<u>Development of an agent based model for predicting arsenic flow and uptake through a small-scale constructed wetland</u>

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Arsenic contamination in soil resulting from anthropogenic activities causes significant health risks to humans and animals. Phytoremediation in constructed wetlands is a cost-effective technology that is fast emerging as the method of choice to treat arsenic contamination. Treatment efficiency of a wetland is determined by the interaction between various soil processes and parameters that affect arsenic flow and its uptake by plants. The complex fate of arsenic in a wetland was modeled using an Agent Based Model. Agent based modeling is a computer based simulation technique in which individual agents that have their own parameter values, can interact with each other and represent a complex system. The goal of this project was to simulate movement of arsenic solution in wetland soil and its' uptake by plants, with a focus on spatial variability in soil properties at a small scale. Our specific objectives are: 1) Develop a conceptual model of arsenic flow and uptake in a small-scale wetland that incorporates the most important parameters and processes that affect fate of arsenic in a wetland 2) Develop an ABM that mimics the behavior of arsenic flow of an experimental wetland with and without plants to compare the efficiency of plant-arsenic-uptake.

The models were constructed using Netlogo 4.1.2, which is a modeling platform developed for examining complex systems through time. In both the models the system is saturated with water as a part of initialization. The first Model contains two kinds of agents: water containing arsenic (arsenic solution) and the grid cells (soil patches) where they move or reside. The second model includes all the factors from Model 1 along with a new agent, plants. Both the models include arsenic flow through the system, diffusion and adsorption and their interaction with heterogeneous pH and redox potential in soil. Model 2 also includes uptake rates of plants. The number of plants (modeled after *Juncus effusus)* in the model system is two. The extent of the model world is 60cm by 8cm. The model world is two-dimensional and shows the horizontal cross-section of the sub-surface. pH and redox are properties of the soil patches. The pH and the redox values are specified based on intermediate segments (every 25 cm) according to Rahman et al. (2011). Adsorption is dependent on redox potential and occurs if the redox potential value is positive. The initial setup of the water containing arsenic is randomized. Arsenic adsorption is calculated as a function of soil pH and probability of arsenic being adsorbed in a patch is modeled as a stochastic process. Parameter values for the model were obtained from the literature and the model will be validated with laboratory data.

Preliminary results of the model show at a lower pH and higher redox potential, soil adsorbs more arsenic than at higher pH and low redox potential. The breakthrough point in Model 1 is earlier than in Model 2 suggesting that presence of plants enhances the treatment efficiency. Plant uptake rate increases with arsenic, at a lower pH before reaching a stage of little variation.

This model is a cost-efficient and interactive tool to manipulate and predict effects of various parameters on arsenic flow and uptake by plants.