Modeling Microbial Transport in Soil and Groundwater

Microbiologists can assist in the development of models of contaminant transport

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Federal, state, and local govermnent agencies are issuing more and more regulations to protect groundwater from microbial contamination. Regulations being proposed include the establishment of wellhead protection zones, drinking-water standards for viruses and parasites, and septic tank placement ordinances.

Microbiologists are being called upon more frequently than ever to work with the engineers, hydrologists, geologists, and soil scientists who are developing and using predictive models of contaminant transport. Because microbiologists frequently lack training in modeling and the modelers have little or no knowledge of microbiology, communication problems can develop. Modelers require information about the factors that affect microbial transport, but many times that information is not available in a directly usable form. With a better appreciation of what modelers need to know, microbiologists can help overcome some of these communication problems.

The use of contaminant transport models for purposes of groundwater protection and bioremediation will likely increase in the future. Such use can help in establishing wellhead protection zones within which potential sources of contamination may not be placed and in granting variances *from* a mandatory groundwater disinfection requirement (to inactivate viruses and ***Giardia*** spp. in drinking water) that the U.S. Environmental Protection Agency plans to publish in the near future.

Typical contaminant transport models are designed to predict how many microorganisms applied to the soil at point A reach point B. Point B may be a source of drinking water, such as a well, at which the type and number of microorganisms represent a health threat. Models can provide useful information about the extent of movement as well as the time required for the microorganisms to move to the desired location. Generally, the more accurate the input data, the more accurate the prediction that can be made by using a model.

A large body of literature describes the processes affecting the fate of microorganisms in the subsurface environment (i.e., soil and groundwater). The fate of microorganisms depends on two main components: survival and transport. Both components must be considered when determining whether there is a hazard to human health associated with the contamination of the groundwater. If a microorganism can survive in the subsurface but is not readily transported through the soil, it likely does not pose a large threat. Similarly, if it is easily transported but does not persist, it may not be of much concern. However, if a microorganism survives in an infective form long enough to be transported through the soil and into the groundwater, it may contaminate the water supply.

Components of a Contaminant Transport Model

The four primary processes involved in contaminant transport that must be characterized quantitatively are decay, advection, dispersion, and adsorption. Contaminant transport is commonly modeled by using an advection-dispersion equation.

Information on the survival characteristics of a microorganism is usually included in a model in the form of a net decay rate. Decay, or inactivation, is the irreversible destruction of the contaminant by chemical, physical, or biological processes. *Any* growth of microorganisms offsets a portion of the decay and can be accounted for by using the net decay rate (i.e., net decay = decay rate – rate of growth). In many models,

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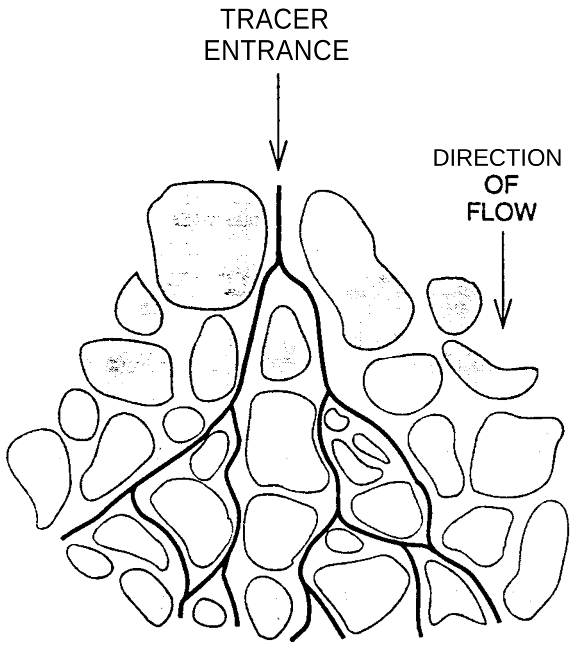
Figure 1. Mechanical Dispersion of Water and Contaminant as Water Flows through the Porous Medium



the net decay rate is considered a constant, making no allowance for any change in decay rates due to changing environmental conditions, The decay rate is determined by a relatively simple process in the laboratory, using conditions that resemble field conditions as closely as possible.

The transport process is described in terms of the three remaining factors: advection, dispersion, and adsorption. Advection is the process by which a contaminant is transported with the bulk flow of the groundwater. In a simple model, advection is equal to the average velocity of the groundwater, which may be determined in several ways. For instance, a soluble, nonreactive substance such as chloride, bromide, or fluorescein (a dye) may be added to the water. In the laboratory, water is applied to the top of a soil column and samples are collected and analyzed for the tracer as a function of time. Assuming that the dissolved tracer mimics the behavior of the water, the average velocity of the water can be calculated.

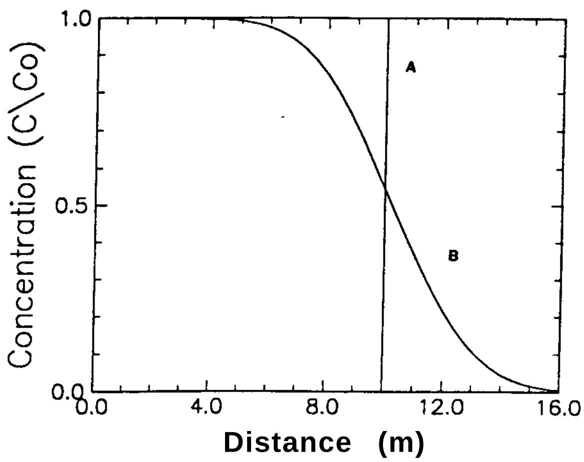
Field tracer tests are much more difficult to perform. Although an average value for the velocity can be obtained over a large area in the field, the velocity from location to location may vary greatly even when two sites are just a few feet apart. Velocity may vary with time because of changes in the porous medium (e.g., shrink@ and swelling materials), boundary conditions (e.g., application of water), and changes in the environmental settings (e.g., temperature changes or a lowering of the hydraulic head and therefore gradients).

Dispersion is another very important process for describing transport. As water moves through soil, it generally does not follow a straight path unless it is flowing through a fracture. Two distinct processes are operating in dispersion: diffusion and mechanical mixing. Diffusion, the spreading out of a solute because of concentration gradients, is a relatively unimportant component of dispersion, compared to mechanical mixing, which occurs when water moving through soil pores diverges around particles. Sometimes the two streams of water will converge on the other side of the particle, and other times the two streams will impinge on another particle and separate again. After traveling around a number of particles the (initially) concentrated water spreads out (Figure 1). The amount of spreading depends upon the type of soil and velocity of the groundwater.

Dispersion can also occur in nonhomogeneous porous media when a contaminant flows faster in one area than another. For example, given a homogeneous porous medium with a single fracture, contaminated water will flow faster in the fracture than in the porous medium. Because the contaminant in the fracture moves ahead of the main contaminated zone, the faster-moving water spreads the contaminant much farther than in a completely homogeneous porous medium. This process is especially important in field soils since heterogeneities such as old root channels and worm and ant holes can also cause dispersion.

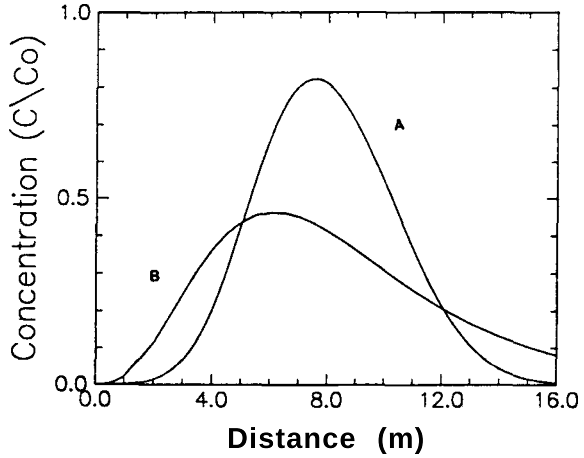
Like advection, dispersion can be measured by using a tracer test. Rather than calculating the average velocity of the water or contaminant, the arrival history of tracer at the column outflow (i.e., the shape of the concentration versus time curve) is determined. Dispersion enables some of the tracer to leave the column before the tracer that is traveling at the average velocity. Without dispersion, all of the contaminant travels through the column at the same rate Figure 2). Dispersion causes the front to spread out, so

Figure 2. Breakthrough Curve of a Contaminant



A, Advection only; B, advection and dispersion.

Figure 3. Effects of Scale-Dependent Dispersion on Contaminant Transport



A, Constant dispersion; B, scale-dependent dispersion

that some of the contaminant travels faster than average and some travels ***slower.***

Dispersion values calculated from soil column experiments generally are not applicable to field situations because the scale in the field is much larger. Compounding this problem, the dispersion of a contaminant changes as water moves farther through a field. Generally, dispersion values increase over larger distances as a tracer encounters more and more heterogeneous features, and the scale of these features increases.

The transport model described here assumes that dispersion remains constant (Figure 3). If, however, the dispersion varies (and linearly increases with the average travel distance), the model predicts a much different distribution (Figure 3), with the contaminant predicted to move much farther than when a constant value for dispersion is used.

The third factor needed to describe the transport process is adsorption, the chemical binding of a contaminant to the surface of a solid medium (e.g., soil). Such binding to a soil surface may be reversible or irreversible and equilibrium or diffusion controlled, depending upon the properties of the contaminant and the subsurface medium. Because adsorption removes contaminants from the fluid phase, even if only temporarily, it slows the movement of the contaminant. The term “retardation” is commonly used to describe the effects of contaminant adsorption.

Adsorption is often measured by calculating a batch adsorption isotherm. The contaminant is added to a flask containing a mixture of soil and water. The mixture is agitated and allowed to reach equilibrium, and then the distribution of the contaminant in the adsorbed and free state is determined at several contaminant concentrations. The results are usually described by using either a Freundlich or Langmuir isotherm.

Many times, however, the adsorption information from batch experiments is not particularly applicable to flowing systems. In flowing systems, the adsorption process may be diffusion controlled When the diffusion of the chemical from the flowing liquid to the liquid adjacent to the adsorption sites governs the adsorption process, laboratory column or field tracer experiments rather than static batch experiments can prove useful.

General Considerations

Characterizing the subsurface medium is key to obtaining an accurate picture of transport in porous media. Heterogeneities such as cracks, fractures, wormholes, and other large openings or soils with markedly different physical properties profoundly affect the flow of water and, hence, the transport of any contaminant. Because analyzing these nonuniformities is both time-consuming and very expensive, other methods for modeling transport in heterogeneous porous media are being sought.

Currently used models usually are too simple to describe the complex nature of field sites, except where the variation in physical properties is small or where comparisons are to be made between different contaminants for hypothetical situations (e.g., screening models).

Although in simple models the chemical and hydrological parameters are constants, in more comprehensive numerical models these parameters can vary over space and time. Such numerical models still suffer from many shortcomings. For example, errors may result from the numerical approximations used. In addition, numerical models can be very time-consuming and expensive to use and may require extensive training in mathematics and computer techniques.

Application of Contaminant Transport Models to Microorganisms

Of all of the information needed for the model, more is known about microbial decay rates than any other factor. Some of the more important factors affecting survival include soil texture (i.e., the amounts of sand, silt, and clay), organic matter in soil, moisture in the soil, pH, temperature, and the chemical composition of the soil-water.

The type of microorganism has a profound impact on the decay rates, which vary by several orders of magnitude. If wastewater is under study, several genera of bacteria, viruses, and parasites are involved. Thus, the decay rate for ***Escherichia coli, for*** example, may not be representative of the decay rates of all microorganisms present. With such a mixed population of microorganisms, it might be prudent to choose the lowest decay rate to be on the safe side. However, this could lead to unrealistically restrictive predictions. Alternatively, the decay rates of each microorganism could be determined, their transport behavior calculated separately, and the results combined.

Another problem is simply finding an applicable decay rate. Many published decay rates are based on laboratory experiments using a liquid medium at one or two different temperatures. Such decay rates differ from those determined in mixtures. Soil-water adjustments should be made so that the value is relevant to environmental settings. In some instances, specific inactivation studies may be required.

Values for the velocity and dispersion of a contaminant are generally obtained from tracer tests. However, the use of a soluble tracer may not give appropriate values for microorganisms. In several laboratory and field studies, the average velocity of the microorganisms was greater than that of a conservative tracer such as chloride.

Pore size exclusion may explain this phenomenon. The advectiondispersion equation assumes that the contaminant is in solution with the same average velocity as the groundwater. If, however, the contaminant is a particle, it may not move through all the pores. A large microorganism may be excluded from the smaller pores and thus may be forced to travel only through the larger pores where their average velocity would be greater than that of the medium taken as a whole. The situation is analogous to that of gel chromatography, in which the largest molecules emerge from the gel first. To counter this problem, tracer tests using microorganisms or other particles with similar characteristics should be conducted. If the microorganisms are large in comparison to the pores in the soil matrix, filtration becomes an important removal mechanism.

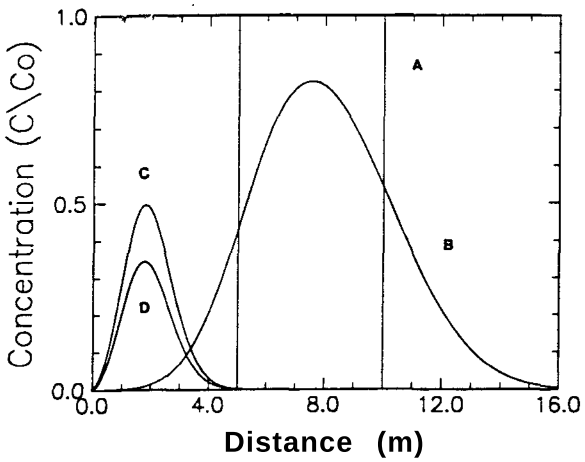
The adsorption of microorganisms to soil materials varies greatly. Attempts to predict the degree of adsorption on the basis of soil properties or characteristics of the microorganisms have not been entirely successful. Therefore, it may be necessary to determine the adsorption characteristics of the microorganism by using the soil at the site of interest.

The degree of adsorption of a particular ***microor*-**ganism may also affect its decay rate. Adsorption of some microorganisms to a solid surface may protect them from some types of inactivation. Thus, some microorganisms have two decay rates: one for the suspended state and another for the adsorbed state.

Illustration of the Effects of These Processes **on** Model Predictions

Advection, dispersion, adsorption, and decay influence the transport of microorganisms in distinctive ways (Figure 4). Assume that microorganisms are added to water for 12 hours and that the water is moving at a rate of 10 meters per day. If the only process affecting transport is advection (A), the first microorganisms travel 10 meters in one day while those added at the end of 12 hours travel only 5 meters.

Figure 4. Effects of Various Processes on Contaminant Transport



A, Advection; B, advection and dispersion; C, advection, dispersion, and adsorption; D, advection, dispersion, adsorption, and decay.

The concentration of microorganisms in the region 5 to 10 meters from the source is constant and is equal to the applied concentration (C/Co = 1). The concentration at 10 meters will remain constant for 12 hours (the time required for the microorganisms added last to travel to 10 meters). After 12 hours, the concentration of microorganisms at 10 meters again drops to zero because all of them are traveling through the soil at the same velocity.

If both advection and dispersion influence the transport process (B), the area under the curve is the same as in A, because all of the microorganisms are still present. However, the microorganisms are not all traveling at the same rate through the soil. Some travel farther than 10 meters in 24 hours, while others take longer than 24 hours to move the same distance. Although the average velocity is the same as in the previous case, individual rates vary more widely.

When adsorption is added to the advection and dispersion processes (C), the area under the curve is reduced because some microorganisms are adsorbed onto the solid medium. Not only does adsorption act to decrease the total number of microorganisms in the water, it slows their movement. The more strongly a microorganism is absorbed, the longer the lag before the first microorganism reaches the lo-meter point.

Because decay of the microorganisms during the transport process permanently removes microorganisms from the system (D), the area under the curve is decreased. However, decay has no effect on the rate of movement of the microorganisms. In terms of modeling microbial transport, this curve (D) is the most realistic of the group. ❑