

PROTECTING OUR GROUNDWATER RESOURCES: EFFICIENT MODELING OF CONTAMINANT TRANSPORT

Through my research I explore and predict the movement of substances dissolved in groundwater (solutes) to better protect and manage this water resource. Small-scale variations of geology affect the transport of solutes in groundwater at larger-scales. I investigate methods of efficiently describing solute transport affected by these small-scale variations.

Groundwater is an integral part of our environment. It significantly affects plant and animal ecology and provides a water resource for human use and consumption. The mismanagement of groundwater, however, can pose serious hazards. Contaminants applied to the land surface or disposed of beneath the ground (such as pesticides, landfill waste, etc.) can dissolve in groundwater. Groundwater can then carry the contaminants to water-supply wells or sensitive ecosystems, where they may cause health or environmental problems. An understanding of the movement of dissolved substances (solutes) through the subsurface is essential to our ability to protect and manage this natural resource.

The subsurface geology of an area significantly affects the movement of solutes through groundwater. To properly manage and protect our groundwater resources, we must have a thorough understanding of the effect of geology on solute transport. The characteristic of the geology that has the greatest effect on groundwater transport is the hydraulic conductivity, which is analogous to electrical conductivity; *i.e.*, it is a measure of how easy it is for water to flow through a particular rock or sediment. The hydraulic conductivity of sand is much higher than the hydraulic conductivity of granite or clay or shale.

There are three major strategies for exploring how solutes move through the ground. Conducting experiments in the field is one way. One must drill many wells and sample them frequently to obtain a satisfactory description of the subsurface and the transport of solutes through it. Therefore, direct observation of groundwater is difficult and very costly. Laboratory experiments are another way to examine these effects. With a laboratory setup, one has greater control over the experiment, but the range of problems that can be investigated is limited and the experiments are costly and time-consuming. Numerical models provide a third way of exploring the interactions of geology and groundwater transport. With this strategy, one describes the relations between the transport of water and solutes and the hydraulic conductivity with mathematics and equations. Generally, these equations are too complicated to be solved analytically, and one must use a computer to obtain solutions. Investigating solutions for different geologic environments gives one an understanding of the impacts of geology on solute transport. Numerical modeling provides an inexpensive and fast way to investigate solute transport. The utility of a numerical model, however, hinges on the accuracy of the underlying mathematical description of the problem.

To use a numerical model successfully, one must know the equations that describe the transport of solutes, and one must have an adequate description of the geology. The equations that describe how water and solutes move through the ground when the hydraulic conductivity is homogeneous, *i.e.*, the same everywhere, are well known. If one is interested in transport through an area or domain where the hydraulic conductivity is spatially varying, or heterogeneous, one can divide that domain into sub-regions within which the hydraulic conductivity is constant (or nearly constant). For example, if the geology of interest is a heterogeneous sedimentary deposit, one can separate the entire formation into regions of

gravel, sand, silt, and clay. This is akin to representing a visual image with discrete pixels. One can then solve the equations that govern transport within each sub-region and link them together to get the solution for the entire domain. A model in which one accounts for all of the geologic variability is termed a fully resolved model. As the number of these sub-regions increases, the computational time and effort required to model transport also increases.

For questions regarding the protection, remediation, and management of our groundwater resources, often the domain of interest is much larger than the size of the sub-regions over which the hydraulic conductivity can be considered constant. For example, the geology may change every meter or so, but one may be interested in knowing how long it will take a contaminant to reach a well that is a kilometer away. Therefore, many sub-regions are required to accurately characterize the geology within the area of interest, and, consequently, the time required to solve the transport equations for a fully resolved model is prohibitive.

One way to circumvent this difficulty is to sacrifice the small-scale details of the solution; we are often most interested in the large-scale behavior. By coarsening the model resolution, we reduce the computational effort required. Though we may be willing to lose the details of the small-scale behavior, we must have a way to account for its effect on the larger-scales. Therefore, we modify or scale-up the governing equations. A common example of scaling-up comes from the world of finance. If you have money in a savings account in which the interest is compounded daily, and you would like to determine the amount of money you will have after one year, you have two choices. You can calculate the amount you will have at the end of the next day, using a simple equation, and do this 365 times. Alternately, you can go directly to the solution by using the formula for compound interest. In the latter case, you have lost the details of the day-to-day variability of your account, but the upscaled equation accounts for the effect of compounding daily on the result for one year. Using upscaled equations reduces the computational cost required to determine the transport of solutes at scales of interest to us. Obtaining accurate upscaled equations, however, is difficult.

The geologic environments that I study consist of high-conductivity sands and gravels, with distinct regions of low-conductivity silt and clay. Such environments are usually found close to the ground surface and are susceptible to contamination. As dissolved substances move through these environments, most of the solutes travel through the sands and gravels. Some solutes, however, make their way into the low-conductivity silts and clays, where they can remain for extended periods of time. Some researchers have adopted upscaled models from chemical engineering to describe this transport behavior. The range of geologic conditions for which these models are appropriate is unclear, however.

Using hypothetical examples of these geologic environments, I examine the ability of the proposed models to accurately describe solute transport. I first use a fully resolved model of a small area to determine the transport behavior. In the fully resolved models, I divide the domain into hundreds of thousands of sub-regions. I compare these results with those from the upscaled models in which the domain is treated as a single unit. By varying the hydraulic conductivity, size, shape, orientation, and spatial arrangement of the silt and clay regions in my numerical models, I look to determine under what conditions one may be able to use these upscaled models. With these numerical experiments, I hope to determine more

effective and efficient ways of predicting solute transport, leading to better protection and management of our groundwater resources.