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

ALGORITHM FOR THE INTERPRETATION OF GROUNDWATER FIELD EXPERIMENTS

A. Grassia

CSIRO Division of Water Resources Research, Private Bag, Wembley, 6014 Australia

ABSTRACT

Field experiments on the depth distributions of a solute in sandy soil under general conditions are discussed. Special consideration is given to the effects of multiple pulses and the proximity of the solute to the phreatic zone. The depth distribution of a tracer is analysed utilizing a general mathematical model proposed in a previous paper by the author, and applied to two illustrative examples.

INTRODUCTION

In an earlier paper Grassia (1988, this volume) proposed a general model for the study of soil water transport in field experiments using tracers. Emphasis was placed on the effects of a near-surface phreatic zone and the presence of multiple pulses of tracer concentration. This latter aspect is discussed in this paper.

The model proposed requires as input tracer concentrations of cored sections of field soils (weighted or unweighted by moisture levels). For each pulse these concentrations, c(ppm), are assumed to be proportional to the ordinates of a normal or truncated normal probability (Gaussian) function. A curve with ordinates which are the sums of ordinates for individual pulses arises with multiple pulses.

A slightly modified version of a Program NONLIN (McIntyre and Ward, 1970) is used to fit the curve to estimate soil parameters. Two illustrative examples are given:

(a) two pulses, with a phreatic zone at infinite depth; and
(b) three pulses, with a phreatic zone at 8m depth.

Core sections of equal length, ΔZ, are assumed in the examples; however, the procedure can be easily extended to core sections of unequal length.

MATHEMATICAL FORMULATION

Tracer distribution may be used to estimate pore water velocity V $[LT^{-1}]$ and the dispersion coefficient D $[L^2T^{-1}]$.

Where the phreatic zone lies at infinite depth, the depth distribution of the concentration of the tracer will be simply

$$c(Z;t) = \sum_i c_i^* \exp\{-[Z-V(t-t_i)]^2/4D(t-t_i)\}/[4\pi D(t-t_i)]^{1/2} \quad (1)$$

where t is the time from application of the tracer at core sampling time for the earliest pulse and therefore known, while t_i is the time from the date of tracer application for the successive pulses, i=1, 2, . . . m−1 for the last, second last, . . ., second pulse assuming m pulses. Evidently $t_m=0$. c_i^* is some function of the ith pulse tracer concentration and will be discussed later.

For a near-surface phreatic zone the expression for estimating c(ppm) becomes more complicated, as the tracer nears the phreatic zone.

If Z_b is the depth of the phreatic zone ($Z \leq Z_b$), the expression for the distribution of the tracer concentrations may have up to three terms present for a pulse:

$$c(Z;t,Z_b) = \sum_{i}^{m} c_i^* \{\exp\{-[Z-V(t-t_i)]^2/4D(t-t_i)\}/[4\pi D(t-t_i)]^{1/2}\}$$

$$[1+\exp\{-Z_b(Z_b-Z)/D(t-t_i)\}]$$

$$+\frac{V}{D}\exp\{-\frac{V}{D}(Z_b-Z)^{1}\,\mathrm{erfc}\,(\frac{2Z_b-Z-V(t-t_i)}{2[D(t-t_i)]})\} \qquad (2)$$

Two Pulses, Phreatic Zone at Infinite Depth

The concentration distribution consists of the sum of m elementary concentrations arising from each of the m pulses or

$$c_j = \sum_{i}^{m} c_{ij}$$

where c_j is the concentration of the jth core.

We observe c_j, and not the c_{ij}'s. If $c_{io} = \sum_j c_{ij}$ and $c_o = \sum c_{io}$, we know c_o but not the c_{io}'s.

Let f_{ij} be the ordinate of the normal distribution for the ith pulse and jth core.

For the ith pulse we have for the total probability

$$p_i = \sum_j f_{ij} \frac{(\Delta Z)_j}{\sigma_i} \qquad (3)$$

where $p_i = 1$ for a non-truncated distribution and $p_i < 1$ for a truncated distribution.

For a $(\Delta Z)_j = \Delta Z$ (constant), from (3) we obtain

$$\sum_j f_{ij} = p_i \frac{\sigma i}{\Delta Z} \qquad (4)$$

Some problems arise for non-constant (ΔZ) as we cannot arrive at expression (4). For constant intervals we expect the following equality:

$$\frac{f_{ij}}{\Sigma f_{ik}} = \frac{c_{ij}}{\sum_k c_{ik}} = \frac{c_{ij}}{c_{io}} \qquad (5)$$

from which

$$c_{ij} = \frac{f_{ij}}{\sum_k f_{ik}} c_{io} \tag{6}$$

and from (4)

$$c_{ij} = \frac{f_{ij} c_{io}}{p_i \left(\frac{\sigma_i}{\Delta Z}\right)} \tag{7}$$

It is not so for unequal intervals. Instead of (6) and (7), from

$$\frac{f_{ij} \quad (\Delta Z)_j/\sigma_i}{\sum_k f_{ik}(\Delta Z)_k/\sigma_i} = \frac{c_{ij} \quad (\Delta Z)_j}{\Sigma_k c_{ik}(\Delta Z)_k} \tag{8}$$

we obtain

$$c_{ij}(\Delta Z)_j = \frac{f_{ij} \quad (\Delta Z)_j/\sigma_i}{\Sigma f_{ik}(\Delta Z)_k/\sigma_i} \sum_k c_{ik}(\Delta Z)_k \tag{9}$$

or

$$c_{ij} = \frac{f_{ij}/\sigma_i}{\sum_k f_{ik} (\Delta Z)_k/\sigma_i} \sum_k c_{ik}(\Delta Z)_k \tag{9'}$$

Also from (3)

$$c_{ij} = \frac{f_{ij}/\sigma_i}{p_i} \sum_k c_{ik}(\Delta Z)_k \tag{10}$$

Usually only a couple of interval sizes, in, for example, a simple relation of 1 to 2, are used in core sampling. The average or the most common length can then be taken as standard, say $\overline{\Delta Z}$, and all intervals expressed as $(\Delta Z)_j = w_j(\overline{\Delta Z})$where the w_j's are weights proportional to size, i.e.

$$w_j = \frac{(\Delta Z)_j}{\overline{\Delta Z}} \tag{11}$$

Then (10) can be written in a form

$$c_{ij} = \frac{f_{ij}}{p_i \left(\frac{\sigma_i}{\overline{\Delta Z}}\right)} \sum_k w_k c_{ik} \tag{12}$$

or in a form close to (7)

$$c_{ij} = \frac{f_{ij}}{p_i\left(\frac{\sigma_i}{\Delta Z}\right)} c'_{io} \tag{13}$$

where $c'_{io} = \Sigma w_k c_{ik}$

Trial value p_i of p_i are required for truncated distributions to use in (7) and (13). From (2) the estimate $\hat{c}_j$ of c_j becomes

$$\hat{c}_j = \Sigma_i \hat{f}_{ij} \left(\frac{\Delta Z}{\sigma_i}\right) \left(\frac{c_{io}}{p_i}\right) \tag{14}$$

For unequal intervals

$$\hat{c}_j = \sum_i \hat{f}_{ij} \left(\frac{\Delta Z}{\sigma_i}\right) \left(\frac{c_{io}}{p_i}\right) \tag{15}$$

Two approaches can be used to fit c_j. We can use

$$\hat{c}_j = \left(\sum_i \hat{f}_{ij} r_i\right) (c_o \Delta Z) \tag{16}$$

for equal core sections, where $c_o = \sum_i c_{io}$ and

$$r_i = \frac{c_{io}/\sigma_i p_i}{\sum_i c_{io}/\sigma_i p_i} \tag{17}$$

or

$$\hat{c}_j = \left(\sum_i \hat{f}_{ij} r_i\right) (c'_o \overline{\Delta Z}) \tag{16'}$$

for unequal core sections, where $c'_o = \sum_i c'_{io}$ and

$$r_i = \frac{c'_{io}/\sigma_i p_i}{\sum_i c'_{io}/\sigma_i p_i} \tag{17'}$$

where $\sum_i r_i = 1$. Hence m–1 r parameters are involved. (Notice ΔZ and Δz occur in both numerator of (17) and denominator of (17′), and cancel out.)

Alternatively we can fit the expression (16) and (16′) for equal core lengths

$$\hat{c}_j = \left(\sum_i \hat{\phi}_{ij} r_i\right) (c_o \Delta Z) \tag{18}$$

and for unequal core lengths

$$\hat{c}_j = (\sum_i \hat{\phi}_{ij}\, r_i')\, (c_o' \Delta Z) \qquad (18')$$

where the $\phi_{ij} = f_{ij}/\sigma_i$ are values obtained from the components of expression (1), and

$$r_i' = \frac{c_{io}/p_i}{\sum_i c_{io}/p_i} \qquad (19)$$

for equal intervals, and

$$r_i' = \frac{c_{io}'/p_i}{\sum c_{io}'/p_i} \qquad (19')$$

for unequal intervals, with $\Sigma r_i' = 1$.

Evidently c_i^* in (1) or (2) is given by

$$c_i^* = r_i'\, c_o\, \Delta Z \qquad (20)$$

for equal core lengths, and

$$c_i^* = r_i'\, c_o' \overline{\Delta Z} \qquad (20')$$

for unequal ones.

If we have m pulses, then besides the two main parameters V and D, m–1 time parameters t_i, and m–1 parameters r_i' are involved in the model as

$$r_m' = 1 - \sum_{i=1}^{m-1} r_i' \qquad (21)$$

Three pulses, with a phreatic zone at 8m depth

Complications arise when sufficient time has elapsed from application of the solute that the earliest pulse of solute has approached the phreatic zone that is, when expression (2) applies.

We discussed the functions of the c_i's; these also arise in (2) but c_m includes contributions of the second and third components. Some complications arise in determining the appropriate expression to estimate soil water transport parameters. Expression (18) is more appropriate, except that ϕ_{mj} involves three

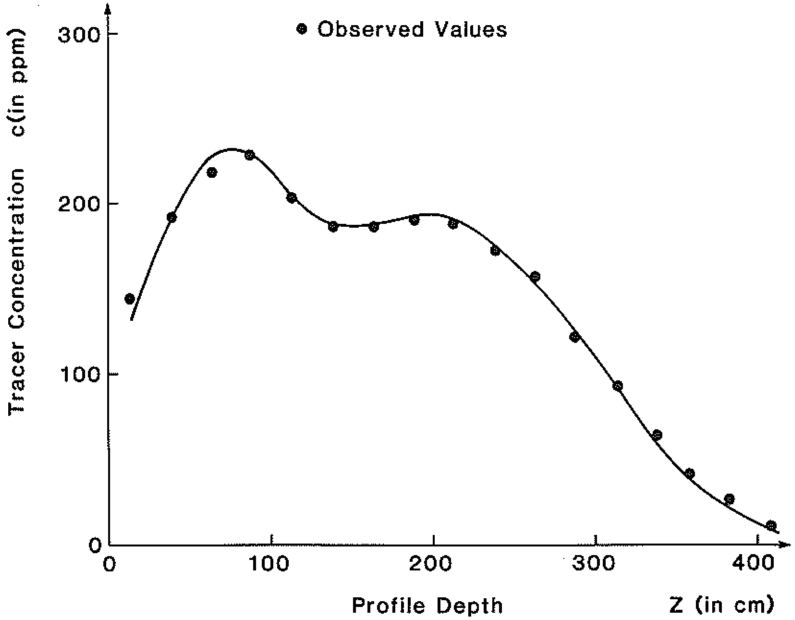

FIG. 1—Tracer distribution in soil profile after 25 days from application of a solution with total tracer concentration of $c_0 = 2500 \times 25$. Two pulse model (not approaching the phreatic zone)

components and we need to derive the appropriate trial values for r_i ($i=1,2,\ldots,m-1$). For that purpose we take,

$$c_{mo} = 1 - \sum_{i=1}^{m-1} c_{io}$$

and the trial values for p_m, $p_m=1$, for use in expression (19) to determine r_i for equal intervals, and similarly, for unequal intervals, use c_{io} and expression (19′).

Illustrative Examples

Two examples will be discussed, using data typical of that leading to the averages of figures 2 and 3 of Grassia (1988, this volume), derived from Sharma *et al* (1985). An equal core length of 25 cm was adopted for simplicity of graphical representation and computer fitting. For both examples it is assumed that the phreatic zone occurs at about 8 m depth.

Example 1

The data were constructed by roughly sketching two Gaussian curves and then adding ordinates for chosen depths assuming the following values: $V=8$, $D=160$, $t=25$, $t_l=18$ ($t-t_l=7$), $c_0=2500$ of which $r_l=0.30$ of c_0 for the sum of the ordinates of second pulse. No random errors were added to the c_{ij}'s.

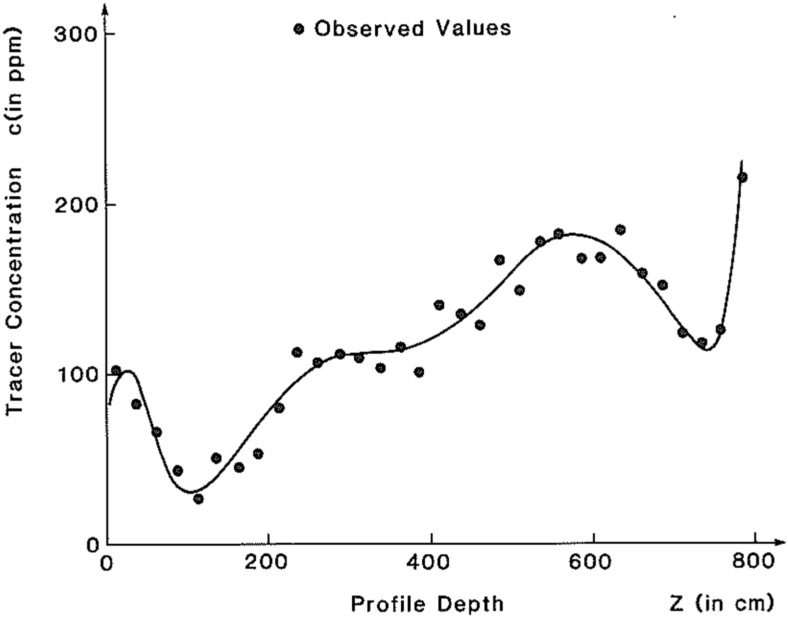

FIG. 2—Tracer distributions in soil profile after 80 days from application of a solution with total tracer concentration of $c_0 = 4000 \times 25$. Three pulse model with the phreatic zone, assumed at about 8m depth, being approached by the earliest pulse.

There are four parameters to estimate:
V, D, t_1 and r_1. Expression (18) was fitted.

The following estimates were obtained for these parameters: V=8.25, D=169.7, t_1=17.9 and r_1=0.325. The fit is shown in Figure 1.

Notice that the value of t is small and therefore no tracer has neared the phreatic zone.

Example 2

The data were constructed as in Example 1 except that three pulses have been assumed, with the tracer distribution approaching the phreatic zone for the earliest pulse. The following parameter values were assumed:
V=7.5, D=130, t=80, t_1=75 (or $t-t_1$=5), t_2=45 (or $t-t_2$=35), c_0=4000, with r_1=0.10 and r_2=0.20 of c_0 being accounted by the third and second pulses, the three components arising for the first pulse accounting for 0.70 of c_0. Some random errors were added to the c_{ij}'s.

The following parameter estimates were obtained: V=7.38, D=140.9, t_1=76.4, t_2 = 43.7, r_1=0.08 and r_2=0.22. See Figure 2 for the fit and shape of the curve.

COMMENTS

It is not uncommon for hydrologists presented with a two pulse curve as shown in Figure 1 to fit to it a left-truncated Gauss function with disastrous consequences on the estimates of the two parameters V and D. When presented with a curve as shown in Figure 2, they often do not know what to do. Attention should be paid to the possible presence of multiple pulses and to the proximity of the phreatic zone by examining the curve.

Changes of the curve from a downward to an upward or flattening trend (as at about 130 cm depth for Figure 1 and at about 100 cm, 400 cm depths for Figure 2) indicate the presence of two and three pulses respectively. A downward trend changing sharply to upward (as at about 750 cm depth in Figure 2) indicates proximity to the phreatic zone.

Factors such as heavy rainfalls following application of the tracer, or knowledge from previous experiments of the approximate depth of the phreatic zone should be taken into consideration to confirm changes in trends of the tracer concentration distribution function.

CONCLUSION

Hydrologists, estimating soil water transport parameters using tracers, should be careful of the choice of the appropriate model for the data at hand. Failure to do so can lead to incorrect estimates of pore water velocity and dispersion.

NOTATION

$c(Z, t)$	tracer concentration at depth Z after time t
c_{ij}	average tracer concentration (ordinate of centre point) for the jth core and ith pulse
c_j	average tracer concentration for ith core for all pulses combined
V	pore water velocity
D	D dispersion coefficient
t	Time elapsed since application of tracer
t_i	time of occurrence of the ith pulse since initial application of the tracer
c_{io}	sum of all average tracer concentrations for the ith pulse
f_{ij}	the ordinate of normal (Gauss) distribution for the ith pulse and jth core
p_i, p^*_i	total probability of the ith pulse tracer for non-truncated and truncated distributions respectively
σ_i	standard deviation of the distribution of the ith pulse
Z	depth (cm)
ΔZ	core section length or interval
$(\Delta Z)_j$	core section length or interval of jth core (unequal intervals used)
$\overline{\Delta Z}$	average or most common length of core section
w_j	weight for jth interval as a function of length
c_o	sum of the average tracer concentrations for all pulses
C_o	total tracer concentration for all pulses ($=c_o \Delta Z$)
c'_{io}	"weighted" sum of all average tracer concentration for the ith pulse when unequal intervals are used
r_i, r'_i	proportion of total tracer for the ith pulse for equal and unequal intervals respectively
c^*_i	function of tracer concentration for the ith pulse
$\hat{}$	"estimate of"

REFERENCES

Grassia, A. 1988: On the depth distribution of an applied tracer in groundwater field experiments. *Journal of Hydrology (NZ) 27 (1), pp..*

McIntyre, G. A.; M. M. Ward 1970: CSIRO Division of Mathematics Statistics Technical Report 3.

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