

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

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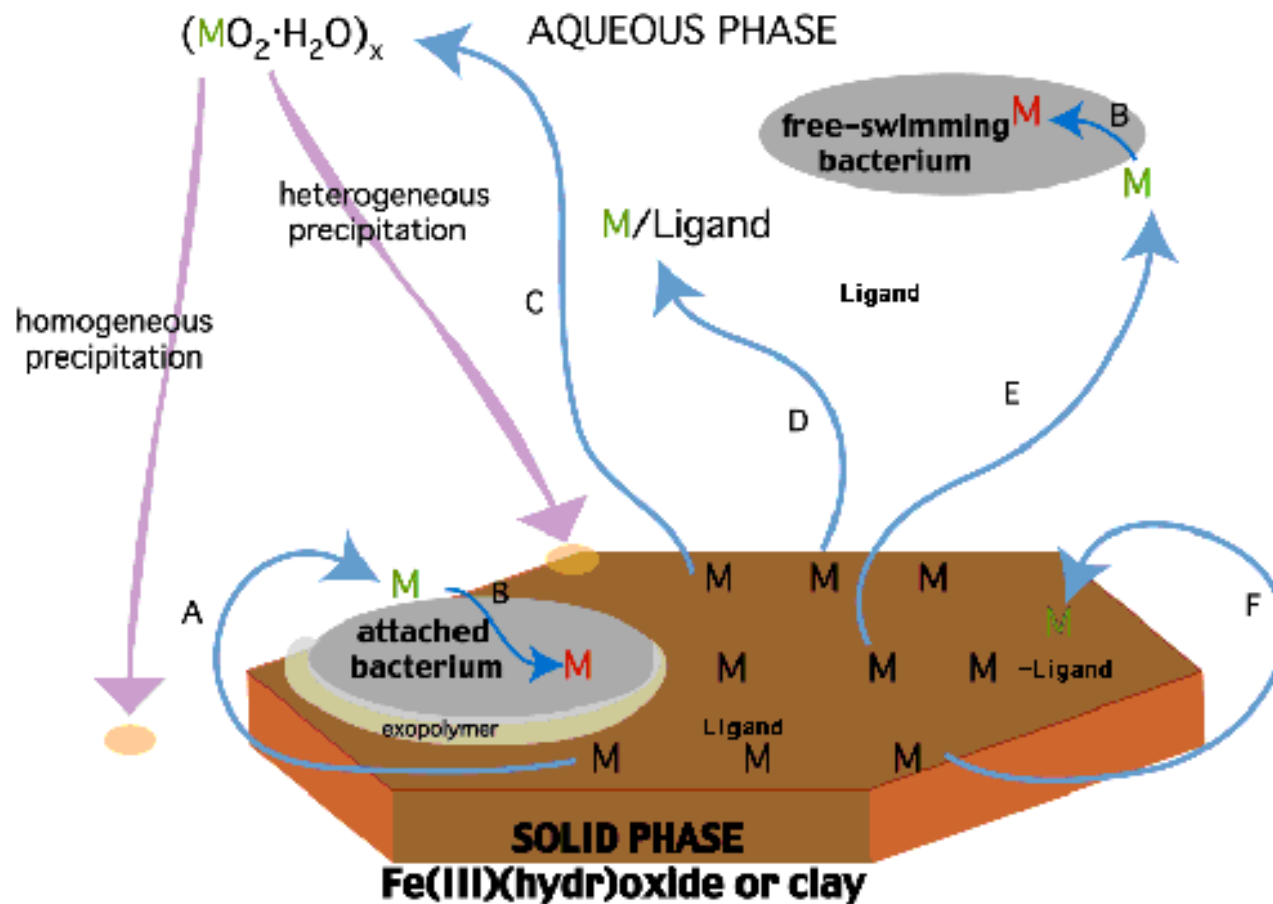
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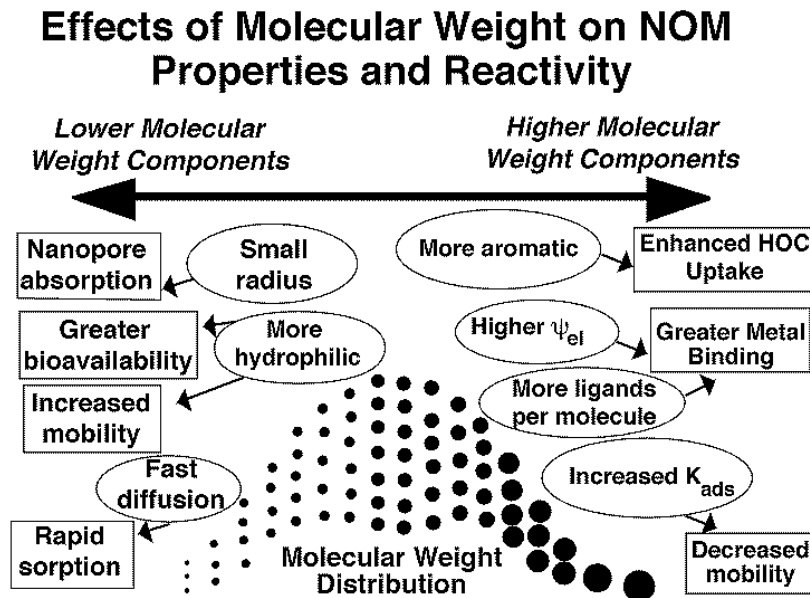
At the mineral-water interface, natural organic matter (ligands), metals, and bacteria undergo



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.

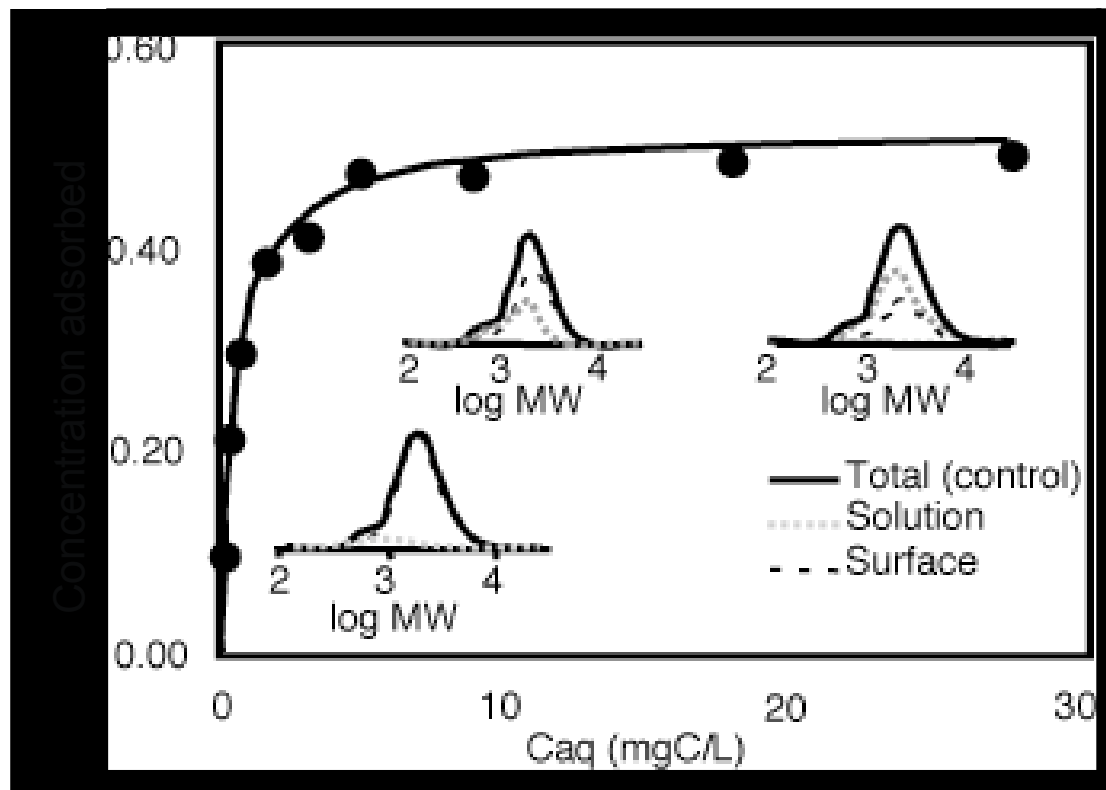
The molecular weight of NOM determines the reactivity of its polydisperse components.



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

‘sorpative 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

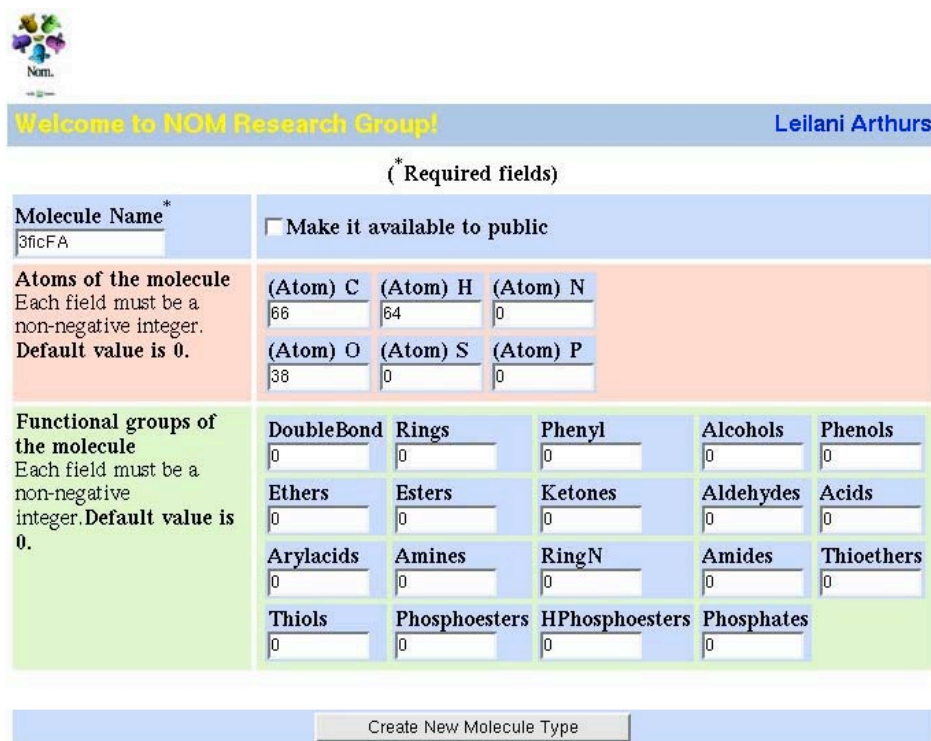
In order to utilize the NOM Simulator to model the preferential adsorption of higher molecular weight NOM components and sorptive fractionation, we first had to formulate appropriate equations to define the probability of these reactions. We are currently using the following equations:

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

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

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.



The screenshot shows the NOM Simulator input interface. At the top left is a logo with the text 'Nom.'. A blue header bar contains 'Welcome to NOM Research Group!' on the left and 'Leilani Arthurs' on the right. Below the header, a note indicates '* (Required fields)'. The form is divided into several sections:

- Molecule Name***: A text input field containing '3ficFA'. To its right is a checkbox labeled 'Make it available to public'.
- Atoms of the molecule**: A section with a light orange background. It contains a text input field with '66' for '(Atom) C', '64' for '(Atom) H', and '0' for '(Atom) N'. Below these are fields for '(Atom) O' (38), '(Atom) S' (0), and '(Atom) P' (0). A note states: 'Each field must be a non-negative integer. Default value is 0.'
- Functional groups of the molecule**: A section with a light green background. It contains a grid of input fields for various functional groups: DoubleBond, Rings, Phenyl, Alcohols, Phenols, Ethers, Esters, Ketones, Aldehydes, Acids, Arylacids, Amines, RingN, Amides, Thioethers, Thiols, Phosphoesters, HPhosphoesters, and Phosphates. Each field contains the number '0'. A note states: 'Each field must be a non-negative integer. Default value is 0.'

At the bottom of the form is a button labeled 'Create New Molecule Type'.

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

Please provide the following information.

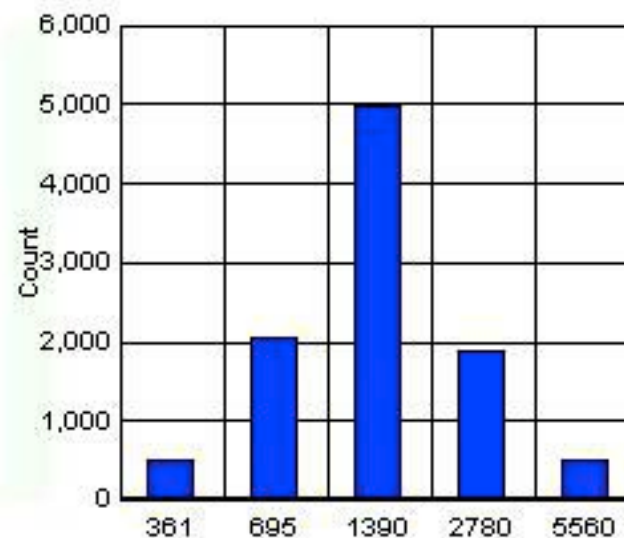
Current Time Step is: 1969 [Refresh](#)

Time Step: 1969
Status: adsorbed
Start Y: 0
End Y: 299

Generate Reports

Generate XML file

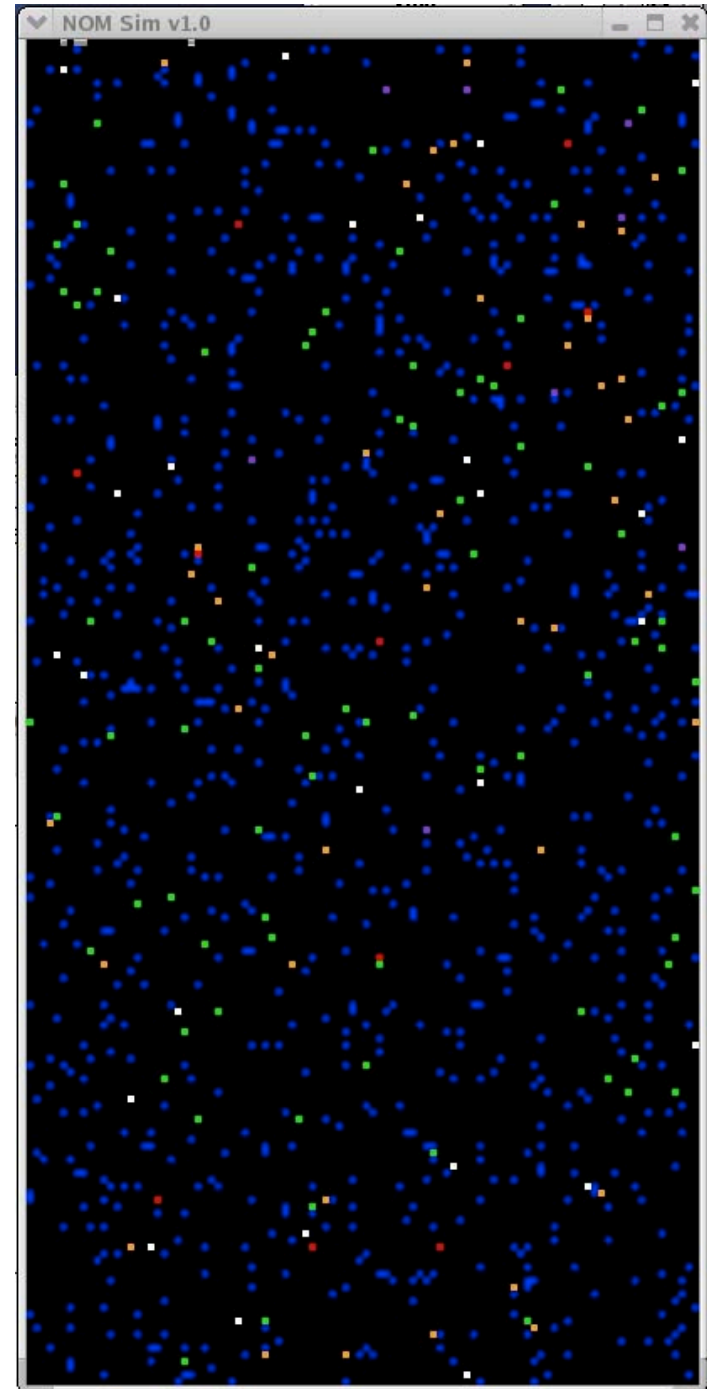
Weight Distribution



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 (represented by black).
- Different colors represent sorbed molecules of different molecular weights.



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