AGENT-BASES SIMULATION OF REACTIVE SOLUTE TRANSPORT

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Natural organic matter (NOM), a heterogeneous mixture of compounds produced by the breakdown of plant material and microbial activity in the environment, plays an important role in the transport of many natural and anthropogenic pollutants, including organic compounds, heavy metals, and radionuclides. Given its heterogeneous composition and structure, models assigning bulk or average properties to the ensemble of NOM components are too simplistic to capture the complex behavior of NOM in the environment. Stochastic models based on an agent-based approach, in which individual NOM fractions are assigned behavioral properties and simulated as distinct reactive agents, can investigate the heterogeneous aspects of NOM transport.

The molecular weight (MW) of aquatic NOM is well-described by a log-normal distribution, and strongly correlated to the reactive behavior of NOM (Cabaniss et al., 2000). High-MW fractions preferentially adsorb to mineral surfaces, therefore are less mobile in porous media than their more hydrophilic, low-MW counterparts. Within the agent-based approach, the MW distribution is sampled to assign behavioral properties to individual "particles" of NOM. These particles are then released into a simulation environment representing the laboratory sand column. Additional properties, such as mean particle velocity, are determined from the hydraulic properties of this environment (porosity, hydraulic conductivity, flow rate), as well as ambient chemical conditions (ionic strength, pH). Particle transport through the column is thus governed by a set of probabilistic rules that relate to the physiochemical properties of the fluid, solute, and porous medium.

Advantages of the agent-based approach include: (1) efficiency – it can be less computationally intensive than explicit simulation of the sorption kinetics of each NOM fraction, (2) flexibility – it is readily adaptable to a wide variety of conditions, and (3) fidelity – by simulating solute particles individually, agent-based models are able to capture observed aspects of NOM transport that are not reproduced by models based on average ensemble behavior.