ADVECTION, DISPERSION, SORPTION, DEGRADATION, ATTENUATION

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Summary

The transport of chemical compounds in porous homogenous media is well understood and the theoretical framework well developed. However, most geological media do not fall in this category. Even the intrinsic heterogeneity in most porous geological media can not be quantified adequately. Neither deterministic nor stochastic models currently do a good job of characterizing the transport of chemical compounds in natural groundwater systems. The situation is even bleaker when evaluating solute transport in fractured or karstic media. Future development has to be geared to better quantify subsurface characteristics in regard to fluid flow and transport. Without it, prediction of the movement of chemicals in the subsurface will not exceed the quality of vague estimates. Recently a lot of effort has been made to understand the transport of bacteria and viruses in the subsurface. Much still needs to be understood, especially in regard to the interactions of microbes with the geological substrate. Nevertheless, much progress has been made considering that about 20 years ago, most scientists did not believe that

microbes existed below the soil zone. More studies need to be done on the distribution of microbial species in the subsurface, their metabolic pathways, and how they can be used to degrade harmful compounds in our drinking water supply and in the subsurface in general. Humankind has just barely opened the door to understanding the immense physical, chemical, and biological complexity of the subsurface starting a few meters below ground surface.

1. Introduction

The physical, chemical, and biological processes of advection, dispersion, diffusion, sorption, and degradation discussed in this chapter have to be considered when evaluating the transport of chemical contaminant compounds, radioactive compounds, bacteria, and viruses in the subsurface. These processes affect the transported substance as well as the transport medium (rocks or sediments in the subsurface) and result in complex distributions of the substance in natural groundwater systems. This contribution will focus on these processes and their effect on groundwater transport.

2. Advection

2.1. Concept of Macroscopic Groundwater Velocity

A geological medium is any type of rock or sediment in the subsurface. If groundwater flow occurs through the pore spaces between the grains of the rock or sediment, that geological medium is called a porous medium. Examples of porous media are sandstone, gravel and sand aquifers. In some geological media groundwater flow occurs through fractures (e.g. granite) or conduits (e.g. karstic limestone) or through a combination of pores, fractures, and conduits (e.g. basalt).

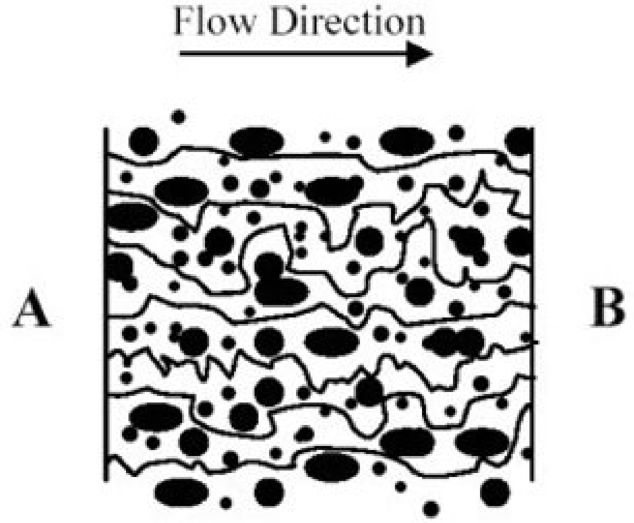

Figure 1. Different pathways through a porous, geological medium. The average linear groundwater velocity is the straight-line distance from A to B divided by the average time needed to travel this distance by all water particles.

When groundwater flows through a porous medium, individual particles of water may choose different pathways around the grains of a geological medium (Figure 1). A particle of water may need a longer or a shorter period of time to move from plane A to B depending on the chosen pathway. It is impossible to measure the time it takes for each water particle. Only the average time for water traveling from A to B can be measured experimentally. Thus, we have to accept a macroscopic viewpoint of the problem and define a macroscopic average travel time, a linear distance between plane A and B, and an average linear groundwater velocity for water moving from A to B. The average linear groundwater velocity is defined by dividing the straight-line distance from A to B by the average time it takes for water to travel from A to B.

2.2. Advective Transport

The term advection refers to the transport of a solute by the bulk movement of groundwater, the movement of particles within flowing water. The velocity of the bulk movement of groundwater is nothing else than the average linear groundwater velocity, also called the advective velocity when referring to the transport of solutes in a groundwater medium. The one-dimensional flux of a solute through a porous medium can be expressed by the equation below:

$$J = v_x \cdot C\, n_e \qquad (1)$$

where:
J= mass flux per unit area per unit time
v_x= average linear groundwater velocity in the direction of flow
C= concentration in mass per unit volume of solution
n_e= effective porosity of the geological medium.

Eq. (1) assumes that the transport of mass does not affect the pattern of flow. The assumption is not true if for example solute and groundwater have a significantly different density, causing the flow of mass and water to diverge. Also, there are some instances where the linear average groundwater velocity differs from the advective velocity of the mass. Bacteria may move faster than solutes through the groundwater medium just because of their size. While water flows along pathways of both low and high microscopic velocity (Figure 1), bacteria of a certain size can only move along large enough pore spaces through which they fit. This in effect causes bacteria to move along preferred pathways of high microscopic velocity and a cloud of injected bacteria may travel from A to B faster than the average time water needs. A larger advective velocity has also been noted for negatively charged ions. Electrical charges due to the presence of clay minerals may force these anions to remain in the center of the pores where the microscopic velocity is large. If the negatively charged ions are large, a cumulative effect due to both size and electrical charges can occur, causing the solute to move at a maximum microscopic velocity by choosing preferred pathways and remaining in the center of the pores. On the other hand, solutes can move at a slower velocity than the average linear groundwater velocity if the geological medium takes on properties of a semi-permeable membrane or if sorption is involved (which will be discussed later). For most practical problems, however, it can be assumed that dissolved mass and groundwater will move at the same advective rate. The effective porosity n_e in Eq. (1) is the porosity through which flow can occur. Not-interconnected and dead-end pores are not included in the effective porosity.

If advection was the only process affecting the transport of a solute in an idealized, homogeneous porous medium, the result would be that the solute would move in the form of a distinct, sharp concentration front through the groundwater medium (Figure 2). Two different cases of injecting a solute into the groundwater medium can be distinguished. The injection can be either in form of a continuous source (Figure 2a) or as a point source in which the solute is injected as a sudden slug (a slug of bacteria, for example, would maintain the same size and concentration during transport, Figure 2b).

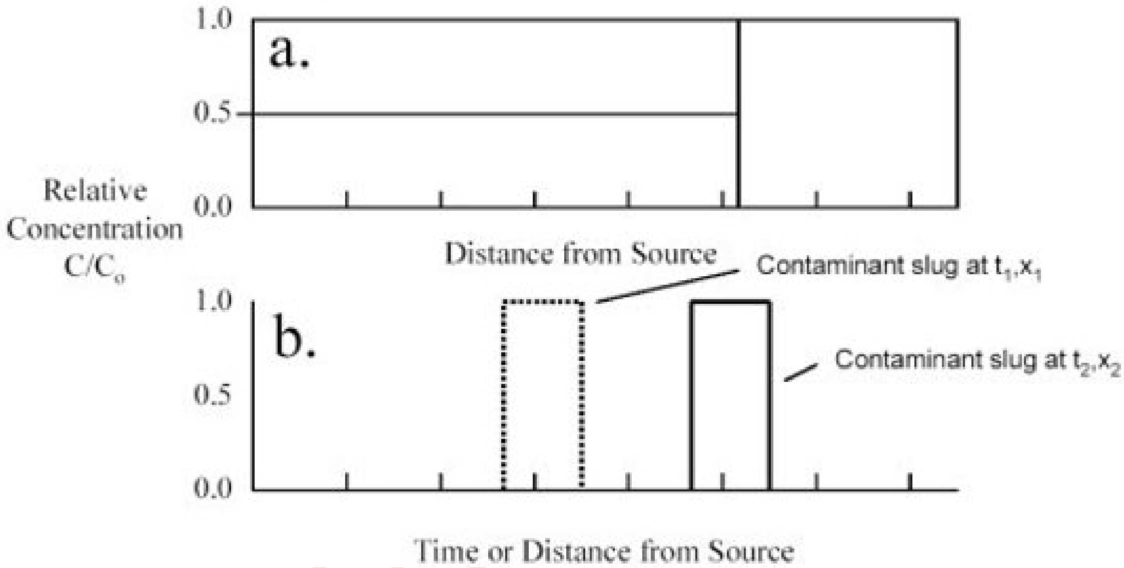

Figure 2. Solute transport by advection only in an isotropic, homogeneous porous medium: (a) continuous source, solute is continuously applied at an initial concentration; (b) point source, a slug of solute concentration is released during a short time interval.. C_o denotes the initial concentration of the solute, C denotes the concentration of solute at time and distance shown in figure.

3. Dispersion and Diffusion

3.1. Mechanical Dispersion

Mechanical dispersion is caused by the different flow paths water particles take in a geological medium (Figure 1). Some of the flow paths are faster because they follow a more direct path or because they are going through larger pores or through the center of pores in which water flows faster because less friction is involved. Other flow paths may be slower because they are closer to the grain boundaries, thus being exposed to more friction in the pore throat, slowing down the water particles. The different flow paths of the water particles cause the mechanical dispersion, a mechanical mixing and dilution of the solute within the bulk movement of groundwater.

The numerical value of mechanical dispersion is the product of advective groundwater velocity and the dispersivity. The dispersivity is a characteristic property of the geological medium, and differs in value for each of the spatial components. For examples, if all the pores are nearly the same size, dispersivity of the rock or sediment would be low. Dispersivity in the direction of flow is referred to as longitudinal dispersivity (in x-direction), dispersivity perpendicular to flow is referred to as transverse dispersivity both in a horizontal plane to flow (in y-direction) and in a vertical plane to flow (in z-direction, flow up or down in a groundwater medium).

It is generally assumed that longitudinal dispersivity is about 10 times larger than transverse dispersivity because the local variation in the velocity field is much more dominant in the direction of flow rather than perpendicular to it. Transverse dispersivity is primarily caused by flow paths that branch out from the centerline of solute movement due to the tortuosity of the geological medium. Concentration distributions (plumes) of a point source form ellipsoids of revolution in three dimensions. If vertical transverse dispersivity is smaller than horizontal transverse dispersivity, as is often the case in layered sedimentary rocks, the plumes take on a surfboard shape.

3.2. Molecular Diffusion

Molecular diffusion is caused by random molecular motion due to the thermal kinetic energy of the solute. The molecular motion in liquids is smaller than in gases but larger than in solids. The coefficient of molecular diffusion is smaller for liquids in a porous medium than in a pure liquid because a collision with the solids of the groundwater medium hinders diffusion. The value of the coefficient of molecular diffusion depends on the type of solute in the groundwater medium, but for major anions and cations it usually ranges between 10^{-10} and 10^{-11} $m^2 s^{-1}$.

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Bibliography

Chapelle F.H. (1993) *Groundwater Microbiology and Geochemistry*. 424 pp. New York: John Wiley and Sons. [This presents a comprehensive discussion of microbial processes in the subsurface and biochemical degradation pathways.]

Fetter C.W. (1999) *Contaminant Hydrogeology*. 500 pp. Upper Saddle River, NJ: Prentice-Hall. [This presents a comprehensive discussion of the movement of contaminant compounds in groundwater.]

Freeze R.A. and Cherry J.A. (1979) *Groundwater*. 604 pp. Englewood Cliffs, NJ: Prentice-Hall. [This presents the best-written book for the understanding of basic concepts in groundwater flow and transport.]

Lyman W.J., Reehl W.F., and Rosenblatt D.H. (1990) *Handbook of Chemical Property Estimation Methods*. Washington, DC: American Geochemical Society. [This presents a comprehensive summary of chemical estimation methods, numbered differently with 1-1 to 1-54, 2-1 to 2-52 and so on: altogether 26 chapters with 3 appendices.]

Wiedemeier T.H., Wilson J.T., Kampbell D.H., Miller R.N., and Hansen E. (1995) *Technical Protocol for Implementing Intrinsic Bioremediation with Long Term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Groundwater*. San Antonio, TX: US Air Force Center for Environmental Excellence.. [This presents a guide for the monitoring of natural attenuation along with a discussion of the primary metabolic pathways of microbes to degrade hydrocarbons.]

Biographical Sketch

Dr. Schulze-Makuch is Assistant Professor and chief scientist of the GeoBiological Groundwater Research Group at the Department of Geological Sciences of the University of Texas at El Paso (UTEP). His interests range from hydrogeology to contaminant transport, and from geobiology to astrobiology. Prior to his employment at UTEP he worked at the Wisconsin Branch Office of Envirogen, Inc. as Senior Project Hydrogeologist, where his major tasks were to investigate and coordinate the remediation of hydrocarbon spills in the subsurface. During that time he also taught as Adjunct Professor at the University of Wisconsin-La Crosse. Dr. Schulze-Makuch received his doctoral degree in geosciences from the University of Wisconsin-Milwaukee and a Diploma and Vordiploma degree (M.Sc. and B.Sc. equivalent, respectively) from the Justus-Liebig-University in Giessen, Germany.