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CONVECTIVE TRANSPORT OF SOLUTES BY STEADY FLOWS
I. GENERAL THEORY

P.A.C. RAATS

Agricultural Research Service, U.S. Salinity Laboratory, U.S. Department of Agriculture, P.O. Box 672, Riverside, Calif. 92502 (U.S.A.)

Present address: Institute for Soil Fertility, Oosterweg 92, Haren (Gr.) (The Netherlands)

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ABSTRACT

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A comprehensive theory describing convective transport of solutes is presented. The time required for a parcel of water to move from one point to another along a streamline is determined, and this basic information is then used to describe collections of parcels of water forming a surface. Input/output relationships are determined in terms of the distribution of the solute over the inflow and outflow surfaces. A simple geometric transformation is used to extend the theory to anisotropic media. Applications to specific flow problems will be treated in Part II.

INTRODUCTION

The two major objectives of research related to the management of water quality are

— to find the space-time trajectories of parcels of water;
— to determine the changes in quality of these parcels.

To meet the first objective, one can turn to a large body of experience with movement of water in saturated and in unsaturated soils. In the past, most concern has been with describing what happens at given places in the course of time. But recently interest has turned more and more to describing what happens to given parcels of water in the course of time. In other words, there is a switch from a spatial to a material description. The progress of a parcel of water in the course of time can be determined by integrating its speed along its path. In this paper it will be shown how this basic information can be used to describe the fate of collections of parcels of water forming a surface or occupying a region and to formulate input/output relationships characterizing transport across a region. Some applications of the theory will be treated in Part II (Raats, 1978).

The second objective of research related to the management of water quality has many aspects:
— to determine the change in the concentration of a parcel of water due to evaporation at or near the soil surface and due to selective uptake of water by plant roots (Raats, 1975);
— to determine the gain or loss of solutes by parcels of water as a result of diffusive and dispersive mixing with their surroundings (Raats, 1978);
— to determine the retardation of solutes relative to the water resulting from adsorption;
— to determine whether solutes precipitate or dissolve.

These aspects will not be pursued in this paper or in the companion paper on applications. All results can be easily extended to solutes subject to radioactive decay or linear adsorption. Unfortunately, nonlinear adsorption and diffusion or hydrodynamic dispersion are usually more difficult to handle.

The key elements of the theory are the treatment of the movement of interfaces by Muskat (1934, 1946) and the transfer function approach to industrial processes by Danckwerts (1953) and to tracers in hydrology by Ericksson (1961, 1971). The present theory unifies and generalizes the two approaches in many respects. It also provides a framework for comparing and for utilizing more fully numerous results for special flow problems that can be found in the literature, as will be shown in Part II. The concepts are of interest in a wide variety of water management problems: leaching of saline soils; development of saline seeps; appearance of salts, nutrients, and pesticides in streams, ditches, and tile lines; movement of water bodies injected in aquifers; the use of temperature and radioactive substances as tracers in hydrology.

The outline of this paper is as follows. In Section 1 I will discuss several methods that can be used to evaluate the time required for a parcel of water to move from one point to another along a streamline. This basic information is used in Section 2 to describe collections of parcels of water forming a surface or occupying a region. In Section 3, I will introduce concepts that are useful for characterizing the integral aspects of transport across a region. In Section 4, I will discuss input/output relationships for entire regions. The global theory in Sections 3 and 4 generalizes concepts developed originally for reactors in chemical engineering and for tracers in biological experiments. The distribution of the solute over the inflow surface and the flow pattern between the inflow and outflow surfaces play a dominant role in the present theory. In Section 5, the theory is extended to anisotropic media.

In Part II I will use a very simple model for flow from a water table to a drain to illustrate the concepts introduced in the first paper. A detailed evaluation of the literature on other problems will also be given in Part II.

1. DISTRIBUTION OF TRAVEL TIMES

The distribution of travel times is basic to all subsequent developments. In essence, it depends on the distribution of the velocities, which in turn depends on the dynamics. Following the definition of the travel time between two points in Section 1.1, I present a kinematical interpretation based upon the balance of mass in Section 1.2, a dynamical interpretation based upon Darcy's law in Section 1.3, and a summary of methods that can be used to calculate travel times in Section 1.4.

1.1. Definitions

Let χ be the place occupied by a parcel (differential volume element) of water in some reference configuration, like time t_0. The places χ at time t_0 may be regarded as labels of parcels. To describe the motion, one needs to know for any parcel, χ, the place, $\mathbf{x}$, it occupies at any time, t:

$$\mathbf{x} = \mathbf{x}\,[\chi, t]. \tag{1.1}$$

The velocity, $\mathbf{v}$, is defined as

$$\mathbf{v} = \partial \mathbf{x}/\partial t|_\chi. \tag{1.2}$$

A curve everywhere tangent to the velocity field is called a streamline. The streamlines of plane and axisymmetric, steady flows can be characterized by a single stream function ψ.

Let s denote the arc-length parameter along a streamline. The vector field, $\mathbf{v}$, is characterized by its magnitude field, v, and unit tangent vector field, τ, defined by (cf. Fig. 1)

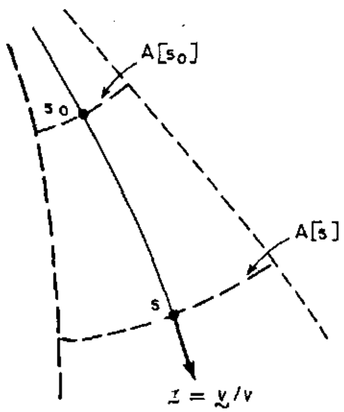

Fig. 1. Infinitesimal stream tube.

$$v = \partial s/\partial t|_\chi, \tag{1.3}$$

$$\tau = \mathbf{v}/v. \tag{1.4}$$

Integration of (1.3) from some reference point, s_0, to some point, s, gives the travel time, $t - t_0$, between two points on a streamline:

$$t - t_0 = \int_{s_0}^{s} v^{-1} \, ds. \tag{1.5}$$

1.2. Kinematical expressions

A purely kinematical expression for the distribution of v along a streamline can be obtained by integrating the balance of mass along this streamline. For steady flow without sources and sinks, the balance of mass is given by

$$\nabla \cdot (\theta \mathrm{v}) = 0, \tag{1.6}$$

where θ is the volumetric water content. Introducing (1.4) into (1.6) and integrating the resulting equation gives [Raats, 1974, Eqs. (14) to (16)]

$$\theta v = (\theta v)_0 \exp\left[- \int_{s_0}^{s} \nabla \cdot \tau \, ds \right]. \tag{1.7}$$

According to (1.7), the magnitude, θv, of the flux at any point, s, along a streamline can be calculated from its value $(\theta v)_0$ at some other point, s_0, and the distribution of $\nabla \cdot \tau$ between s_0 and s. Dividing both sides of (1.7) by θ and introducing the resulting expression for v into (1.5) gives

$$t - t_0 = (\theta v)_0^{-1} \int_{s_0}^{s} \theta \exp\left[\int_{s_0}^{s} \nabla \cdot \tau \, ds \right] ds. \tag{1.8}$$

According to (1.8) the travel time $t - t_0$ is inversely proportional to the flux $(\theta v)_0$ at s_0 and a function of the distribution of θ and $\nabla \cdot \tau$ between s_0 and s. The divergence of the unit tangent vector field, $\nabla \cdot \tau$, is a characteristic of the flow pattern and is a measure of the divergence or convergence of infinitesimal stream tubes. It can be shown that [Raats, 1974, Eq.(10)]

$$\nabla \cdot \tau = \frac{1}{A} \frac{\delta A}{\delta s} = \frac{\delta \ln A}{\delta s}, \tag{1.9}$$

where A is the cross-sectional area of an infinitesimal stream tube, and $\delta \cdot / \delta s$ is the directional derivative along a streamline. Integration of Eq.(1.9) gives

$$A[s] = A_0 \exp\left[\int_{s_0}^{s} \nabla \cdot \tau \, ds \right], \tag{1.10}$$

where A_0 is the area of the stream tube at s_0. According to (1.10), the area of a stream tube at some point s along a streamline is proportional to A_0 and a function of the distribution of $\nabla \cdot \tau$ between s and s_0. The cross-sectional area increases if $\nabla \cdot \tau > 0$ and decreases if $\nabla \cdot \tau < 0$. Introducing (1.10) into (1.7) and (1.8) gives

$$\theta v = (\theta v)_0 A_0 / A, \tag{1.11}$$

$$t - t_0 = (\theta v)_0^{-1} \; A_0^{-1} \int_{s_0}^{s} \theta \; A \; \mathrm{d}s. \tag{1.12}$$

On the right-hand side of (1.12), the integral corresponds to the total amount of water in the stream tube between the points, s_0 and s, while $(\theta v)_0 A_0$ corresponds to the steady flux. Obviously, the ratio of these two quantities is equal to the travel time between s_0 and s. If $\theta = \theta_0$ all along the stream tube, then (1.12) reduces to

$$t - t_0 = (v_0 A_0)^{-1} \int_{s_0}^{s} A \; \mathrm{d}s, \tag{1.13}$$

where the integral corresponds to the volume of the stream tube between s_0 and s. Given a flow pattern, this volume and the area A_0 can be easily evaluated from graphical integration. For a given stream tube, the time $t - t_0$ is inversely proportional to the velocity v_0.

Sometimes it is more convenient to evaluate the progress along a streamline in terms of its projection onto a coordinate line or curve. Clearly

$$t - t_0 = \int_{s_0}^{s} v^{-1} \; \mathrm{d}s = \int_{x_{i0}}^{x_i} v_i^{-1} \; \mathrm{d}x_i, \tag{1.14}$$

where x_i is a coordinate line or curve, and v_i is the component of the velocity along x_i. This form is particularly convenient, if the component of the velocity in a certain direction is known along a given streamline explicitly as a function of just the coordinate corresponding to that direction. If the x_i's form a rectangular Cartesian coordinate system, then it is easily shown that

$$t - t_0 = (\theta_0 \; v_{i0} \; A_{i0})^{-1} \int_{x_{i0}}^{x_i} \theta \; A_i \; \mathrm{d}x_i, \tag{1.15}$$

where A_i is the intersection of the stream tube with the coordinate plane perpendicular to x_i.

The above discussion establishes the link between approximate graphical analyses based on (1.12), (1.13), and (1.15) and a precise analytical description of the flow pattern in terms of the unit tangent vector field $\boldsymbol{\tau}$. These interpretations enhance the intuitive understanding of analytical or numerical solutions of specific flow problems.

1.3. Dynamical expressions

The results obtained thus far are purely kinematic. They apply to any steady flow independent of its dynamics. The first dynamical expression that

I will consider is Darcy's law for flow in a saturated or unsaturated, isotropic porous medium:

$$v = -k/\theta \; \nabla H, \tag{1.16}$$

where k is the hydraulic conductivity, and H is the total head, which is the sum of the pressure head, h, and the gravitational head, z. If the soil is unsaturated, k will be a function of θ. Introducing (1.16) into (1.5) gives

$$t - t_0 = - \int_{s_0}^{s} (\theta/k)|\nabla H|^{-1} \, ds. \tag{1.17}$$

Transforming from integration with respect to s to integration with respect to H gives

$$t - t_0 = - \int_{H_0}^{H} (\theta/k)|\nabla H|^{-2} dH, \tag{1.18}$$

and

$$t - t_0 = - \int_{H_0}^{H} (\theta k) \, v^{-2} \, dH, \tag{1.19}$$

where the integrations are to be performed along a stream line. The integrals in (1.18) or (1.19) can be evaluated easily if θ and k are constants, and ∇H or v are known as functions of H along a streamline. Similar to (1.14) and (1.15), Eqs.(1.18) and (1.19) can be written in component form:

$$t - t_0 = - \int_{H_0}^{H} (\theta/k)|\partial H/\partial x_i|^{-2} \, dH, \tag{1.20}$$

and

$$t - t_0 = - \int_{H_0}^{H} (\theta k) \, v_i^{-2} \, dH, \tag{1.21}$$

where the integrations are to be performed along the coordinate x_i.

Eq. (1.18) suggests a simple graphical method for evaluating travel times. The finite difference version of (1.18) is

$$\Delta t = \frac{\theta}{k} \frac{(\Delta s)^2}{\Delta H}. \tag{1.22}$$

From a flow net, one can determine graphically the varying increments Δs corresponding to fixed increments ΔH. For given θ and k, and a fixed increment ΔH, the increment of Δt is proportional to the *square* of the increment of Δs. This is consistent with the well-known fact that for plane flow equidistant streamlines and equipotentials divide the flow region in similar, curvilinear rectangles. Thus, any nonuniformity in the flow becomes amplified in the distribution of travel times.

1.4. Recapitulation

In summary, the following methods can be used to calculate travel times:

(1) *Analytical.* (a) If $|\nabla H|$ or v is known as a function of the stream function, ψ, and the total head, H, then (1.18) or (1.19) can be used. (b) If $\partial H/\partial x_i$ or v_i is known as a function of ψ and x_i, then (1.20) or (1.21) can be used.

(2) *Graphical.* If the flow pattern and the distribution of θ are known, then (1.12) or its coordinate version (1.15) can be used.

(3) *Numerical.* If the distributions of k, θ, and H are known, a variety of numerical schemes can be set up to calculate the progress of particles along streamlines. For example, one could use the finite difference equation (1.20) as a basis.

2. DISTRIBUTION OF FAMILIES OF ISOCHRONES

In Section 1 I outlined the methods that can be used to evaluate the time required for a parcel of water to move from one point to another along a streamline. That basic information will be used to describe the movement of collections of parcels of water forming a surface. Examples of such surfaces are discrete inputs of solute into the region of interest and interfaces between regions occupied by waters of different qualities. Eq. (1.1) describes the configurations of such surfaces, with the velocity of parcels, χ, on the surface given by (1.2). Elimination of the parameter χ gives

$$f(\mathbf{x}, t) = 0. \tag{2.1}$$

Given a spatial representation, like (2.1), it is not possible to calculate a unique form (1.1), since the points on the successive configurations can be mapped continuously infinitely many ways. However, given (1.1), differentiation of (2.1) with respect to t gives (Muskat, 1934)

$$\dot{f} = \frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f = 0. \tag{2.2}$$

Lagrange showed that (2.2) is the necessary and sufficient condition for the surface $f(\mathbf{x}, t) = 0$ to be material (Truesdell and Toupin, 1960, Section 74). The normal velocity or speed of displacement of the surface, v_n, is given by

$$v_n = \mathbf{v}\cdot\mathbf{n} = \partial\mathbf{x}/\partial t|_\chi \cdot \mathbf{n}, \tag{2.3}$$

where $\mathbf{n}$ is the unit normal to the surface.

In terms of the arc-length parameter, s, along the streamlines, Eq. (2.2) can be written as

$$\partial f/\partial t + v\,\partial f/\partial s = 0. \tag{2.4}$$

If v is independent of time, integration of (2.4) gives (Muskat, 1934)

$$f = \gamma t - \gamma \int v^{-1}\, ds + g = \text{constant}, \tag{2.5}$$

where γ is an arbitrary constant, and g is an arbitrary function to be adjusted so that f assumes its initial form at the reference time, t_0. All the later history of the parcels lying initially on this line may then be found by simply plotting Eq.(2.5) for successive values of t. Comparison of (2.5) and (1.5) shows that $(f-g)/\gamma$ corresponds to t_0. Without any loss of generality, the parameter, γ, can be taken as unity. Using results from the previous section, many other forms of (2.4) and (2.5) can be obtained. For example, Muskat (1934) gave a version with the integral in (2.5) replaced by the right-hand side of (1.18).

A region, in which a steady flow occurs, is generally bounded by inflow surfaces, stream surfaces, and outflow surfaces. The stream tubes connect the inflow and outflow surfaces. The subscripts α and ω will, respectively, denote quantities associated with the inflow and outflow surfaces.

Let t_α and t_ω be the times at which a parcel enters and leaves the system, respectively. With each stream tube is associated a unique *transit time*, τ, defined by

$$\tau = t_\omega - t_\alpha. \tag{2.6}$$

With each parcel in the system is associated a unique *residence time* defined by

$$\tau_\alpha = t - t_\alpha \tag{2.7}$$

and a unique *residual transit time* defined by

$$\tau_\omega = t_\omega - t. \tag{2.8}$$

Eqs.(2.6), (2.7), and (2.8) imply that the transit time is equal to the sum of the residence and residual transit times:

$$\tau = \tau_\alpha + \tau_\omega. \tag{2.9}$$

Contours of equal τ_α and τ_ω form two families of *isochrones*. Any isochrone of the τ_α family (τ_ω family) represents a collection of parcels entering (leaving) the system simultaneously.* The inflow and outflow surfaces serve as reference surfaces. Of course, Eq.(2.5) suggests that one can take any surface $g(u, v)$ as a reference surface and determine a family of isochrones representing its past and future configurations. The travel time distributions along streamlines discussed in Section 1 uniquely determine all such families. In view of the great interest in convective transport of solutes, it seems desirable that solving a steady flow problem would include determining at least one family of isochrones.

*In population dynamics t_α is the time of birth; t_ω is the time of death; τ is the life time; τ_α is the age; τ_ω is the residual life time.

With each streamline, ψ, is associated a unique transit time, τ. Therefore, any point in the flow region can be characterized by values of the residence time, τ_α, and the transit time, τ. In view of (2.9), equivalent characterizations consist of giving the residence time, τ_α, and the residual transit time, τ_ω, or the transit time, τ, and the residual transit time, τ_ω.

Any point in the flow region is characterized by its location on a certain streamline and on a certain member of *any* family of isochrones. Stream tubes with a certain flux and isochrones differing by a fixed time increment will partition the flow region into subregions of equal volume. For plane flows, uniformly spaced streamlines and isochrones will partition the plane of flow into subregions of equal area. This contrasts sharply with the curvilinear, similar rectangles formed by uniformly spaced streamlines and equipotentials.

Following the shape of a subregion during its course along a stream tube gives a clear idea of the deformation of such a subregion. The orientation of the isochrones with respect to the streamlines usually changes in the course of time. In particular, parcels situated upon an iso-H surface at a certain time will generally not have occupied such a surface in the past and will not remain on such a surface in the future. This can be demonstrated by considering the time rate of change of the total head, $\mathrm{d}H/\mathrm{d}t$, of a parcel,

$$\mathrm{d}H/\mathrm{d}t = \partial H/\partial t + \mathbf{v}\cdot\nabla H. \tag{2.10}$$

Using (1.16) in (2.10) and noting that for steady flow $\partial H/\partial t = 0$ gives

$$\mathrm{d}H/\mathrm{d}t = -(k/\theta)|\nabla H|^2. \tag{2.11}$$

Eq.(2.11) shows that parcels situated upon an iso-H surface will remain upon such a surface if and only if $|\nabla H|$ is constant on each iso-H surface (Muskat, 1946, p.458). This condition is satisfied for linear flow, two-dimensional radial flow, and spherical flow; it seems that the condition is not satisfied in any other cases. In such flows, the inflow and outflow surfaces are equipotential surfaces and the transit time will be the same for each stream tube. The general trend can also be deduced from (1.22), which shows that for a fixed increment, ΔH, the corresponding increment, Δt, is proportional to the square of the corresponding increment, Δs.

3. THE CUMULATIVE TRANSIT TIME DENSITY DISTRIBUTION AND RELATED CONCEPTS

In this section I will interpret the frequency distribution of transit times, i.e., of travel times between points of input surfaces and points of output surfaces. The immediate result is an integral characterization of simple leaching processes in flow systems with arbitrary geometry. The key concept of transit time density distribution will also be used in the next section, where the output of solutes will be related more fully to the initial distribution over the entire system and the subsequent distribution over the input surface.

The *cumulative transit time distribution function*, q, is defined as the fraction of the stream tubes with transit times smaller than τ. (See Fig. 2 which illustrates many of the concepts introduced in this section.) At any time a fraction q of the output will be younger than τ and a fraction $(1-q)$ of the output will be older than τ. The derivative $dq/d\tau$ is *the transit time density distribution function*. Geometrically, $dq/d\tau$ corresponds to the frequency distribution of the volume of the stream tubes. The function q can be determined by measuring the concentration of the solute or the tracer in the output after a step change of the concentration in the input. The function $dq/d\tau$ can be determined by measuring the output resulting from a pulse distributed uniformly in the input. It will be shown later that $dq/d\tau$ may be regarded as a transfer function of the flow system for solutes distributed uniformly in the input.

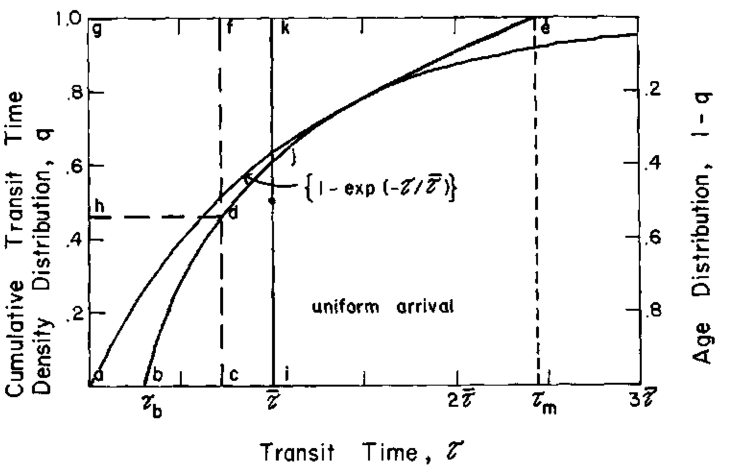

Fig. 2. Integral properties of leaching processes.

Generally, the transit time will be different for each stream tube (Fig. 2). The shortest transit time, τ_{min}, for the smallest stream tube, gives the *breakthrough time* for a given input. The longest transit time, τ_{max}, for the largest stream tube, gives the *memory time* for a given input. If the inflow and outflow surface intersect each other, then the transit time along the intersection will be zero. In flow systems with such intersections, the breakthrough time for a given input will be zero. For streamlines with stagnation points, the transit time is infinite. Hence, in flow systems with stagnation points, the memory time for a given input is infinite.

The *bypass* B is defined as

$$B = F \int_0^{\tau} q \, d\tau, \tag{3.1}$$

where F is the integral, steady flux of water across the system. The bypass B

is the amount of water that was applied after time t_0 and that has already left the flow system at time $t_0 + \tau$. The bypass B at time $t_0 + \tau$ is equal to F times the area under the q vs. τ curve between 0 and τ (Fig. 2). The *displacement* D is defined as

$$D = F \int_0^\tau (1 - q)\, d\tau = F\tau - B, \tag{3.2}$$

that is, D is the amount of water that was applied after time t_0 and that has displaced water present in the system at time t_0. The displacement D at time $t_0 + \tau$ is equal to F times the area above the q vs. τ curve between 0 and τ (Fig. 2). Note that $F\tau$ is the *total amount of water applied* after t_0 and that

$$F\tau = B + D. \tag{3.3}$$

The concepts just introduced provide a basis for defining two *efficiency* parameters characterizing a leaching process. The *overall leaching efficiency* over the time interval t_0 to $t_0 + \tau$ is defined as the ratio of the displacement and the total amount of water applied:

$$E_a = \frac{D}{F\tau} = \frac{\int_0^\tau (1 - q)\, d\tau}{\tau} = 1 - \frac{B}{F\tau} = \frac{D}{B + D}. \tag{3.4}$$

The fraction $B/(F\tau)$ could be called the *overall leaching inefficiency* because it is the fraction of the applied water that has bypassed. The *marginal leaching efficiency* at time $t_0 + \tau$ is the ratio of the time rate of change of the displacement to the rate at which the water is applied:

$$E_m = \frac{dD/dt}{F} = 1 - q. \tag{3.5}$$

The total volume, V, of the flow system is given by

$$V = F \int_0^\infty (1 - q)\, d\tau = F\bar{\tau}, \tag{3.6}$$

where $\bar{\tau}$ is the turnover time of the system. According to (3.6), V is equal to F times the total area above the q vs. τ curve. The amount of water $V - D$ not yet displaced at time τ is given by

$$V - D = F \int_\tau^\infty (1 - q)\, d\tau, \tag{3.7}$$

that is $V - D$ is equal to F times the area above the q vs. τ curve between τ and ∞. At time $t_0 + \tau$, the displacement D may also be written as the sum of two parts

$$D = D_1 + D_2$$

$$= F \int_0^{q[\tau]} \tau \, dq + F \tau (1 - q[\tau]). \qquad (3.8)$$

On the righthand side of (3.8), the first term represents stream tubes from which all the water present at time t_0 has been displaced at time $t_0 + \tau$; while the second term represents water displaced from stream tubes, from which only part of the water present at time t_0 has been displaced at time $t_0 + \tau$.

Table I summarizes some particular values of B, D, E_a, and E_m. For times smaller than $t_0 + \tau_{min}$ the bypass is zero, the displacement is $F\,\tau$, and the efficiencies E_a and E_m are unity. At the breakthrough time, $t_0 + \tau_{min}$, the displacement is $F\,\tau_{min}$. At the memory time, $t_0 + \tau_{max}$, the bypass is $(F\,\tau_{max} - V)$, the displacement is V, the overall efficiency is $\bar{\tau}/\tau_{max}$, and the marginal efficiency is zero. If the memory time approaches infinity, then as $t \to t_0 + \tau_{max}$, the bypass approaches infinity and the overall efficiency approaches zero. The leaching process will be most efficient if the transit times are narrowly distributed around $\bar{\tau}$. The hydraulic efficiencies account only for the influence of the transit times. The net efficiency also depends on diffusion, hydrodynamic dispersion, and exchange processes.

TABLE I

Summary of some particular values of B, D, E_a, and E_m

t	$< t_0 + \tau_{min}$	$t_0 + \tau_{min}$	$t_0 + \tau_{max}$	$t_0 + \tau_{max} \to \infty$
q	0	0	1	1
B	0	0	$F\,\tau_{max} - V$	∞
D	$F\,\tau_{min}$	$F\,\tau_{min}$	V	V
E_a	1	1	$\bar{\tau}/\tau_{max}$	0
E_m	1	1	0	0

The diagram of q versus τ shown in Fig. 2 can be used to summarize the displacement process for a given geometry and for given boundary conditions. The times τ_b, $\bar{\tau}$, and τ_m are the breakthrough, turnover, and memory times, respectively. The area above the curve bde corresponds to the total amount of water in the system. The area acfg corresponds to the total amount of water applied at time τ. This water is divided into three parts: water that has bypassed (bcd), water present in completely leached stream tubes (abdh), and water present in partially leached stream tubes (hdfg). The area def represents water yet to be displaced from the partially leached stream tubes. At the turnover time, $\bar{\tau}$, this area is equal to the area representing bypass. The curve $q = \{1 - \exp(-\tau/\bar{\tau})\}$ applies to an apparently well-mixed system and will be discussed in detail in Part II.

Each of the functions q, $dq/d\tau$, B, or D completely characterizes the convective transport across a region. Consider a line parallel to the vertical axis and intersecting the horizontal axis at a certain value τ (Fig. 2). The area to the left of this line and above the $q[\tau]$ curve represents water in the system younger than τ, while the area to the right of this line and above the $q[\tau]$ curve represents water in the system older than τ. This internal age distribution is not the same as the age distribution in the output. In the output, the fractions younger and older than τ correspond to the fractions of the vertical line below and above the $q[\tau]$ curve, respectively. This shows that the efficiencies, E_a and E_m, are closely related to the internal age distribution and the age distribution in the output, respectively.

4. INPUT—OUTPUT RELATIONSHIPS

In this section it will be shown how the output of solutes is related to the initial distribution over the entire region and the subsequent distribution over the input surface.

The input function $f_\alpha\,[q,t]$ describes the flux of solute into the region as a function of the cumulative transit time distribution function, q, and the time, t (Fig. 3). The cumulative input into the region from time t_0 up to time t is given by

$$Q_\alpha = \int_{t_0}^{t} \int_0^1 f_\alpha \, \mathrm{d}q \, \mathrm{d}t. \tag{4.1}$$

The rate of input into the region at time t is given by

$$\frac{\mathrm{d}Q_\alpha}{\mathrm{d}t} = \int_0^1 f_\alpha \, \mathrm{d}q. \tag{4.2}$$

The cumulative input into any stream tube is given by

$$\frac{\mathrm{d}Q_\alpha}{\mathrm{d}q} = \int_{t_0}^{t} f_\alpha \, \mathrm{d}t. \tag{4.3}$$

In many applications, the input function is separable

$$f_\alpha\,[q,t] = f_{\alpha q}[q] \cdot f_{\alpha t}[t]. \tag{4.4}$$

If the input function is separable, it can be written as the product of the rate of input $\mathrm{d}Q_\alpha/\mathrm{d}t$ and the input density distribution $r[q]$:

$$f_\alpha[q,t] = r[q]\,\frac{\mathrm{d}Q_\alpha}{\mathrm{d}t}, \tag{4.5}$$

where

$$r = \frac{f_{\alpha q}}{\int_0^1 f_{\alpha q}\,\mathrm{d}q}. \tag{4.6}$$

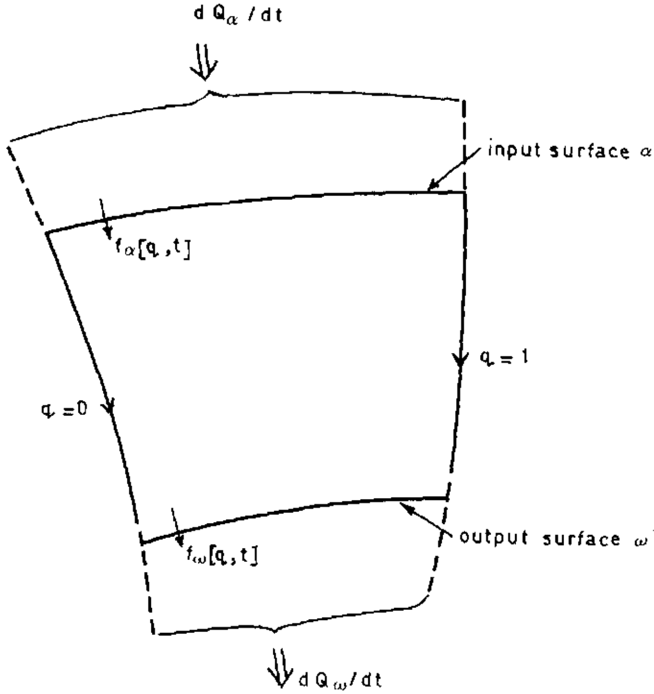

Fig. 3. Input/output relationships.

The following special cases are of particular interest:

(1) If the solute is introduced with the water, and, at any instant, the concentration of the solute in the input is uniform, then $f_{\alpha q}[q]$ is a constant.

(2) If the solute is not introduced with the water, but is applied directly to the inflow surface, then the amount of solute in a given stream tube is the amount applied to the intersection of the stream tube and the inflow surface. If the solute is applied uniformly over the input surface, then the density distribution of the areas of these intersections determines the density distribution of the solute over the stream tubes; more specifically, $f_{\alpha q}[q]$ may then be taken as proportional to $(\mathrm{d}a_\alpha/\mathrm{d}q)/A_\alpha$, where $\mathrm{d}a_\alpha$ is an element of inflow surface and A_α is the total inflow surface. Of course, the rate of input $\mathrm{d}Q_\alpha/\mathrm{d}t$ will depend on the process of dissolution.

(3) In treatments of soils with chemicals for pest control or reclamation, it may be desirable to distribute the chemical over the stream tubes in accordance with their volumes or, equivalently, in accordance with their transit times, i.e., $f_\alpha\,[q] \sim \tau$.

(4) The function $f_{\alpha t}[t]$ may be a constant, a delta function, expressible in terms of a Fourier series, etc.

The output function $f_\omega\ [q,t]$ depends upon the initial distribution $\rho\ [q,\tau_\omega]$ and upon the input function, with the travel time distribution providing the connection. For a given stream tube, the output at time t derives from an input at time $t-\tau$ if $t-t_0 \geqslant \tau$; otherwise it derives from initial storage along the isochrone with $\tau_\omega = t - t_0$:

$$f_\omega\ [q,t] = \begin{cases} f_\alpha\ [q,\ t-\tau] & \text{if } t-t_0 \geqslant \tau, \\ \rho\ [q,\tau_\omega = t-t_0] & \text{if } t-t_0 < \tau. \end{cases} \tag{4.7}$$

The cumulative output from the region is given by (cf., Fig. 3):

$$Q_\omega = \int_{t_0}^{t} \int_0^1 f_\omega\ \mathrm{d}q\ \mathrm{d}t. \tag{4.8}$$

The rate of output from the region is given by

$$\frac{\mathrm{d}Q_\omega}{\mathrm{d}t} = \int_0^1 f_\omega\ \mathrm{d}q$$

$$= \int_0^l f_\alpha\ [q,\ t-\tau]\ \mathrm{d}q + \int_l^1 \rho\ [q,\ \tau_\omega = t-t_0]\ \mathrm{d}q, \tag{4.9}$$

where

$$l = \begin{cases} 1 & \text{if } \tau_{\max} \leqslant t-t_0, \\ q[\tau = t-t_0] & \text{if } \tau_{\max} \geqslant t-t_0. \end{cases} \tag{4.10}$$

In (4.9), the first term represents a flux of solutes across the flow region; the second term represents leaching of solutes present at time t_0. The cumulative output from any stream tube is given by

$$\frac{\mathrm{d}Q_\omega}{\mathrm{d}q} = \int_{t_0}^{t} f_\omega\ \mathrm{d}t$$

$$= \int_{t_0}^{t_\star} \rho\ [q,\tau_\omega = t-t_0]\ \mathrm{d}t + \int_{t_\star}^{t} f_\alpha\ [q,\ t-\tau]\ \mathrm{d}t, \tag{4.11}$$

where

$$t_\star = \begin{cases} t & \text{if } t-t_0 \leqslant \tau, \\ t_0+\tau & \text{if } t-t_0 > \tau. \end{cases} \tag{4.12}$$

In (4.11), the first term represents leaching of solutes present in the stream tube at time t_0; the second term represents a flux of solutes across the flow region.

If the input function is separable, then substitution of (4.5) into (4.9) and changing in the first term of the resulting equation from integration with respect to q to integration with respect to τ gives

$$\frac{dQ_\omega}{dt} = \int_{t_0}^{t} T[\tau]\,\frac{dQ_\alpha}{dt}\,[t-\tau]\,d\tau + \int_{l}^{1} \rho\,[q,\tau_\omega = t - t_0]\,dq, \tag{4.13}$$

where the transfer function $T[\tau]$ is the product of the input and transit time density distribution functions:

$$T[\tau] = r\,dq/d\tau. \tag{4.14}$$

Three special cases are of particular interest:

(1) Unit pulse input and $\rho\,[q,\,\tau_\omega = t - t_0] = 0$. The output will correspond to the transit time density distribution function, $dq/d\tau$. Tracers are often used in this context.

(2) Step function input of solute dissolved in the water and $\rho\,[q,\,\tau_\omega = t - t_0] = 0$. The output will correspond to the cumulative transit time distribution function, $q\,[\tau]$. Leaching involves a step change of the input.

(3) A periodic input of solute dissolved in the water given by

$$\frac{dQ_\alpha}{dt} = \bar{a} + a_0 \cos\ \Omega t, \tag{4.15}$$

where $\bar{a}$ is the average rate of input, a_0 is the amplitude of the input variation, and Ω is the frequency of the input variation. Introducing (4.15) in (4.13) and taking the limit $t \to \infty$ gives

$$\frac{dQ_\omega}{dt} = \bar{a} + a \cos(\Omega t - b), \tag{4.16}$$

where the amplitude a and the phase shift b are given by

$$a = a_0 \left(\left\{ \int_0^\infty T[\tau]\,\cos\ \Omega\tau\,d\tau \right\}^2 + \left\{ \int_0^\infty T[\tau]\,\sin\ \Omega\tau\,d\tau \right\}^2 \right)^{1/2}, \tag{4.17}$$

$$b = \tan^{-1} \frac{\int_0^\infty T[\tau]\,\sin\ \Omega\tau\,d\tau}{\int_0^\infty T[\tau]\,\cos\ \Omega\tau\,d\tau}. \tag{4.18}$$

In principle, the transfer function $T[\tau]$ can be determined from measurements of a and b as functions of Ω. Alternatively, if $T[\tau]$ is known, then the frequency can be evaluated from (4.16), (4.17), and (4.18). Eqs.(7.16) and (7.17) of Part II give the amplitude and phase shift for a uniform, periodic input into a system with an exponential transit time density distribution.

5. EXTENSION TO ANISOTROPIC MEDIA

The simplest approach to flows in anisotropic soils is to transform the problem for the anisotropic soil into an equivalent problem for an isotropic soil. Let x_i ($i = 1, 2, 3$) be the principal directions and k_i ($i = 1, 2, 3$) be the associated principal hydraulic conductivities. A new coordinate system, $x_i^\star$, can be defined by

$$x_i^\star = (k_0/k_i)^{1/2}\, x_i, \tag{5.1}$$

where k_0 is an arbitrary, constant conductivity. The transformed components of the velocity are given by

$$v_i^\star = -k^\star \frac{\partial H}{\partial x_i^\star} = \left(\frac{k^{\star 2}}{k_0\, k_i}\right)^{1/2} v_i = \left(\frac{k_1\, k_2\, k_3}{k_0\, k_0\, k_i}\right)^{1/2} v_i, \tag{5.2}$$

where

$$k^\star = \left(\frac{k_1\, k_2\, k_3}{k_0}\right)^{1/2}. \tag{5.3}$$

Introducing (5.3) and (5.2) into (1.5) gives the transformed travel time distribution

$$t^\star - t_0^\star = \int_{x_{i0}^\star}^{x_i^\star} v_i^{\star\,-1}\, \mathrm{d}x_i^\star = \frac{k_0}{k^\star}\,(t - t_0). \tag{5.4}$$

Eq. (5.4) shows that once the travel time distribution $t^\star - t_0^\star$ for a given flow in an isotropic medium is known, then the travel time distribution for corresponding flows in all anisotropic media can be determined immediately from knowledge of the principal hydraulic conductivities k_1, k_2, and k_3.

Since the travel time distribution is basic to the entire analysis presented in this paper, the simple Eq. (5.4) can be used to extend all results to anisotropic porous media. In particular, the transit time for a given stream tube, and the residence time and residual transit time of a parcel will transform according to

$$\tau^\star = \frac{k_0}{k^\star}\,\tau, \qquad \tau_\alpha^\star = \frac{k_0}{k^\star}\,\tau_\alpha, \qquad \tau_\omega^\star = \frac{k_0}{k^\star}\,\tau_\omega. \tag{5.5}$$

The stretching and shrinking transformations given by (5.1) will also properly transform sequences of material surfaces associated with any flow problem.

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