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AGENT-BASED SIMULATION OF NOM: PREDICTING ION BINDING, LIGHT ABSORPTION AND MICROBIAL UTILIZATION

The production, transformation and mineralization of natural organic matter (NOM) has been simulated using a stochastic, agent-based approach which produces mixtures with bulk composition consistent with NOM. To be useful in an ecological or biogeochemical context, the model must also be able to predict environmentally important properties like acidity, metal ion binding and microbial utilization rates, and light absorption. Acidity and Cu(II) binding can now be estimated using a series of empirical structure-activity relationships developed using simple molecules without any 'calibration' to environmental data. Similar prediction methods are being developed and improved for light absorption and bacterial utilization. Results to date show that 1) proton and Cu(II) binding by simulated NOM is similar to that observed for isolated NOM samples; 2) predicted rates of microbial NOM utilization are quantitatively similar to observed field rates and 3) simulated exposure of NOM to sunlight increases microbial utilization rates. Simulated NOM ultraviolet and visible light absorbance spectra will be compared to spectra from filtered water samples and from isolated NOM.

 TS21 TS44 GS08

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