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Multidimensional transport of solutes in saturated and in unsaturated soils

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Summary

The theory for multidimensional, convective transport of ideal tracers is extended to solutes subject to linear adsorption and/or linear production or decay. Some aspects of nonlinear adsorption, linear dispersion, and the influence of plant roots are also discussed. Expressions are derived relating the tracer velocity, the speed of isoconcentration surfaces, and the speed of shock waves to the velocity of the water and the shape of the adsorption isotherm. The response in the ditches or drains to a uniform periodic input of solute in the water is discussed in some detail for situations with no ponding on the soil surface, a relatively flat water-table, and the distance between the ditches or tile drains large relative to the depth of the impermeable layer.

Introduction

In two recent papers I discussed transport of solutes (Raats, 1978 a, b), the first paper dealing with the general theory, the second paper with specific flow problems. The time required for a parcel of water to move from one point to another along a streamline was determined and this basic information was then used to describe collections of parcels of water forming a surface. For any geometry and boundary conditions, the cumulative transit time distribution function, q, was defined as the fraction of the stream-tubes with transit times smaller than τ. The transit time density distribution was defined as the derivative of q with respect to τ. The function q can be determined by measuring the concentration of an ideal tracer in the output following 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. Inputs distributed nonuniformly over the input are characterized by an input density distribution function, r. It was shown that the product of this input density distribution function, r, and the transit time density distribution function, $dq/d\tau$, may be regarded as a transfer function of the flow system:

$$T(\tau) = r\, dq/d\tau, \tag{1}$$

where the square brackets denote functional dependence. The general relationship between the input I and output O, can be written as

$$O(t) = \int_{t_0}^{t} T(\tau)\, I\,(t\text{-}\tau)\mathrm{d}\tau + \text{ a contribution of solutes present at time } t_0. \qquad (2)$$

In this paper I will show that the entire theory can be extended to solutes subject to linear adsorption and/or to linear production or decay. Some aspects of nonlinear adsorption, linear dispersion, and the influence of plant roots will also be discussed.

The capacity relationship and the flux

The differential balance of mass of a solute can be written as

$$\frac{\partial \mu}{\partial t} = -\nabla . \underset{\sim}{F} + \sigma, \qquad (3)$$

where t is the time, ∇ is the vector differential operator, μ is the bulk density, $\underset{\sim}{F}$ is the flux of the solute, and σ is the rate of production. The total bulk density is the sum of the bulk densities μ_a in the adsorbed phase, and θc in the aqueous phase:

$$\mu = \mu_a + \theta c, \qquad (4)$$

where θ is the volumetric water content and c is the local density in the aqueous phase. Assuming that the adsorption isotherm describes a unique relationship between μ_a and c, the time rate of change of μ_a at any point can be written as

$$\frac{\partial \mu}{\partial t} = \varkappa \frac{\partial c}{\partial t} + c \frac{\partial \theta}{\partial t}, \qquad (5)$$

where

$$\varkappa = \frac{\mathrm{d}\mu_a}{\mathrm{d}c} + \theta. \qquad (6)$$

The total capacity, $\varkappa$, is the sum of the capacity of the absorbed phase, $\mathrm{d}\mu_a/\mathrm{d}c$, and the capacity of the aqueous phase, θ. The average of $\varkappa$ over the range c_1 to c_2 is defined as

$$\bar{\varkappa}_{12} = \frac{\int_{c_1}^{c_2} \varkappa \, \mathrm{d}c}{\int_{c_1}^{c_2} \mathrm{d}c} \qquad (7)$$

$$= \frac{\mu_2 - \mu_1}{c_2 - c_1} = \frac{\mu_{a1} - \mu_{a2}}{c_2 - c_1} + \theta. \qquad (8)$$

Geometrically, $\varkappa$ is the slope of a plot of μ versus c and $\bar{\varkappa}_{12}$ is the slope of the chorde between the points (c_1, μ_1) and (c_2, μ_2) in the same plot (Fig. 1). For the special case with $c_1 = 0$ and $c_2 = c$ the average capacity will be denoted by $\varkappa$ and will be given by

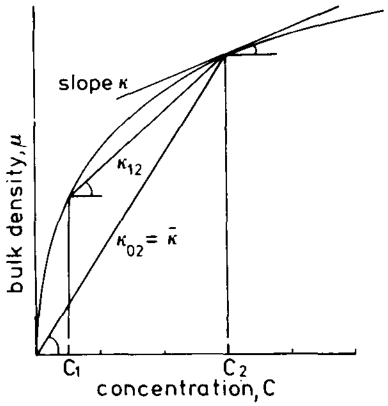

Fig. 1. The adsorption isotherm.

$$\bar{\kappa} \equiv \frac{\mu}{c} = \frac{\mu_a}{c} + \theta. \tag{9}$$

Geometrically, the average capacity $\bar{\kappa}$ corresponds to the slope of the chorde running from (0, 0) to (c, μ) in a plot of μ versus c (Fig. 1).

The flux $\underset{\sim}{F}$ is assumed to be the sum of a convective component $\theta \underset{\sim}{v}_w c$ and a dispersive component $-D\nabla c$:

$$\underset{\sim}{F} = \theta \underset{\sim}{v}_w c - D\nabla c. \tag{10}$$

Introducing Eq. 10 and Eq. 5 into Eq. 3 gives

$$\kappa \frac{\partial c}{\partial t} = -\theta \underset{\sim}{v}_w . \underset{\sim}{\nabla} c + \nabla . D \nabla c - \left(\frac{\partial \theta}{\partial t} + \underset{\sim}{\nabla} . \theta \underset{\sim}{v}_w \right) c + \sigma. \tag{11}$$

If the solution is dilute, then to a first approximation no distinction need to be made between the movement of the water and the soil solution as a whole, so that the balance of mass of the aqueous phase can be written as:

$$\frac{\partial \theta}{\partial t} = - \nabla . \theta \underset{\sim}{v}_w + \lambda, \tag{12}$$

where λ is the volumetric rate of uptake. Introducing Eq. 12 into Eq. 11 gives

$$\kappa \frac{\partial c}{\partial t} = -\theta \underset{\sim}{v}_w . \nabla c + \nabla . D \nabla c - \lambda c + \sigma. \tag{13}$$

Many qualitative and some quantitative aspects of solutions of Eq. 13 are presented in this paper.

The velocity of tracers and of surfaces of constant c

The velocity $\underset{\sim}{v}$ of the isotopically exchangeable solute, or, for short, the tracer velocity, is defined as the mass flux $\underset{\sim}{F}$ divided by the total density μ of the isotopically exchangeable solute

$$\underset{\sim}{v} = \underset{\sim}{F}/\mu. \tag{14}$$

Introducing Eq. 10 into Eq. 14 and using Eq. 9 gives

$$\underset{\sim}{v} = \frac{1}{\bar{\varkappa}}\left(\theta \underset{\sim}{v}_{w} - D\ \nabla \ln c\right). \tag{15}$$

According to Eq. 15 the tracer velocity vector is the sum of two components; (1) a convective component proportional to the reciprocal of the average capacity $\bar{\varkappa}$, to the water content θ, and to the velocity $\underset{\sim}{v}_{w}$ and (2) a diffusive component proportional to the reciprocal of the average capacity $\bar{\varkappa}$, to the dispersion tensor D, and to the negative of the relative concentration gradient $(\nabla c)/c = \nabla \ln c$ (Fig. 2). *The reciprocal of the average capacity $\bar{\varkappa}$ is a retardation factor for the tracer velocity $\underset{\sim}{v}$.* The retardation accounts for the average time spend by the solute in the absorbed phase.

Surfaces of constant c satisfy the kinematic condition

$$\frac{\mathrm{D}c}{\mathrm{D}t} = \frac{\partial c}{\partial t} + \underset{\sim}{v}_{c} \cdot \nabla c = 0, \tag{16}$$

where $\underset{\sim}{v}_{c}$ is the velocity vector of points on a surface of constant c. Eq. 16 can also be written as

$$\frac{\mathrm{D}c}{\mathrm{D}t} = \frac{\partial c}{\partial t} + v_{c}\ |\nabla c| = 0, \tag{17}$$

where the speed of propagation v_{c} of the surface of constant c is defined as

$$v_{c} = \underset{\sim}{v}_{c} \cdot \underset{\sim}{n}_{c} = -\frac{\partial c/\partial t}{|\nabla c|}, \tag{18}$$

where $\underset{\sim}{n}_{c}$ is the unit vector normal to the surface of constant c. Introducing Eq. 13 into Eq. 18 gives

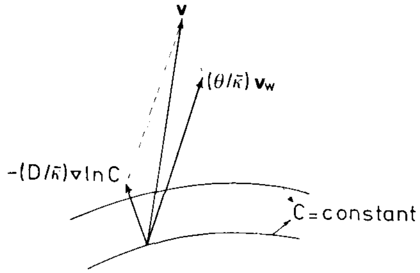

Fig. 2. The tracer velocity and its components.

$$v_c = \frac{\theta \underset{\sim}{v}_w \cdot \underset{\sim}{\nabla} c - \nabla \cdot D \nabla c + \lambda c - \sigma}{\varkappa \, |\nabla c|} \tag{19}$$

According to Eq. 19, the speed of the surface of constant c is proportional to the reciprocals of the capacity $\varkappa$ and of the magnitude of ∇c and to the sum of four contributions to the local rate of change of the concentration with time, $\partial c/\partial t$, respectively due to convection, dispersion, selective uptake by plant roots, and production. *The reciprocal of the capacity* $\varkappa$ *is a retardation factor for the speed* v_c *of the isoconcentration surface.* Since $\varkappa$ is a function of c, this retardation factor is different for each iso-c surface, but independent of time for any given iso-c surface.

Transport of a solute subject to linear production or decay and to linear adsorption

The rate of production is assumed to be given by

$$\sigma = - \alpha \mu, \tag{20}$$

where α is the rate constant which is < 0 for production and > 0 for decay. From Eq. 20 and Eq. 9 it follows that

$$\sigma = - \alpha \bar{\varkappa} c. \tag{21}$$

If the adsorption isotherm is linear, then $\varkappa$, $\bar{\varkappa}_{12}$, and $\bar{\varkappa}$ are constants and equal to each other:

$$\varkappa = \bar{\varkappa}_{12} = \bar{\varkappa} = k. \tag{22}$$

This means that *the retardation factors for the tracer velocity and for the speed of the iso-concentration surfaces are equal to each other.*

Introducing Eq. 21 and Eq. 22 into Eq. 13 gives

$$\frac{\partial c}{\partial t} = -\frac{\theta}{k} \underset{\sim}{v}_w \cdot \nabla c + \nabla \cdot \frac{D}{k} \nabla c - \left(\frac{\lambda}{k} + \alpha \right) c. \tag{23}$$

Introducing the transformation

$$c = c_0 \exp(-\alpha t) \tag{24}$$

into Eq. 23 gives

$$\frac{\partial c_0}{\partial t} = -\frac{\theta}{k} \underset{\sim}{v}_w \cdot \underset{\sim}{\nabla} c_0 + \nabla \cdot \frac{D}{k} \nabla c_0 - \frac{\lambda}{k} c_0. \tag{25}$$

In the absence of decay the distribution of the concentration will be given by $c_0(\underset{\sim}{x}, t)$. According to Eq. 23, 24 and 25, *linear production or decay simply causes an overall exponential decrease of the concentrations at all points in the system.*

Purely convective transport

If the transport is purely convective then Eq. 10, 15 and 19 reduce to, respectively,

$$\underset{\sim}{F} = \theta \underset{\sim}{v}_{w}\, c, \tag{26}$$

$$\underset{\sim}{v} = (\theta \underset{\sim}{v}_{w}) / \bar{\varkappa}, \tag{27}$$

$$v_{c} = \frac{\theta \underset{\sim}{v}_{w} . \underset{\sim}{\nabla} c + \lambda c - \sigma}{\bar{\varkappa} \mid \nabla c \mid} . \tag{28}$$

From Eq. 27 and 28 it follows that, if λ and σ are zero, in the direction along the unit normal $\underset{\sim}{n}_{c}$ the ratio R of the speed of the tracer and of the isoconcentration surface is given by

$$R = \frac{\underset{\sim}{v}_{w} . \underset{\sim}{n}_{c}}{v_{c}} = \frac{\varkappa}{\bar{\varkappa}} . \tag{29}$$

Eq. 29 implies that $R < 1$ if the adsorption isotherm is convace and $R > 1$ if the adsorption isotherm is convex with respect to the c axis.

For purely convective transport Eq. 13 reduces to

$$\varkappa \frac{\partial c}{\partial t} = \theta \underset{\sim}{v}_{w} . \nabla c - \lambda c + \sigma. \tag{30}$$

Purely convective transport of a solute subject to linear production or decay and to linear adsorption in the absence of uptake of water by plant roots

For this case Eq. 25 reduces to

$$\frac{\partial c_{0}}{\partial t} = \underset{\sim}{v} . \nabla c_{0}, \tag{31}$$

with the tracer velocity $\underset{\sim}{v}$ given by

$$\underset{\sim}{v} = (\theta / k) \underset{\sim}{v}_{w} . \tag{32}$$

Once the distribution of c_0 is known, the distribution of c can be calculated from Eq. 24.

Eq. 1 gives the transfer function T for water or an ideal tracer as the product of a transit time density distribution function $\mathrm{d}q/\mathrm{d}\tau$ and an input density distribution function r. The transit time density distribution for the solute can be found immediately from the transit time density distribution for the water by multiplying the turnover time $\bar{\tau}_{\text{water}}$ for the water bij a factor k:

$$\bar{\tau}_{\text{solute}} = k\, \bar{\tau}_{\text{water}} . \tag{33}$$

Recall that the turnover time $\bar{\tau}_{\text{water}}$ is equal to the volume of water in the system divided by the rate of input. Eq. 23, 24 and 25 imply that the reduction in the output with respect to the input due to linear production or decay can be accounted for by a multiplicative factor exp ($-\alpha t$) in the transfer function. The transfer function for the solute thus becomes

$$T_{\text{solute}} = r(dq/\mathrm{d}\tau)_{\text{solute}} \exp(-\alpha t). \tag{34}$$

Shock waves

Consider a shock wave between regions α and β. Let the subscripts α and β denote quantities in the respective regions. The speed of a shock wave, v_s, is determined by the condition that the net rate of transport to the shock, $\theta \underset{\sim}{v}_w . \underset{\sim}{n}_s (c_\alpha - c_\beta)$, is equal to the rate of accumulation at the shock, $(\mu_\alpha - \mu_\beta)\underset{\sim}{v}_s$:

$$v_s = \frac{\theta\,(c_\alpha - c_\beta)}{(\mu_\alpha - \mu_\beta)}\, \underset{\sim}{v}_w . \underset{\sim}{n}_s . \tag{35}$$

Using Eq. 7 in Eq. 35 gives

$$v_s = \theta \underset{\sim}{v}_w . \underset{\sim}{n}_s / \bar{\varkappa}_{\alpha\beta} . \tag{36}$$

According to Eq. 36 *the average capacity* $\bar{\varkappa}_{\alpha\beta}$ *over the range* c_α *to* c_β *serves as retardation factor for the velocity of shock waves.* The transit time density distribution for the shock wave can be found immediately from the transit time density distribution for the water by multiplying the turnover time by a factor $\bar{\varkappa}_{\alpha\beta}$:

$$\bar{\tau}_{\text{shock}} = \bar{\varkappa}_{\alpha\beta}\, \bar{\tau}_{\text{water}} . \tag{37}$$

Apparently well-mixed systems

For steady flow to ditches or tile drains the transit time density distribution is approximately exponential, provided water is not ponded on the surface, the water-table is relatively flat, and the distance between the ditches or tile drains is large relative to the depth of the impermeable layer. Eq. 34 then reduces to

$$T_{\text{solute}} = (r/\bar{\tau}) \exp(\tau/\bar{\tau}) \exp(-\alpha\tau), \tag{38}$$

$$= (r/\bar{\tau}) \exp(1 - \alpha\tau)(\tau/\tau), \tag{39}$$

where $\bar{\tau}$ is the turnover time for the solute defined by Eq. 33. Introducing the apparent turnover time $\bar{\tau}^*$ defined by

$$\bar{\tau}^* = \bar{\tau}/(1 - \alpha\bar{\tau}), \tag{40}$$

Eq. 39 can be rewritten as

$$T_{solute} = r(1-\alpha\bar{\tau})^{-1} (\bar{\tau}^*)^{-1} \exp(\tau/\bar{\tau}^*). \tag{41}$$

If $r = 1$ and $\alpha = 0$ then (41) reduces to the transfer function discussed in detail in an earlier paper (Raats, 1978b).

Consider a uniform, periodic input of solute dissolved in the water, i.e., an input I whose input density distribution $r(q)$ is unity and whose time dependence is described by:

$$I = \bar{c} + a_0 \sin(\Omega t), \tag{42}$$

where $\bar{c}$ is the average concentration of the input, a_0 is the amplitude of the input variation, and Ω is the frequency of the input variation. The response to such an input by a system with an initial concentration c_i and a response function given by Eq. 41 is:

$$O = \bar{c} + a \sin(\Omega t - b) + A \exp(-t/\bar{\tau}^*), \tag{43}$$

with the amplitude a, the phase angle b, and the factor A given by

$$a = a_0 (1-\alpha\bar{\tau})^{-1} (1 + \Omega^2 \bar{\tau}^{*2})^{-1/2}, \tag{44}$$

$$b = \tan^{-1}(\Omega\bar{\tau}), \tag{45}$$

$$A = c_i - \bar{c} - a \sin(-b). \tag{46}$$

The last term on the right hand side of Eq. 43 is negligible for $t \gg \bar{\tau}$. This limiting case, including plots of the dimensionless amplitude a/a_0 and phase angle b was discussed

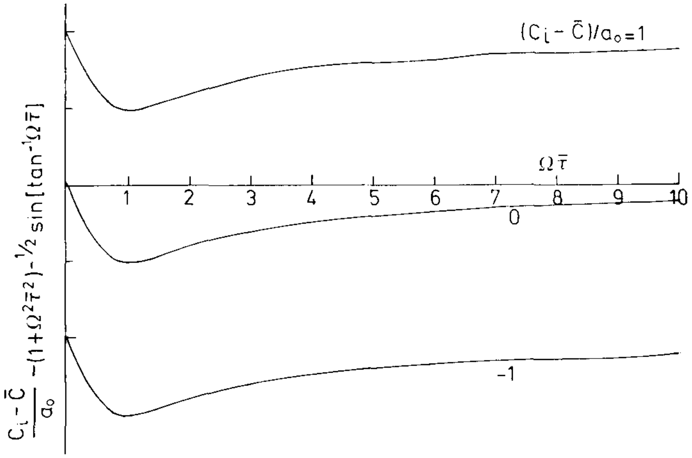

Fig. 3. The dimensionless amplitude of the transient component of the response to a sinusoidal oscillation of an apparently well-mixed system as a function of the dimensionless frequency.

earlier (Raats, 1978b, Fig. 6). Substituting Eq. 44 and 45 into Eq. 46 and dividing both sides by a_0 gives

$$\frac{A}{a_0} = \frac{c_i - \bar{c}}{a_0} - (1 + \Omega^2\bar{\tau}^2)^{-1/2} \sin(-\tan^{-1}(\Omega\bar{\tau})). \tag{47}$$

Fig. 3 shows a plot of A/a_0 as a function of $\Omega\bar{\tau}$ with $(c_i - \bar{c})/a_0$ as a parameter. The results show that for small values of A/a_0 the factor A in Eq. 43 depends strongly on the frequency.

Discussion

In two recent papers I presented a comprehensive theory for steady, multidimensional, convective transport of solutes, the first paper dealing with the general theory, the second paper with specific flow problems (Raats, 1978a, b). Rice & Raats (1979) used the same type of theory to predict minimum underground detention times and attenuation of nitrate peaks for two types of systems: (1) shallow aquifers where the renovated water is collected with horizontal drains, and (2) deep aquifers where the renovated water is collected with wells. The analysis presented above attempts to extend such theories to solutes subject to adsorption, production or decay, and dispersion. The results generalize some obtained earlier for one-dimensional flows (Reiniger & Bolt, 1972; Bolt, 1979). Also, the results indicate that for solutes subject to dispersion, nonlinear adsorption, and nonlinear production or decay detailed numerical calculations will often be needed. Finite element methods appear to be best suited for this purpose. The influence of uptake by plant roots can be treated analytically for some simple, one-dimensional cases (Raats, 1975, 1977) but will in general also have to be treated numerically.

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