Journal of Hydrology (N.Z.) Vol. 27, No. 1, 1988

ON THE DEPTH DISTRIBUTION OF AN APPLIED TRACER IN GROUNDWATER FIELD EXPERIMENTS

A. Grassia

CSIRO Division of Water Resources Research, P.O. Wembley 6014 Australia

ABSTRACT

A general mathematical model is proposed for the study of water transport in soil, in field experiments using tracers. The model can be used with tracer concentrations having different distributions, as might occur either shortly or sometime after tracer application, in field experiments where the phreatic zone lies close to the surface. Procedures are suggested for dealing with multiple peaks caused by multiple pulses of varying tracer concentration.

INTRODUCTION

Sharma *et al.* (1985) investigates recharge rates to groundwater in an area of vegetated land on the Swan Coastal Plain of Western Australia. The soil type there is a deep, well-drained, coarse-textured, grey san in the Bassendean dune system (McArthur and Bettenay, 1960). The phreatic surface lies about 8 m below the ground surface (for further details see Sharma *et al.*, 1985).

Potassium bromide was used as a tracer and applied to an area of 0.04 ha. The concentration of bromide was measured in a number of profiles at different depths, at four times following application of the bromide to the soil surface.

Two recharge models were applied by Sharma *et al.* to their data: the deterministic model widely discussed in water resources literature (e.g. see Rose *et al.*, 1982), and a stochastic model put forward in more recent times (Jury, 1982, Jury *et al.*, 1982).

This study critically examines these currently-used models, to determine if their mathematical formulation and boundary conditions are appropriate, or if conditions in the study area reequire a different mechanism, and hence different boundary conditions.

These models also assume uniform moisture content although dealing with natural rainfall instead of artifical-watering experiments, and ingore possible interfence by surface vegetation or pockets of poor surface-sand wettability.

Mathematical Model

The model for the distribution of a solute in a soil with a uniform water content is expressed by a well-established second-order partial differential equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial Z^2} - V\frac{\partial C}{\partial Z} \qquad (1)$$

where C is the solute concentration as a function of the profile depth Z

(measured positively downward) and time t, D [L^2 T^{-1}] is pore water velocity. Notice that D has two components. In fact $D = D_o + \epsilon V$ where D_o is the molecular diffusion co-efficient and ϵ [L] is the proportionally factor referred to as dispersivity.

The following initial and boundary conditions have been used in the literature (e.g. De Smedt and Wierenga, 1978) for pulse input

$$C(z,o) = o \qquad Z > o \tag{2a}$$
$$C(o,t) = c_o \qquad o < t < t_o \tag{2b}$$
$$C(o,t) = o \qquad t > t_o \tag{2c}$$

(t_o = pulse time length).

The solution of (1) obtained with these conditions is satisfactory for values of t when negligible concentrations of the tracer have approached the water table. However, with time, the tracer nears as the water table D becomes small, as $V \rightarrow O$ and $D \rightarrow D_o$.

In most stuides the water table is assumed to be at infinite depth, and the theroretical solutions obtained with the above conditions would lead to a fairly satisfactory fit to the experimental data.

In the Swan Coastal Plain study, the water table is fairly close tot he soil surface, at about 8 m depth. Solutions derived from heat conduction theory for a bar with one end at infinity, and with conditions (2a)→(2c), are in appropriate when the solute approaches the water table. A different mechanism approximating the transport process could be required. One mechanism is that pertaining to "the study of effect of gravity on the Brownian Motion" or the phenomenon of sedimentation (Chandrasekar, 1943). Instead of (2a)→(2c) the following boundary condition is used (in our notation and with being the Dirac's Delta function)

$$\frac{C}{C_o} \rightarrow \delta(Z\text{-}0) \text{ as } t \rightarrow o \tag{3a}$$

and

$$D\left(\frac{\partial C}{\partial Z}\right) - VC = o \tag{3b}$$

at $Z = Z_b$ for all $t \rightarrow o$, where Z_b is the depth of the phreatic zone.

Conditions (3b) implies that no particle of the solute will move beyond the phreatic surface. This is not true. But, as a tracer particle reaching the water table is subject only to a diffiusion process, as pore water velocity $V \rightarrow o$, transport would be slowed considerably. As a consequence tracer particles would accumulate near the phreatic surface, leading to an acceptable approximation of the correct solution. The correct solution for the transport process would require the assumption of a discontinuous medium requiring a more complicated approach. While expression (1) would be appropriate up to a certain depth above the water table, for tracer particLes reaching the phreatic surface the following diffusion process equation should be used

$$\frac{\partial C}{\partial t} = D_o \frac{\partial^2 C}{\partial Z^2} \quad (Z \geq Z_b) \tag{4}$$

This has the solution

$$C = C_b \text{ erfc } ((Z-Z_b)/2\sqrt{D_o t}) \tag{5}$$

(Freeze and Cherry, 1979), where C_b and t are successive concentrations and times of the tracer reaching the phreatic surface.

This should be combined with the solution of (1) for $Z < Z_b$. This would be difficult as there is no clear separation between the two zones near the phreatic surface. Therefore the assumption of an impermeable surface implied by condition (3) could provide a better solution for $Z \leq Z_b$, with a value of t conveniently large, but not too large. The solution of (1) would then reduce to

$$\frac{C(Z;t,Z_b)}{C_o} \quad \frac{1}{2(\pi Dt)^{1/2}} \exp(-[-Z+Vt]^2/4Dt)$$

$$+ \frac{1}{2(\pi Dt)^{1/2}} \exp(-(-Z+2Z_b)^2/4Dt) \exp\left(\frac{2VtZ}{4Dt} - \frac{V^2t^2}{4Dt}\right)$$

$$+ \frac{V}{D} e^{-\frac{V}{D}(Z_b-Z)} \frac{1}{\sqrt{\pi}} \int_{L}^{\infty} \exp(-x^2)dx \tag{6}$$

where $L = (-Z+2Z_b-Vt)/2(Dt)^{1/2}$
or

$$\frac{C(Z;t,Z_b)}{C_o} = \frac{1}{2(\pi Dt)^{1/2}} \exp(-[-Z+Vt]^2/4Dt)$$

$$(1+\exp[-Z_b (Z_b-Z)/Dt])$$

$$+ \frac{V}{D} \exp\{-\frac{V}{D}(Zb-Z)\} \frac{1}{2} \text{erfc}\left(\frac{-Z+2Z_b - Vt}{2(Dt)^{1/2}}\right) \tag{7}$$

The second and third terms are negligible for small values of t, but as t increases their contribution cannot be ignored, especially as Z approaches Z_b. Shapes of the curves for some increasing values of t (=1, . . .,7) are shown in Figure 1.

In the field V and D might not be constant for all depths; both could be functions of depth. D can be expressed as $D = D_o + \epsilon V$. If we assume D_o constant with Z, then changes in ϵ with Z can be used to determine D.

A possible function is

$$V(Z) = \frac{V_o}{1+aZ} \qquad (a > o)$$

Hence for Z=Z* we have for the mean velocity

$$\bar{V}(Z) = \frac{1}{Z^*_o} \int_{0}^{Z^*} V(Z)dZ = V_o \frac{\log(1+aZ^*)}{aZ^*} \tag{8}$$

Evidently $\bar{V}(Z^*) \rightarrow V_o$ as $Z^* \rightarrow o$ (i.e. for small core sections).

In field experiments the tracer solution, of concentration C_o when applied to the surface, may enter the soil profile as a number of different pulses of unequal concentrations $C_o^{(i)}$, where $C_o = \Sigma_i C_o^{(i)}$. This could be due to factors such as vegetation, poorly-wettable sandy soils, organic matter, preferred pathways and the interaction between poor wettability and organic matter content.

The movement of the solute into the soil appears in the data as a sequence of unequal-size pulses in the curve. The irregular periodicity depends on the frequency, duration, and amount of rain at each event (Rose D. A., 1977).

Even at distances far from the water table (or assuming $Z_b \approx \infty$), when expression (7) can be simplified to

$$\frac{C(Z;t)}{C_o} = \frac{1}{2(\pi Dt)^{1/2}} \exp\{-[-Z+Vt]^2/4Dt\} \tag{9}$$

a sequence of more-or-less irregular curves would be observed. In fact

$$\frac{C(Z;t,Z_b)}{C_o} = \Sigma \frac{C_o^{(i)}}{C_o} \frac{1}{2[\pi D(t-t_i)]^{1/2}} \exp\{-[-Z+V(t-t_i)]^2/4D(t-t_i)\} \tag{10}$$

(t_i time from application of the solute of the ith pulse of size $C_o^{(i)}$; $C_o^{(i)}$ = for $t-t_i \leq o$).

To study dispersion (D) and pore water velocity (V) in field experiments a sufficient length of time should pass that the distribution of the concentration of the tracer in the soil approaches curve 4 of Figure 1, i.e. a normal distribution, and expressions (6) or (7) can be reduced to (9). If a short time has passed and the distribution of concentration of the tracer is similar to curves 2 and 3, or if a long time has passed and the distribution is similar to curves 5-7 of Figure 1, complications may lead to poorer estimates of the properties, especially in the latter case.

Parameter Estimation

Let us assume a homogeneous field or a single core.

(a) *Single Peak*

When a single peak is present for t, such that the tracer has not neared the water table, the first term in expression (7) would be involved. Only a negligible contribution would occur from the third term. As t increases and the tracer nears the water table the second and especially the third terms become important.

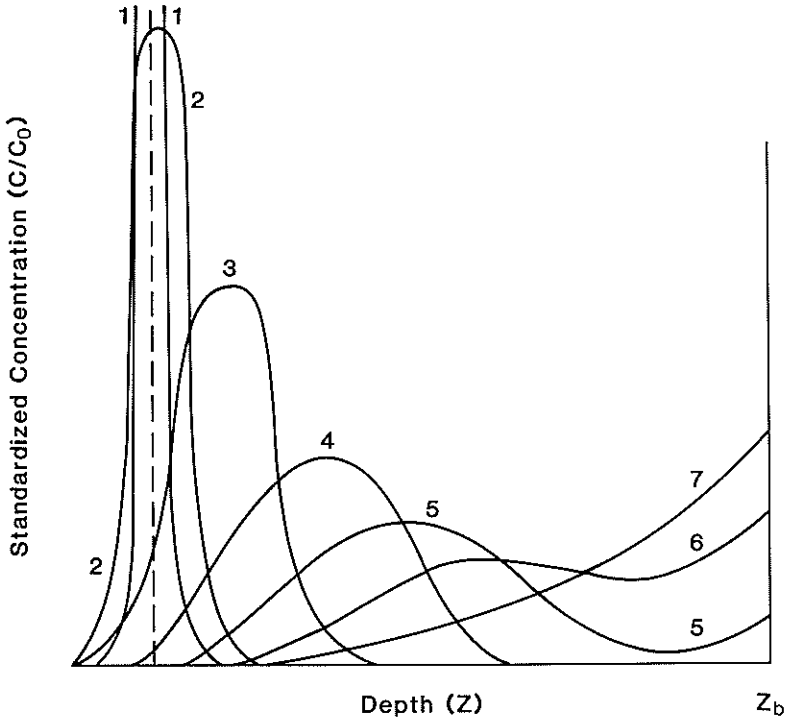

FIG. 1—Distribution of concentrations at different times from trace application (Z_b=depth of phreatic zone).

(b) *Multiple Peaks*

When several peaks are present and t is not large, expression (10) is the appropriate model to fit, requiring a computer programme for peak separation. Unfortunately we do not know t_i. However, infiltration parameters can be estimated from the curve with the lowest peak due to the first pulse. If information is available on rainfall, perhaps other pulse information and expression (10) could be used.

Let us assume a heterogeneous field and a number of cores.

Complications arise when the transport or other properties are heterogeneous, and, for a given time span, averages of raw data for several individual cores are used. For that time span, two or more consecutive curves may be averaged (Fig. 1). Further complications arise when averaging several cores, if non-uniform multiple pulses occur, as distinguished contributions from the various pulses can't be.

An examination of Figures 2 and 3 (derived from Sharma *et al.*, 1985), in which the raw data are means of 6 and 25 cores, 21 and 76 days after tracer application respectively, shows the complications. Multiple pulse and flow patterns at different stages appear in the individual sample cores. At least two pulses (Fig. 2) or three or four pulses (Fig. 3) appear to be present.

Confidence limits indicate some of the differences in tracer concentration curves for individual cores. Higher limits at some depths could reflect different curve patterns, leading to greater variability at these depths.

The data in Figure 2 approach curve 4 of Figure 1 and the simplified expression (9) could be used to obtain approximate parameter estimates. The data of Figure 3, apart from multiple pulses, seem to consist of a mixture of curves 5, 6 and 7 of Figure 1, i.e. the tracer is near the phreatic zone. For each of these curves the full expression (7) should be appropriate. However,

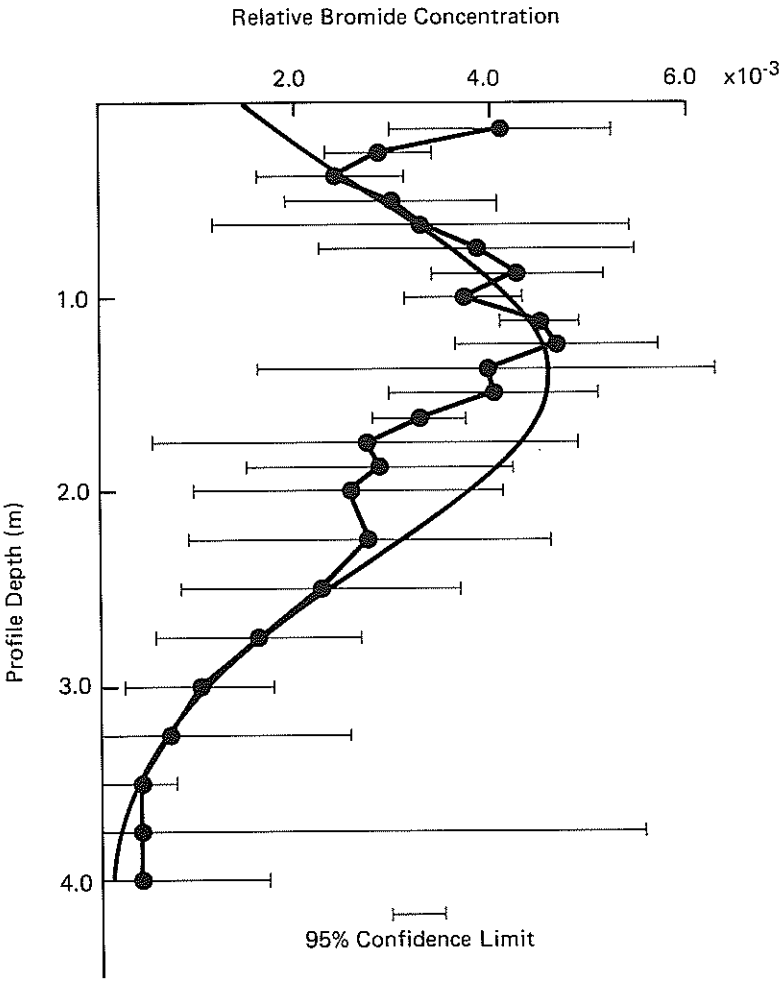

FIG. 2—Depth distribution of experimentally measured relative bromide concentration and its associated variability (shown by 95% confidence limits), and the theoretically fitted function. This solute profile was measured 21 days after application of bromide.

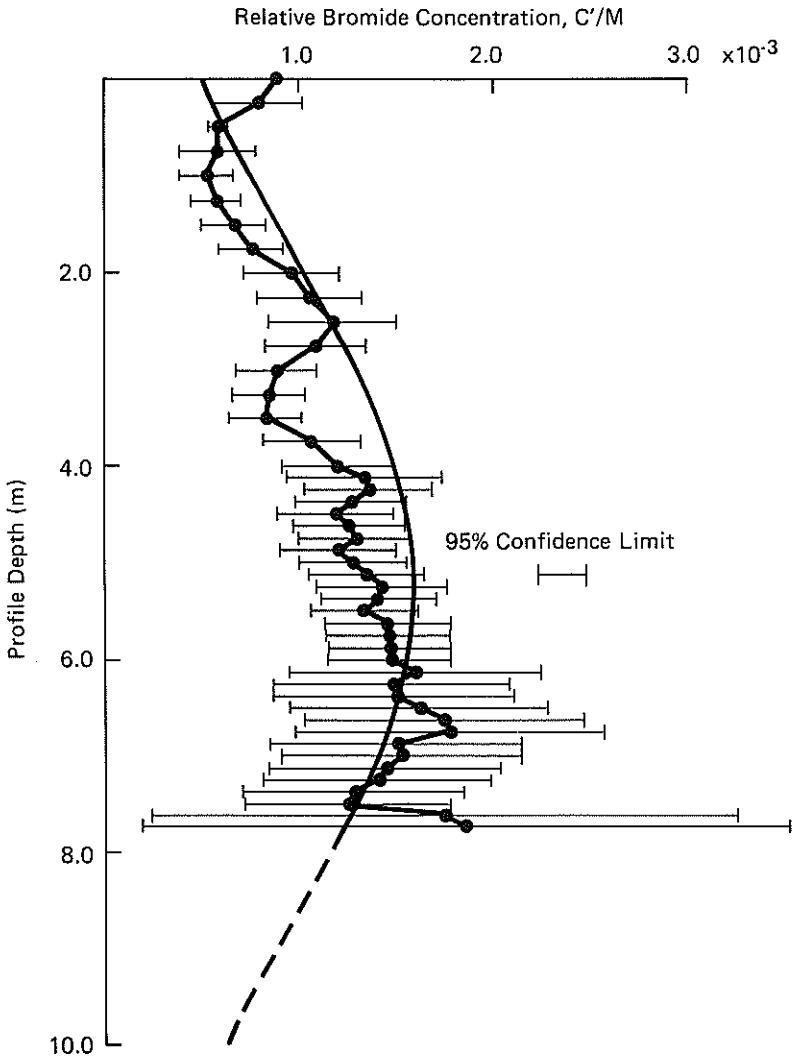

FIG. 3—Depth distribution of experimentally measured relative bromide concentration and its associated variability, measured 76 days after solute application. The smooth curve shows the corresponding predicted bromide distribution based on our model.

the use of (7) to fit the data of Figure 3 is likely to lead to poor estimates of the parameters.

The averaging of parameter estimates obtained from individual cores for field experiments should provide better estimates of soil transport properties in the study area than estimates based on averages of raw data.

Further Remarks

The shapes of curves 5, 6 and 7 of Figure 1, at or near the depth of the phreatic surface, would be correct if an impermeable layer is assumed at the depth of the phreatic surface. This is not so here, as a diffusion process replaces the original transport process. Therefore shapes may change near this depth. Instead of increasing monotonically as shown in Figure 1, they may flatten or have a local maximum.

So far we have not discussed the most suitable form of $\underline{c}$ for estimating the parameters V and D. In expressions (6) or (7) some unscaled frequency functions are involved in field data. Therefore, if continuous sampling is assumed, in

$$\frac{1}{C_o} \int_o^{Z_b} c(Z;t)\, dZ = k \qquad (11)$$

or, if core sample sections of length h_j are used, in

$$\frac{1}{C_o} \Sigma\, h_j C_j(Z;t) = k \qquad (12)$$

then $k \neq 1$, due to sampling variability or other uncontrollable environmental factors. Moreover, the experimental procedure might measure some variable C* function of C, for which $k \neq 1$ would be the rule. However, values of C can often be obtained from C* by scaling, when it is expected that $k = 1$ in (11) or (12).

CONCLUSION

The mathematical model presented in this paper better approximates the physical conditions of heterogeneous soils and a shallow water table than models used previously, and deals with multiple peaks. To obtain estimates of the average dispersion coefficient and pore water velocity, it is better to average the estimates of the parameters than to average raw data. Standardisation may be achieved by scaling. The only limitation of the model is that an impermeable layer is assumed at or near the depth of the phreatic zone, instead of a change from a transport to a diffusion process.

ACKNOWLEDGEMENT

I wish to thank the following officers of the Division of Water Resources Research, CSIRO, Western Australia: R. Barron for useful discussions at the development stage for the investigation; Kathy McGuckin for her excellent typing of the manuscript; and Dr G. Davis for valuable comments on the manuscript.

REFERENCES

Chandrasekar, S. 1943: *Stochastic Problems in Physics and Astronomy. 15*: 1-86. (See Wax, N. (1954). *Selective Papers on Noise and Stochastic Processes*: Dover, New York.)

De Smedt, F.; P. J. Wierenga 1978: Solute transport through soil with nonuniform water content. *Soil Science Society America Journal 42*: 407-412.

Freeze, R. A.; J. A. Cherry 1979: *Groundwater*. Prentice-Hall, Englewood Cliffs, pp. 113.

Jury, W. A. 1982: Simulation of solute transport using a transfer function. *Water Resources Research 18*: 363-368.

Jury, W. A.; L. H. Stolzy; P. Shrouse 1982: A field test of the transfer function model for predicting solute movement. *Water Resources Research 18*: 369-375.

McArthur, W. M; E. Bettenay 1960: Development and distribution of soils of the Swan Coastal Plain, W.A. *CSIRO, Soil Publ. No. 16*, Melbourne.

Rose, C. W.; F. W. Chichester; T. R. William; J. T. Ritchie 1982: Application of an approximate analytic method of comparing solute profiles with dispersion in soils. *Journal Environment Quality 11:* 151-155.

Rose, D. A. 1977: Hydrodynamic dispersion in porous materials. *Soil Science 123*: 277-283.

Sharma, M. L.; I. D. Cresswell; J. D. Watson 1985: Estimates of natural groundwater recharge from the depth distribution of an applied tracer. *Proceedings* of 21st Congress of International Association for Hydraulic Research. Vol. 1, pp. 64-70. Institute of Engineers. Australia.