Researchers study role of natural organic matter in environment

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The decomposition of plant, animal and microbial material in soil and water produces a variety of complex organic molecules, collectively called natural organic matter. These compounds play many important roles in the environment.

By studying the molecular mechanisms responsible for the complex behavior of natural organic matter, researchers at the University of Illinois at Urbana-Champaign are finding new ways to prevent the compounds from fouling water purification and desalination facilities.

Natural organic matter is ubiquitous in soils, waters and sediments. In agriculture, natural organic matter is important because of its positive effects on the structure, water retention and nutrient properties of soils.

Natural organic matter also interacts with metal ions and minerals to form complexes of widely differing chemical and biological nature. Solubility, mobility and toxicity of many trace metals are strongly correlated with the concentration of natural organic matter in soil and water.

Natural organic matter creates problems for the water supply industry, however, requiring removal to minimize water color and giving rise to potentially harmful chemical byproducts as a result of chlorination. Through a process called "bio-fouling," natural organic matter is also a major culprit in degrading the performance of membrane filtration systems used for water purification and desalination.

However persistent and universal natural organic matter molecules are in the environment, they are little understood. Natural organic matter has no unique structure or composition, cannot be crystallized and is extremely difficult to characterize.

Illinois researcher Andrey Kalinichev and geology professor James Kirkpatrick have used computer simulations and nuclear magnetic resonance spectroscopy to investigate some of the factors that contribute to the complex behavior of dissolved natural organic matter. They will present their findings at the American Geophysical Union meeting in San Francisco, Dec. 11-15. A paper reporting their findings has been accepted for publication in the European Journal of Soil Science.

"Bio-fouling is one of the most important problems in developing advanced membrane technologies for water purification and desalination," Kalinichev said. "It creates great complications for the industry."

Because of its acidic nature, natural organic matter can form complexes with dissolved metal ions. The binding of ions such as calcium, sodium, magnesium and cesium to natural organic matter, and their potential effects on bio-fouling were studied using molecular dynamic computer simulations performed by Kalinichev, and nuclear magnetic resonance measurements performed by Kirkpatrick and former student Xiang Xu.

"Membrane researchers know that when calcium is present, bio-fouling occurs very fast and filters clog quickly," Kalinichev said. "But when only magnesium or sodium is present, the filters clog more slowly, if at all."

Using relatively simple but realistic molecular models of natural organic matter dissolved in ionic solutions, Kalinichev and Kirkpatrick found that sodium and magnesium ions have very weak interactions with natural organic matter. Cesium interacts more strongly, but calcium has the strongest interaction with natural organic matter.

The strength of the interactions of ions with natural organic matter is dependent upon multiple factors such as ion size, electric charge, and the energy it takes to break the hydration shell of water molecules around the ions, Kalinichev said.

Metal ions in water are usually hydrated, which means they are surrounded by water molecules. For these ions to form strong complexes with natural organic matter, the attached water molecules must be removed.

When this happens, several negatively charged molecules of natural organic matter can simultaneously attach to the same ion, creating much larger aggregates. These aggregates are responsible for the formation of bio-fouling layers on membrane surfaces.

In addition to clogging filters, natural organic matter can change the mobility of certain toxic metals in soil and water.

"We performed our experiments and computer simulations with ions such as sodium and calcium because their behavior in water is already well studied," Kalinichev said. "Our next step is to use these models to study the effects of natural organic matter interaction with less common but more toxic metals such as strontium, lead, mercury, zinc and nickel."

Source: University of Illinois at Urbana-Champaign

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