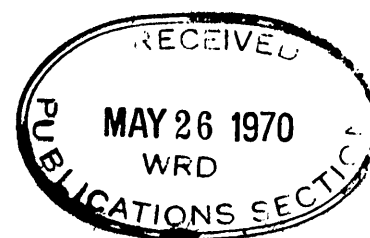


1970

Theory of Dispersion in a Granular Medium

GEOLOGICAL SURVEY PROFESSIONAL PAPER 411-I



Theory of Dispersion in a Granular Medium

By AKIO OGATA

FLUID MOVEMENT IN EARTH MATERIALS

GEOLOGICAL SURVEY PROFESSIONAL PAPER 411-I

*A review of the theoretical aspects of
dispersion of fluid flowing through a
porous material*



UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1970

UNITED STATES DEPARTMENT OF THE INTERIOR

WALTER J. HICKEL, *Secretary*

GEOLOGICAL SURVEY

William T. Pecora, *Director*

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402 - Price 45 cents (paper cover)

CONTENTS

	Page		Page
Symbols.....	iv	Field equation for two-fluid systems.....	19
Abstract.....	I 1	Adsorption.....	10
Introduction.....	1	Mathematical treatment of the dispersion equation.....	12
Acknowledgments.....	2	Nature of the dispersion coefficient.....	23
Historical development.....	2	Evaluation of dispersion coefficient by analytical methods.....	25
Derivation of the basic field equations.....	4	Evaluation of dispersion coefficient by experimental methods.....	27
Isotropic dispersion.....	5	Summary.....	32
Anisotropic dispersion.....	6	References cited.....	33
Some useful transformations.....	7		
Dispersion equation in cylindrical and spherical coordinates.....	8		

ILLUSTRATIONS

	Page
FIGURE 1. Diagram illustrating mass balance in a cubic element in space.....	I 5
2. Schematic diagram of coastal aquifer system.....	9
3. Schematic diagram of transport in porous medium.....	11
4. Definition sketch of one-dimensional system.....	12
5-8. Graphs showing—	
5. Concentration distribution; plane source at $x=0$ maintained at constant concentration.....	14
6. Concentration distribution; region $x \leq 0$ initially at constant concentration.....	15
7. Steady-state concentration distribution; circular surface source at constant strength.....	16
8. Steady-state concentration distribution; circular surface source maintained at constant concentration.....	17
9. Definition sketch of radial flow.....	17
10. Graph showing concentration distribution for radial-flow system.....	19
11. Definition sketch of system depicting no dispersion in x direction.....	20
12. Approximate concentration profile due to lateral dispersion; radially symmetrical model.....	20
13. Approximate concentration profile due to lateral dispersion; two-dimensional model.....	21
14. Graph showing comparison of examples 3, 4, and 6.....	22
15. Concentration profile showing dispersion in an adsorbing medium with $\partial S/\partial t = bC$	24
16. Concentration profile showing dispersion in an adsorbing medium with $\partial S/\partial t = b(C - mS)$, $D_x \partial^2 C/\partial x^2 = 0$, and $\frac{\partial S}{\partial t} \gg \frac{\partial C}{\partial t}$	25
17. Sketch showing random path chosen by a fluid particle moving through the canal system.....	26
18. Sketch showing typical setup for column experiment.....	28
19. Plot of the Schmidt number versus the Reynolds number.....	30
20. Plot of the Peclet number versus the Reynolds number.....	31
21. Graph showing example of comparison between theoretical and experimental results.....	32

SYMBOLS

Q	total rate of flow	Inverse Laplace transform	$L^{-1}[f(p)] = f(t)$
u, v, w	velocities in the x, y , and z directions, respectively (the Darcy velocity divided by porosity)		$= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} f(p) dp$
C	Concentration in mass of solute per unit volume of fluid	$\text{erf}(x)$	error function defined by $\text{erf}(x)$
C_0	reference concentration		$= \frac{2}{\pi} \int_0^x e^{-\eta^2} d\eta,$
C'	ratio C/C_0	$\text{erfc}(x)$	complimentary error function defined by $1 - \text{erf}(x)$
D_i	dispersion coefficient in the $i = x, y, z$ directions	$J_1(x)$	Bessel function of the first kind of order ,
F_i	mass flux of dissolved component per unit area in the i th direction	$Y_1(x)$	Bessel function of the second kind of order ,
x, y, z	space dimensions of Cartesian system	$I_1(x)$	modified Bessel function of the first kind of order ,
t	time	$K_1(x)$	modified Bessel function of the second kind of order ,
A	cross-sectional area	$J(x, y)$	$1 - e^{-y} \int_0^x e^{-t} I_0[2(yt)^{1/2}] dt$, or
r	radial space coordinate		$1 - x^2 \int_0^\infty e^{-yt - x^2} J_0[2(yt)^{1/2}] J_1[2(xt)^{1/2}] dt$
K	hydraulic conductivity	l	length of elementary canal
k	intrinsic permeability	ρ	density (also r/a)
p	pressure	$\gamma = \rho g$	specific weight
g	gravitational constant	μ	viscosity
q	flux per unit area	ν	kinematic viscosity
f	porosity	ψ	stream function
d	diameter of the particle making up the solid matrix	ξ, η, ζ	transformed coordinates as specified
y_0	thickness of the aquifer	T	ut/x
S	concentration per unit volume of solid material	X	D/ux
b, m	constants related to linear adsorption rates	Pe_r	ud/D_r , radial Peclet number
\bar{n}	number of steps in a random walk analysis	Pe_x	ua/D_r , axial Peclet number
\exp	exponential		
Laplace transform	$L\{f(t)\} = \int_0^\infty e^{-pt} f(t) dt$		

THEORY OF DISPERSION IN GRANULAR MEDIUM

By AKIO OGATA

ABSTRACT

This report is a presentation of the theoretical aspects of the investigations and a few confirmatory laboratory studies of the dispersion process. The basic assumptions associated with the development of the dispersion equation, based on the applicability of a heuristic expression similar to Fick's law, are described. In general, these assumptions limit its application to a homogeneous medium in which the dispersion process is anisotropic. The present level of knowledge is made apparent through the presentation of several solutions for the differential equation that approximates the dispersion process. Adsorption and its effect on the fate of a contaminant is given only limited discussion because of the lack of formal studies, on a macroscopic scale, applicable to the hydrologic regimen. The equations approximating dispersion in a two-fluid system (salt-fresh water) are also presented.

INTRODUCTION

The rapidly growing need to dispose of radioactive waste products, and the increased rate of pollution of the ground-water resource by other chemical compounds, make it increasingly apparent that a much more detailed description of flow in porous media must be sought. Because of the dangers inherent in the presence of contaminants in the water supply, their fate and mode of travel downstream from their sources must be predicted. The fate of a contaminant depends on both the macroscopic and microscopic behavior of the fluid under the existing flow conditions and the physico-chemical conditions within the environment of the granular material. The discussion to follow presents a simplified treatment of dispersion phenomenon, and a mathematical expression, in the form of a differential equation, is developed. As the medium becomes more complex, the flow description becomes indeterminate (Skibitzke and Robinson, 1963), since the description of the transport mechanism, owing to convection and dispersion, requires first a correlation between properties of the porous medium and the flow conditions.

The present-day study of dispersion may be separated into three categories (C. V. Theis, written commun., Oct. 1967):

1. The mathematical problem.

2. The laboratory problem for confirmation of (1) and its extension to include parameters that cannot be included in the mathematical model.
 3. The field—that is, the natural aquifer—problem which introduces larger variations in parameters.
- Much progress has been made in segment (1) in recent years, and because of availability of electronic computers, complex mathematical equations can now be readily analysed. The problem (segment 3) is not clearly understood because of large variations in the parameters controlling the mixing mechanisms. Segment (2), on the other hand, is effectively used as a method to confirm mathematical analysis, but as yet, is limited in its use as a physical model of the real system. Bachmat (1967) pointed out that both the geometric and time-scale ratio for the model and prototype must be 1:1.

This paper is limited to the theory of dispersion or category (1) as described above. Because existing literature on the subject is extensive, a thorough review is beyond the scope of this paper.

The mechanisms associated with the transport of a dissolved substance in porous media are listed below. Some of these mechanisms are of little significance in natural ground-water bodies, but they are important in exchange systems that are used in the chemical industry. The mechanisms are as follows:

1. Molecular diffusion—the transport of mass in its ionic or molecular state due to differences in concentration of a given species in space. The gross transport obeys Fick's first and second laws of diffusion (Bird and others, 1960, p. 502).
2. Mechanical dispersion—the mixing mechanism that is present because of the variations in the microscopic velocity within each flow channel and from one channel to another. Microscopically, there is no mixing; however, if the average concentration of a given volume of fluid is considered, an apparent dilution or spreading is present. The gross transport, as in eddy diffusion, is given by an expression similar to Fick's law.

3. Eddy diffusion—the mixing process that is due to the random fluctuation of fluid mass or the occurrence of eddies in the condition described as turbulent flow. In porous media these eddies exist only to a slight extent, if at all, because of the small size of the pores; but in media consisting of large grains, such as gravel, eddies may occur to some degree. In the more common types of media, however, the existence of low gradients tends to limit or preclude turbulence.
4. Mixing due to structural controls—the apparent mixing mechanism due to large-scale structural variations in the granular material. These variations control the direction of movement of a given fluid particle; hence, if an average concentration is taken along a given plane parallel or transverse to the direction of flow, a large-scale mixing is observed. Whether this type of mixing can be treated in a manner analogous to that of mechanical dispersion is questionable, and, in any event, such a treatment would likely require a complete description of changes in the properties of the porous medium. The analysis would probably require the use of the Lagrangian concept in which each fluid particle must be traced along its path of flow.
5. Adsorption—a process which differs from the others in that the amount of mass transported depends on the physicochemical interaction of the transported substance and the solid of the medium. The existence of an unbalanced force field causes migration of a liquid-borne contaminant from the liquid to the solid surface. In some instances the contaminant is permanently fixed on the surface, whereas in others it moves continuously from liquid to solid, or vice versa. Hence, the measurement of the liquid phase concentration shows a diminution of the concentration. Also, the contaminant does not travel at the same rate as the fluid.

At present, there are basically two related methods of analysis that are useful in depicting dispersion. The first is a microscopic study of a fluid particle which employs the concepts of statistical analysis. The second is a microscopic analysis of dispersion or transport of mass which is expressed in terms of a heuristic law analogous to Fick's first law of diffusion. The microscopic analysis, which predicts the position of the fluid particle at any given time, is completely dependent on the mathematical model chosen to represent the medium. The most satisfactory model to date is the representation based on the assumption of pore channels located with complete randomness and multiply connected at some end points. On the other hand, the

heuristic approach requires that a partial differential equation similar to all transport systems be solved.

Acknowledgments

This review of the Theory of Dispersion was initiated while the author was associated with the Phoenix Research Office of the U.S. Geological Survey. The author gratefully acknowledges the detailed discussions and suggestions of R. H. Brown, H. H. Cooper, H. E. Skibitzke, C. V. Theis, and others in the review of the manuscript.

Historical Development

Perhaps the first to recognize the occurrence of dispersion phenomena was Slichter (1905) in his investigation of the use of salt as a tracer in ground-water flow. He noted that at a point away from the source the salt concentration increased gradually rather than abruptly, as would be predicted by Darcy's expression. That is, a gradation of salt concentration in the fluid occurred as the front moved past a given point of measurement. Slichter explained this by noting that in flow through capillary tubes the velocity of the fluid varies across the cross section of each tube and that, because the soil complex is composed of a great number of these tubes, the sum of the deviation in each tube is likely to cause the mixing that he observed. Following the same line of reasoning, lateral dispersion—dispersion perpendicular to the direction of the average flow—was attributed to the repeated branching of the individual flow tubes within the solid matrix. This explanation is most commonly used today to describe the mechanical component of the dispersion phenomenon.

Earlier papers dealing with two-fluid systems have been concerned with the economically important problem of salt-water invasion in coastal aquifers. The first analytical descriptions and investigations were based on the supposition that the fluids could be treated as though they were immiscible. However, in the middle and later 1930's, a zone of diffusion which could not be explained by immiscible-fluid theory, was noted. This diffusion zone prompted recognition of the dispersion process as a possible cause for its occurrence. This phenomenon was treated theoretically by Kitagawa in 1934 when he made theoretical and experimental studies of dispersion in a porous system. The physical model he chose was that of dispersion of a salt tracer emitted from a line source within a horizontal flow field. The experimental model, like most laboratory models, was composed of sand. The theoretical analysis was based on the assumption that, at some distance from the source, the concentration distribution would conform with the normal probability curve.

Before Kitagawa's treatment became widely accepted, refinements of the displacement theory for a coastal aquifer came about largely through the efforts of Wentworth (1948). He postulated a "rinsing theory" based on the hypothesis that the pores of the medium act as mixing cells and that the ocean tides cause the alternate filling of the pore by salt and fresh water, thereby creating a partial mixing of the fresh and salt water. Wentworth derived an approximate expression for numerical computation.

Accelerated field investigations in the latter part of the 1950's and in the early 1960's indicated that instability of the salt water-fresh water front posed a threat to the water-supply systems in many coastal regions. The results of these studies were recorded in various publications; for example, Cooper (1959) and Kohout (1960, 1961) described the conditions in Florida with supplementary information on the Hawaiian Islands to provide evidence of a dispersion-induced circulation of sea water into the zone of diffusion and back to the sea.

The results of these investigations gave impetus to the development of analytical methods designed to predict the dispersive effects of ocean tides. Results of other analytical studies have been published by Carrier (1958), Jong (1959), Henry (1960), and Bear and Todd (1960). The limitations of these investigations lie in the incomplete knowledge of the flow system in heterogeneous coastal aquifers and in the necessary oversimplification of such a system. Hence, the theoretical results were correlated only with those from a laboratory model designed to conform with the mathematical model.

It was argued that, because of the discrepancy between the medium of the mathematical model and the real medium, the mathematical model cannot be expected to depict what actually took place. Because of this several investigators have preferred a statistical model to develop expressions for the dispersion coefficient. Two statistical models were used: the completely disordered flow of Scheidegger (1954) and the randomly oriented flow channels of Jong (1958) and Saffman (1959, 1960). Experiments on laboratory models, however, indicated a variance in the completely disordered model which could not be reconciled with the laboratory data. An important limitation of Scheidegger's model was that it did not include a directionally variable coefficient of dispersion. The assumption of random fluid paths did, however, provide for the directionally variable coefficient, because of the lateral components of the flow velocity. The difficulties that precluded a model description of the aquifer were apparent, and a variety of postulates were introduced

to simplify the flow regime so that an analysis was possible. The assumption that the medium can be described limited the analysis to an isotropic medium.

Most of the articles published assumed that the field equation, similar to Fick's second law of diffusion in a moving medium, was a good first-order approximation. Although the assumption that the transport equation consists of two modes—the Darcy component and the dispersion component—avoided the requirement that the individual flow paths be known, it required that the average direction and magnitude of the flow be defined and that the dispersion coefficient be determined experimentally. Because the flow through a columnar model is readily defined, this type of analysis is especially useful in predicting the behavior of reactor columns or ion-exchange columns employed in the chemical industry. Dankwerts (1953) gave a comprehensive discussion of the analysis of a columnar model and described the types of flow found in experiments on packed columns. In most industrial applications, the flow rate in the exchange process is much higher than that of ground water in nature; therefore, the analysis may not be useful in the field of hydrology. The differential equation which describes the field is valid, but the nature and magnitude of the dispersion coefficient are altered.

An analysis which employs a "perfect mixture model" described, for example, by Aris and Amundson (1957), may also be used for the higher fluid velocities. This mathematical model assumed that each pore cell within the porous medium constituted a mixing chamber, within which the two fluids were perfectly mixed. The analysis differed from that of the low-flow model in that the laboratory experimental data indicate a concentration breakthrough curve which was more nearly approximated by the Poisson distribution.

In the middle and later 1950's there were many studies of dispersion in sand-filled columns, which were related to hydrology. Day (1956) investigated a salt-water replacement system and based his analysis on the diffusion equation and Scheidegger's disordered model to explain data obtained in the laboratory. Rifai and others (1956) published what was perhaps one of the most comprehensive laboratory and theoretical studies to that time. The theoretical part of their study employed both the capillary-tube and the disordered-medium models. As was expected, the two models gave identical results because of the applicability of the central limit theorem (Beran, 1957) in the disordered-medium model. In essence, the application of the central limit theorem indicated that the diffusion equation was valid. Both laboratory and theoretical results indicated that the dispersion coefficient in the

direction of flow was nearly proportional to the first power of the average velocity, which confirmed Scheidegger's prediction.

The results of studies by Rifai and others have been largely confirmed by many investigators; however, there are some indications that the dispersion coefficient is proportional to a power of the velocity which is slightly greater than one. It will be shown in a subsequent section that, if the flow similitude is specified by the Reynolds number and the mass transport by the Schmidt number, this power is very near one. Studies of friction losses in consolidated media (Muskat, 1946), indicated that the Reynolds number, unless modified to some extent, did not adequately specify the similitude conditions. Efforts to extend the Reynolds number concept to flow in other than isotropic unconsolidated material have not been successful.

Experimental evidence indicated that the magnitude of the dispersion coefficient was not equal in all directions. In fact, the very nature of the flow system makes it highly unlikely that the magnitudes would be the same. Hence, Jong (1958) and Saffman (1959, 1960) developed a model of random flow paths to compute the magnitude of the dispersion in directions both parallel and transverse to the flow. The mere existence of individual grains in porous material gave rise to microscopic velocity components transverse to the direction of the average flow, thereby creating the lateral movement of the contaminant and the velocity dependency of the dispersion coefficient.

This concept was extended by Bear (1961) in a paper on the tensor form of the dispersion coefficient. He verified the tensor characteristic of the coefficient experimentally by observing the dispersion of a tracer from a point source. Although there was little doubt that the coefficient was a tensor, Bear's experiment did not correct for the spread due to the volume of the tracer injected. On the basis of experience in other fields, such as heat flow and molecular diffusion, it can be assumed that the generalized transport coefficient may be characterized as a tensor.

The magnitude of the dispersion coefficient was dependent not only on the fluid velocity but also on the characteristics of the porous medium. Many experiments reported in the literature show this to be true. Among these were experiments by Orlob and Radhakrishna (1958), who explored the effect of entrapped air in a granular material, and by Biggar and Nielsen (1960), who examined sands and other types of naturally occurring soils to determine the effect of inhomogeneity and variations of particle sizes. Also, Skibitzke and Robinson (1963) obtained qualitative laboratory results that demonstrated the importance of heterogeneity of the medium.

To date, both theoretical and experimental investigations have been confined primarily to unidirectional flow. Although the experimental data indicated that dispersion was directionally dependent, they were not sufficient to enable a statement as to how the ratio of the magnitudes of the two components of the coefficient can be predicted in advance of an experiment. To depict transverse dispersion, Ogata (1961) developed a simplified mathematical model for steady flow, principally to analyze experimental results given in a later report (Ogata, 1964a; also Skibitzke, 1964). Harleman and Rumer (1962) used a similar mathematical model to correlate results of their experiments. Many results published in chemical journals will not be mentioned because they involved flow rates higher than those of interest here. Articles have appeared also in petroleum journals, but most of these articles are reviews of previous works generally with additional experimental data to supplement results of others so that empirical expressions can be developed.

DERIVATION OF THE BASIC FIELD EQUATIONS

The equation derived in this section is a statement of the law of conservation of mass. For simplicity, the development will be in terms of Cartesian (x, y, z) coordinates. The field equations can then be obtained readily in terms of other coordinate systems through known transformation.

The description of the mechanism of mass transport through a complex porous medium necessitates the adoption of a fictitious model such that average conditions can be more easily expressed. The first general assumption is that Darcy's law applies. This is corollary to the assumption that a piston-type flow occurs. In other words, 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 employed to approximate the real system. For the dispersion mechanism, this refinement involves a transport component that is analogous to Fick's first law. The justification for the use of this type of expression is given by Taylor (1953) in his study of laminar flow through pipes.

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.

ISOTROPIC DISPERSION

To establish the mathematical statement of the conservation of mass, consider a cubic element in the three-dimensional Cartesian space, as represented in figure 1. The two modes of transport of a fluid within

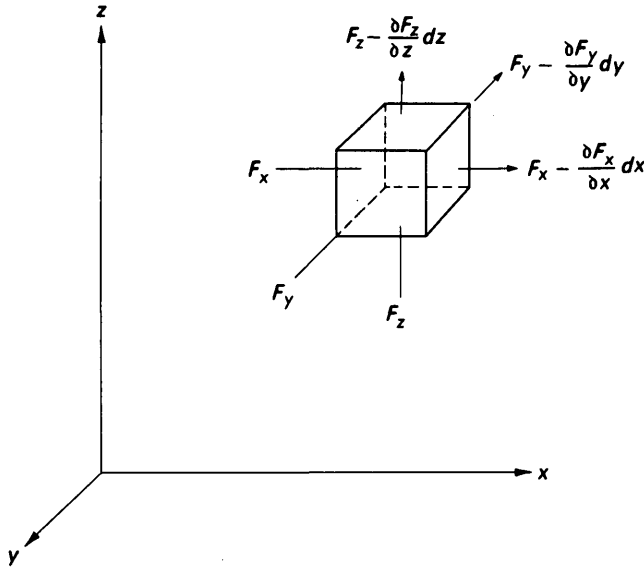


FIGURE 1.—Mass balance in a cubic element in space.

a porous medium have been described as (a) convection and (b) dispersion. In mathematical terms these modes for direction x (say) are expressed:

$$\text{Transport by convection} = uCdA$$

$$\text{Transport by dispersion} = D_x \frac{\partial C}{\partial x} dA,$$

where dA is an elemental cross-section area of the cubic element. 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

$$F_x = uC - fD_x \frac{\partial C}{\partial x},$$

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

870-887 Q-70—2

Similarly, expressions in the other two directions are written

$$F_y = vC - fD_y \frac{\partial C}{\partial y}$$

$$F_z = wC - fD_z \frac{\partial C}{\partial z}.$$

From figure 1, the total amount of solute entering a cubic element in space is

$$F_x dzdy + F_y dzdx + F_z dxdy.$$

The total amount leaving the cubic element is

$$\left(F_x - \frac{\partial F_x}{\partial x} dx\right) dzdy + \left(F_y - \frac{\partial F_y}{\partial y} dy\right) dzdx + \left(F_z - \frac{\partial F_z}{\partial z} dz\right) dxdy$$

where the partial terms indicate the spatial change of the fluid mass in the specified direction. Accordingly, the difference in the amount entering and leaving the cubic element is

$$\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dxdydz.$$

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

$$f \frac{\partial C}{\partial t} dxdydz.$$

The equating of the difference of outflow and inflow to the amount of dissolved substance accumulated within the cubic element leads to the relationship

$$\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = f \frac{\partial C}{\partial t}. \quad (1)$$

Equation 1 is a mathematical statement of the law of conservation of mass under the conditions stipulated. Vectorially, the equation is written

$$\nabla \cdot \mathbf{F} = f \partial C / \partial t.$$

Substituting the expressions for F_x , F_y , and F_z and assuming that $D_x = D_y = D_z = D = \text{constant}$ and since $\nabla \cdot \mathbf{q} = 0$, equation 1 becomes

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

where $\frac{d}{dt}$ is the operator $\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z}$. Equation 2

applies to both diffusion and heat transfer within a moving medium. Note that the terms u , v , and w as used in equation 2 now represent average velocities or the Darcy velocity divided by the porosity.

Because the characteristics of the dispersion coefficient other than its directional nature are not well understood, equation 2 was developed on the assumption that D was a constant. If D is a function of concentration, that is, if $D=f(C)$, equation 2 is written

$$\frac{dC}{dt} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right). \quad (3)$$

Equation 3 is nonlinear for $D=f(C)$ and can be solved only for simple expressions of $f(C)$, generally by numerical methods. These types of problems are encountered in the analysis of soil moisture and in some other types of diffusive processes. Excellent discussions of the numerical methods applicable in obtaining solutions for the one-dimensional equations are presented by Crank (1956) and also in many articles relating to soil-moisture movement.

ANISOTROPIC DISPERSION

All experiments conducted in two dimensions indicate that the magnitudes of the dispersion coefficient depend on the reference direction, with the larger value oriented in the direction parallel to the flow. To include this directional dependency in the equations requires that the coefficient D be represented by a more general mathematical construct known as a tensor. The complex properties of tensors are better described in texts on advanced mathematics and need not be included here.

In generalizing the dispersion coefficient into a tensor, Bear (1961) assumed an analogy with a tensor representing elastic deformation or tensor of the fourth rank. In three dimensions this tensor has 81 components, but because of symmetry the tensor has 21 nonzero components (Jeffreys, 1961, p. 78). Scheidegger (1961), in a verification of Bear's tensor, assumed dispersion to be analogous to turbulence rather than to elasticity. Because turbulence is not symmetrical to the same extent as elasticity, its tensor consists of 36 rather than 21 nonzero components. For unidirectional flow in an isotropic medium, however, the results of both Bear's and Scheidegger's analyses show that the dispersion coefficient is described completely by longitudinal and transverse components—in other words, by a tensor composed of only two components.

The difficulties inherent in the application of the tensor to evaluate mass transport arise from difficulties in measuring the various components. Thus, as in heat flow or diffusion, it is generally necessary to assume

that the dispersion coefficient is characterized by three independent components parallel to the chosen reference axes. Under this assumption the dispersion tensor is a second-rank tensor consisting of nine components. Jost (1960, p. 4), in discussing diffusion systems, argued that the existence of components other than those making up the main diagonal of the matrix is doubtful. However, this argument cannot readily be extended into the study of dispersion in granular media. Thus, for simplicity it is assumed that the dispersion coefficient is approximated by a tensor composed of, at most, nine components.

Using the standard notation for second-order tensors, the dispersion component of the transport equation can be expressed

$$-G_i = D_{ij} \frac{\partial C}{\partial x_j}, \quad i, j = 1, 2, 3. \quad (4)$$

In other words, the three components of mass transport are written

$$\begin{aligned} -G_1 &= D_{11} \frac{\partial C}{\partial x_1} + D_{12} \frac{\partial C}{\partial x_2} + D_{13} \frac{\partial C}{\partial x_3}, \\ -G_2 &= D_{21} \frac{\partial C}{\partial x_1} + D_{22} \frac{\partial C}{\partial x_2} + D_{23} \frac{\partial C}{\partial x_3}, \\ -G_3 &= D_{31} \frac{\partial C}{\partial x_1} + D_{32} \frac{\partial C}{\partial x_2} + D_{33} \frac{\partial C}{\partial x_3}, \end{aligned}$$

and the dispersion tensor D_{ij} can be represented by the matrix

$$D_{ij} = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}.$$

The advantage of the tensor notation is that it provides a shorthand method of describing, in general, the physical phenomena. Equation 4 describes the most useful case of dispersion in a porous medium and indicates that the three components of mass transport are determined not only by the direction of the maximum concentration gradient but also by the gradients at right angles to this direction. In an anisotropic medium, because the dispersion constant is dependent on the fluid and medium properties, the elements forming the matrix can be both time and space dependent. The dispersion tensor can be described by a single number, as in isotropic dispersion, or by a matrix which reflects the complexity of the porous medium itself. Only for isotropic media has the coefficient of dispersion been described successfully by experimental methods.

If the medium is isotropic and the Darcy velocity is constant, the transport equation in the x direction is $F_x = uC - G_x$; where G_x is the dispersion component.

The substitution of the transport equation into the continuity equation results in the field equation

$$\begin{aligned} \frac{dC}{dt} = & D_{11} \frac{\partial^2 C}{\partial x^2} + D_{22} \frac{\partial^2 C}{\partial y^2} + D_{33} \frac{\partial^2 C}{\partial z^2} \\ & + (D_{23} + D_{32}) \frac{\partial^2 C}{\partial y \partial z} + (D_{13} + D_{31}) \frac{\partial^2 C}{\partial z \partial x} \\ & + (D_{12} + D_{21}) \frac{\partial^2 C}{\partial x \partial y} \end{aligned} \quad (5)$$

Equation 5 describes the field distribution for a system of anisotropic mass transport. If $D_{11} = D_{22} = D_{33} = \text{constant}$ and $D_{ij} = 0$ for $i \neq j$, equation 5 is identical with equation 2. This results from the fact that equation 2 was developed under the assumption that D was a tensor of zero rank.

Equation 5 is known as a quadric, and by use of standard transformations it can be reduced to the form of equation 3. This transformation involves rotating the coordinate axes so that the reference axes parallel the principal axes of dispersion. Recent experimental and analytical studies point to the important fact that in isotropic and homogeneous media the principal axes of dispersion are oriented parallel and transverse to the mean direction of regional flow. This indicates that for such media the mass transport system can be defined by two characteristic dispersion components that are specified when the mean direction of regional flow is known.

Assuming that the principal axes can be defined, the dispersion tensor can be transformed so that only the elements of the major diagonal remain, all others being zero. The matrix representation of the tensor then becomes

$$D_{ij} = \begin{bmatrix} D_x & 0 & 0 \\ 0 & D_y & 0 \\ 0 & 0 & D_z \end{bmatrix}$$

In unidirectional flow, symmetry about the mean flow line exists so that $D_y = D_z$.

The possible representation of the dispersion coefficient in the manner depicted by the matrix is significant because of the internal complexity of the porous environment. Actually, the dispersion of a fluid flowing through a homogeneous porous medium is the result of the averaging process necessary to describe the flow of ground water. In essence, this signifies that provided all the possible microscopic changes in the magnitude and the direction of the pore channels can be expressed quantitatively, the components of the dispersion tensor can be computed by statistical means.

SOME USEFUL TRANSFORMATIONS

The diffusion, or heat-flow, equation where $\text{grad } \vec{q}C = 0$ has been studied extensively and published in detail by Carslaw and Jaeger (1959), Crank (1956), and Jost (1960). For various types of boundary-valued problems it is expedient to transform the field equation so that the convective terms do not appear explicitly.

Two methods can be used to remove the explicit convective terms for problems in which the boundary conditions involve media of infinite extent. These transformations require the introduction of a new coordinate system or a change in the independent variables. First consider the transformation of a standard-rectilinear coordinate system into a new system called moving coordinates. The dispersion equation including the directional properties of coefficient D is

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \quad (6)$$

A transformation similar to one commonly used in the study of wave equations is given by the expressions

$$\xi = x - ut, \quad \eta = y - vt, \quad \zeta = z - wt, \quad \text{and } \tau = t.$$

Using the chain rule of partial differentiation, the above expressions are substituted in equation 6. For example, the transformation of $\partial C / \partial x$ is given by

$$\frac{\partial C}{\partial x} = \frac{\partial C}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial C}{\partial \tau} \frac{\partial \tau}{\partial x} = \frac{\partial C}{\partial \xi}$$

Two similar expressions for η and ξ coordinates can be obtained in the same manner. The time differentiation follows the same rule and is given by

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial C}{\partial \tau} \frac{\partial \tau}{\partial t} = \frac{\partial C}{\partial \tau} - u \frac{\partial C}{\partial \xi}$$

A similar method is utilized to determine the second differentiation with respect to the x , y , and z coordinates. Substitution in equation 6 reduces it to the form

$$\frac{\partial C}{\partial \tau} = D_x \frac{\partial^2 C}{\partial \xi^2} + D_y \frac{\partial^2 C}{\partial \eta^2} + D_z \frac{\partial^2 C}{\partial \zeta^2}, \quad (7)$$

which is analogous to the heat conduction or diffusion equation. The transformation of coordinates did not involve rotation of the coordinate axes; hence, the dispersion coefficient D_i is still oriented in the original x , y , and z or the new ξ , η , and ζ directions.

Introduction of the above transformation in effect creates a system based on coordinates that move in

space at a rate dependent on the magnitudes of the average fluid-flow velocities. Physically, this may be pictured as an observer moving along with a velocity \vec{q} while watching the process of dispersion. The choice of this new coordinate system is possible because the transport due to convection is a conservative process; hence, stopping the fluid movement to simplify the analysis of the dispersion process is permissible. However, the transformation does pose difficulties as, for example, in problems where certain conditions are specified at an initial point. In such problems the transformation tends to increase the difficulty of inserting the specified conditions in the solution of the differential equation. To illustrate, consider the problem where the concentration C is specified at the point $x=y=z=0$; say, $C(0,0,0,t)=C_0$, where C_0 is a constant. It is noted that when $x, y, z=0$; $\xi, \eta, \zeta=-qt$, where $q=u, v, w$, respectively. The problem now becomes one of describing the concentration for a system in which the concentration is specified at points in space depending on the time. This tends to increase the complexity of the mathematical analysis, unless there is symmetrical distribution of concentration about the source of fluid at $x=0$.

The second transformation method involves the substitution of a new dependent variable. In this instance, it is assumed that the solution of the problem can be expressed functionally by

$$C = \exp \left[\frac{u}{2D_x} \left(x - \frac{ut}{2} \right) + \frac{v}{2D_y} \left(y - \frac{vt}{2} \right) + \frac{w}{2D_z} \left(z - \frac{wt}{2} \right) \right] \Gamma(x, y, z, t),$$

where $\Gamma(x, y, z, t)$ is an unspecified function. Assuming that, generally, the solution of the diffusion equation is of this nature, the next step is to determine the function $\Gamma(x, y, z, t)$. The solution must satisfy equation 6; hence, substitution gives the expression

$$\frac{\partial \Gamma}{\partial t} = D_x \frac{\partial^2 \Gamma}{\partial x^2} + D_y \frac{\partial^2 \Gamma}{\partial y^2} + D_z \frac{\partial^2 \Gamma}{\partial z^2}, \quad (8)$$

which is the diffusion equation. The boundary conditions, as given in the preceding paragraph, must be written as a time-dependent variable at a specified point in space. Because Γ_0 (say) is specified at a given point in space, an analysis using equation 8 introduces no further difficulties.

In general, the transformations leading to equations 7 and 8 work well for dispersion in media of infinite extent. In the event of a finite boundary—the concentration is specified along $x, y, z=L$ —some other transfor-

mation of equation 6 must be utilized to circumvent the specification of concentration at infinity.

Usually, mathematical solutions are readily found for the dispersion equation describing isotropic conditions; that is, for $D_x=D_y=D_z=D$. Thus, introducing the independent variable

$$x' = x\sqrt{\frac{D}{D_x}}, \quad y' = y\sqrt{\frac{D}{D_y}}, \quad z' = z\sqrt{\frac{D}{D_z}}$$

and substituting these independent variables in equation 6 gives

$$\frac{\partial C}{\partial t} + \text{div } q' C = D \nabla^2 C,$$

where

$$q' = iu\sqrt{\frac{D}{D_x}} + jv\sqrt{\frac{D}{D_y}} + kw\sqrt{\frac{D}{D_z}}$$

$$\nabla^2 = \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2}$$

i, j, k = unit vectors in the x, y , and z directions. To reduce this relation to the form of equations 7 and 8, the transformations previously discussed can be used.

DISPERSION EQUATION IN CYLINDRICAL AND SPHERICAL COORDINATES

The field equation as previously written is in rectangular or Cartesian coordinates. For some problems the cylindrical or the spherical coordinates may be more suitable for analysis. The fundamental equations governing the dispersion process are readily derived in much the same manner as before by stating the mass balance within a reference space as defined by the given coordinate system. Similarly, coordinate transformations are readily accomplished because the interrelationships between any given coordinate systems are known.

In cylindrical coordinates the isotropic dispersion equation is

$$\begin{aligned} \frac{\partial C}{\partial t} + q_r \frac{\partial C}{\partial r} + q_\theta \left(\frac{1}{r} \right) \frac{\partial C}{\partial \theta} + q_z \frac{\partial C}{\partial z} \\ = D \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2} \right]. \quad (9) \end{aligned}$$

And in spherical coordinates the equation is

$$\begin{aligned} \frac{\partial C}{\partial t} + q_r \frac{\partial C}{\partial r} + q_\theta \left(\frac{1}{r} \right) \frac{\partial C}{\partial \theta} + q_\phi \left(\frac{1}{r \sin \theta} \right) \frac{\partial C}{\partial \phi} \\ = D \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial C}{\partial \theta} \right) \right. \\ \left. + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 C}{\partial \phi^2} \right]. \quad (10) \end{aligned}$$

FIELD EQUATION FOR TWO-FLUID SYSTEMS

In the development of the dispersion equation the density and viscosity of the contaminant fluid was assumed to be the same as the surrounding original or uncontaminated fluid. In cases where high concentrations of a contaminant occur, as in an aquifer subject to salt-water encroachment in coastal regions, this assumption is no longer valid. In such an environment both the viscosity and the specific weight of the contaminated fluid change. Addition of the gravity force is now necessary for analyzing the concentration distribution along the interface between the contaminated and uncontaminated fluids. The gravity force exerts so large an influence on the flow field that the position of a particle of contaminated fluid at any given time is largely predetermined by this force. That is, the description of the velocity field is dependent on the dynamic equilibrium position of the interface between the two fluids. Thus, definition of the dispersion process in a two-fluid system requires complete knowledge of both the fluid properties and the flow field.

When no chemical reaction between the fluids and the solids take place, the dispersion equation is the same as previously described with the provision that velocity is space dependent. Hence, the field equation is written

$$D_z \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} = \frac{\partial C}{\partial t} + \text{div } \vec{q}C. \quad (11)$$

Equation 11 indicates that the field equation is completely specified provided the flux \vec{q} is determined. Although conditions depart somewhat from those studied by Darcy, it is assumed that the flow equation may be generalized such that

$$\vec{q} = -\frac{K}{\rho g} (\nabla p - \rho \vec{g}). \quad (12)$$

The schematic diagram of a two-fluid model under dynamic equilibrium conditions is shown in figure 2. The description of the transport of salt requires the complete solution of equation 11 subjected to equation 12. Inasmuch as equation 11 is nonlinear it is virtually unsolvable without the use of numerical methods or various simplifications. For example, Jong (1959) defined the flow system in terms of curvilinear coordinates oriented with respect to the assumed position of the interface, thereby enabling the use of a two-dimensional system. Paralleling the classical hydrodynamics, a stream function is introduced into the analysis. The pertinent components of the stream function are defined as

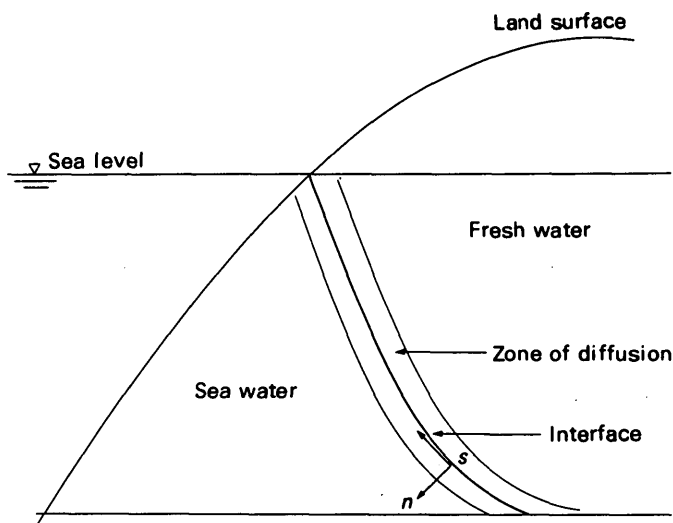


FIGURE 2.—Schematic diagram of coastal aquifer system.

$$q_s = -\partial\psi/\partial n$$

$$q_n = \partial\psi/\partial s$$

where s and n denote the directions parallel and normal to the interface, respectively, as shown in figure 2. The components of flow in the specified reference frame (eq 12) are

$$\begin{aligned} \frac{\mu}{k} q_s &= -\frac{\partial p}{\partial s} - \gamma \frac{\partial y}{\partial s} \\ \frac{\mu}{k} q_n &= -\frac{\partial p}{\partial n} - \gamma \frac{\partial y}{\partial n}, \end{aligned} \quad (13)$$

where $k = \frac{K\mu}{\rho g}$. Accordingly, substituting the stream function in equation 13, the continuity equation may be written

$$\nabla^2 \psi = \frac{k}{\mu} \frac{\partial \gamma}{\partial x} - \frac{1}{\mu} \left[\frac{\partial \mu}{\partial x} \left(\frac{\partial \psi}{\partial x} \right) + \frac{\partial \mu}{\partial y} \left(\frac{\partial \psi}{\partial y} \right) \right]. \quad (14)$$

The terms in the brackets are included to show the effect of viscosity μ which is dependent on the salt concentration in the fluid. The right side of the equation describes the effects of changes in density and viscosity.

Equation 14 is analogous in form to a vorticity equation that frequently appears in the potential theory in hydrodynamics. This vorticity equation has been studied in classical hydrodynamics, and methods of solution for various boundary conditions are described in a number of texts; for example, Milne-Thomson (1961, p. 564). Equation 14 is also substantially the same equation derived by Henry (1960) in evaluating the two-fluid system. Henry used the same basic flow equation, expressed the specific weight γ in terms of the salt concentration C , and assumed that the viscosity

change due to that concentration is small. Hence, the equation he derived is in the form

$$\nabla^2 \psi = \frac{k_1 y_0}{Q} \frac{\partial C'}{\partial x'}, \quad (15)$$

where $k_1 = k \left(\frac{\rho_1 - \rho_0}{\rho_0} \right)$, y_0 is the aquifer thickness, Q is the aquifer discharge, C' is the ratio between the concentration of salts in the aquifer water and the sea water C/C_s , and x' is the dimensionless length x/y_0 . Equations 14 and 15 differ only in that the first specifies possible effects of the viscosity changes.

To simplify the analysis, Jong (1959) dealt with the vorticity equation (eq 14), excluding the terms in brackets since the change in viscosity is small. He showed that the analysis can be carried out by replacing real fluids with fictitious fluids and by introducing singularities parallel to the interface of the system. The characteristics of the singularities are determined by the actual observed velocity distribution; in other words, the singularities are chosen so that the original velocity distribution in the two fluids is reproduced. The method, thus, makes possible computation of the position of the interface between two fluids of different densities. Because the equations are derived for steady-state conditions, the final position of the interface can be computed for any given flow conditions.

Equation 15 describes the flow conditions, in terms of a stream function, for the change in specific weight of the fluid with the change in salt content. However, the transport of the salt is also dependent on mechanical dispersion; thus, equation 15 specifies only a part of the problem. In other words, equation 15 describes the flow field within the transition zone containing fluids of different densities, and the transport of mass within this zone needs to be described by the dispersion equation. The solution of the vorticity equation given by Jong makes it possible to compute the location of the interface for any specified time, from which the stream function can be determined for the whole flow field. When unsteady conditions prevail, these solutions may still be used as long as the changes in the flow field are small. The transport system, however, must be described subsequent to description of flow in order to determine the dispersion effects on the frontal zone.

Since by definition $q_x = \partial \psi / \partial y$ and $q_y = -\partial \psi / \partial x$, substitution into the two-dimensional steady-state transport or dispersion equation leads to

$$\frac{D}{Q} \nabla^2 C' = \frac{\partial \psi}{\partial y'} \frac{\partial C'}{\partial x'} - \frac{\partial \psi}{\partial x'} \frac{\partial C'}{\partial y'}. \quad (16)$$

Equation 16 is thus an approximation of the steady-state mass transport process which can be completely

specified, provided ψ is specified by equation 15. Henry (1960) has developed solutions for two special instances of the transport equation and has evaluated them numerically.

ADSORPTION

In the discussion and development of dispersion equations to this point, no means of mass transport has been considered other than mechanical dispersion and convective transport. In the isotropic systems usually studied in the laboratory, the spread of tracers in the fluid is generally observed to be small, which indicates that the magnitude of the dispersive term is small. All soil complexes display an additional component of mass transfer generally termed "adsorption." Adsorption is a chemical reaction in which mass transfer occurs by actual removal of the dissolved substance from the liquid phase owing to mutual attraction between the substance and the solid phase of the porous medium. Generally speaking, in natural flow systems this process is of major magnitude with the fate of any contaminant introduced into the soil or the ground-water system dependent to a large extent on the capacity of the solid matrix material to adsorb the dissolved component. This is recognized by most workers in the field of radioisotope disposal; however, the major research is confined to surface chemistry which takes into account the microscopic aspects of the adsorption process.

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

$$\frac{u_T}{u} = \frac{1}{1+M}; M = \frac{S\rho}{Cf},$$

where

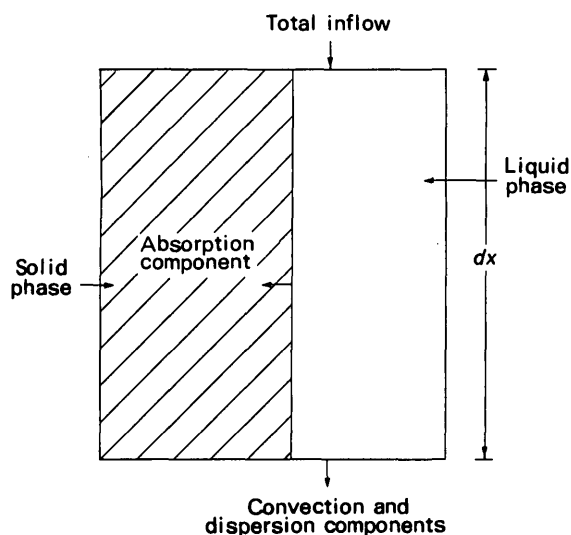
S = trace component adsorbed per gram of solid matrix,

ρ = bulk density of solid matrix, and

u_T = velocity of tracer.

This expression was established empirically and has 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 by equation 3. The adsorption component in the physical model can be pictured as a mathematical sink or source with its strength dependent on the difference of concentration of the liquid phase and the solid phase. A simplified model is illustrated in figure 3. Here, it is



(From Bird and others, 1960)

FIGURE 3.—Schematic diagram of transport in porous medium.

assumed that the adsorption component is in one direction only.

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

$$D\nabla^2 C = \frac{dC}{dt} + \frac{\partial S}{\partial t}, \quad (17)$$

where S is defined simply as the concentration of the solid phase. The function S has the same dimension as C .

The analysis of dispersion in adsorbing media—that is, the use of equation 17—depends on the representation of S in terms of C , where it is assumed that the relationship $\partial S/\partial t = f(C)$ holds. To describe this phenomenon completely requires a macroscopic study of the energy state at any equilibrium condition as prescribed by thermodynamic principles. Because of the complexity of the subject, especially when the kinetics of transfer rates is included, no detailed discussion is presented. Excellent discussions are included in Glassstone (1961) and Adamson (1960). This discussion is limited to the use of simplified expressions that have been applied in studies of reaction columns.

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

$$\frac{\partial S}{\partial t} = b(C - mS), \quad (18)$$

where b and m are constants. As indicated by Crank (1956), this equation describes a first-order reversible reaction and is applicable to some ion-exchange proc-

esses in fluids flowing in porous substances. Note that, when the term mS is much smaller than C , the expression reduces to a form similar to Langmuir's equilibrium isotherm for low concentrations or

$$\frac{\partial S}{\partial t} = bC. \quad (19)$$

Equation 19 is applicable to a first-order irreversible reaction wherein the soil particle may be thought to act as a mathematical sink.

Extending the expression given as equation 18 a little further, it may be written

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

where $n \leq 1$. Note that for the special case of $n=1$, this is equation 18. The need to determine three unknown parameters makes the above equation difficult to evaluate even under the rather idealized conditions encountered in a laboratory. Again assuming that $mS \ll C$, the equation may be written in the simpler form

$$\frac{\partial S}{\partial t} = bC^n, \quad (20)$$

which is virtually the expression for Freundlich's equilibrium isotherm.

The three types of reaction rates represented by equations 19–21 are discussed by Crank (1956, p. 121) in reference to a diffusion system involving various boundary conditions. The solution of the simultaneous equations represented by equations 3 (for a constant D), 18, and 19 can be determined by operational methods. A numerical method, however, must be used to solve equation 20. When equation 19 is used to represent the reaction rate, direct use can be made of solutions for various boundary conditions in heat flow reported extensively by, for example, Carslaw and Jaeger (1959). The reversible reaction system, equation 20 for diffusion in a plane sheet, has been analytically determined by Crank (1956, p. 132) for the boundary conditions

$$S = C = 0, \quad -a \leq x \leq a, \quad t = 0$$

$$L \frac{\partial C}{\partial t} = \mp D \frac{\partial C}{\partial x}, \quad x = \pm a, \quad t > 0.$$

The solution, however, is too complex to be reproduced. Ogata (1964b) obtained a solution for a semi-infinite medium, which will be presented as one of the mathematical examples.

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 ground-water reservoir is largely dependent on the amount transferred between the liquid and solid phases. Perhaps the most realistic macroscopic appraisal available is in the results of reaction-tower experiments. The analytical difficulties that appear whenever the adsorption isotherm is nonlinear are formidable, however, not insurmountable.

MATHEMATICAL TREATMENT OF THE DISPERSION EQUATION

The analytical treatment of dispersion phenomena within a porous matrix, based on the preceding theoretical development, presupposes that the dispersion coefficient is a known parameter. Thus, the full definition of the physical system depends on accumulation of data concerning this specific parameter. It will become apparent in the following discussion that only the simpler dispersion systems are treated primarily because of the need for laboratory confirmation. The discussion is, therefore, not intended to be a complete presentation of all known solutions of the differential equation. Also, this section presents methodology considered useful in the analysis of the dispersion equation.

The analytical methods, namely, Laplace transforms, the product solution, and the point source solution are the principal tools used in the study of the differential equation. These techniques are discussed to some extent in the work of Carslaw and Jaeger (1959) and in many texts in advanced calculus.

All the examples to follow are limited to flow in a semi-infinite medium. The use of more complex boundaries adds little to the study of the fundamental characteristics of the mass transport system because of the complexity of the final expression. The principal objective is to investigate initially the nature of dispersion. Hence, the convective term— $\text{div } \vec{q}C$ —will be assumed to be given by $u \partial C / \partial x$; in other words, the flow field is assumed constant and unidirectional. Space dependency of the dispersion coefficient is not considered; variation is limited to directional dependency only. In systems involving an adsorptive solid medium, the problem becomes highly complex and thus no analysis has yet been attempted for anything more complex than one-dimensional mass transport.

The examples given are intended only as samples of solutions available and may not be physically realistic. This is especially true in examples 3 and 4 where a system involving a disk source was chosen to depict a two-dimensional case. Example 3 actually may not be physically realistic; however, it may possibly occur when the velocity u is small. That is, example 3 implies that a concentration gradient occurs at $x=0$.

Numerous solutions available in the published literature are presented in the following pages. Whenever possible, a reference is given so that the complete development can be consulted by those who are interested. In addition a limited number of functions, which the author arranged to have computed, are presented in graphical form as appropriate.

The first two examples considered are for dispersion within a semi-infinite medium in a unidirectional flow field. It is postulated that the concentration is specified at $x=0$ and at the initial time $t=0$. The system is defined schematically in figure 4. For the specified field conditions, the field equation (eq 6), omitting the subscript x , becomes simply

$$D \frac{\partial^2 C}{\partial x^2} = u \frac{\partial C}{\partial x} + \frac{\partial C}{\partial t} \quad (21)$$

The subscript x has been dropped in equation 21, since dispersion occurs only in the x direction.

Example 1.—The plane $x=0$ is maintained at a concentration $C=C_0$.

The boundary conditions are given by

$$\begin{aligned} C(x,0) &= 0, & x &\geq 0 \\ C(0,t) &= C_0, & t &\geq 0 \\ C(\infty,t) &= 0, & t &\geq 0. \end{aligned}$$

The method best suited is the Laplace transforma-

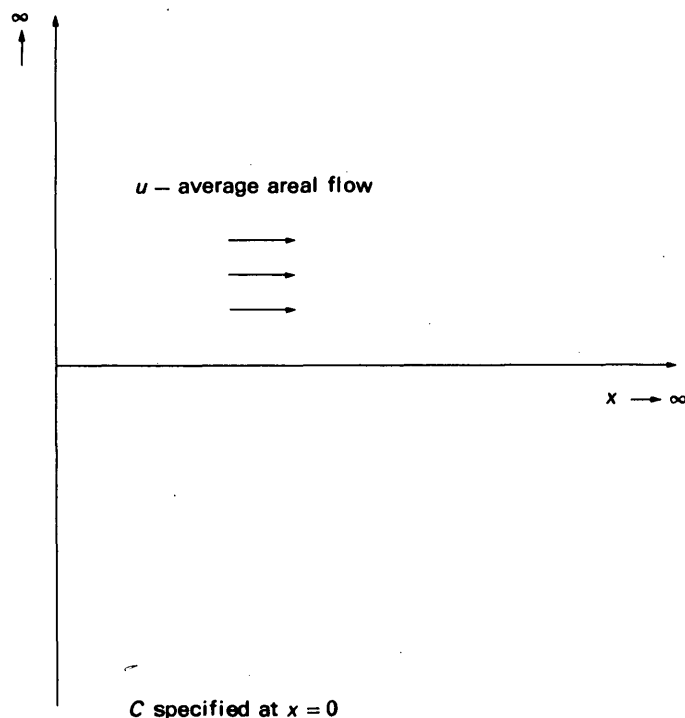


FIGURE 4.—Definition sketch of one-dimensional system.

tion; substitution of the transform leads to the subsidiary system given by the equation

$$D \frac{d^2 \bar{C}}{dx^2} = u \frac{d\bar{C}}{dx} + p\bar{C}.$$

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

$$\frac{\bar{C}}{C_0} = \frac{1}{p} \exp \left[\frac{ux}{2D} - x \left(\frac{u^2}{4D^2} + \frac{p}{D} \right)^{1/2} \right].$$

The inverse transform as given by Erdelyi and others (1954, p. 246) is readily determined as

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left(\frac{x-ut}{2\sqrt{Dt}} \right) + \frac{1}{2} \exp \left(\frac{ux}{D} \right) \operatorname{erfc} \left(\frac{x+ut}{2\sqrt{Dt}} \right). \quad (21a)$$

Example 2.—The region $x \leq 0$, initially at concentration C_0 .

The boundary conditions of interest are specified by

$$\begin{aligned} C(x, 0) &= C_0, \quad x < 0, \\ C(x, 0) &= 0, \quad x > 0, \\ C(\infty, t) &= 0, \quad t \geq 0, \\ C(-\infty, t) &= C_0, \quad t \geq 0. \end{aligned}$$

Again, various analytical methods are available; the simplest and most straightforward method involves the use of a plane-source solution as the fundamental solution. The concentration at any point in space (see, for example, Rifai and others, 1956, p. 54) is given by the expression

$$C = \frac{C_0}{2\sqrt{\pi Dt}} e^{-\xi^2/4Dt}.$$

Summing over all possible values of ξ , gives

$$\begin{aligned} \frac{C}{C_0} &= \frac{1}{2\sqrt{\pi Dt}} \int_{-\infty}^{\infty} e^{-\xi^2/4Dt} d\xi = \frac{1}{\sqrt{\pi}} \int_{\xi/2\sqrt{Dt}}^{\infty} e^{-\eta^2} d\eta \\ &= \frac{1}{2} \operatorname{erfc} (\xi/2\sqrt{Dt}), \end{aligned} \quad (21b)$$

where $\xi = x - ut$.

The graphical representation of the solutions given for examples 1 and 2 appears in figures 5 and 6. Note that because a constant concentration is maintained at $x=0$, example 1 exhibits an asymmetrical concentration distribution about $x=ut$. However, it has been shown that the conditions of flow through porous media are such that the second term in equation 21a is negligible (Ogata and Banks, 1961). Hence, the two systems exhibit no difference at some distance from the source.

Consider now, the system that is described within a two-dimensional frame of reference because of symmetry about a given axis. The definition plane is given in figure 4. Because of the mathematical complexities, this system is illustrated using circular surface sources maintained at constant strength and constant concentration. The results are sufficiently complex that in a discussion on evaluation of the dispersion coefficient (p. I30-I32) an approximation is used to simplify the computations.

Assuming again a unidirectional ground-water flow field with parameters D_x and u oriented in the x direction and D_r in the r direction normal to x , the field equation for the radially symmetrical system becomes

$$\frac{D_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) + D_x \frac{\partial^2 C}{\partial x^2} = u \frac{\partial C}{\partial x} + \frac{\partial C}{\partial t}. \quad (22)$$

Equation 22 is equation 9 when symmetry exist about the axis x ; in other words, the variation in concentration with respect to the angle θ is zero.

Example 3.—A disk source, $0 \leq r \leq a$ located at $x=0$ emitting at constant rate $F=F_0$.

The boundary conditions are

$$\begin{aligned} F &= F_0 \text{ at } x=0, \quad 0 \leq r \leq a, \quad t \geq 0 \\ F &= 0 \text{ at } x=0, \quad r > a, \quad t > 0. \end{aligned}$$

Initially, the fluid in the porous medium is at zero concentration.

The solution of this system is readily determined by use of the point source. Using the method described by Carslaw and Jaeger (1959, p. 266), the expression applicable for an instantaneous disk source is

$$\frac{C}{F_0} = \frac{a}{2\sqrt{\pi D_x t}} \exp \left(-\frac{\xi^2}{4D_x t} \right) \int_0^\infty e^{-D_r \lambda^2} J_0(r\lambda) J_1(a\lambda) d\lambda,$$

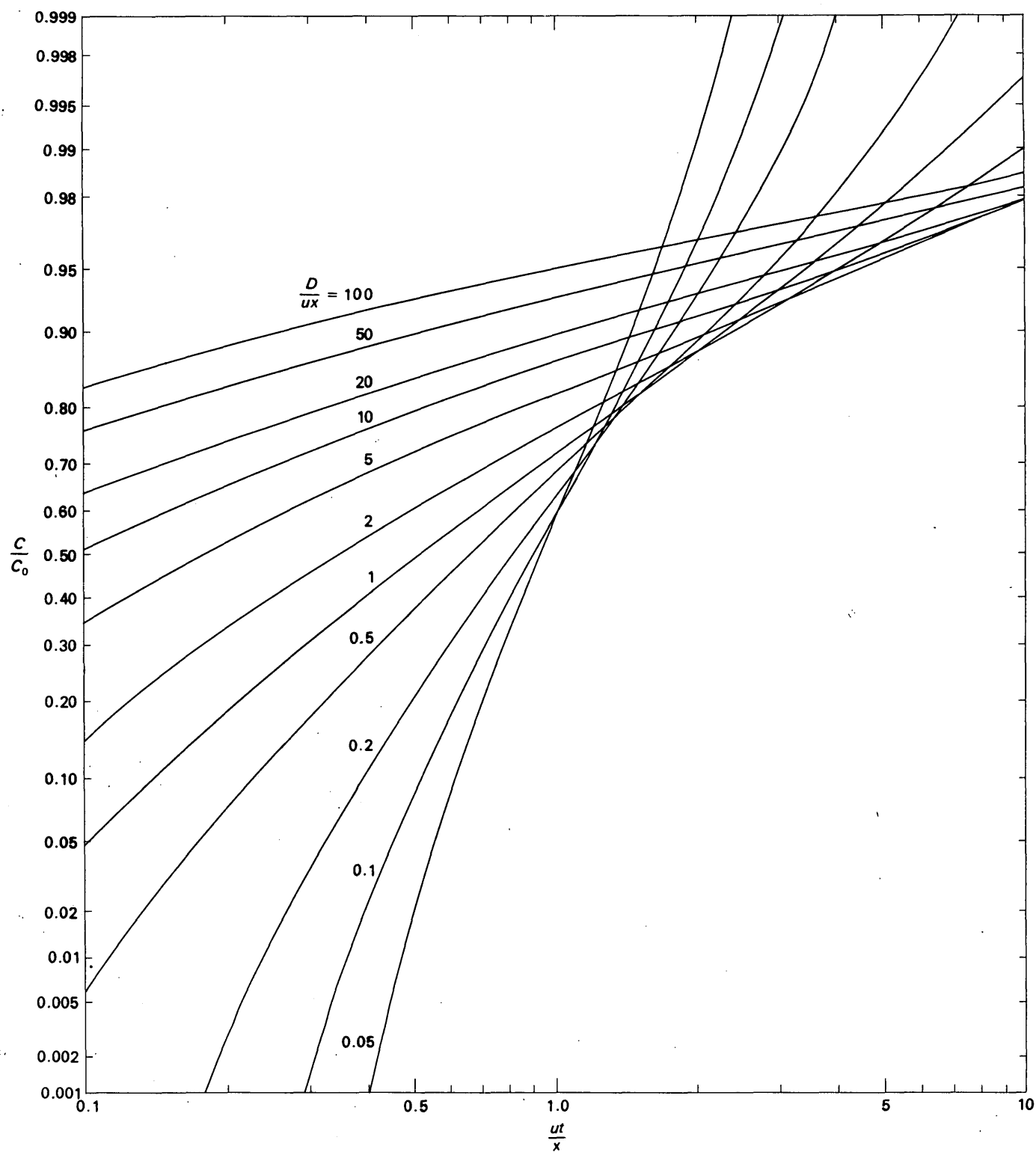
where $\xi = x - ut$. For the special case $D_r = D_x = D$ and $u=0$, the expression is the same as equation 9, page 260, in Carslaw and Jaeger (1959).

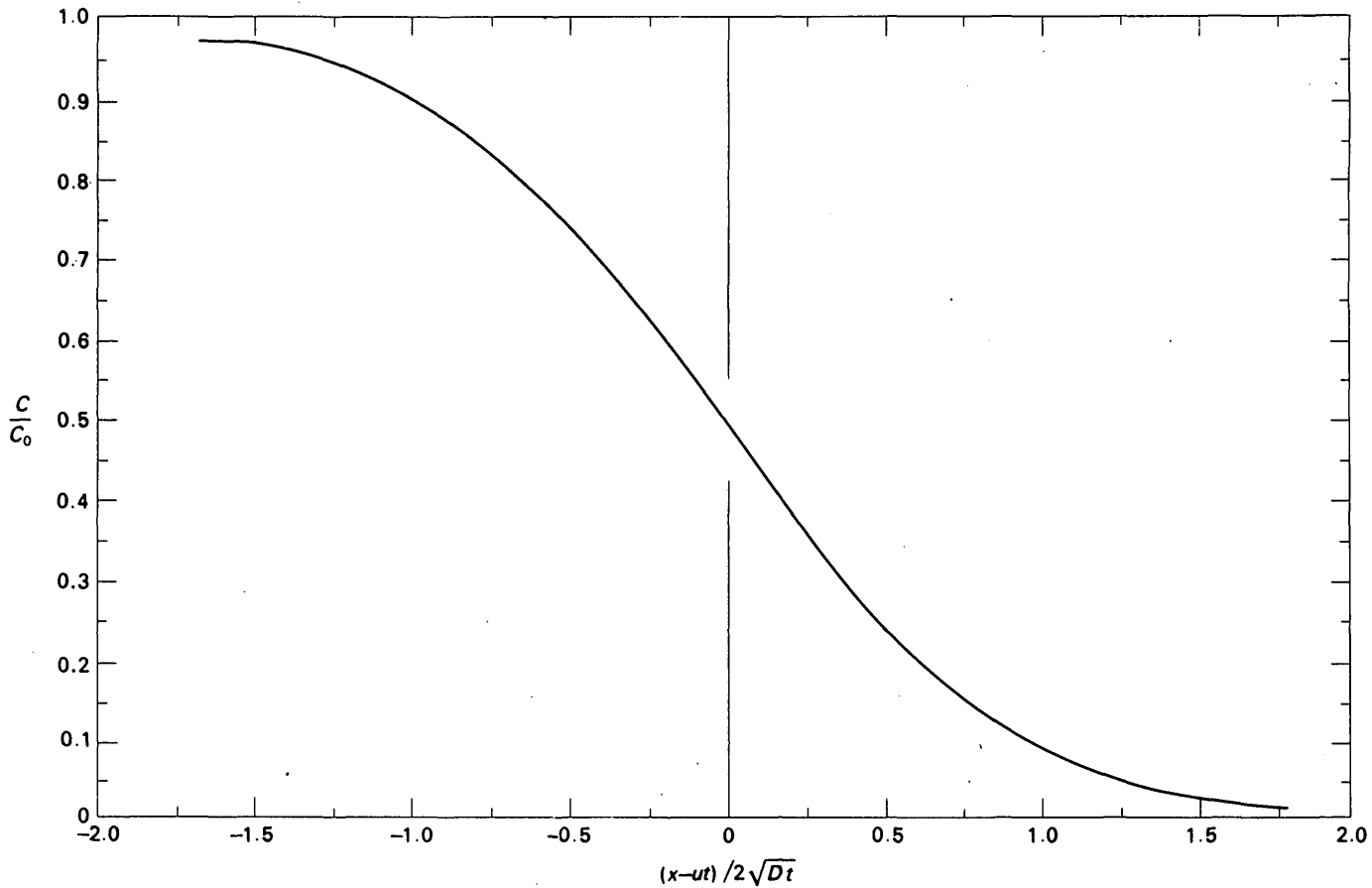
To obtain an expression for the continuous disk source, the above equation is integrated between the limits 0 to some time t . After some algebraic manipulation the integral equation is written

$$\frac{C}{F_0} = \frac{2ae^{\beta\alpha}}{u\sqrt{\pi}} \int_0^\beta e^{-\gamma^2 - \alpha^2/\gamma^2} \int_0^\infty e^{-\gamma^2 r^2 \lambda^2} J_0(r\lambda) J_1(a\lambda) d\lambda d\gamma,$$

where

$$\beta = \frac{u}{2} \sqrt{\frac{t}{D_x}}, \alpha = \frac{ux}{4D_x}, \text{ and } \gamma^2 = \frac{4D_x D_r}{u^2}.$$

FIGURE 5.—Concentration distribution; plane source at $x=0$ maintained at constant concentration.

FIGURE 6.—Concentration distribution; region $x \leq 0$ initially at constant concentration.

The above expression may be written in two alternative ways, or

$$\frac{C}{F_0} = \frac{2e^{2\alpha}}{u\sqrt{\pi}} \int_0^\beta e^{-t^2 - \alpha^2/\zeta^2} \left[1 - J\left(\frac{a^2}{4\gamma^2\zeta^2}, \frac{r^2}{4\gamma^2\zeta^2}\right) \right] d\zeta,$$

where

$$1 - J(x, y) = x^{1/2} \int_0^\infty e^{-\tau} J_0(2\sqrt{\tau y}) J_1(2\sqrt{\tau x}) \frac{d\tau}{\tau},$$

and

$$\frac{C}{F_0} = \frac{ae^{2\alpha}}{2u} \int_0^\infty J_0(r\lambda) J_1(a\lambda) \left\{ \exp(-2\alpha\sqrt{1+\gamma^2\lambda^2}) \operatorname{erfc}\left[\frac{\alpha}{\beta} - \beta\sqrt{1+\gamma^2\lambda^2}\right] - \exp(2\alpha\sqrt{1+\gamma^2\lambda^2}) \operatorname{erfc}\left[\frac{\alpha}{\beta} + \beta\sqrt{1+\gamma^2\lambda^2}\right] \right\} \frac{d\lambda}{\sqrt{1+\gamma^2\lambda^2}}.$$

For the steady-state condition, that is, letting $t \rightarrow \infty$ in the above expression, the equation obtained is

$$\frac{C}{F_0} = \frac{a}{u} \int_0^\infty \exp[2\alpha(1 - \sqrt{1+\gamma^2\lambda^2})] J_0(\lambda r) J_1(\lambda a) \frac{d\lambda}{\sqrt{1+\gamma^2\lambda^2}}.$$

The steady-state solution, although simpler, cannot be integrated and must be evaluated numerically. Along the axis $r=0$, the integral equation can be expressed in terms of an elementary function or,

$$\frac{uC}{F_0} = 1 - \exp(2\alpha - 2\sqrt{\alpha^2 + \gamma^2}).$$

Example 4.—A disk surface source $0 \leq r \leq a$ located at $x=0$ and maintained at a constant concentration C_0 .

This example considers the steady state only since the solution is not available for the transient system. The boundary conditions for this specific problem are

$$C(0, r) = C_0, \quad 0 < r < a$$

$$C(0, r) = 0, \quad r > a$$

$$C(\infty, r) = 0, \quad r \geq 0.$$

$$C(x, \infty) = 0, \quad x \geq 0.$$

To analyze this problem, it is assumed that the solution is represented by the product of two functions of single variables, that is,

$$C = R(r)X(x),$$

where $R(r)$ is a function of r only, and $X(x)$ is a function of x only. Substitution for C in equation 22, noting that for steady state $\partial C/\partial t = 0$, the partial differential equation is reduced to the subsidiary equations

$$D_r \frac{d^2 R}{dr^2} + \frac{dR}{dr} + \zeta^2 R = 0$$

$$D_x \frac{d^2 X}{dx^2} - u \frac{dX}{dx} - \zeta^2 X = 0,$$

where ζ^2 is an unspecified constant.

The solutions of the subsidiary equation are readily obtained. The solutions are

$$R(r) = A_1 J_0(r\zeta/\sqrt{D_r})$$

$$X(x) = A_2 \exp [2\alpha (1 \pm \sqrt{1 + 4D_x \zeta^2/u})].$$

Because of the condition specifying C be zero as $x \rightarrow \infty$, the positive sign before the radical in the second equation is discarded. The solution is thus

$$C = A(\zeta) \exp [2\alpha (1 - \sqrt{1 + 4D_x \zeta^2/u})] J_0(r\zeta/\sqrt{D_r}).$$

The method of determining $A(\zeta)$ is described fully by Sneddon (1951, p. 59), the result is

$$\frac{C}{C_0} = a \int_0^\infty \exp [2\alpha (1 - \sqrt{1 + \gamma^2 \lambda^2})] J_0(\lambda r) J_1(\lambda a) d\lambda.$$

A similar solution for $D_r = D_x = D$ and $u = 0$ is given by Carslaw and Jaeger (1959, p. 214).

The steady-state solutions to examples 3 and 4 are almost identical, except for the factor $1/\sqrt{1 + \gamma^2 \lambda^2}$. The two solutions, presented as examples 3 and 4, are represented graphically in figures 7 and 8. The numerical computations for the integrals in examples 3 and 4 were accomplished by integrating under a curve with a polar planimeter. In both examples the function could not be integrated into a readily calculable form. However, the integrals can be evaluated by numerical methods for various values of $\eta = r/a$, which may be used in evaluating experimental data.

The previous examples considered dispersion in flow systems described by a single-space variable and by two-space variables. Examples 3 and 4 considered a radially symmetrical system with flow occurring along the cylindrical axis. Consider now, a line sink or a line source at $r = 0$ in a cylindrical reference frame. This is generally termed "a radial flow system." The definition of the geometrical configuration is presented in figure 9, and the applicable differential equation follows.

Writing the expression for the conservation of mass, with reference to the definition sketch (fig. 9), the differential equation is

$$\frac{\partial}{\partial r} \left(D \frac{\partial C}{\partial r} \right) + \frac{D}{r} \frac{\partial C}{\partial r} - u \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t}. \quad (23)$$

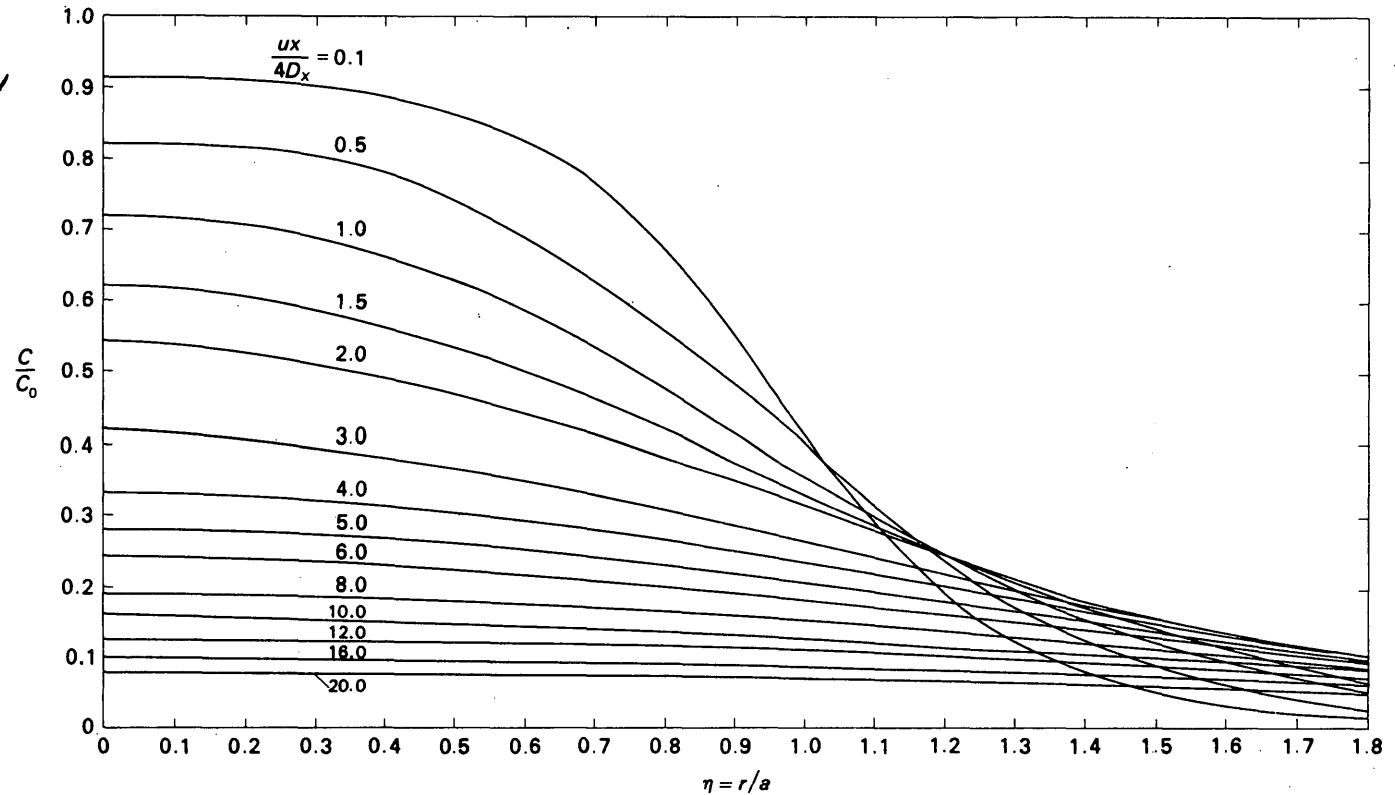


FIGURE 7.—Steady-state concentration distribution; circular surface source of constant strength.

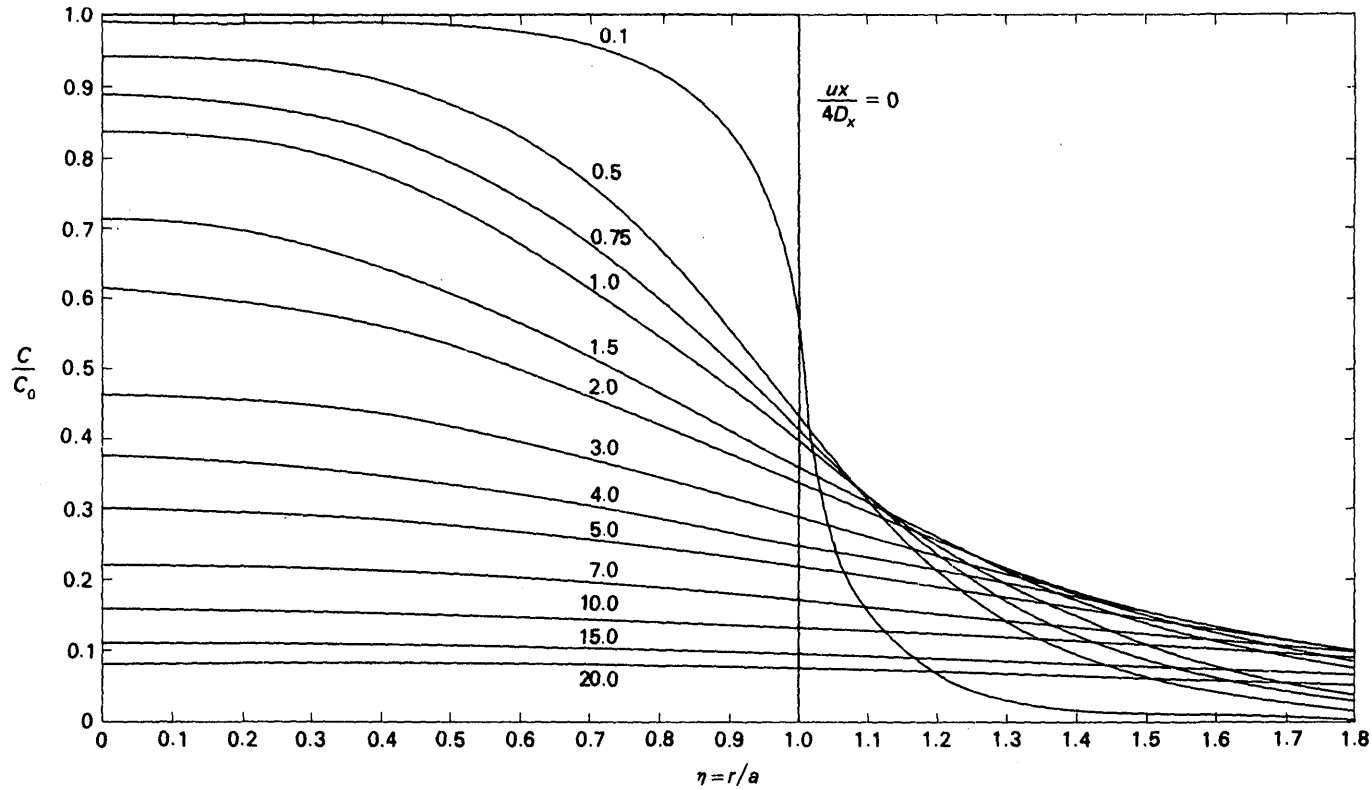


FIGURE 8.—Steady-state concentration distribution; circular surface source maintained at constant concentration.

Here, the concentration and the dispersion coefficient do not vary with the angle θ nor with the distance z which is normal to r . Equation 23 is written to allow for a possible space dependency of the dispersion coefficient D in the direction r . The basis of this space dependency comes from experimental and statistical findings that D is directly proportional to the velocity of the fluid stream. Since it is readily seen that the velocity is

inversely proportional to the distance from the source at $r=0$, this same relationship is assumed to hold for the dispersion coefficient.

The expression for fluid velocity may be formulated provided the quantity of flow or flux is specified at some value of $r=r_0$, generally near the source. Since flow is assumed steady, continuity requires that the velocity at any point is given by the expression $u=u_0 r_0/r$, where u_0 is the average velocity at $r=r_0$. Substituting the variable velocity into equation 23 leads to the expression

$$\frac{\partial}{\partial r} \left(D \frac{\partial C}{\partial r} \right) + \frac{D - u_0 r_0}{r} \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t} \quad (24)$$

Experimental evidence indicates that the dispersion coefficient D in a homogeneous medium varies very nearly with the first power of velocity; thus, D can be written

$$D = D_m u = D_m u_0 r_0 / r = D_0 / r,$$

where D_m is a constant related to the solid and liquid properties. Substituting the preceding expression into equation 24 gives

$$\frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial C}{\partial r} \right) + \frac{1 - \frac{a}{D_0} r}{r^2} \frac{\partial C}{\partial r} = \frac{1}{D_0} \frac{\partial C}{\partial t},$$

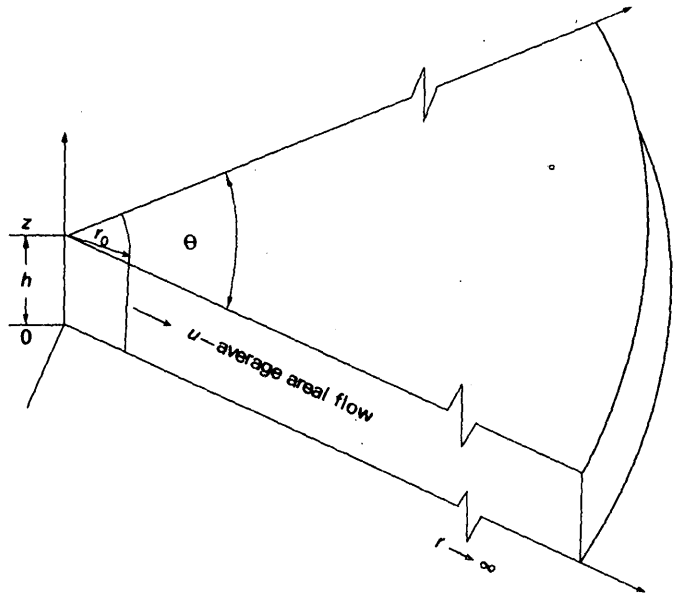


FIGURE 9.—Definition sketch of radial flow.

where $a = u_0 r_0$. Accordingly, collecting the terms leads to the equation

$$\frac{\partial^2 C}{\partial r^2} - \frac{a}{D_0} \frac{\partial C}{\partial r} = \frac{r}{D_0} \frac{\partial C}{\partial t} \quad (25)$$

Example 5.—Dispersion in a fluid flowing radially from a line source at $r=0$.

The boundary conditions to be satisfied are

$$C(r_0, t) = C_0, \quad t \geq 0$$

$$C(r, 0) = 0, \quad r > r_0$$

$$C(\infty, t) = 0, \quad t \geq 0.$$

The method of analysis because of convenience and simplicity in determining the coefficient of the solution is the Laplace transform. Equation 25 transforms to

$$\frac{d^2 \bar{C}}{dr^2} - \frac{a}{D_0} \frac{d\bar{C}}{dr} = \frac{pr}{D_0} \bar{C}.$$

The solution of the transformed problem is

$$\frac{\bar{C}}{C_0} = \sqrt{z} \exp \left[\frac{a}{2D_0} (z - z_0) \right] \left\{ K_{\frac{1}{2}} \left(\frac{2}{3} \sqrt{\frac{pz^3}{D_0}} \right) / p \sqrt{z_0} K_{\frac{1}{2}} \left(\frac{2}{3} \sqrt{\frac{pz_0^3}{D_0}} \right) \right\},$$

where $z = r - a/4D_0 p$, $z_0 = r_0 - a/4D_0 p$ and $K_{\frac{1}{2}}(x)$ is the modified Bessel function of the second kind of order $\frac{1}{2}$.

The inversion of the Laplace transformed system has been obtained by the use of the inversion theorem (Ogata, 1958, p. 88). The final expression is given by

$$\frac{C}{C_0} = 1 + \frac{2}{\pi} \exp \left[\frac{a}{2D_0} (r - r_0) \right] \int_0^\infty \left[\frac{\xi^2 r - \alpha}{\xi^2 r_0 - \alpha} \right]^{\frac{1}{2}} \exp(-\xi^2 t) M(\xi) \frac{d\xi}{\xi},$$

where

$$M(\xi) = \frac{J_{\frac{1}{2}}(\sigma) Y_{\frac{1}{2}}(\sigma') - Y_{\frac{1}{2}}(\sigma) J_{\frac{1}{2}}(\sigma')}{J_{\frac{1}{2}}^2(\sigma') + Y_{\frac{1}{2}}^2(\sigma')}$$

$$\sigma = 2(\xi^2 r - \alpha)^{\frac{1}{2}} / 3\xi^2 \sqrt{D_0}, \quad \alpha = a^2/4D_0$$

$$\sigma' = 2(\xi^2 r_0 - \alpha)^{\frac{1}{2}} / 3\xi^2 \sqrt{D_0}$$

and $J_{\frac{1}{2}}(x)$, $Y_{\frac{1}{2}}(x)$ are Bessel functions of the first and second kind of order $\frac{1}{2}$, respectively.

The solution in its present form has not been evaluated; however, a finite difference scheme has been applied to the differential equation. The integral in its present form is cumbersome to evaluate because of the appearance of the Bessel function in both numerator

and denominator. Shamir and Harleman (1967) have obtained an approximate solution of equation 25, numerically. Experimental analysis of this problem has been done by Lau, Kaufman, and Todd (1959); however, certain fundamental simplifications were required for the comparison of experimental with theoretical results. A result of the finite difference computation for the value $D_0/u_0 r_0 = 1 \times 10^{-2}$ is presented in figure 10.

The solutions for dispersion in one-dimensional, two-dimensional, and the special case of radial-flow systems have been presented. Continuation of this analytical trend would suggest that dispersion in a three-dimensional system should be considered next. However, the relative difficulties in coping with a three-dimensional ground-water system renders the attempt hardly worthwhile. Thus, it seems more useful in the final two examples of dispersion without chemical reaction to consider approximate solutions for two-directional dispersion. In the two-dimensional field equations (eq 22) it is assumed that, if the term $D_x \partial^2 C / \partial x^2$ is small compared to the other terms, the system can be described as consisting of flow and dispersion that are orthogonal to each other. This is signified in the definition sketch presented as figure 11.

For dispersion process from a disk source, the field equation is

$$D_r \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) = \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} \quad (26)$$

For the plane source in which $y > 0$ initially at a constant concentration, the appropriate field equation is

$$D_y \frac{\partial^2 C}{\partial y^2} = \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} \quad (27)$$

Equation 27 is identical with the diffusion through a wall, and equation 26 is identical with diffusion from a cylinder moving in the direction x at the rate u .

Example 6.—Approximate radially symmetrical model of lateral dispersion.

The approximation of lateral dispersion, equation 27, in which the justification of its use is given, was treated by Ogata (1961). In previous discussion on transformation of the coordinates, it was pointed out that the coordinate transformation $\xi = x - ut$ may be used to eliminate the convective term. Equation 26 may thus be written

$$D_r \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) = \frac{\partial C}{\partial t}.$$

Although C depends on x , this need not be specified in the boundary conditions since x does not appear

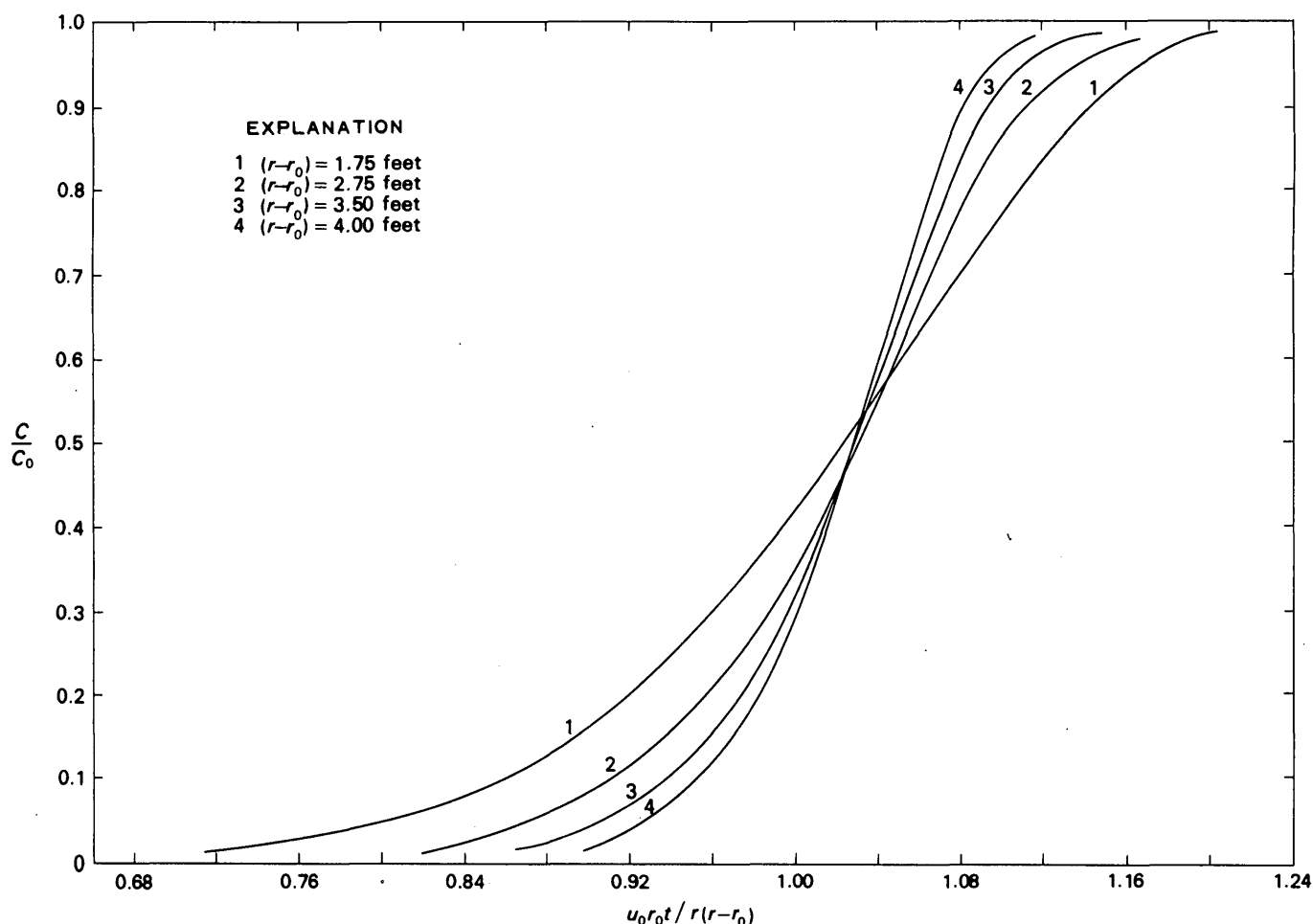


FIGURE 10.—Concentration distribution for radial-flow system.

explicitly in the differential equation. Hence, the boundary conditions are stated

$$C(r, 0) = C_0, r < a,$$

$$C(r, 0) = 0, r > a,$$

$$(\partial C / \partial r)_{r=0} = 0, t > 0.$$

The solution of the above differential equation for the specified boundary condition is obtained by Laplace transformation. The subsidiary equations for $r > a$ and $r < a$ are

$$\frac{d^2 \bar{\lambda}}{dr^2} + \frac{1}{r} \frac{d\bar{\lambda}}{dr} - q^2 \bar{\lambda} = 0; r < a,$$

$$\frac{d^2 \bar{C}}{dr^2} + \frac{1}{r} \frac{d\bar{C}}{dr} - q^2 \bar{C} = 0; r > a,$$

where $\bar{\lambda} = \bar{C} + \frac{C_0}{p}$ and $q^2 = p/D$. The two regions are described by identical equations when $\bar{\lambda}$ is used.

Particular solutions valid for the region of interest with the specified constraints are

$$\bar{C} = \frac{C_0}{p} \left[1 - \frac{K_1(qa)I_0(qr)}{I_0(qa)K_1(qa) + K_0(qa)I_1(qa)} \right]; r < a$$

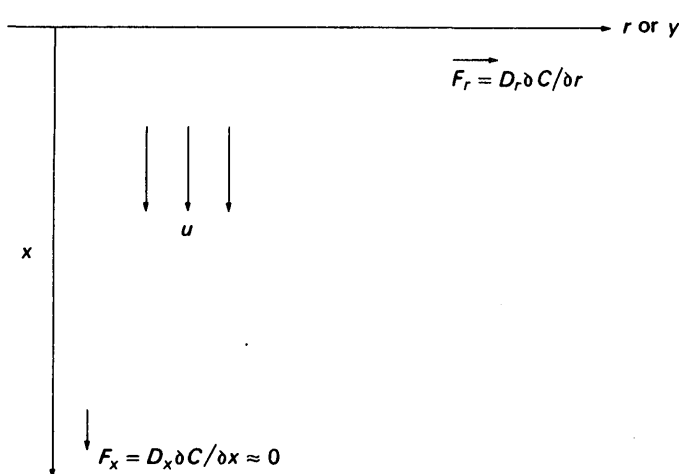
$$\bar{C} = \frac{C_0}{p} \left[\frac{I_1(qa)K_0(qr)}{K_0(qa)I_1(qa) + K_1(qa)I_0(qa)} \right]; r > a.$$

The inverse of the above expression is given by Carslaw and Jaeger (1959, p. 346). The solution for all values of r is given by

$$\frac{C}{C_0} = a \int_0^\infty \exp(-D\alpha^2 t) J_1(\alpha a) J_0(\alpha r) d\alpha.$$

From equation 27, it is immediately apparent that for steady-state conditions the solution can be obtained by replacing t with $\frac{x}{u}$. The steady-state conditions are thus computed from the same expression.

Example 7.—Approximate steady-state model of lateral dispersion in a unidirectional flow field.

FIGURE 11.—Definition sketch of system depicting no dispersion in x direction.

The model considered is dispersion in a fluid moving in the direction x with the plane $y=0$ initially at a constant concentration C_0 . This special case was treated by Harleman and Rumer (1962, p. 24). Equation 27 is the appropriate differential equation and the boundary conditions are

$$C(0, y) = C_0, \quad 0 < y < \infty$$

$$C(0, y) = 0, \quad -\infty < y < 0$$

$$\left(\frac{\partial C}{\partial y}\right)_{y=\pm\infty} = 0, \quad x \geq 0.$$

The application of Laplace transform in equation 27 leads to the subsidiary equation

$$u \frac{d\bar{C}'}{dx} = -D_v p^2 \bar{C}',$$

where $\bar{C}' = \bar{C}/C_0$.

The solution of this subsidiary equation is readily determined as

$$\bar{C}' = \frac{1}{\sqrt{2\pi}} (ip)^{-1} \exp\left(-\frac{D_v x}{u} p^2\right).$$

Hence, using the complex inversion theorem, the solution obtained is,

$$\frac{C}{C_0} = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{y}{2\sqrt{D_v x/u}} \right) \right].$$

The expression for example 6 has been computed numerically for various values of $\frac{a^2 u}{4D_v x}$. The expression for example 7, on the other hand, is a standard tabulated function; hence, numerical values are available. These two expressions are presented graphically as figures 12 and 13. Because of the simpler nature of these expressions, as compared with those obtained in examples 3 and 4, their use, whenever applicable, is favored for computing numerical values of the dispersion coefficient for any given experiment. Figure 14

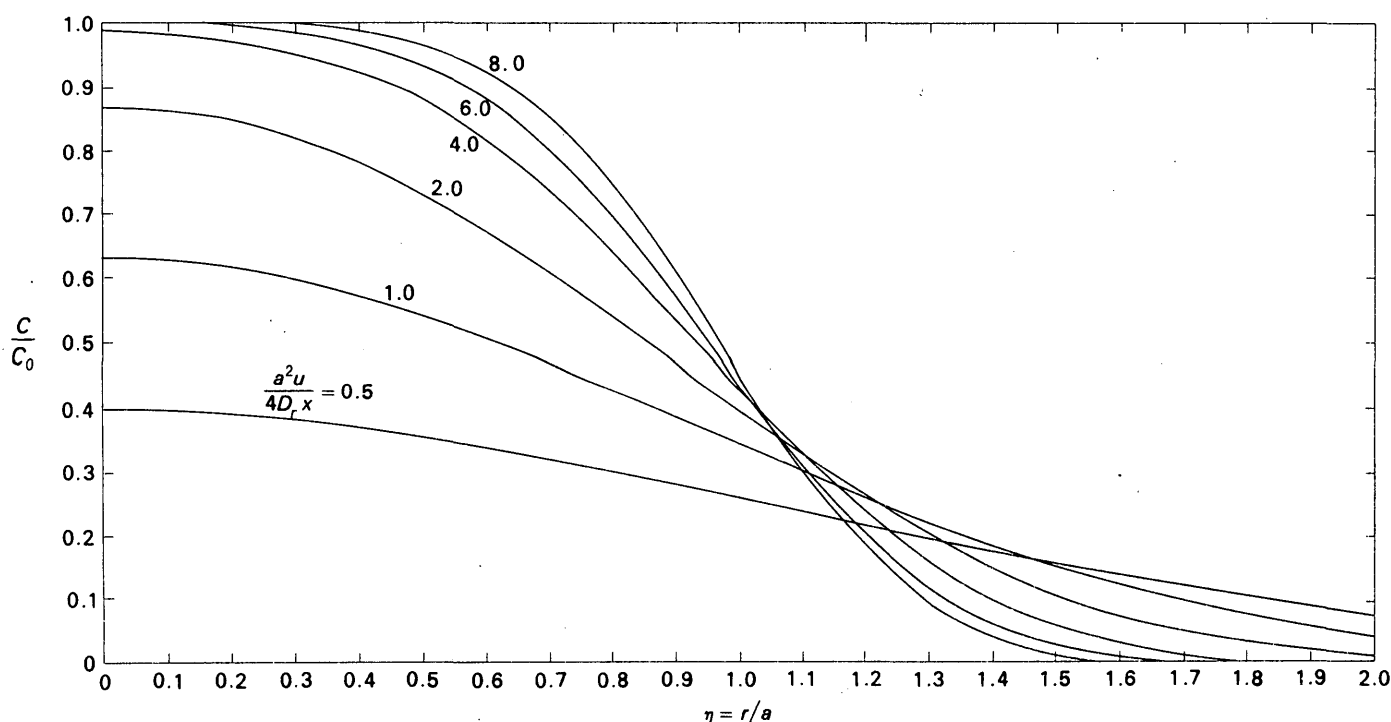


FIGURE 12.—Approximate concentration profile due to lateral dispersion; radially symmetrical model.

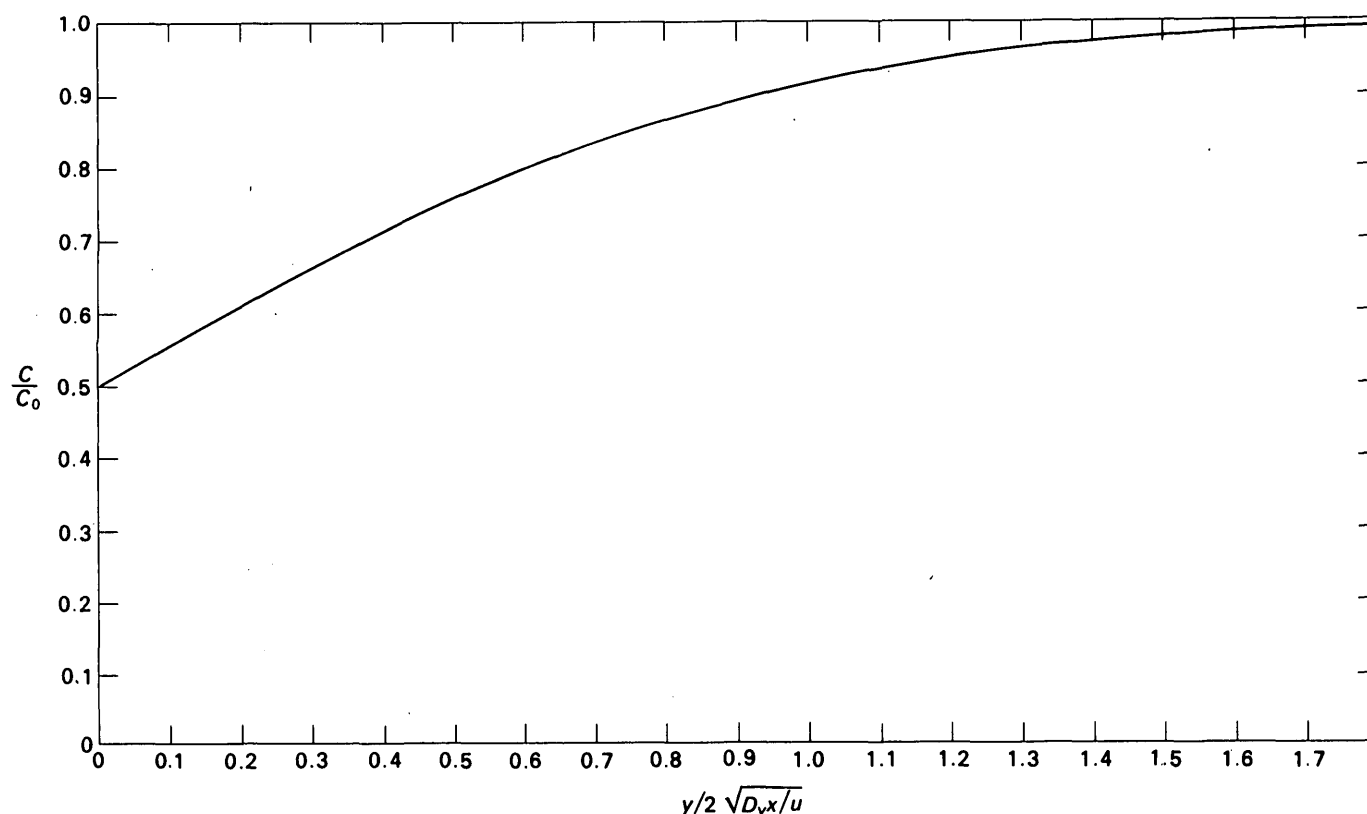


FIGURE 13.—Approximate concentration profile due to lateral dispersion; two-dimensional model.

shows the curves for examples 3, 4, and 6 for two values of $4D_y x/ua^2$. As expected for higher values of $4D_y x/ua^2$, the difference between the three functions become appreciable. For a first approximation, however, the use of the solution obtained in examples 6 or 7 would be simpler and of sufficient accuracy.

The following examples of mathematical analysis of dispersion consider an adsorbing medium. The system will be limited to a semi-infinite medium. The adsorption rate is assumed to be linear or more specifically of the form $\partial S/\partial t = b(C - mS)$. For flow in a medium with finite boundaries, the reader is referred to several examples given by Crank (1956) as the complete solutions are too complex to be reproduced here.

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 differential equation

$$D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} + \frac{\partial S}{\partial t}. \quad (28)$$

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

$$\frac{\partial S}{\partial t} = b(C - mS). \quad (29)$$

In the examples to follow, equations 28 and 29, 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

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

$$C(x, 0) = 0, \quad x > 0,$$

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

$$S(x, 0) = 0, \quad x > 0.$$

Example 8.—Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t = bC$, ($m=0$).

The solution of simultaneous equations 28 and 29 (with $m=0$) for the prescribed conditions can be determined by assuming that it may be written in the form

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

Substituting the above expression into equation 33 leads to an equation with Γ as the dependent variable, or

$$D \frac{\partial^2 \Gamma}{\partial x^2} = \frac{\partial \Gamma}{\partial t}.$$

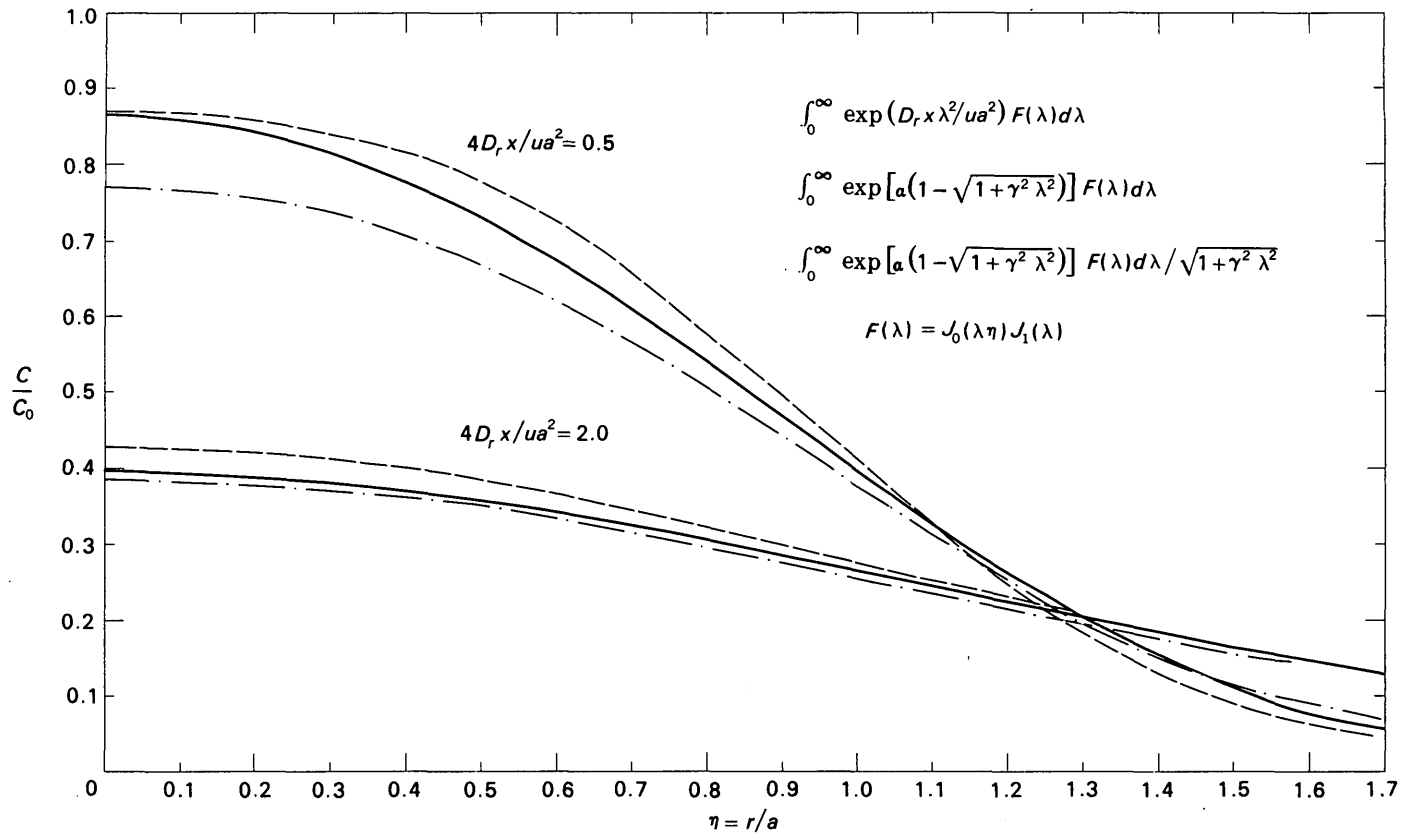


FIGURE 14.—Comparison of examples 3, 4, and 6.

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

$$\Gamma(0, t) = C_0 \exp \left[\left(\frac{u^2}{4D} + k \right) t \right].$$

The general solution of the equation above is given by Carslaw and Jaeger (1959, p. 63). For this specific case the solution is

$$\Gamma(x, t) = \frac{2}{\sqrt{\pi}} C_0 \exp \left[\left(\frac{u^2}{4D} + b \right) t \right] \int_{x/2\sqrt{Dt}}^{\infty} \exp \left[-\left(\frac{u^2}{4D} + b \right) \frac{x}{4D\eta^2} - \eta^2 \right] d\eta.$$

The integral above is a well-tabulated function called the error function, or

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

where

$$M = \sqrt{1 + 4Db/u^2}.$$

Example 9.—Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t = k(C - mS)$ with $D_x \partial^2 C/\partial x^2 \cong 0$ and $\partial C/\partial t < \partial S/\partial t$.

The differential equation for the specified condition is reduced to $-u \partial C/\partial x = \partial S/\partial t$. Using the Laplace transform, the subsidiary equations obtained are

$$u \frac{d\bar{C}}{dx} = -p\bar{S}$$

$$p\bar{S} = b\bar{C} - bm\bar{S}.$$

The solution satisfying these simultaneous equations is

$$\frac{\bar{C}}{C_0} = \frac{1}{p} \exp \left[-\frac{bx}{u} \left(\frac{p}{p + km} \right) \right].$$

The inverse of the above expression is available in tables of the inverse transform. The solution obtained by Houghton and Marshall (1947) is

$$\frac{C}{C_0} = 1 - \exp(-bmt) \int_0^{bx/u} \exp(-\xi) J_0(2i\sqrt{bmt\xi}) d\xi.$$

Example 10.—Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t = b(C - mS)$, with $\partial S/\partial t \gg \partial C/\partial t$.

The postulated conditions reflect primarily the mathematical viewpoint of looking toward a simplified equation. Again, the use of the Laplace integral

transform reduces the partial differential equations to the subsidiary expressions

$$D \frac{d^2 \bar{C}}{dx^2} - u \frac{d\bar{C}}{dx} = p\bar{S}$$

$$p\bar{S} = b(\bar{C} - m\bar{N}).$$

The solution of these simultaneous equations, obtained by classical methods, is

$$\frac{\bar{C}}{C_0} = \frac{1}{p} \exp \left[\frac{ux}{2D} (1 - \sqrt{1 + 4Dpk/u(p+bm)}) \right].$$

The inverse is obtained by standard means and is described by Ogata (1964b). The expression obtained is

$$\begin{aligned} \frac{C}{C_0} &= \frac{2e^{\alpha - bmt}}{\sqrt{\pi}} \int_0^\infty \exp(\xi^2 - \alpha^2/4\xi^2) \int_0^{\beta/\xi^2} e^{-\lambda} I_0(2\sqrt{bmt\lambda}) d\lambda d\xi \\ &= \frac{2e^{\alpha}}{\sqrt{\pi}} \int_0^\infty \exp[-\xi^2 - \alpha^2/\xi^2] J(\beta/\xi^2, bmt) d\xi, \end{aligned}$$

where $\alpha = ux/2D$, $\beta = Db\alpha^2/u^2$, and $J(x, y)$ is the Goldstein J function which has been defined in example 3.

Example 11.—Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t = b(C - mS)$, with $Dx\partial^2 S/\partial x^2 \cong 0$.

The equation considered is again a variation of the complete field equations 28 and 29 with the condition that dispersion in the direction of flow is small. The method of analysis again involves application of the Laplace integral transform. The subsidiary equations for this case are

$$u \frac{d\bar{C}}{dx} + p\bar{C} + p\bar{S} = 0$$

$$p\bar{S} = b(\bar{C} - m\bar{S}).$$

The solution of these simultaneous equations can be determined by elementary means, and the resulting expression is

$$\frac{\bar{C}}{C_0} = \frac{1}{p} \exp \left[-\left(\frac{x}{u}\right) \frac{(p+bm+b)}{(p+bm)} \right].$$

The solution as given by Ogata (1964b) is

$$\begin{aligned} \frac{C}{C_0} &= 1 - \exp \left[-bm \left(t - \frac{x}{u} \right) \right] \int_0^{kx/u} e^{-\lambda} I_0 \left[\sqrt{bm \left(t - \frac{x}{u} \right) \lambda} \right] d\lambda \\ &= J \left[\frac{bx}{u}, bm \left(t - \frac{x}{u} \right) \right]. \end{aligned}$$

Note that the preceding solution is the same as that for example 9 when $(t - x/u)$ is replaced by t .

Example 12.—Dispersion in an adsorbing medium; adsorption rate given by $\partial S/\partial t = b(C - mS)$.

This final example employs equations 29 and 30. The subsidiary equations, obtained by use of the Laplace transform, are

$$D \frac{d^2 \bar{C}}{dx^2} - u \frac{d\bar{C}}{dx} = p\bar{S} + p\bar{C}$$

$$p\bar{S} = b(\bar{C} - m\bar{N}).$$

The particular solution of the transformed equations for the specified boundary conditions is given by the expression,

$$\bar{C} = \frac{C_0}{p} \exp \left\{ \frac{x}{2D} \left[u - \sqrt{u^2 + 4Dp \left(1 + \frac{b}{p+bm} \right)} \right] \right\}.$$

The process of inversion is described by Ogata (1964b), and the final expression is written

$$\frac{C}{C_0} = \frac{2e}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^\infty \exp(-\xi^2 - \alpha^2/4\xi^2) J(\epsilon, \tau) d\xi,$$

where $\epsilon = b\gamma^2/\xi^2$, $\tau = bm(t - \gamma^2/\xi^2)$, $\alpha = ux/2D$, $\gamma^2 = x^2/4D$ and $J(\epsilon, \tau)$ is the Goldstein J function as defined previously.

Note that this solution is identical with the solution in example 10 when the term $(t - \gamma^2/\xi^2)$ is replaced by t .

Because the development of the solutions for examples 10–12 is relatively recent, their numerical evaluation has not been completed. The solution for example 8 can be readily computed, whereas the solution for 9 has been used in analyzing reactor columns. Figures 15 and 16 are graphical representations of the expressions for these two examples.

The number of conditions, other than the one-dimensional system, that have been investigated are relatively few. Because of the similarity between equations describing dispersion in ground water and those describing diffusion and heat-conduction systems, numerous analytical solutions are available. And with the increased use of digital computers, a variety of more complex mathematical problems can now be solved numerically.

NATURE OF THE DISPERSION COEFFICIENT

In the analytical development of the macroscopic theory of dispersion it is assumed that the characteristics of the dispersion coefficient are known, and that it is virtually a constant. In reality, the nature of this coefficient is unknown and is the subject of considerable

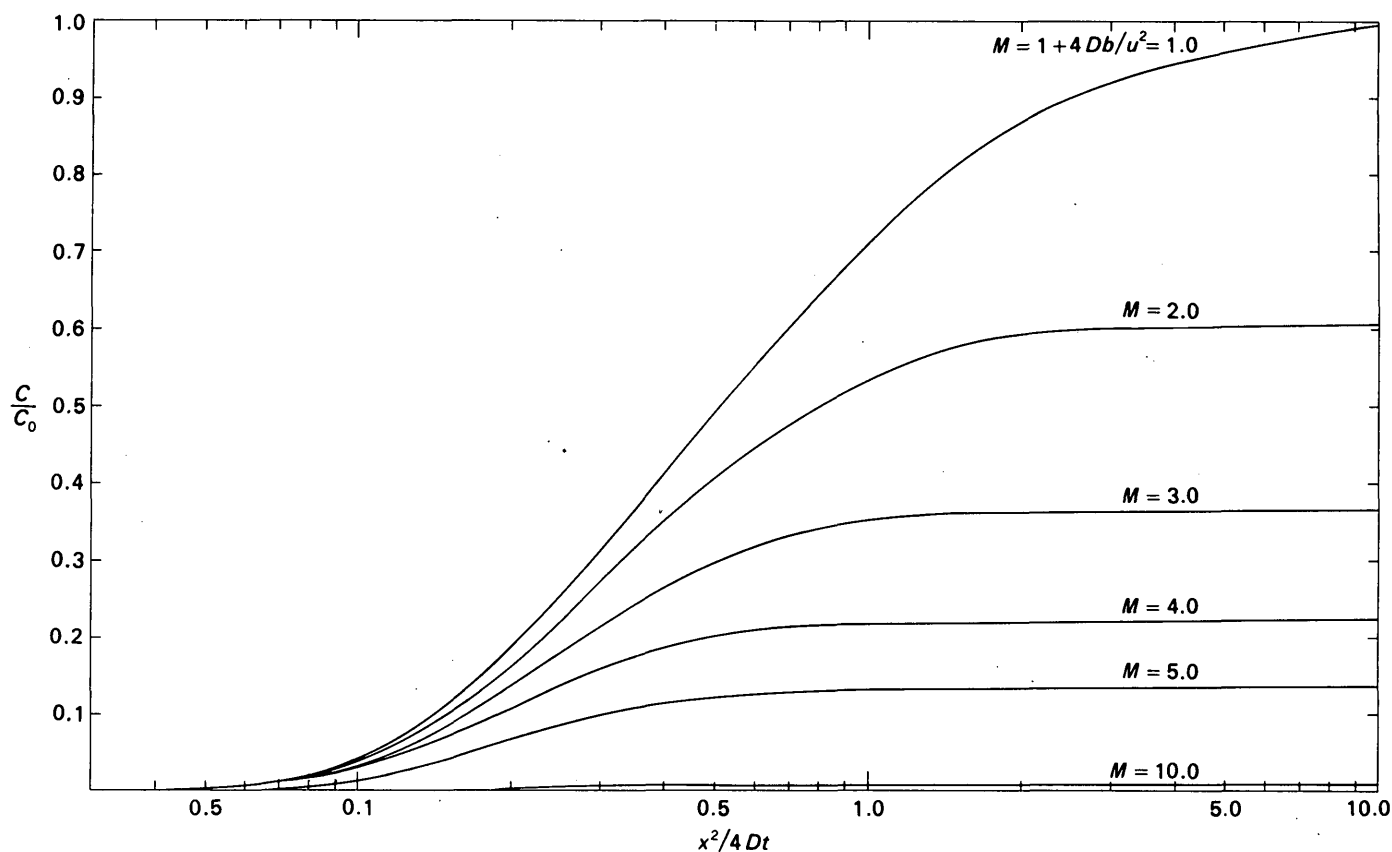


FIGURE 15.—Concentration profile of dispersion in an adsorbing medium with $\partial S/\partial t = bC$.

investigation. Extension of the theory describing dispersion in a porous medium, or the ability to use dispersion equations for systems other than isotropy, is entirely dependent on the evaluation of this coefficient by either analytical or laboratory means. Further, this critical evaluation depends entirely on the ability to describe analytically the physical properties of the porous medium. This stage of investigation has not been reached as yet; thus, the discussion to follow is limited to evaluation of the dispersion process in isotropic material.

Many experimental and analytical papers published in journals show the dependency of the magnitude of the dispersion coefficient on the flow rate and the effective grain size—diameter—of the porous medium. This dependency comes about because, provided the sand is uniform, the geometric characteristics are described by a single parameter—the sand-grain diameter. But, whenever the materials that make up the matrix depart from isotropic conditions, the representation of the medium by a so-called characteristic length becomes a difficult task, as experienced in attempts to generalize the concept of a friction factor in fluid flow through porous media (Carman, 1956). Generalization of the results of laboratory and analytical studies cannot be

realized unless a porous matrix can be described in its generality, including parameters such as the grain distribution and degree of cementation. This need is reflected in all problems involving the granular medium and in some quarters gave rise to such correction terms as “tortuosity.” However, the only route opened at present is to assume that the Reynolds number establishes flow similitude and the Schmidt number establishes similitude in the diffusion. Then, the correlation of these two similarity criteria makes it possible to write an analytical expression for the functional relationship between the flow and diffusion processes.

Characteristics of the dispersion coefficient for conditions encountered in the laboratory are generally studied through statistical evaluation, or by correlation of the experimental data with results of a mathematical model. The statistical model is important in that to a limited extent it does point out the parameters that control the magnitude of the coefficient. Its weakness lies in the need to reduce the porous matrix to an extremely simplified structure in order to render the problem mathematically tractable. The use of the macroscopic model is, however, a little more difficult since the nature of the coefficient is only specified as a constant. Thus, any correlation of these coefficients with

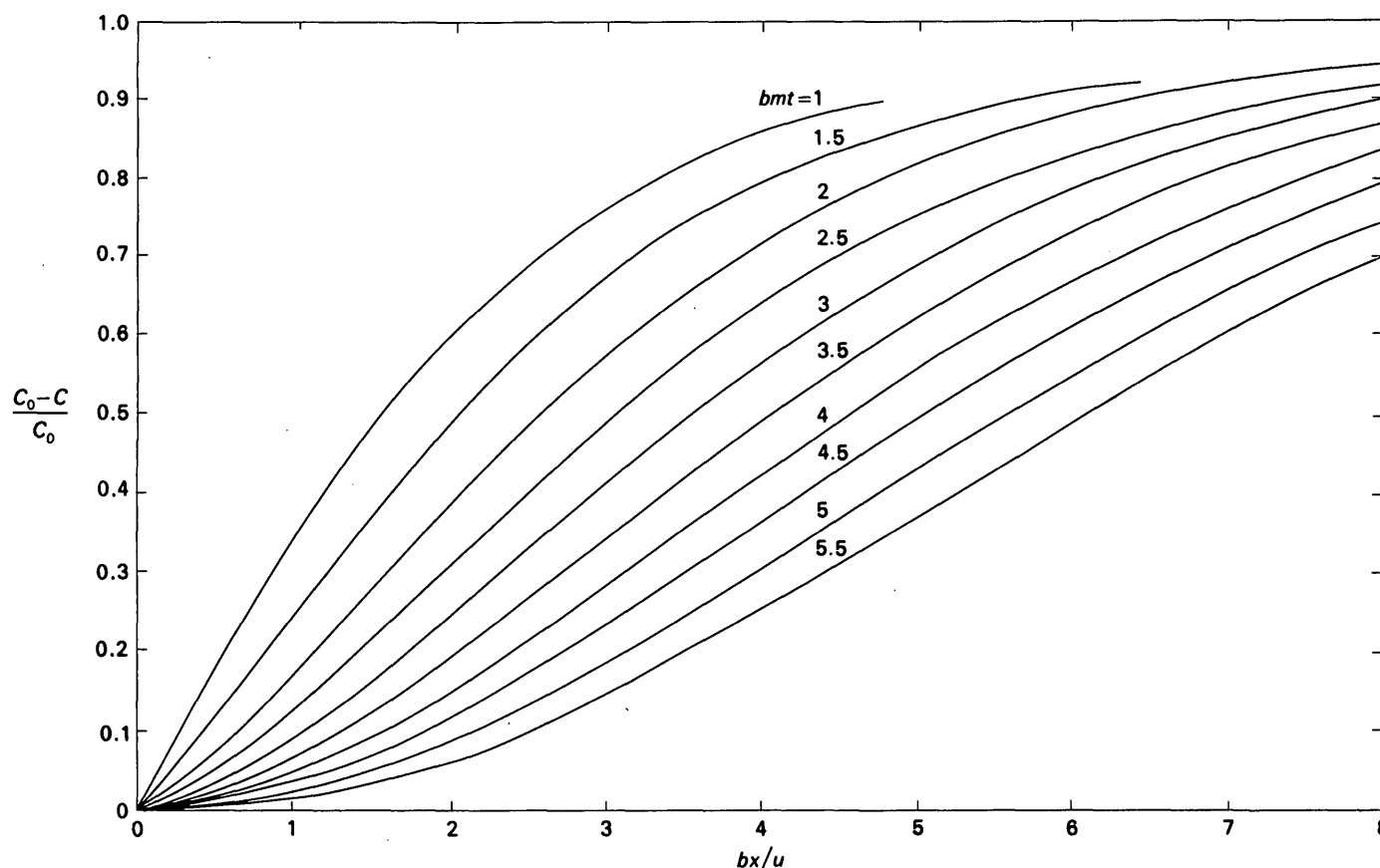


FIGURE 16.- Concentration profile of dispersion in an adsorbing medium with $\partial S/\partial t = b(C - mS)$, $D_x \partial^2 C/\partial x^2 \approx 0$, and $\frac{\partial S}{\partial t} \gg \frac{\partial C}{\partial t}$.

various parameters must be accomplished by methods of regression, unless similarity can be established between the various flow conditions in the laboratory and the field.

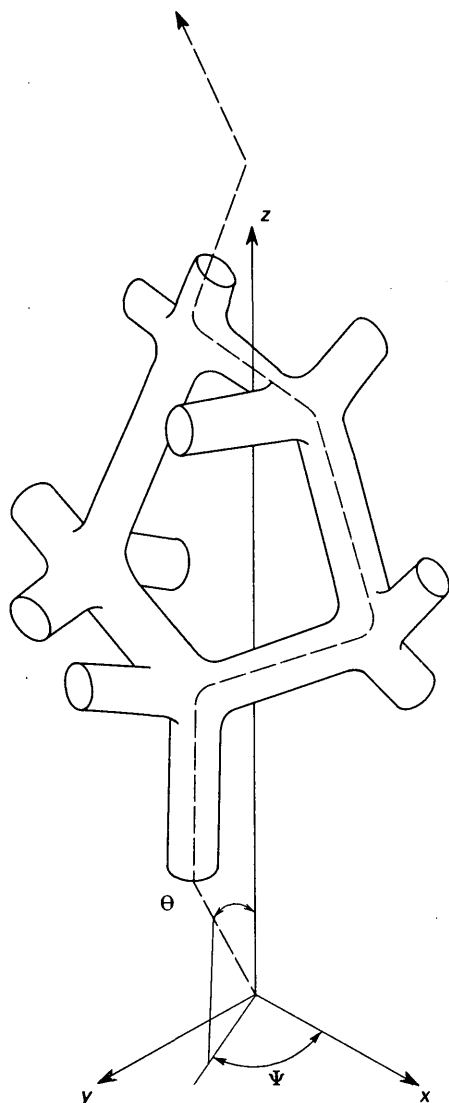
Numerous experiments indicate that the use of the Reynolds number and Schmidt number are useful in establishing results comparable to those obtained by statistical analysis, provided the porous matrix is isotropic. However, in natural soils, or when air entrapment occurs in flows, the dispersion coefficient cannot be readily correlated to an effective diameter or a characteristic length. Thus, the expression for the D is written $D_t = D_m u$, where D_m is an experimental constant that depends on characteristics of the porous medium.

EVALUATION OF DISPERSION COEFFICIENT BY ANALYTICAL METHODS

The statistical development of the dispersion theory is of interest because it reveals the dependence of the magnitude of the dispersion coefficient on the characteristics of the flow and the porous medium. Stringent conditions, however, must be postulated to simplify the model so that the mathematical concept can be utilized. As is generally true in most mathematical development, the mathematical model adopted has little resemblance

to the actual porous matrix. The basic theory of the statistical analysis is described in four papers published in separate scientific journals. These papers were written by Scheidegger (1954), Jong (1958), and Saffman (1959, 1960). Saffman's and Jong's models are similar in nature; however, Scheidegger, who introduced the concept of statistical hydrodynamics, chose a mathematical model that assumed random motion of the fluid particles.

The results of both Jong and Saffman are reproduced. The porous medium model of Jong is reproduced as figure 17. The pore channels are assumed to be capillary tubes multiply connected at some end points and uniformly distributed in all directions in space. The medium is assumed to be made up of spherical particles that form polyhedral cavities connected by triangular capillary tubes. The velocity within a tube varies according to the position of the fluid particle within the canal; however, for simplicity it is postulated that the mean velocity is represented by the rate at which the fluid particle containing, say, a contaminant or tracer, passes from point to point. The multiple connections at the tube-end points represent a limited choice of direction confronting an arriving particle of fluid containing the contaminant or tracer. This postulate, to some degree,



(From Jong, 1958)

FIGURE 17.—Random path chosen by a fluid particle moving through the canal system.

indicates randomness of the particle path, and together with the fact that the pressure gradient is proportional to $\cos \theta$ (fig. 17), makes it possible to trace or determine the probable location of the fluid particle at any given time.

The complete analysis presented by Jong (1958) is not repeated here inasmuch as it is basically a justification for the use of a given probability function. Of immediate interest, however, is the end result which follows and indicates the functional dependency of the dispersion coefficient on the flow field and the pore characteristics. The use of average velocity to characterize the flow makes it possible to characterize the pore system by a length parameter defined here as the elementary

length l . The final results of Jong's analysis are the statements that the dispersion coefficients are related to the flow and media parameters according to the expressions

$$\begin{aligned} D_r &= 3u l / 16 \\ D_z &= u l (\lambda + \frac{3}{4} - \ln \gamma) / 6. \end{aligned} \quad (30)$$

In equation 30, the symbols are defined as follows:

u = average velocity,
 l = length of elementary canal,
 λ = function of Z_0 where Z_0 is the distance along the z direction at which the maximum number of particles are located at time T_0 ,

$\ln \gamma$ = Eulers constant ≈ 0.577 .

The elementary length of the porous medium, and the residence time of the tagged fluid therein, constitute the variables of the statistical analysis. Although the elementary length may be used to describe the medium, the magnitudes of the dispersion coefficient cannot be computed directly unless there is a relating measurable parameter associated with the characteristic length. Jong reports that for his experimental model, in which the medium was composed of glass beads, the calculated value of l was one-third of the mean grain diameter. For conditions other than isotropy, it is expected that the value of l will depend on the grain-size distribution and the mode of packing.

Staffman (1959), in his first paper on the theory of dispersion, used a statistical model identical with that of Jong's. The basis of his analysis is the visualization of the fluid path as a random walk process where the length, the direction, and the duration of each step are random variables. The expressions for radial and axial dispersion derived from this mathematical model are

$$\begin{aligned} D_r &= 3u l / 16 \\ D_z &= \frac{1}{2} u l F^2, \end{aligned} \quad (31)$$

where

$$F^2 = \frac{1}{3} \log \left(\frac{3ut_0}{l} \right) - \frac{1}{12}, \text{ if } \frac{ut_0/l}{\sqrt{n} \log (3ut_0/l)} \ll 1$$

or

$$F^2 = \frac{1}{6} \log \left(\frac{27ut}{2l} \right), \text{ if } \log \sqrt{n} \gg 1, \frac{3ut_0/l}{\sqrt{n} \log \sqrt{n}} \gg 1.$$

The symbols in equation 31 and the related expressions are defined as follows:

- t = time,
 t_0 = estimate of time for appreciable diffusion to take place along the pore,
 u = average velocity in the x direction,
 l = pore length, and
 n = number of steps in the random walk analysis.

Equations 30 and 31 indicate a slightly different result for D_x , but the radial diffusion coefficients D_r derived by these two methods are identical

Saffman (1960), in a later paper, investigated dispersion phenomena by using a Lagrangian correlation function in an attempt to compute values of dispersion coefficients for a more generalized condition in terms of the dimensionless number $u l/D$, where D is the molecular diffusivity. The results of the analysis are much more complex, and the expressions are not reproduced here. Saffman states that comparisons of these results with experimental analysis show a large discrepancy, probably attributable to nonuniform packing of the granular material within the experimental column and possible channeling along the boundary between container and porous material. Or this discrepancy may be the consequence of oversimplifying the existing mathematical model in order to render the analysis tractable. The conclusion that can be drawn is that too much weight is being placed on the single parameter l —the elementary canal length. Differing somewhat from Jong, Saffman calculated the value of the coefficient on the assumption that the magnitude of l equals the mean diameter of the sand grains.

In an attempt to reconcile some of the discrepancies noted, especially transverse to the flow direction, Saffman (1960) pointed out that in a strictly two-dimensional system, as depicted by the mathematical model, two of the basic assumptions may not represent good approximations. Physically, because of the prevailing steady-state laminar flow, there can be no intertwining of the streamlines except in a three-dimensional flow system. Hence, the variation of the width of the stream tubes is on the order of the diameter of the sand grain or less. Thus, the assumptions of statistical independence of each streamline, and the uncorrelated nature of the mean displacement transverse to the flow, cannot be strictly valid. Using statistical models these investigations find that at some time after the introduction of the contaminant, or at some distance from the contaminating source, dispersion is described by equation 6. This conclusion based on the assumption that the central limit theorem is applicable was first stated by Beran (1957).

It is apparent that the choice of the mathematical model in the statistical analysis is limited entirely by

the mathematical difficulties, and thus cannot in any way represent a true porous medium. The departure from the physical features of the actual granular material may be the primary reason for the poor correlation between calculated and observed values. These difficulties are inherent because of limited knowledge in the statistics of sedimentation and other geologic processes. This differs to a large degree from other transport systems in which the kinetic theory of gases or the statistical mechanics is applicable. In systems where these theories are applicable, meaningful statistical averages can be derived from the mathematical model, making possible the computation of the relationship between the coefficient and the various parameters. Certain limitations are imposed by the chosen mathematical model, but they are not so severe as in the analysis of flow through a porous matrix.

The generalization of the expressions for the dispersion coefficient cannot be readily achieved at present. However, the statistical studies may be used as a guide in an attempt to formulate empirical expressions. Articles such as that of Perkins and Johnston (1963) give a number of empirical expressions that have been used to describe systems of specific interest.

EVALUATION OF DISPERSION COEFFICIENT BY EXPERIMENTAL METHODS

Analysis in the preceding section indicates that the magnitude of the coefficient is dependent on the velocity of fluid flow and the elementary canal length used to describe the porous material. The validity of the dispersion equation is also established, although no proof was given. The magnitude of the dispersion coefficient is obtained by correlation of the solution of equation 6 with experimental data. This section discusses the use of the dispersion equation as the tool in the experimental determination of the magnitude of the dispersion coefficient. The difference between the two methods is that the statistical method requires experimental determination of the medium characteristic, whereas the macroscopic method requires evaluation of the coefficient itself.

Many solutions have been presented in a previous section to indicate the nature and extent of theoretical investigations of transport phenomena. These solutions were obtained for boundary conditions which involved semi-infinite porous media, readily amenable to representation by laboratory test models. The verification of theoretical results has generally been confined to the analysis of one-dimensional models that are easier to build and test. These models are most appropriate for experimentally establishing the magnitude of the longitudinal dispersion coefficient. Accordingly, the quanti-

fication of the coefficient is based on the conditions specified by

$$C(0,t) = C_0, t > 0,$$

$$C(x,0) = 0, x > 0,$$

$$\lim_{x \rightarrow \infty} C(x,t) = 0, t > 0.$$

The first statement indicates that over a defined plane, say $x=0$, the concentration is to be maintained at a known and feasible value. The second condition is merely a statement of the concentration of the fluid which initially fills the porous matrix. This condition can be established to be either zero or any known value C_0 .

For the conditions depicted, the solution of the differential equation is as given in example 1. Most studies indicate that the second term in that equation is generally small, so that the solution presented as example 2 gives a good approximation (Ogata and Banks, 1961). Thus, for purpose of correlation, the expression to be used (see eq. 26b) is

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left(\frac{1-T}{2\sqrt{XT}} \right),$$

where $T=ut/x$ and $X=D/ux$.

The laboratory model constructed to conform with the specified boundary conditions consists of a tubular column filled with unconsolidated sand. Except for the contact at the wall of the tube, where some flow channeling may occur, the model satisfies the conditions specified for a semi-infinite porous medium. The tracer chosen depends on the nature of the investigation. Common salt has proven the easiest to measure and is used whenever density is not a critical factor. Because of its electrolytic characteristic, in-place measurement of the salt concentration can be obtained by means of an electric probe. At points where large enough samples of fluid may be taken, however, chemical methods represent an economical and rapid means of determining the concentration at any specified time. In either event the requirement is that measurements be taken at some distance from the tracer source, at a location and in a manner which does not disturb the flow. A typical setup for a columnar model is presented in figure 18.

Since the solution is available, the magnitude of D can be rapidly computed. The simplest means of calculating this result is to establish the value of the ratio $X=\theta/\phi$, where $\phi=(1-T)/2\sqrt{XT}$ and $\theta=(1-T)/2\sqrt{T}$. For any value of C/C_0 , ϕ can be determined from

the tables of the error function. By definition, $\theta=\sqrt{X}\phi$; thus, since $T=ut/x$ and T is known for any

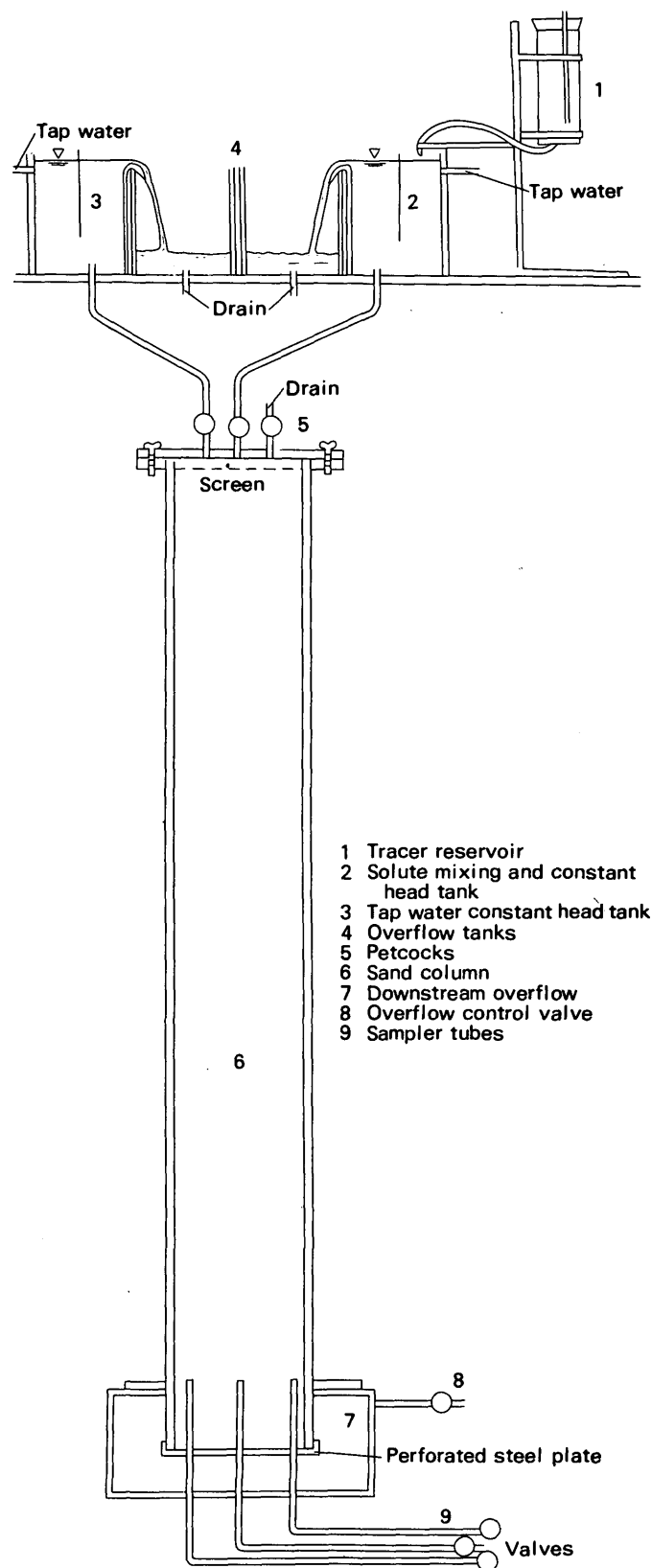


FIGURE 18.—Typical setup for column experiment.

given series of tests, the values of θ and ϕ are available. The values of these two parameters are plotted on rectangular coordinates that associate θ and ϕ with a given value of C/C_0 . The resulting plot can be analyzed by a straight-line correlation that relates the ϕ and θ values. The slope of the straight line is readily determined and by noting that the average slope is $\theta/\phi = \sqrt{X} = \sqrt{\frac{D}{ux}}$, the value of D can be computed.

This method affords a simple means for computing the value of the dispersion coefficient directly from any given series of tests.

The results obtained from any such analysis, however, yield simply a number applicable to a particular series of tests. A generalized expression for the results of all such tests cannot be realized unless relating parameters that hold for all conditions are identified. One method for obtaining these parameters is by rewriting equation 6 in dimensionless form. For this purpose let,

$$\chi = x/d, \tau = ut/d, \text{ and } C' = C/C_0$$

where d is defined simply as a characteristic length. Substituting the dimensionless variables in equation 22 results in the expression

$$\frac{D}{ud} \frac{\partial^2 C'}{\partial \chi^2} = \frac{\partial C'}{\partial \tau} + \frac{\partial C'}{\partial \chi}$$

Accordingly for the postulated conditions, the generalization of the test results depend on the single parameter D/ud . The rewriting of the field equation in its dimensionless form permits identification of a parameter which, in effect, is the similarity criterion for the process described by the equation.

The resulting parameter, however, is not a familiar one in fluid mechanics literature. To resolve this, consider the flow mechanism in a porous matrix. Dimensional analysis like that described by Muskat (1946, p. 56) indicates that the flow is characterized by a parameter known as a Reynolds number, which appears frequently in the hydraulics. Since flow in a porous medium is virtually flow in capillary tubes, it is not surprising that the Reynolds number describes the similarity conditions. Assuming the medium is described by a characteristic length d , the Reynolds number may be written, ud/ν , where d for a homogeneous medium is either the pore channel diameter or the grain diameter and ν is the kinematic viscosity of the fluid. Accordingly, the parameter D/ud may be rewritten as $\frac{D}{\nu}/\text{Re}$. The parameter D/ν is the familiar dimensionless group appearing in the study of isothermal diffusion and is called the Schmidt number (Bird, and others,

1960, p. 512). The coefficient of the differential equation in terms of these two dimensionless groups may be written

$$D/ud = 1/(\text{Sc})(\text{Re}) = 1/\text{Pe},$$

where Sc is the Schmidt number; Re, the Reynolds number; and Pe, the Peclet number. Thus, based on the various assumptions made in the development of the differential equation, the dispersion process in a porous medium is characterized by the Schmidt number and the Reynolds number.

For purpose of generalization, the magnitudes of the dispersion coefficient resulting from computation of experimental observations are correlated by plotting the Schmidt number against the Reynolds number. An illustration of this correlation method is given as figure 19. The plot is on a log-log scale and produces a straight line having a slope of nearly unity over the range of Reynolds numbers less than one.

Another common practice in evaluating an exchange system is to correlate the Peclet number, ud/D , with the Reynolds number. It can be seen that because $\text{Pe} = (\text{Sc})(\text{Re})$, if similarity in the dispersion phase is represented by the Schmidt number, the correlation will result in a horizontal line. An illustration of a plot of the Peclet number and Reynolds number is given in figure 20.

These are the two methods of correlation most commonly used in analyzing mass transport in a homogeneous granular porous medium. A majority of investigations indicate that a plot of a Reynolds number versus a Schmidt number (fig. 19) results in a straight line of unit slope, thus, indicating a direct relationship of the dispersion coefficient to the velocity and the characteristic length—the average grain diameter—or

David.

The works of Jong and Saffman, however, point out that the proportionality constant includes the residence time of the fluid; hence, the coefficient is generally written $D = D_m u$, where D_m is an unspecified constant. Scheidegger (1960, p. 259) further indicated that the relationship should be written $D = D_m u^n$, where the value n is either 1 or 2, depending on the velocity distribution taken to represent flow in the pore channel. In more recent analysis, Harleman and Rumer (1962) obtained values of $D_m = 0.027$ and $n = 1.10$ for glass beads of 0.39 mm average grain diameter, and $D_m = 0.09$ and $n = 1.18$ for glass beads of 0.965 mm average grain diameter. Because the available data are limited, it is difficult to confirm or refute the validity of this type of expression. The limited data, coupled with ease of computation, popularize the use of $n = 1$ in analyzing dispersion in a homogeneous medium.

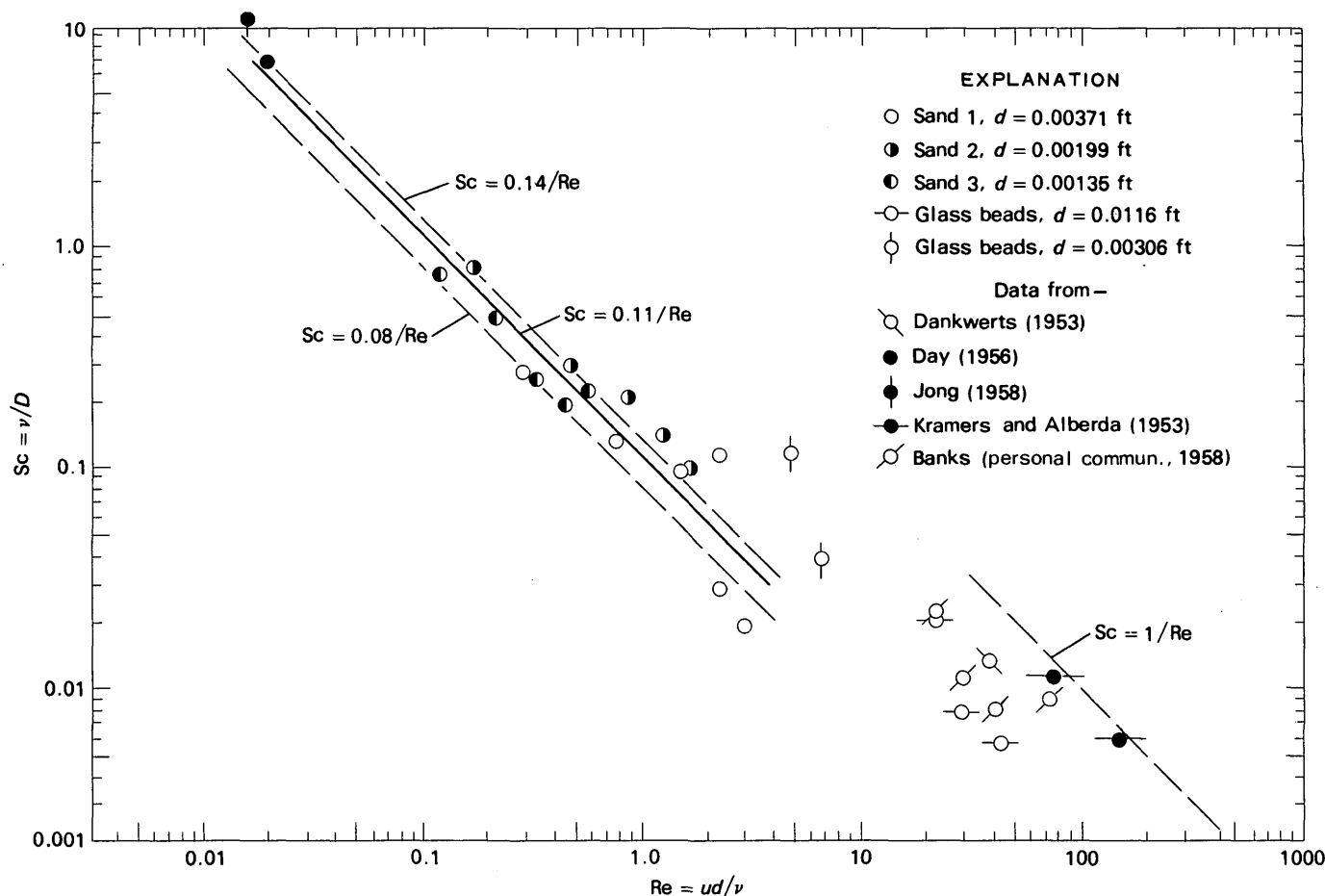


FIGURE 19.—Plot of the Schmidt number versus the Reynolds number.

In the section headed "Field equation for anisotropic dispersion," the directional properties of the dispersion coefficient were discussed. Laboratory observations and analytical studies, like those of Bear (1961), indicate that the magnitude of the coefficient is different in at least two directions, parallel to and transverse to the direction of flow.

The few available laboratory data for transverse diffusion are generalized by a plot of the Peclet number versus the Reynolds number. A general review of the published data relating to oil production is presented by Perkins and Johnston (1963). However, the specific area of interest, as displayed by the analytical and experimental data, is that related to flow conditions for which the Reynolds number >1 . In a ground-water regime, this represents a range of flow that is not normally observed.

For the lower range of the Reynolds number, representative of ground-water flow conditions, the analysis uses the two-dimensional dispersion equation with the constant dispersion coefficient developed previously. The most practical flow system for studying dispersion, because of ready representation in the laboratory, is

the axially symmetrical system described by the equation

$$D_r \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) + D_x \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

Again, D_r and D_x represent the radial and longitudinal dispersion coefficients, respectively, and the fluid flow is in the direction parallel to the x axis.

To determine the grouping of the parameters involved in the process of mass transport, the above equation is rewritten in dimensionless variables. To accomplish this, put $x = \chi d$, $r = \rho d$, and $t = \tau d/u$ where d is a representative or characteristic length describing the porous medium. Substitution of these dimensionless variables leads to the expression

$$\frac{1}{Pe_r} \left(\frac{\partial^2 C'}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial C'}{\partial \rho} \right) + \frac{1}{Pe_x} \frac{\partial^2 C'}{\partial \chi^2} - \frac{\partial C'}{\partial \chi} = \frac{\partial C'}{\partial \tau}$$

where $Pe_r = ud/D_r$ is the radial Peclet number and $Pe_x = ud/D_x$ is the axial Peclet number.

The Schmidt number, for directions r and x , and the Reynolds number characterize the dispersion and convection, respectively, for a radially symmetrical system.

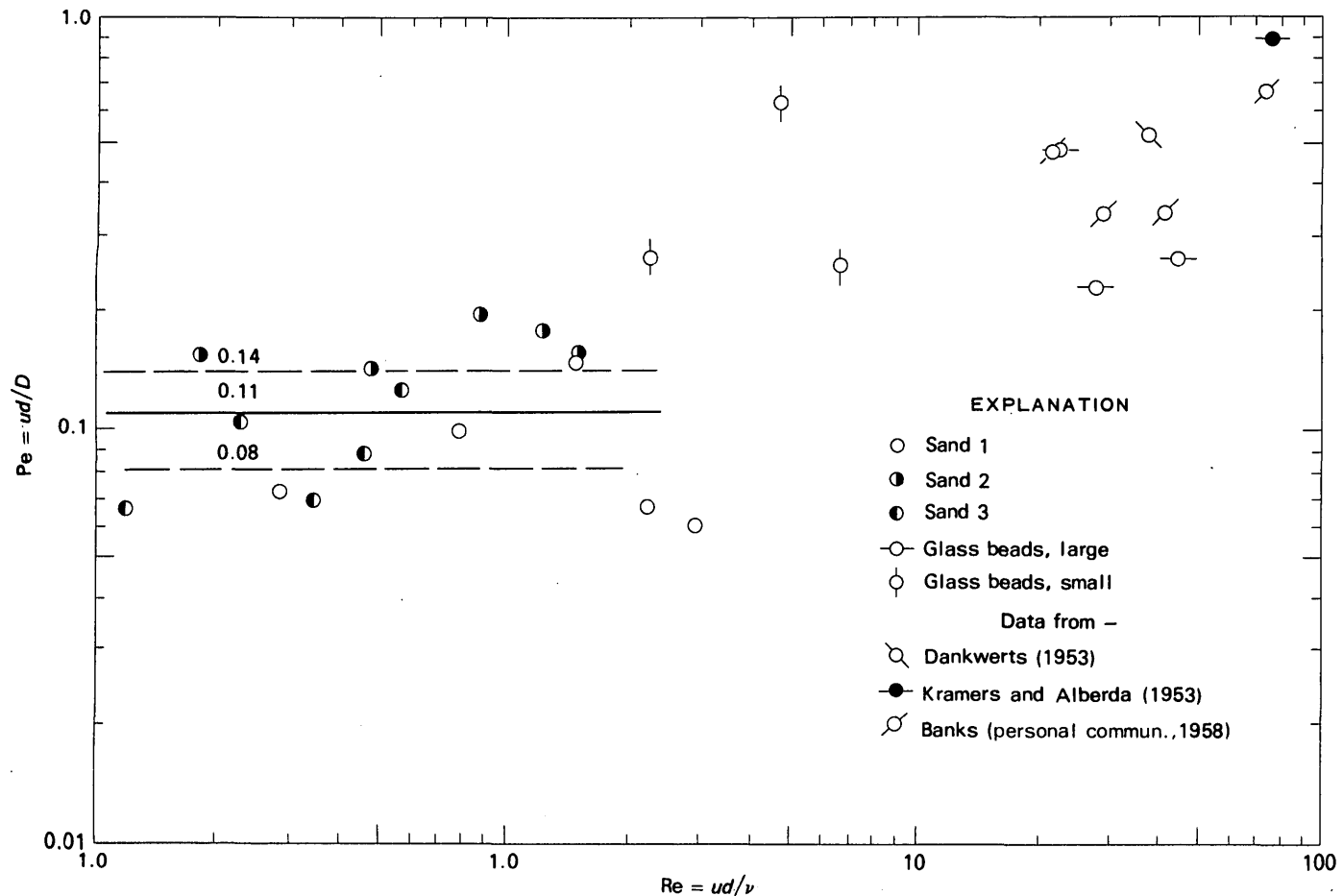


FIGURE 20.—Plot of the Peclet number versus the Reynolds number.

Published articles, for example, Kramers and Alberda (1953), indicate that the longitudinal and radial Peclet numbers are constant. Therefore, both radial and longitudinal dispersion coefficients may be expressed explicitly by the relationship $D = D_m u$, where D_m is a constant for any given granular material.

Because of difficulties in building a two-dimensional physical model, the radial dispersion is investigated by considering a system where the longitudinal dispersion is small. One approximate analysis for steady-state condition is described by Ogata (1961) and may be used to calculate the magnitude of the radial dispersion coefficient from any suite of experimental data. This approximate equation is given in example 6. The complete solution, however, as previously stated, is too complex for rapid computation of the dispersion coefficient; hence, the expression

$$\frac{C}{C_0} = 1 - \exp\left(-\frac{a^2 u}{4 D_r x}\right)$$

applicable for $r=0$ may be used.

Evaluation of the experiment conducted in Phoenix by the Geological Survey (Skibitzke and others,

1961) was based on the preceding expression. Because of some variation in the experimental data, only the average value of $\bar{D}_r = 1 \times 10^{-5}$ cm²/sec was determined to be significant. The velocity of the fluid in the experimental model was approximately 4×10^{-4} cm/sec, and the computed value of D compares well with results obtained by others and summarized by Perkins and Johnston (1963). It is also interesting to note that this value of the dispersion coefficient is near that of molecular diffusion of salt in water.

A second model of interest is the one used by Harleman and Rumer (1962). A two-dimensional dispersion model was analyzed both theoretically and experimentally. The mathematics of the mass transport system is described in example 7 where the solution was presented as

$$\frac{C}{C_0} = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{y}{2\sqrt{D_r x/u}} \right) \right]$$

Computed values of the dispersion coefficient, based on the observed and the approximate mathematical models, show a range of D_r from 9×10^{-5} to 6.5×10^{-4} cm²/sec for values of the fluid velocity rang-

ing from 0.012 to 0.28 cm/sec. By correlation of the dispersion coefficient with the Reynolds number, the proposed expression for the dispersion coefficient transverse to the direction of flow was

$$D_v = 0.0015|u|^{0.646}.$$

Using this expression with the results of the Phoenix experiment, a value of 0.96×10^{-5} cm²/sec was obtained for D_v , which shows good agreement.

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 convection component, as described by Darcy, and a dispersion component. In all investigations the dispersion component is considered to be primarily an effect of the microscopic velocity variation within the pore channel and, hence,

is simply a perturbation from the described, average flow. There are other mechanisms involved in the transport of the dissolved component, but their magnitude is small for normal ground-water flows, excepting adsorption. This mechanism of dispersion is treated to be analogous to eddy diffusion; thus, an expression similar to Fickian law of diffusion is used in the mathematical model to describe the dispersion component.

Evaluation of dispersion theory, based on the stipulated assumptions, entails laboratory investigations that are necessarily simple. Laboratory analysis of a linear flow system can be readily carried out and is especially useful in evaluating the one-dimensional progress of a slug of tracer. Such laboratory investigation is described in the section on determination of the dispersion coefficient. The results comparing theoretical and actual concentration distributions in the frontal zone of a linear flow system are typified in figure 21. For such a flow system there is ample evidence of this nature which indicates that the theory of dispersion in a homogenous medium is a good first approximation.

On the basis of findings from experimental evaluation of the theory of dispersion, the application of the

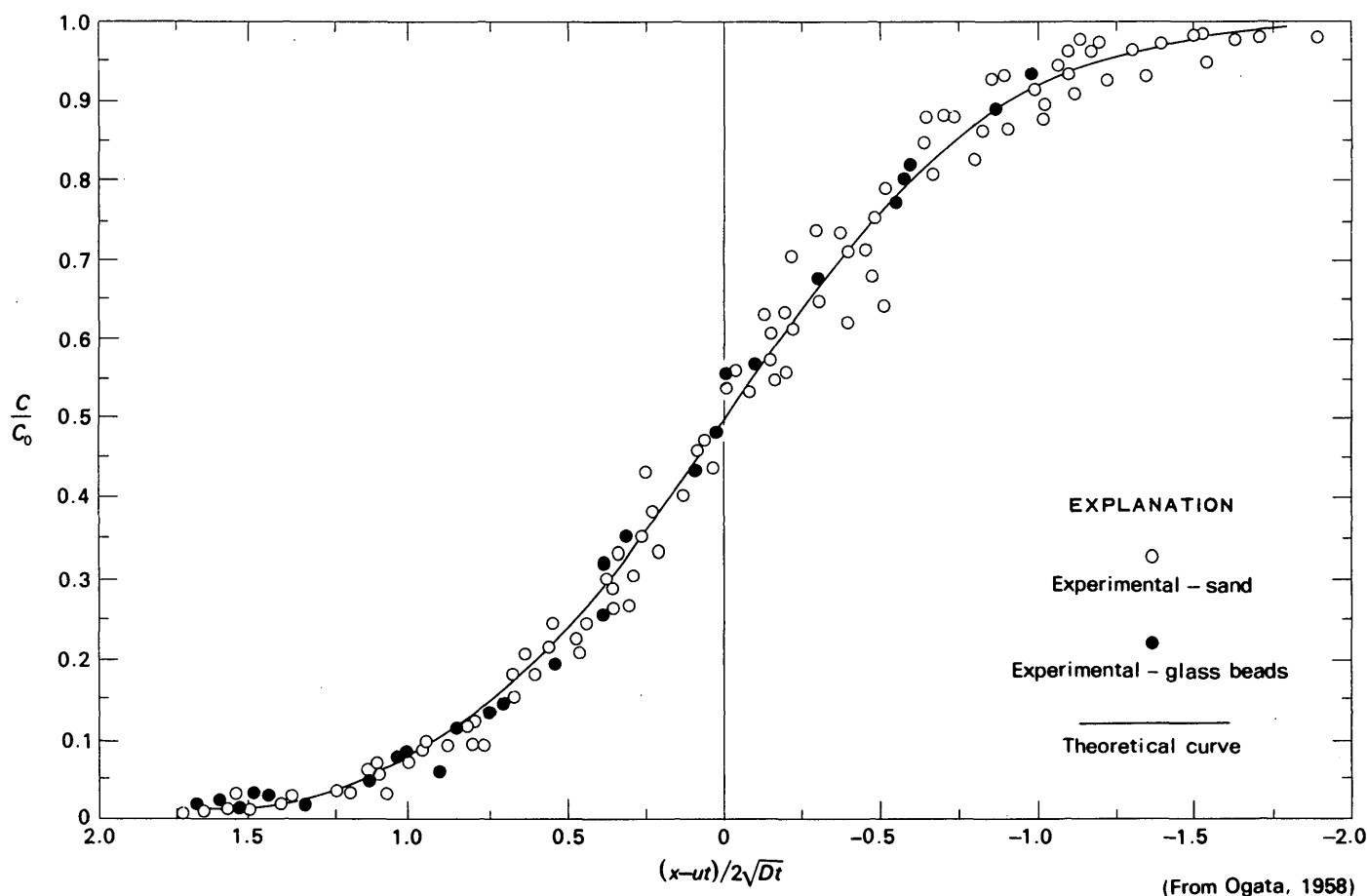


FIGURE 21.—Example of comparison between theoretical and experimental results. From Ogata, 1958.

theory is progressing to more complex flow systems. A good example is the derivation of an analytical expression representing the mixing of two miscible fluids of different densities. This effort is directed particularly toward analyzing the conditions encountered in coastal aquifers where observations reveal the development of a diffused zone between the fresh- and salt-water zones. The theoretical treatment is basically that of a one-dimensional dispersion system in which the coordinates are oriented with the position of the interface between the two fluids.

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. Accordingly, a description of the transport component perpendicular to the direction of flow is imperative. The approach to this description is to assume that the generalization can be accomplished by assigning to the dispersion coefficient the properties of a tensor. Justification of this method is based on experimental evidence which indicates that the magnitude of the dispersion coefficient for a homogeneous medium is different in the directions transverse and parallel to the line of flow. Because the generalization depends on the ability to identify separately all given causes of spreading of the contaminant, such as the effect of the injection source, the tensor components are not yet quantified.

Additional mechanisms, such as mass transfer from the liquid to the solid phase due to adsorption, are of fundamental importance whenever it is required that the fate of a given substance in a ground-water body be determined. The adsorption process may be described by the historical evaluation of the mechanism involved, and its effect on the transport of the given substance through the field of flow. In many instances of transport through a porous medium, the large solid surface area available makes the adsorption phenomenon the most important feature. Description of this phenomenon involves a chemical process; hence, the thermodynamics of the mass transfer must be determined for detailed analysis. At present, for lack of better data, approximation of the adsorption rate is used in the mathematical analysis. There is, as yet, no experimental evidence to indicate the validity of these expressions used in the mathematical model.

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 (Skibitzke and others, 1961). Thus, the limitations placed on the analytical theories of dis-

persion 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.

The investigations of mass-transport phenomena have proceeded along both analytical and experimental lines. The experimental methods have been used to verify the analytical expressions obtained by solving the differential equation of mass transport. Qualitative data defining the phenomenological process have also been obtained in the laboratory to demonstrate the nature of the flow. The analytical developments have proceeded along established lines to obtain expressions for predicting the possible concentration of a given dissolved substance under various specified conditions. As with all analyses, their applicability is limited by the ability to describe the parameters that control the behavior mechanisms; hence, only the most simple linear flow systems are described.

Within a limited range, the theories of dispersion have been verified by the results of experimental analysis. However, these expressions are only useful whenever ground-water investigations can be brought into the laboratory; for example, when the use of tracers is needed in establishing certain details of the fluid flow. Extension of such investigations into more complex porous media depends on successfully directing the research in dispersion theory so that the requisite studies of the controlling parameters are possible.

REFERENCES CITED

- Adamson, A. W., 1960, *Physical chemistry of surfaces*: New York, Interscience Publishers, 629 p.
- Aris, R., and Amundson, N. R., 1957, Some remarks on longitudinal mixing or diffusion in fixed beds: *Am. Inst. Chem. Eng. Jour.*, v. 3, no. 2, p. 280-281.
- Bachmat, Y., 1967, On the similitude of dispersion phenomena in homogeneous and isotropic porous medium: *Water Resources Research*, v. 3, no. 4, p. 1079-1083.
- Bear, Jacob, 1961, On the tensor form of dispersion in porous media: *Jour. Geophys. Research*, v. 66, no. 4, p. 1185-1198.
- Bear, Jacob, and Todd, D. K., 1960, The transition zone between fresh and salt waters in coastal aquifers: *California Univ., Water Resource Center Contribution* 29, 156 p.
- Beran, M. J., 1957, Dispersion of soluble matter in flow through granular media: *Jour. Chem. Physics*, v. 27, no. 1, p. 270-274.
- Biggar, J. W., and Nielsen, D. R., 1960, Diffusion effects in miscible displacement occurring in saturated and unsaturated porous materials: *Jour. Geophys. Research*, v. 65, no. 9, p. 2887-2896.
- Bird, R. B., Stewart, W. E., and Lighfoot, E. N., 1960, *Transport phenomena*: New York, John Wiley & Sons, 780 p.

- Carman, P. C., 1956, Flow of gases through porous media: New York, Academic Press Inc.
- Carrier, G. F., 1958, The mixing of ground water and sea water in permeable subsoils: *Jour. Fluid Mech.*, v. 4, no. 5, p. 479-488.
- Carslaw, H. S., and Jaeger, J. C., 1959, Conduction of heat in solids: London, Oxford Univ. Press, 510 p.
- Cooper, H. H., Jr., 1959, A hypothesis concerning the dynamic balance of fresh water and salt water in a coastal aquifer: *Jour. Geophys. Research*, v. 64, no. 4 p. 461-467.
- Crank, J., 1956, The mathematics of diffusion: London, Oxford Univ. Press, 347 p.
- Dankwerts, P. V., 1953, Continuous flow system distribution of residence times: *Chem. Eng. Sci.*, v. 2, no. 1, p. 1-13.
- Day, P. R., 1956, Dispersion of moving salt-water boundary advancing through saturated sand: *Am. Geophys. Union Trans.*, v. 37, no. 5, p. 595-601.
- Erdélyi, A., Magnus, W., Oberhettinger, F., and Tricomi, F. G., 1954, Tables of integral transforms, v. 1: New York, McGraw-Hill Book Co., 391 p.
- Glasstone, Samuel, 1961, Textbook of physical chemistry: Princeton, N. J., D. Van Nostrand Co., 1320 p.
- Harleman, D. R. F., and Rumer, R. R., Jr., 1962, The dynamics of salt-water intrusion in porous media: Massachusetts Inst. Technology Hydrodynamics Lab. Rept. 55, 125 p.
- Henry, H. R., 1960, Salt intrusion into coastal aquifers: *Internat. Assoc. Sci. Hydrology, Comm. Ground Waters Pub.* 52, p. 478-487.
- Hougen, O. A., and Marshall, W. R., Jr., 1947, Adsorption from a fluid stream flowing through a stationary granular bed: *Chem. Eng. Process*, v. 43, no. 4, p. 197.
- Jeffreys, Harold, 1961, Cartesian tensors: London, Cambridge Univ. Press, 92 p.
- Jong, G. de Josselin de, 1958, Longitudinal and transverse diffusion in granular deposits: *Am. Geophys. Union Trans.*, v. 39, no. 1, p. 67-74.
- 1959, Vortex theory of multiple phase flow through porous media: California Univ. Water Resource Center Contribution 23, 80 p.
- Jost, W., 1960, Diffusion in solids, liquids, gases: New York, Academic Press Inc., 558 p.
- Kitagawa, K., 1934, Sur le dispersement et l'écart moyen de l'éconlement des eaux sonterraines, I. Expériences avec un modèle le laboratoire: Kyoto Imperial Univ., Coll. Sci. Mem. Ser. A, v. 17, p. 37-42.
- Kohout, F. A., 1960, Cyclic flow of salt water in the Biscayne aquifer of southeastern Florida: *Jour. Geophys. Research*, v. 65, no. 7, p. 2133-2141.
- 1961, Fluctuation of groundwater levels caused by dispersion of salts: *Jour. Geophys. Research*, v. 66, no. 8, p. 2429-2434.
- Kramers, H., and Alberda, G., 1953, Frequency response analysis of continuous flow system: *Chem. Eng. Sci.*, v. 2, no. 4, p. 173-181.
- Lau, Leung-Kai, Kaufman, W. J., and Todd, D. K., 1959, Dispersion of a water tracer in radial laminar flow through homogeneous porous media: *Calif. Univ., Inst. Eng. Research Ser.* 93, Issue No. 5, 78 p.
- Milne-Thomson, L. M., 1961, Theoretical hydrodynamics: New York, MacMillan Co., 660 p.
- Muskat, Morris, 1946, The flow of homogeneous fluids through porous media: Ann Arbor, Michigan, J. W. Edwards, Inc., 749 p.
- Ogata, Akio, 1958, Dispersion in porous media: Evanston, Ill., Northwestern Univ., Ph. D. dissert.
- 1961, Transverse diffusion in saturated isotropic granular media: U.S. Geol. Survey Prof. Paper 411-B, 8 p.
- 1964a, The spread of a dye stream in an isotropic granular medium: U.S. Geol. Survey Prof. Paper 411-G, 11 p.
- 1964b, Mathematics of dispersion with linear adsorption isotherm: U.S. Geol. Survey Prof. Paper 411-H, 9 p.
- Ogata, Akio, and Banks, R. B., 1961, A solution of the differential equation of longitudinal dispersion in porous media: U.S. Geol. Survey Prof. Paper 411-A, 7 p.
- Orlob, G. T., and Radhakrishna, G. N., 1958, The effects of entrapped gases on the hydraulic characteristics of porous media: *Am. Geophys. Union Trans.*, v. 39, no. 4, p. 648-659.
- Perkins, T. K., and Johnston, O. C., 1963, A review of diffusion and dispersion in porous media: *Soc. Petroleum Engineers Jour.*, v. 3, no. 1, p. 70-84.
- Rifai, M. N. E., Kaufman, W. J., and Todd, D. K., 1956, Dispersion phenomena in laminar flow through porous media: *Calif. Univ., Inst. Eng. Research Ser.* 93, Issue No. 2, 157 p.
- Saffman, P. G., 1959, A theory of dispersion in a porous medium: *Jour. Fluid Mech.*, v. 6, p. 321-349.
- 1960, Dispersion due to molecular diffusion and macroscopic mixing in flow through a network of capillaries: *Jour. Fluid Mech.*, v. 7, p. 194-208.
- Scheidegger, A. E., 1954, Statistical hydrodynamics in porous media: *Appl. Physics Jour.*, v. 25, p. 994-1001.
- 1960, The physics of flow through porous media: Canada, Univ. Toronto Press, 313 p.
- 1961, General theory of dispersion in porous media: *Jour. Geophys. Research*, v. 66, no. 10, p. 3273-3278.
- Shamir, U. Y., and Harleman, D. R. F., 1967, Numerical solutions for dispersion in porous media: *Water Resources Research*, v. 3, no. 2, p. 557-581.
- Skibitzke, H. E., 1964, Extending Darcy's concept of ground-water motion: U.S. Geol. Survey Prof. Paper 411-F, 6 p.
- Skibitzke, H. E., Chapman, H. T., Robinson, G. M., and McCullough, R. A., 1961, Radio-tracer techniques for the study of flow in saturated porous material: *Internat. Jour. Appl. Radiation and Isotopes*, v. 10, no. 1, p. 38-46.
- Skibitzke, H. E., and Robinson, G. M., 1963, Dispersion of ground water flowing through heterogeneous materials: U.S. Geol. Survey Prof. Paper 386-B, 3 p.
- Slichter, C. S., 1905, Field measurements of the rate of movement of underground water: U.S. Geol. Survey Water-Supply Paper 140, p. 9-85.
- Sneddon, I. N., 1951, Fourier Transforms: New York, McGraw-Hill Book Co., 542 p.
- Taylor, Geoffrey, 1953, Dispersion of soluble matter in solvent flowing slowly through a tube: *Royal Soc. London Proc.*, ser. A, v. 219, p. 187-203.
- Vermeulen, Theodore, and Hiester, N. K., 1952, Ion exchange chromatography of trace elements: *Ind. Eng. Chemistry*, v. 44, p. 636-651.
- Wentworth, C. K., 1948, Growth of the Ghyben-Herzberg transition zone under a rinsing hypothesis: *Am. Geophys. Union Trans.*, v. 29, p. 97-98.