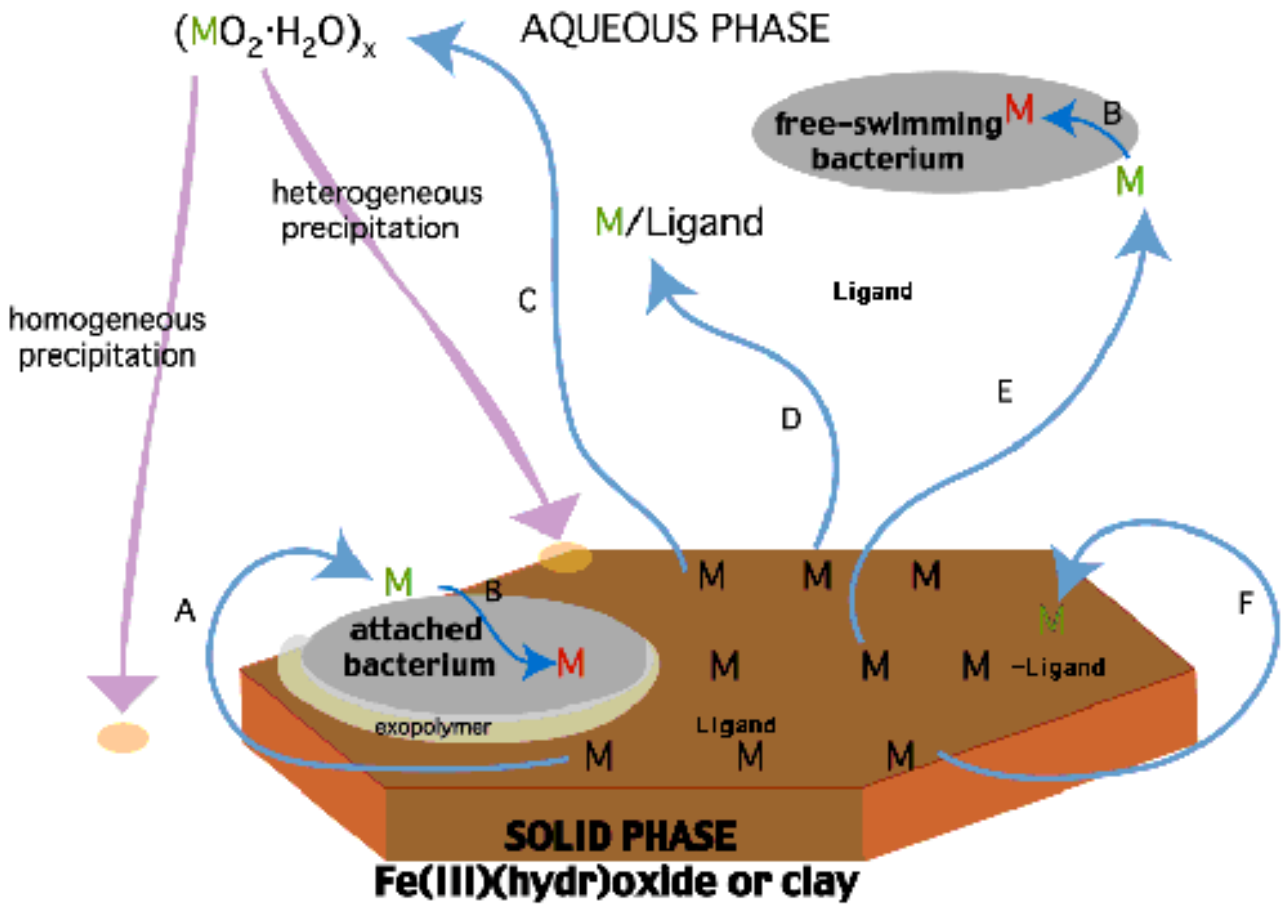
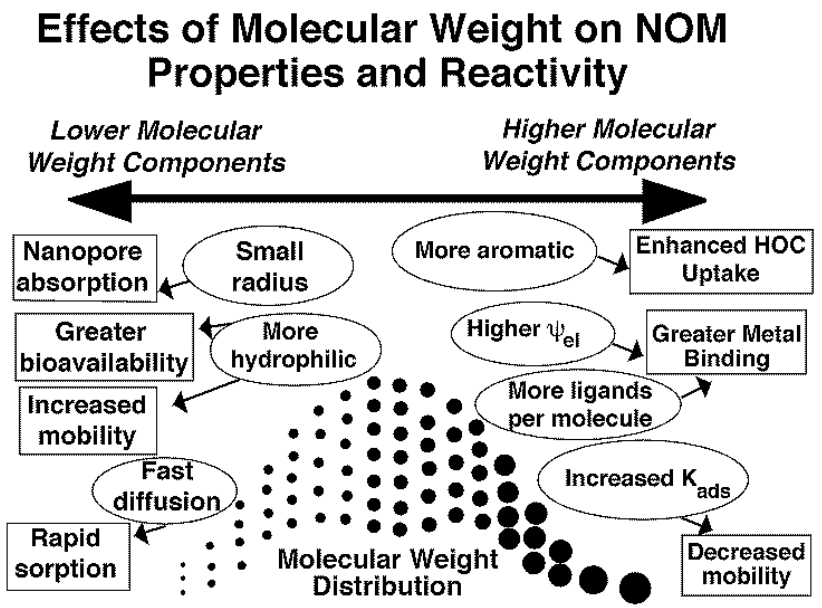
At the mineral-water interface, natural organic matter (ligands), metals, and bacteria undergo



Natural organic matter is a key component of soil biogeochemistry.

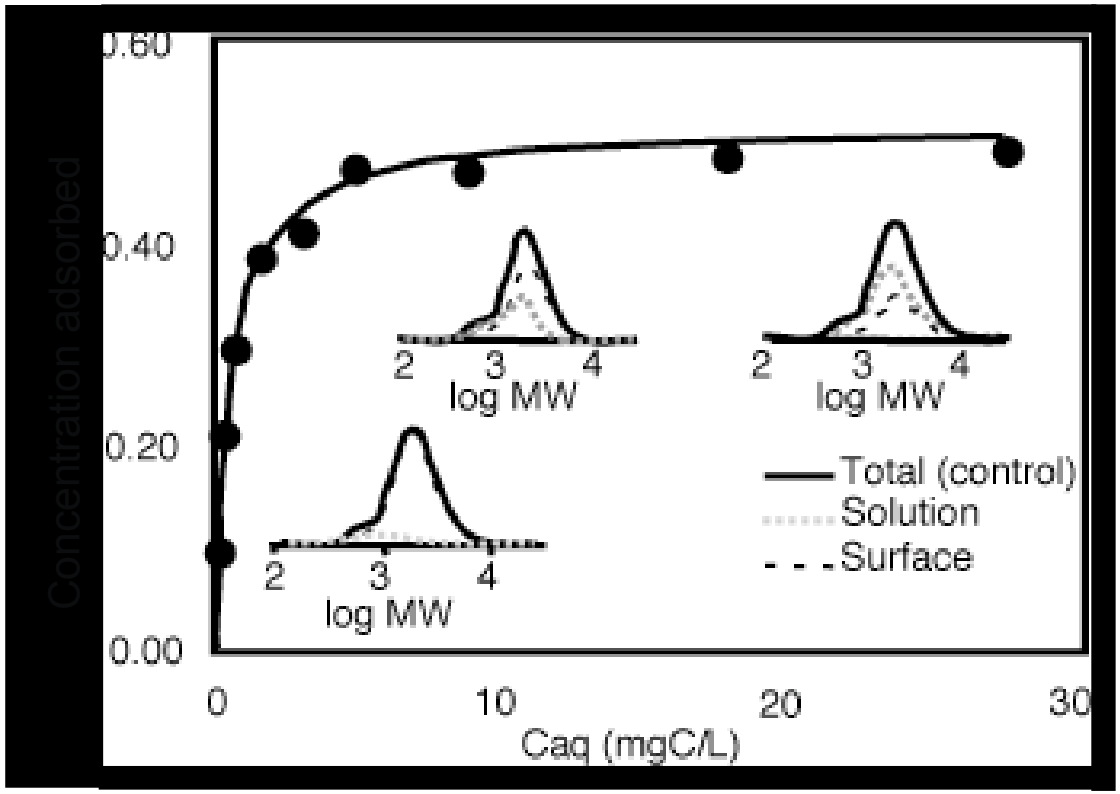
- Natural organic matter (NOM) forms primarily from the breakdown of organic debris, and it is ubiquitous in aquatic and terrestrial ecosystems.
- NOM helps to control the mobility and transport of trace metals, radionuclides, and organic pollutants.
- NOM is a primary source of C to microorganisms.
- The presence of NOM affects drinking-water remediation and treatment operations.

The molecular weight of NOM determines the reactivity of its polydisperse components.



High pressure size exclusion chromatography has shown that NOM has a log-normal distribution of molecular weight.

Adsorption experiments indicate preferential adsorption of higher molecular weight NOM components to mineral surfaces, leading to ‘sorptive fractionation.’



We are modeling results of field and laboratory research that demonstrate and describe this preferential adsorption and sorptive fractionation.

In order to model this process, we are using a computer program capable of stochastically simulating the adsorption of NOM components to soil.

The program is tentatively called the "NOM Simulator."

The NOM Simulator

- The NOM Simulator design is written in Java, based on J2EE architecture, and currently operates in a distributed cluster.
- The cluster processors run both Linux 8.0 and Windows 2000 operating systems.
- Three main components provide the basic structure for the NOM Simulator: a WEB interface, a core simulation engine, and a data analysis package.
- Various servers also contribute to the overall architecture, including a reports server and a data mining server.

Defining the System

- In order to utilize the NOM Simulator to model the preferential adsorption of higher molecular weight components and sorptive fractionation, we first had to define the system to be modeled.

- We modified the program for a constant input and variable output of the number of NOM molecules into and out of the system, with a set distribution of molecular weights defined by the user.

- We currently assume that the porous soil media is composed of high affinity goethite surfaces. Eventually, we'll model other surfaces such as quartz.

- We will modify the program so that larger molecules are represented by more than one cell.

- We are currently testing the simulator on the basis of elemental composition and molecular weight. In the future, we hope to run tests that incorporate molecules that contain a variety of functional groups.

Reaction Probability Equations

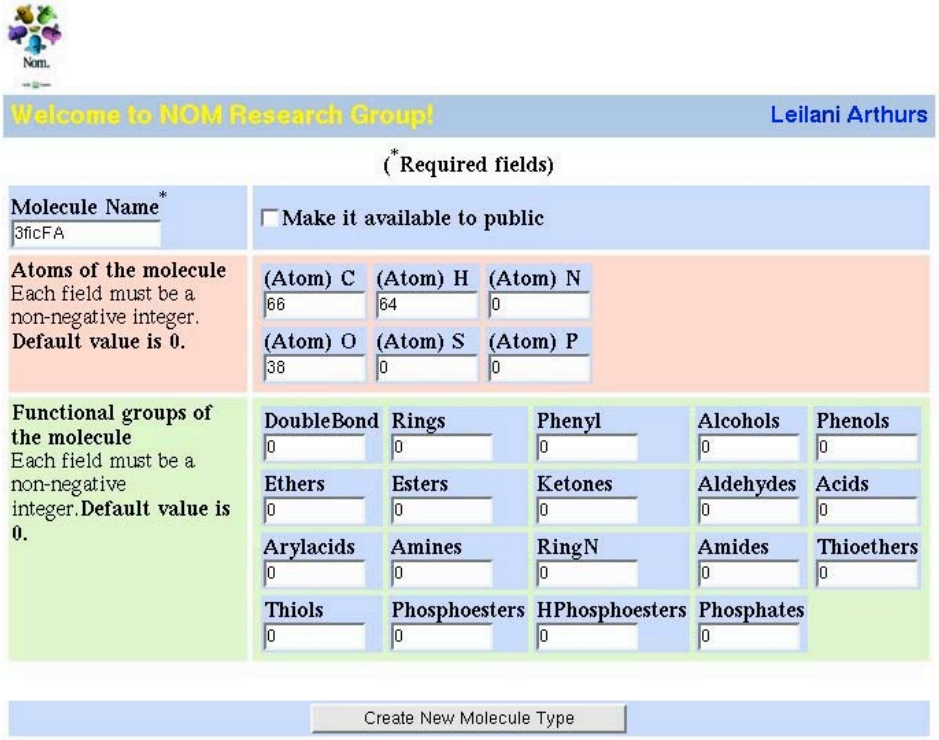
In order to utilize the NOM Simulator to model the preferential adsorption of higher molecular weight NOM components and sorptive fractionation, we first had to formulate appropriate equations to define the probability of these reactions. We are currently using the following equations:

$$P_{adsorb} = C \times \Delta t \times \frac{1}{MW} \times \frac{3}{pH}$$

$$P_{desorb} = C \times \Delta t \times \frac{1}{MW} \times \frac{pH}{3}$$

Testing NOM Simulator

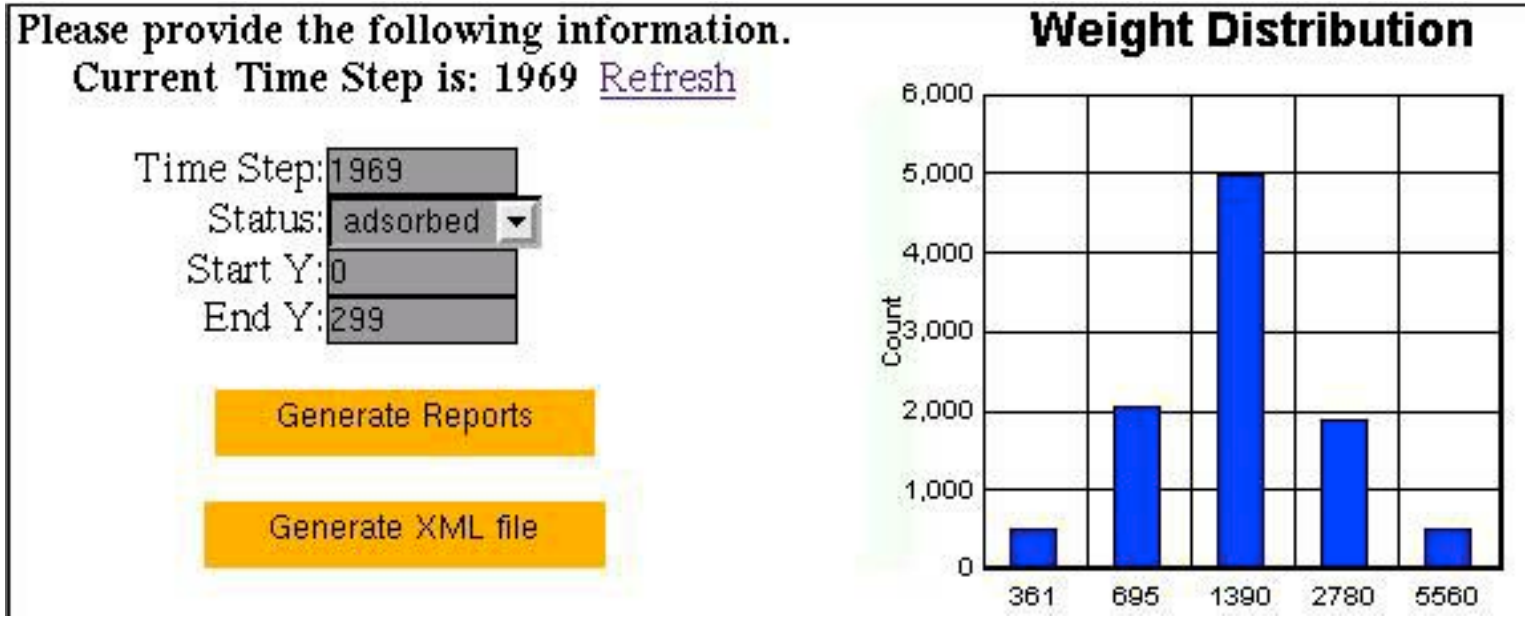
- We are now in the process of testing and concurrently modifying the NOM Simulator so that it illustrates expected trends via desired outputs and results.



Example of an input file.

Desired Outputs & Results

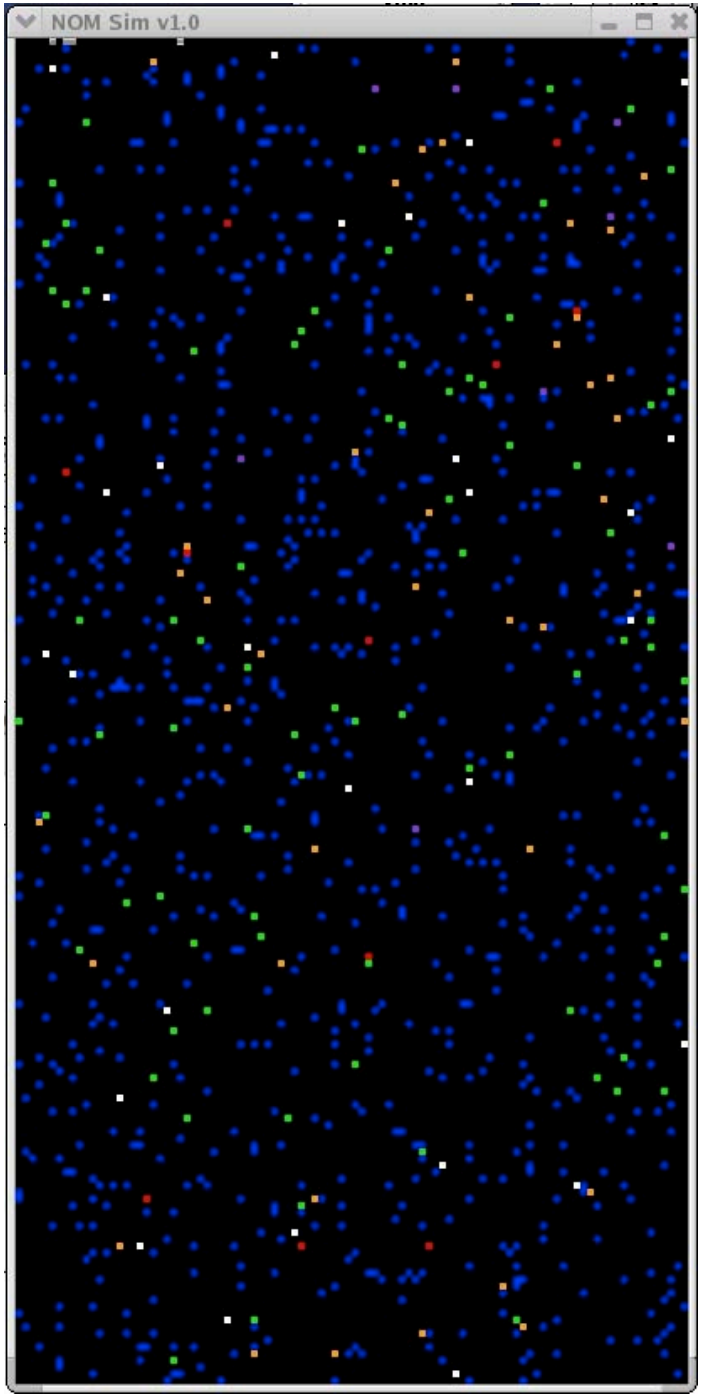
- Fractionation vs. time of NOM adsorbed
- Fractionation vs. time of NOM in solution
- Fractionation vs. space of NOM adsorbed
- Fractionation vs. space of NOM in solution
- Isotherms



Example of an output file.

Graphic Simulation

- This image is a screen capture of our GUI simulation that models NOM transport through, sorption to, and desorption from soil surfaces.
- Blue represents NOM particles moving in water flowing through the soil medium (representd by black).
- Different colors represent sorbed molecules of different molecular weights.



ACKNOWLEDGEMENTS

- Center for Environmental Science and Technology and Environmental Molecular Science Institute at the University of Notre Dame
- National Science Foundation (Information Technology Research and Hydrologic Science Division)