# Dispersion in a Porous Medium with One-Dimensional Dispersion Numerical Model

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## I. Introduction

Concern over the potential for migration of wastes in the subsurface has generated a great deal of interest in the mechanisms responsible for contaminant transport through groundwater systems. Increased attention by both researchers and regulatory agencies to subsurface contamination can be attributed to the growing popularity of waste disposal by means of landfills, sludge lagoons, and deep injection wells and to the concern over subsurface disposal of low to high level radioactive wastes.

To prevent the deterioration of groundwater quality, it has become necessary to develop a methodology for monitoring, analyzing, and predicting the movement of contaminants through the subsurface. The hope of formulating such a methodology has motivated the development of predictive tools in the form of mathematical models designed to simulate the transport of contaminants through groundwater systems.

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The components of transport process are advection, dispersion (including diffusion), and chemical reactions. There are two approaches to the contaminant transport problem as applied to groundwater system. Either an advection-dispersion model is constructed in which the effects of dispersion are included in addition to advection, or an advection model is developed. Both types of models may incorporate chemical reactions.

The major problems associated with modeling contaminant movement in groundwater systems where the effects of dispersion are considered to be significant are measuring dispersivity in the field and overcoming numerical difficulties which can arise when solving the dispersion equation. Incorporating chemical reactions into both advection-dispersion models and advection models is another difficult problem.

## II. Field Determination of Input Parameters

Several investigators have pointed out the difficulties involved in the descriptions of groundwater systems which are sufficiently detailed to allow accurate prediction of contaminant migration. To solve the transport equation, one needs to predict the velocity distribution and the dispersivity of fluid flow. However, to date there are no well-tested, standard techniques for acquiring these critical data.

### 2.1 Velocity

Because it is difficult to measure groundwater velocity directly, groundwater hydrologists like to determine groundwater velocity indirectly using Darcy's Law and measurements of heads and hydraulic conductivity.

When velocity is determined indirectly using Darcy's Law, it is necessary to estimate porosity. However, porosity can vary by several tens of percent within a single sedimentary deposit, laboratory and field experiments may not capture its important spatial variation.

### 2.2 Dispersivity

The magnitude of transfer caused by dispersion is quantified through the use of the coefficient of dispersion. From experiments, it is known that the coefficient of dispersion is proportional to the velocity. Thus, the coefficient of dispersion can be estimated if velocities and dispersivities are known.

When a true dispersivity is not known, researchers generally attempt to solve a problem by assuming constant values for longitudinal and transverse dispersivity.

## III. Numerical Difficulties in Solving the Dispersion Equation

In addition to the difficulties involved in determining the velocity distribution and dispersivities of fluid flow, the other obstacle in developing a methodology to deal with the contaminant transport lies in the fact that numerical solutions of the dispersion equation are frequently characterized by oscillation in the computed concentration front (numerical dissipation or also called numerical diffusion or dispersion). Fig. 1 illustrates the effects of overshoot on a 1-D numerical dispersion problem. Causes of overshoot in numerical dispersion analysis and comparison of different analytical schemes have been discussed by many reseachers, detailed discussions will not be presented here but can be found elsewhere(1,2).

## IV. Derivation of the Basic Field Equations

### 4.1 Isotropic Dispersion

The first general assumption is that Darcy's Law applies. The model is such that all particles of water move at the same rate of speed through the porous medium. Because of this assumption, which neglects microscopic variations in fluid velocity, a refinement must be emplyed to approximate the real system. For the dispersion mechanism, this refinement involves a transport component that is analogous to Fick's first law. The dispersion coefficient that appears in the dispersion component is assumed to be approximated by a constant, whereas it generally is to some extent dependent on the concentration and the type of dissolved or suspended substance. The development of the differential equation, however, is based on the assumption that the concentration is sufficiently small that the dispersion coefficient is independent of concentration. No chemical reaction is assumed to occur between the solid and the liquid phases. This supposes that within the fluid system no loss or addition of matter can take place.

To establish the mathematical statement of the conservation of mass, consider a cubic element in the three-dimensional Cartesian space, as presented in Fig. 2. The two modes of transport of a fluid within a porous medium have been described as (a) convection and (b) dispersion. In mathematical terms

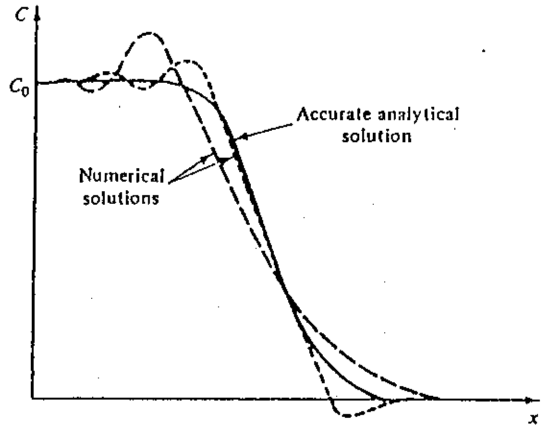

Fig. 1 Schematic illustration of oscillations in numerical solutions of an advancing front (after Bender et al. 1975)

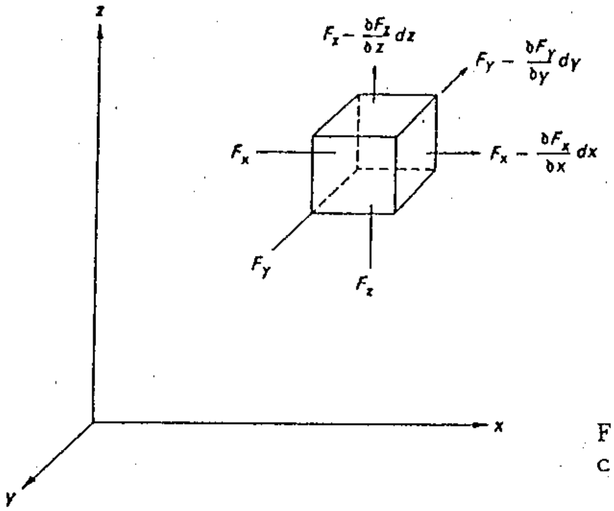

Fig. 2 Mass balance in a cubic element in space

these modes for direction X are expressed:

$$\text{Transport by convection} = u * C * dA$$

$$\text{Transport by dispersion} = D_X * \frac{\partial C}{\partial X} * dA$$

where dA= an elemental cross-section area of the cubic element; C= chemical concentration; $D_x$= diffusion coefficient in X-direction and u= particle speed. Assuming that these two components may be superposed, the total amount of material transported parallel to any given direction is obtained by summing the convective and dispersive transports. Thus, if $F_x$ represents the total amount of mass per unit cross-sectional area transported in the X-direction per unit time, then

$$Fx = u * C - n * D_x * \frac{\partial C}{\partial X}$$

where n= porosity of the medium. The negative sign before the dispersive term indicates that the contaminant moves toward the zone of lower fluid concentration.

From Fig. 2, the difference in the amount of solute entering and leaving the cubic element is

$$\left( \frac{\partial F}{\partial X}x + \frac{\partial F}{\partial Y}y + \frac{\partial F}{\partial Z}z \right) dx\ dy\ dz$$

Because there is no loss in the mass of the liquid, the difference between the amount entering and leaving must be equal to the amount of mass accumulated within the element. The rate of mass change is represented mathematically by the expression

$$n \frac{\partial C}{\partial t} dx\ dy\ dz$$

Equating the two equations as shown above leads to the following relationship

$$\frac{\partial F}{\partial x}x + \frac{\partial F}{\partial y}y + \frac{\partial F}{\partial z}z = n \frac{\partial C}{\partial t} \qquad (1)$$

Equation 1 is a mathematical statement of the law of conservation of mass under the conditions stipulated. Substituting the expressions for $F_x$, $F_y$, and $F_z$ and assuming that $D_x=D_y=D_z$=const., equation 1 becomes

$$D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) = \frac{dC}{dt} \qquad (2)$$

## 4.2 Adsorption

Vermeulen and Hiester(1952), in a macroscopic investigation of ion-exchange columns, specified that the ratio of the tracer velocity under equilibrium conditions may be expressed as:

$$\frac{u_T}{u} = \frac{1}{1+M} \quad ; \qquad M = \frac{S \cdot \rho}{C \cdot n}$$

where S= tracer component adsorbed per gram of solid matrix; $\rho$= bulk density of solid matrix; and $u_T$= velocity of tracer. The relationship shown above was established empirically and had been used to some extent to determine rate of movement of radioactive isotopes.

To develop the transport equation which includes adsorption, it is assumed that the rate of adsorption is the third component in the dispersion equation. This assumption simply implies that the chemical reaction or the rate of adsorption can be superimposed on the dispersion and convection system previously described in equation 2. The adsorption component in the physical model can pictured as a mathematical sink or source with its strength dependent on the difference of concentration of the liquid phase and the solid phase. Fig. 3 shows a simplified model where the adsorption component is assumed in one-direction only.

Superposition of the three components, i.e. adsorption, dispersion, and convection, allows the writing of the continuity or mass-balance equation as follows:

$$D \nabla^2 C = \frac{dC}{dt} + \frac{\partial S}{\partial t} \qquad (3)$$

where S is defined simply as the concentration of the solid phase, which has the same dimension as C. The analysis of dispersion in adsorbing media depends on the representation of S in terms of C, where it is assumed that the relationship $\partial S/\partial t = f(C)$ holds.

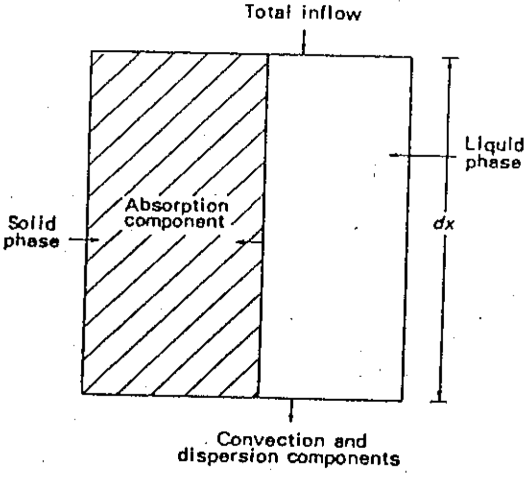

Fig. 3 Schematic diagram of transport in porous media (after Bird and others)

One of the expressions most frequently used in the analysis of ion-exchange is

$$\frac{\partial S}{\partial t} = b( C - mS)$$

where b and m are constants. As indicated by Crand(1956), this equation describes a first-order reversible reaction and is applicable to some ion-exchange processes in fluids flowing in porous substances.

Despite the fact that the adsorption process is generally ill-defined, it is an important factor in the control of mass transport within a porous medium. In most cases the fate of the contaminant in a groundwater reservoir is largely dependent on the amount transferred between the liquid and solid phases.

## 4.3 Mathematical Treatment of the Dispersion Equation

All theexamples illustrated follows are limited to flow in a semi-infinite medium. The principal objective is to investigate initially the nature of dispersion.

The examples given are intended only as samples of solutions available and may not be physically realistic. The first example considered is for dispersion within a unidirectional flow field. It is postulated that the concentration is specified at x=0 and at the initial time t=0. For the specified field conditions, the field equation becomes simply

$$D\frac{\partial^2 C}{\partial x^2} = u\frac{\partial C}{\partial x} + \frac{\partial C}{\partial t}$$

Example 1

The plane x=0 is maintained at a concentration $C=C_0$

The boundary conditions are given by

$$C(x,0) = 0, \qquad x \geq 0$$

$$C(0,t) = C_0, \qquad t \geq 0$$

$$C(\infty,t) = 0, \qquad t \geq 0$$

The method best suited is the Laplace transformation; substitution of the transform leads to the subsidiary system given by the equation

$$D\frac{d^2\bar{C}}{dx^2} = u\frac{d\bar{C}}{dx} + p\bar{C} \qquad (4)$$

The solution of this subdiary equation subjected to the restraints due to the boundary condition is

$$\frac{\bar{C}}{C} = \frac{1}{p}\exp\left[\frac{ux}{2D} - x\left(\frac{u^2}{4D^2} + \frac{p}{D}\right)^{\frac{1}{2}}\right] \qquad (5)$$

The inverse transform as given by Erdelyi and others(1954) is readily determined as

$$\frac{C}{C_0} = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-ut}{2\sqrt{Dt}}\right) + \exp\left(\frac{ux}{D}\right)\operatorname{erfc}\left(\frac{x+ut}{2\sqrt{Dt}}\right)\right] \qquad (6)$$

Because a constant concentration is maintained at $x=0$, example 1 exhibits an asymmetrical concentration distribution about $x=ut$.

When mass transfer due to adsorption is superimposed on the convective and dispersive transport, the continuity consideration in a one-dimensional flow system leads to the following differential equation

$$D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} + \frac{\partial S}{\partial t} \qquad (7)$$

The time rate of change in the solid-phase concentration was previously indicated to be approximated by the linear equation

$$\frac{\partial S}{\partial t} = b( C-mS ) \qquad (8)$$

In the example follows, equations 7 and 8, with suitable modifications, are used to describe the concentration distribution within an adsorbing medium. The flow occurs in a semi-infinite medium; hence, for all following examples the boundary conditions are:

$$C( 0,t ) = C_0, \qquad t \geq 0$$
$$C( x,0 ) = 0, \qquad x > 0$$
$$C( \infty,t ) = 0, \qquad t \geq 0$$
$$S( x,0 ) = 0, \qquad x > 0$$

Example 2

Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t=b$, where $m=0$.

The solution of simultaneous equations 7 and 8 for the prescribed conditions can be determined by assuming that it may

Example 1

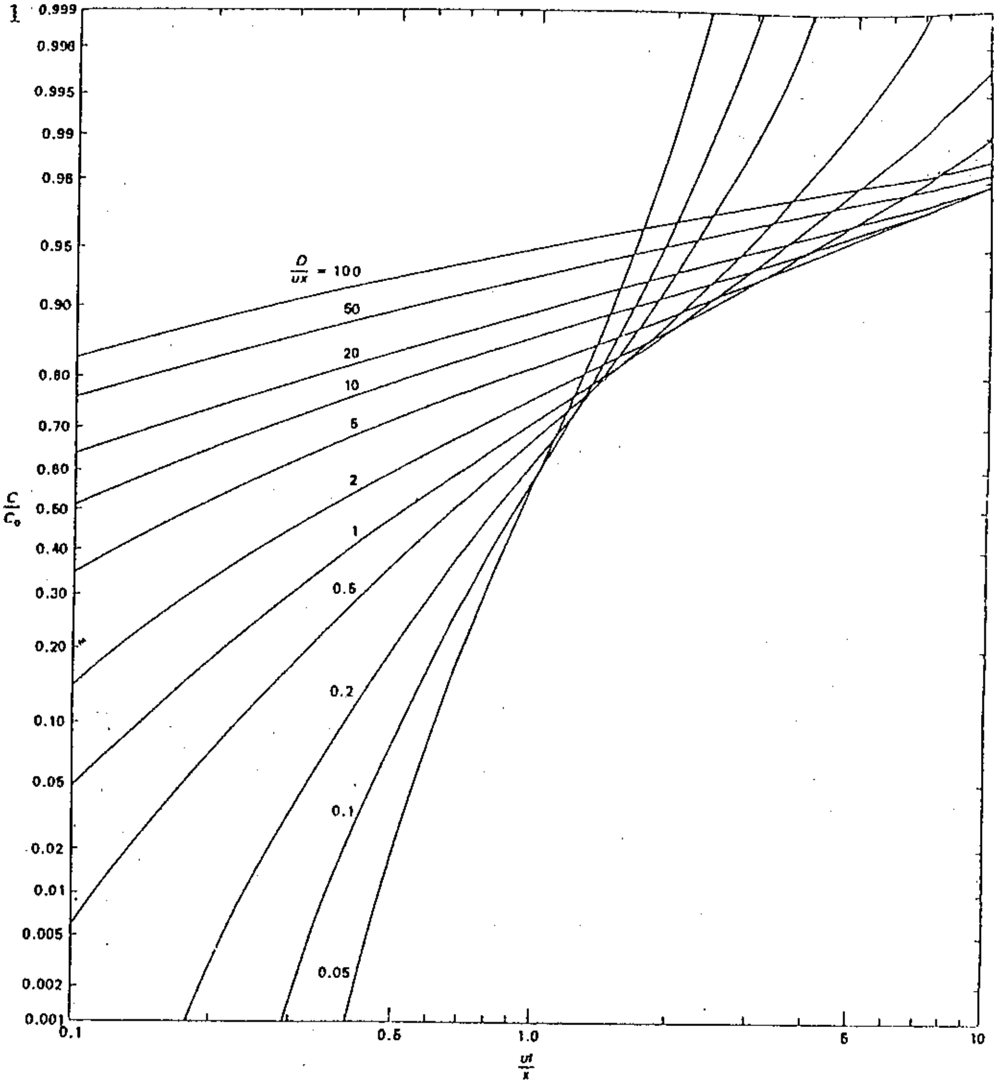

Fig. 4 Concentration distribution; plane source at x=0 maintained at constant concentration

be written in the form

$$C(x,t) = T(x,t)\exp\left[\frac{ux}{2D} - \left(\frac{u^2}{4D} + b\right)t\right] \qquad (9)$$

Substituting the above expression into equation 2 leads to an equation as follows

$$D\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \qquad (10)$$

Example 2

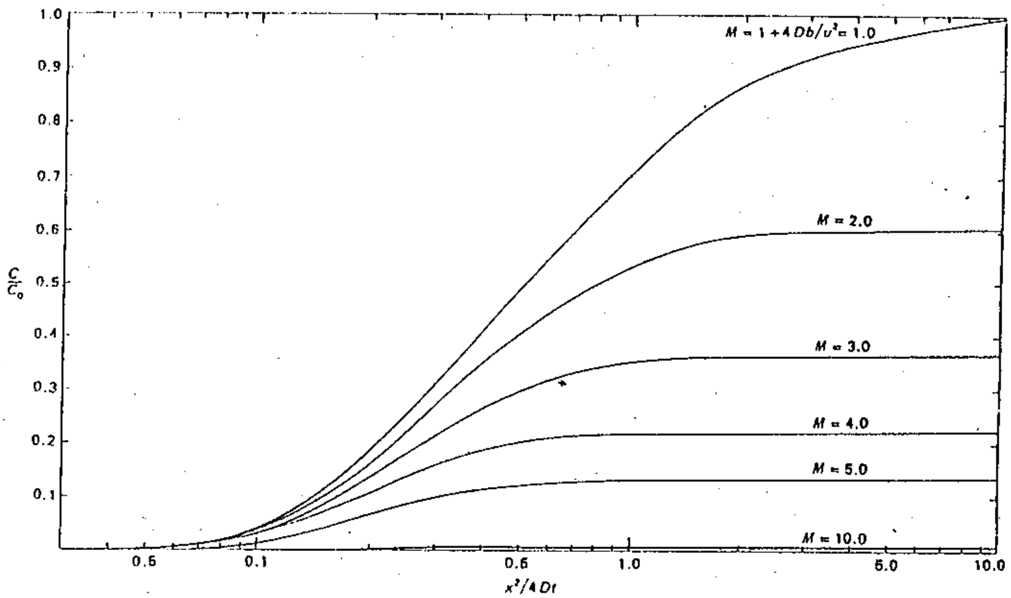

Fig. 5 Concentration profile of dispersion in an adsorbing medium with S/ t=bC

For the function T, the condition at x=0 is given by

$$T(0,t) = C_0 \exp[(\frac{u^2}{4D} + k)t] \qquad (11)$$

The general solution of the equation above has been given by Carslaw and Jaeger(1959), it will not be expressed detailed here.

V. Summary

The theory of dispersion of miscible fluids has been developed extensively for fluid flow within a homogeneous porous medium. In the development, a fluid containing a given dissolved substance is described as moving according to Darcy's Law, provided density differences between that fluid and the natural host fluid are negligible. However, the transportation of the dissolved substance has both a dispersion component, and a convection component as described by Darcy. There are other mechanisms involved in the transport of the dissolved component, but their magnitude is small for normal groundwater flows, excepting adsorption.

The field applicability of the analysis for a unidirectional transport system is limited. For problems involving any injection of contaminant, the dispersion phenomena take place in at least two dimensional space. The approach to this description is to assume that the generalization can be accomplished by assigning the dispersion coefficient to the properties of a tensor.

In all attempts to describe the flow conditions in a porous matrix, it has been found that the generalization of the expression for flow is formidable primarily because of the inability to represent statistically the physical properties of the given medium in relation to the fluid flow. Thus, the limitations placed on the analytical theories of dispersion are apparent. The generalized description of the transport of mass within any heterogeneous porous medium is unattainable by any presently known methods. However, the problems encountered in a real situation do not require complete and rigorous formulation; usually, an engineering estimate of the maximum possible effect under the observed conditions is acceptable.