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Using Global Sensitivity Analysis to Identify Controlling Processes of Complex Systems

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For an open and complex environmental system, it is always difficult, if not impossible, to understand all the processes and their interactions. On the other hand, since the system dynamics are determined mainly by controlling processes, a better understanding of the controlling processes can lead to advanced predictive understanding of the system. Therefore, identifying controlling processes is always the first step for gaining predictive understanding. The identification, however, is challenging because of uncertainty inherent in system processes such as process parameters and conceptualizations. The overarching scientific question to be answered in this project is as follows: *If we are not certain about the choice of process models and model parameters, can we correctly identify the controlling processes of a complex system?* To answer this question, this project introduces the concept of multiple working hypotheses into the identification of controlling processes to explicitly take into account the uncertainty in conceptualizing and simulating individual processes.

In this poster presentation, we will first present a case study that uses sensitivity analysis to improve a nitrogen transport model developed based on the mixing layer theory. The sensitivity analysis considers three parameters, the mixing layer thickness and two mass transfer coefficients from the mixing layer, and identifies that the mixing layer thickness is the most important parameter. In other words, the nitrogen mixing process is more important than the mass transfer process. To improve the nitrogen transport model, a time-dependent equation is derived to estimate the mixing layer thickness to replace the constant mixing layer thickness used in the conventional mixing layer theory. Using the time-dependent mixing layer thickness substantially improves the model fit to observed nitrogen concentrations in a laboratory experiment.

Another achievement made in this project is the improved computational efficiency for calculating the process sensitivity index, which is the key variable for identifying dominating processes. The calculation is based on Monte Carlo simulation, and the original way of calculation is computational expensive because it is based on combinations of model parameter samples. We developed a new method to remove the sample combination, which reduces the number of model simulation from the order of N^2 to N, N being the number of parameter samples. We are implementing the new computational method for uranium reactive transport modeling at Naturita, which involves three processes, i.e., groundwater flow, uranium transport, and uranium surface complexation reaction. The goal is to identify the controlling processes for contaminant remediation.