

NOTA 1404

February 1983

INSTITUUT VOOR CULTUURTECHNIEK EN WATERHUISHOUDING
WAGENINGEN

ALTERRA
Wageningen Universiteit & Research centre
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ANALYSIS OF A MODEL FOR TRANSPORT, ADSORPTION AND
DECOMPOSITION OF SOLUTES IN THE SOIL

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ANNEX HP 97 programme

1. INTRODUCTION

In this report a model for the transport, adsorption and decomposition of solutes in the soil is presented. The model has been described before by RIJTEMA (1981, 1982). Here, a programme for the HP97 calculator is presented and techniques from systems analysis are introduced for finding optimum parameters from experimental results.

In the final section of the report the use of the model will be illustrated with some column experiments reported by HOEKS et al. (1979) and a field research conducted by ABDEL NASSER (1983).

2. MODEL FORMULATION

The soil is subdivided into soil layers with thickness L_n . The model for the one-dimensional case consists of n soil layers in series.

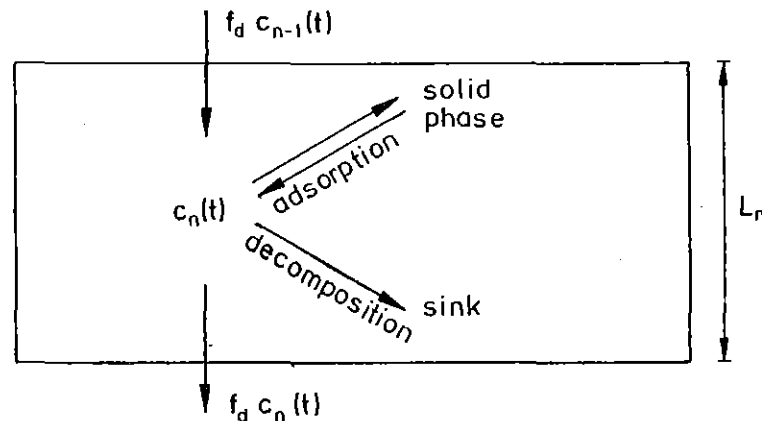


Fig. 1. Soil layer n

- f_d = drainage flux in mm.day^{-1}
- $c_{n-1}(t)$ = concentration incoming flux
- $c_n(t)$ = concentration liquid phase soil layer n
- L_n = thickness layer n in mm

2.1. Processes in the soil

Three processes will be considered: transport (dispersion), adsorption and decomposition.

The change in concentration due to transport in layer n can be formulated (continuity equation):

$$\theta_n L_n \left(\frac{dc_n(t)}{dt} \right)_T = f_d c_{n-1}(t) - f_d c_n(t) \quad (1)$$

where θ_n = effective pore space involved in transport and mixing of solutes

the subscript T refers to transport

The Langmuir equation is frequently used to describe the adsorption of ions to the solid soil phase:

$$S = S_m \frac{k \cdot c}{1 + k \cdot c} \quad (2)$$

where S = quantity of adsorbed solute (in mg or meq/100 gr soil)

S_m = maximum quantity that can be adsorbed

k = constant depending on ion and soil type

c = concentration in the liquid phase in mg/l or meq/l

For low values of c the denominator in eq. (2) approaches unity and the quantity adsorbed is proportional to the concentration. For soil layer n the change in concentration due to adsorption is:

$$\theta_n L_n \left(\frac{dc_n(t)}{dt} \right)_A = -L_n \frac{dS}{dt} = -\theta_n L_n R_n \frac{dc_n(t)}{dt} \quad (3)$$

where the subscript A refers to adsorption

$$R_n = \frac{k \cdot S_m}{\theta_n} - \text{distribution ratio}$$

The distribution ratio R_n gives the ratio of the quantity of the solute in the solid phase (adsorbed) over the liquid phase (in solution).

The first order linear decomposition is given by the equation:

$$c(t) = c(t_0) e^{-\alpha(t-t_0)} \quad (4)$$

where α = decomposition coefficient (day^{-1})

For soil layer n the continuity equation for the decomposition gives:

$$\theta_n L_n \left(\frac{dc_n(t)}{dt} \right)_D = - \alpha_n \theta_n L_n c_n(t) \quad (5)$$

where the subscript D refers to decomposition.

Combining the three effects (super position):

$$\frac{dc_n(t)}{dt} = \left(\frac{dc_n(t)}{dt} \right)_T + \left(\frac{dc_n(t)}{dt} \right)_A + \left(\frac{dc_n(t)}{dt} \right)_D \quad (6)$$

gives the differential equation for layer n :

$$\theta_n L_n \frac{dc_n(t)}{dt} = f_d c_{n-1}(t) - f_d c_n(t) - \theta_n L_n R_n \frac{dc_n(t)}{dt} - \theta_n L_n \alpha_n c_n(t) \quad (7)$$

2.2. One dimensional basic equations

The mass balance equation (7) can be simplified by introducing two parameters:

$$A_n = \frac{f_d}{\theta_n L_n (1+R_n)} \quad \text{and} \quad B_n = \frac{\alpha_n}{1+R_n} \quad (8)$$

Substitution of A_n and B_n into (7) gives:

$$d c_n(t) + (A_n + B_n) c_n(t) dt = A_n c_{n-1}(t) \quad (9)$$

This equation can be solved assuming A_n and B_n constant ($A = A_n$ and $B = B_n$) under the boundary conditions:

$$c_n(t) = c_n(t_0) \quad \text{for } t = 0$$

and

$$c_{n-1}(t) = c_i \quad \text{for } n = 0$$

Integration gives for the concentration in layer n:

$$c_n(t) = \left(\frac{A}{A+B}\right)^{n+1} c_i + e^{-(A+B)t} \sum_{k=0}^n \frac{(At)^{n-k}}{(n-k)!} \{c_k(t_0) - \left(\frac{A}{A+B}\right)^{k+1} c_i\} \quad (10)$$

where c_i = concentration in the irrigation water or in precipitation

Eq. (10) describes the concentration of the soil solution in the layers in a vertical soil column. The concentration of the drainage water equals the concentration in the last layer of this column.

2.3. Pseudo two-dimensional formulation

For the two dimensional case calculations have to proceed along the stream tubes. It has been assumed that no interactions between different stream tubes takes place.

2.3.1. No influence of the aquifer

The streamlines for a saturated soil system with fully flowing surface drains is schematically given in Fig. 2.

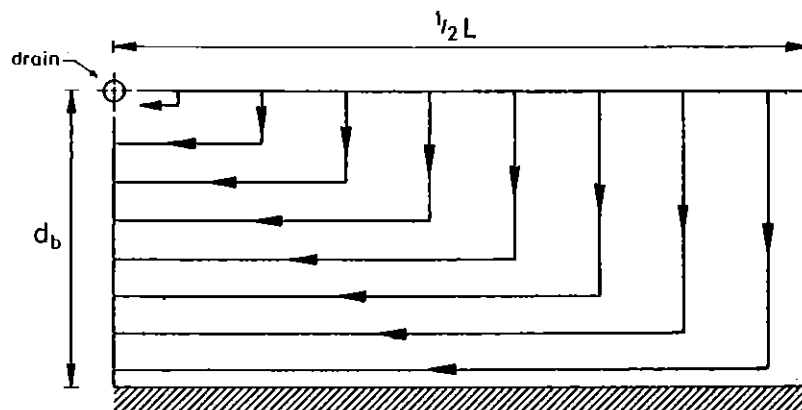


Fig. 2. Schematic flux pattern two dimensional case

Each stream tube consists of a partly vertical and a partly horizontal flow. The choice of soil layers has to be in such a way that N stream tubes with 1, 2, 3, ... N soil layers each results. The soil compartments for vertical flow generally will have different dimensions than those in the horizontal flow pattern. If w is the width of such a

compartment the following condition must be met (assuming θ_n and R_n constant):

$$w_v L_v = w_h L_h \quad (11)$$

where w_v = width of a vertical flow compartment

L_v = length of a vertical flow compartment

w_h = width of a horizontal flow compartment

L_h = length of a horizontal flow compartment

For $d = 0$ (land surface) the following relation for w_v is valid:

$$N w_v = L/2 \quad (12)$$

where $N = n+1$ = number of soil layers along the longest stream tube

L = drain distance

For $L = 0$ (vertical section below the drain) the following relation for w_h holds:

$$N w_h = d_b \quad (13)$$

where d_b = depth of the drainage barrier

and along the stream tube with N layers:

$$N(L_v + L_h) = 2d_b + L - (w_h + w_v) \quad (14)$$

Solution of eqs. (11) - (14) for L_v and L_h gives:

$$L_v = d_b \frac{2N-1}{N^2} \quad \text{and} \quad L_h = L/2 \frac{2N-1}{N^2} \quad (15)$$

Solution of eqs. (11) - (14) for N , taking $L_v = L_n$ gives:

$$N = \frac{d_b}{L_n} + \left\{ \left(\frac{d_b}{L_n} \right)^2 - \frac{d_b}{L_n} \right\}^{1/2} \quad \text{for } L_n \leq d_b \quad (16)$$

The concentration in the soil water solution for the soil layers

is calculated with eq. (10). For the concentration of the drainage water the average of the concentrations has to be taken:

$$c_d(t) = \frac{1}{N} \sum_{n=0}^{N-1} c_n(t) \quad (17)$$

where $c_d(t)$ = concentration of the drainage water

So far the unsaturated flow above drain level has not been taken into account. In the unsaturated zone only vertical flow will be considered. The number of soil layers for vertical unsaturated flow is:

$$N_u = \frac{d_d}{L_n} \quad (18)$$

where N_u = number of soil layers in the unsaturated zone

d_d = drainage depth (\equiv thickness unsaturated zone)

The flux pattern in this case consists of N stream tubes with $N_u+1, N_u+2, \dots, N_u+N$ soil layers each.

Assuming no discharge from the unsaturated zone directly to the drain eq. (17) changes:

$$c_d(t) = \frac{1}{N} \sum_{n=N_u}^{N+N_u-1} c_n(t) \quad (19)$$

2.3.2. Percolation to the aquifer

Deep percolation to the aquifer may occur when the drainage barrier (Fig. 2) is not really impermeable, or when the physical drainage barrier is absent. In this last case the effective drainage barrier is assumed at $L/4$.

The number of stream tubes participating in the deep percolation flux is given by the equation:

$$N_p = \beta N \quad (20)$$

where N_p = number of stream tubes participating in the deep percolation flux

$\beta = f_p/f_d$ = ratio of percolation flux and drainage flux

f_p = deep percolation flux

The flow pattern in this case is given in Fig. 3.

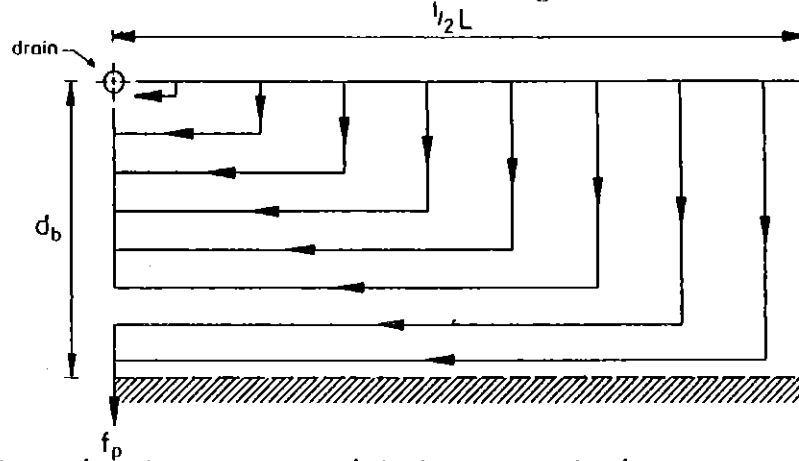


Fig. 3. Schematic flux pattern with deep percolation

For the concentration in the soil water of layer n eq. (10) can be used. The flux reaching the drain equals $f_d - f_p$ in this case and the concentration in the drainage water becomes:

$$c_d(t) = \frac{1}{N - N_p} \sum_{n=N_u}^{N+N_u - N_p - 1} c_n(t) \quad (21)$$

The concentration in the percolation flux f_p can be calculated from the complementary layers:

$$c_p(t) = \frac{1}{N_p} \sum_{n=N+N_u - N_p}^{n+N_u - 1} c_n(t) \quad (22)$$

2.3.3. Seepage from the aquifer

The schematic flux pattern for this case is given in Fig. 4.

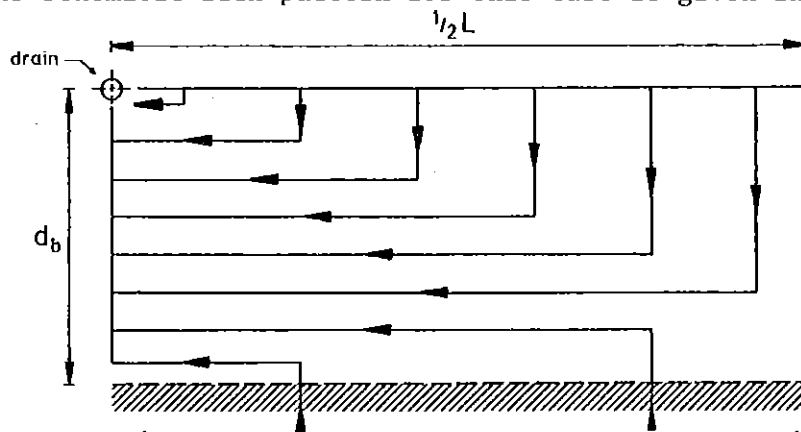


Fig. 4. Schematic flux pattern with seepage from the aquifer

The number of stream tubes participating in the seepage flux is given by the equation:

$$N_s = \gamma N \quad (23)$$

where N_s = number of stream tubes participating in the seepage flux pattern

$\gamma = f_s / (f_s + f_d)$ = ratio of seepage flux and total flux to the drain

f_s = seepage flux

The direction of flow in the soil layers participating in the seepage flux is reversed, and the calculation of the concentration of the soil water in these layers ($n, n-1, \dots, N-N_s$) are calculated with eq. (10) with adapted layer numbering. Using $m = N+N_u-m-1$ and $l = N+N_u-k-1$ as layer number transformation the following expression for the concentration of the soil water is found:

$$c_m(t) = \left(\frac{A}{A+B}\right)^{n+1} c_s + e^{-(A+B)t} \sum_{k=0}^n \frac{(At)^{n-k}}{(n-k)!} \{c_l(t_0) - \left(\frac{A}{A+B}\right)^{k+1} c_s\} \quad (24)$$

for $n = N_{s-1}, N_{s-2}, \dots, 0$

where $A = f_s / \theta L(1+R)$

c_s = concentration of the seepage water

For the concentration of the drainage water the average concentration of the participating soil layers can be calculated using eq. (19).

When the drainage flux is absent ($f_d = 0$) all layers will be involved in the seepage flux pattern ($\gamma = 1$ and $N_s = N$; eq. 23). Considering an unsaturated zone, the seepage flux may reach the top layers if evapotranspiration takes place from these layers. Assuming an evapotranspiration rate equal to the seepage flux to take place from the surface layer the mass balance for layer 0 reads:

$$\frac{dc_o(t)}{dt} + B c_o(t) = A c_1(t) \quad (25)$$

$$\text{where } c_1(t) = \left(\frac{A}{A+B}\right)^n c_s + e^{-(A+B)t} \sum_{k=0}^{n-1} \frac{(At)^{n-k-1}}{(n-k-1)!} \{c_{n-k}(t_o) - \left(\frac{A}{A+B}\right)^{k+1} c_s\}$$

according to eq. (24) taking $N_s = N_u + N = n+1$

Solving eq. (25) gives the following expressions for $c_o(t)$:

$$\begin{aligned} c_o(t) = & \frac{A}{B} \left(\frac{A}{A+B}\right)^n c_s - e^{-(A+B)t} \sum_{k=0}^n \left[\{c_k(t_o) - \left(\frac{A}{A+B}\right)^{n-k} c_s\} \sum_{i=0}^k \frac{(At)^i}{(i)!} \right] \\ & + e^{-Bt} \left[c_o(t_o) - c_s \frac{A+B}{B} \left(\frac{A}{A+B}\right)^n + \sum_{k=1}^n \{c_k(t_o) - \left(\frac{A}{A+B}\right)^{n-k} c_s\} \right] \quad (26a) \end{aligned}$$

for $B \neq 0$

$$\begin{aligned} \text{and } c_o(t) = & c_o(t_o) + At c_s - e^{-At} \sum_{k=0}^n \left[\{c_k(t_o) - c_s\} \sum_{i=0}^k \frac{(At)^i}{(i)!} \right] \\ & + \sum_{k=1}^n \{c_s - c_k(t_o)\} \quad (26b) \end{aligned}$$

for $B = 0$

Assuming the concentration of the flux into layer 0 constant during the calculation time step:

$$\frac{\tilde{c}_1(t)}{c_1} = 1/2 \{c_1(t_o) + c_1(T)\} \quad \text{for } t_o \leq t \leq T \quad (27)$$

where $T-t_o$ is the time step

and solving eq. (25) introducing $\tilde{c}_1(t)$ for $c(t)$ gives for $c_o(t)$:

$$c_o(t) = \frac{A}{B} \tilde{c}_1(t) + e^{-Bt} \{c_o(t_o) - \frac{A}{B} \tilde{c}_1(t)\} \quad (28a)$$

for $B \neq 0$

$$\text{and } c_o(t) = c_o(t_o) + At \tilde{c}_1(t) \quad \text{for } B = 0 \quad (28b)$$

2.4. Systems approach

In system analysis as applied in classic hydrology the system (model) is described in terms of input, system operation, and output. When the model is a linear time invariant system, its operation can be described by the unit hydrograph (impulse response) and the convolution integral.

The summation curve can be defined as the system's response to a unit of input, applied during an infinite time period (VAN DE NES, 1973). The impulse response is defined as the system's output when it is activated by a unit of input applied during an infinitely short period.

In soil chemistry the summation curve is known as the 'breakthrough curve' and is experimentally determined by feeding a soil column with an initial uniform concentration in the soil solution at a fixed rate and a constant concentration in the feed solution. The summation curve being defined as the integral of the impulse response is given by:

$$S(t) = \int_0^t h(t) dt \quad (29)$$

where $S(t)$ = summation curve

$h(t)$ = impulse response

The impulse response is easily obtained as the first derivative of the breakthrough curve with respect to time.

The shape of the impulse response of the system can be characterized by the statistical moments:

$$M_i = \frac{\int_0^{\infty} t^i h(t) dt}{\int_0^{\infty} h(t) dt} \quad (30)$$

where M_i = i^{th} moment relative to the origin

The first moment gives the average time or time lag:

$$\bar{t} = M_1 \quad (31)$$

The second moment gives the variance. The standard deviation of

the impulse response relative to the mean (time lag) can be calculated:

$$\sigma_t^2 = M_2 - (\bar{t})^2 \quad (32)$$

where \bar{t} = average time of outflow

σ_t^2 = standard deviation of outflow

The moments of input, output and impulse response are related (NASH, 1959):

$$M_i\{y(t)\} = M_i\{x(t)\} + M_i\{h(t)\} \quad \text{for } i = 1, 2 \text{ and } 3 \quad (33)$$

where $y(t)$ = systems output

$x(t)$ = systems input

Eq. (33) can be used to find the system parameters, if the moments of the impulse response can be expressed mathematically in the system parameters and if input and output are experimentally determined. If the input is applied during an infinitely short period at $t = 0$ (for the impulse response) the first three moments of the input are zero.

The summation curves for the concentration of the drainage water can be derived by introducing the proper boundary conditions into the pertinent equations (10) for the one dimensional formulation and eq. (17) for the pseudo two dimensional problem. These boundary conditions are:

$$\begin{aligned} c_i &= 1 & \text{for } t \geq 0 \\ c_n(t_o) &= 0 & \text{for } t = 0 \end{aligned} \quad (34)$$

Introduction of these boundary conditions into eq. (10) for the one dimensional formulation gives:

$$S_n(t) = \left(\frac{A}{A+B}\right)^{n+1} - e^{-(A+B)t} \sum_{k=0}^n \frac{(At)^{n-k}}{(n-k)!} \left(\frac{A}{A+B}\right)^{k+1} \quad (35)$$

By differentiating the impulse response is found:

$$h_n(t) = A(At)^n \frac{1}{n!} e^{-(A+B)t} \quad (36)$$

Substitution of eq. (36) into the equations for the moments (30), (31) and (32) gives for the average and standard deviation:

$$\bar{t} = \frac{N}{A+B} \quad (37)$$

and

$$\sigma_t^2 = \frac{N}{(A+B)^2} \quad (38)$$

For a tracer ion, like Cl^- , not involved in adsorption and/or chemical reactions in the soil these equations can be used to find the optimum parameters θ , L_n and N , where L_n and N are related:

$$N L_n = L_T \quad (39)$$

where L_T = column length

Combination of (37), (38) and (39) and taking $R = \alpha = 0$ gives:

$$\theta = \frac{\bar{t} f_d}{L_T} \quad (40)$$

and

$$L_n = L_T \frac{\sigma_t^2}{(\bar{t})^2} \quad (41)$$

Considering, next, a solute involved in adsorption and chemical decomposition, the parameter α may be found directly from eq. (35). It can be proved that the right part of the right hand side of eq. (35) approaches zero for big t values:

$$\lim_{t \rightarrow \infty} S_n(t) = \left(\frac{A}{A+B} \right)^{n+1} \quad (42)$$

The practical meaning of eq. (42) is that the final value of the breakthrough curve after reaching equilibrium is determined by the parameter B . Introducing the expressions for A and B (eq. 8) into (42) it follows for α :

$$\alpha = \frac{f_d}{\theta L} \frac{\{1 - (S_{nc})^{\frac{1}{N}}\}}{(S_{nc})^{\frac{1}{N}}} \quad (43)$$

where $S_{nc} = \lim_{t \rightarrow \infty} S_n(t)$, the final, constant, value of the breakthrough curve.

Using the average time (eq. 37) the parameter R is found:

$$R = \frac{\bar{t}}{N} \left(\frac{f_d}{\theta L} + \alpha \right) - 1 \quad (44)$$

For the two dimensional case the equations are more complicated. The summation curve for the concentration of the drainage water can be derived from eq. (35):

$$S(t) = \frac{1}{N} \sum_{m=0}^n \left\{ \left(\frac{A}{A+B} \right)^{m+1} - \sum_{k=0}^m \frac{(At)^{m-k}}{(m-k)!} \left(\frac{A}{A+B} \right)^{k+1} e^{-(A+B)t} \right\} \quad (45)$$

The impulse response is found by differentiation:

$$h(t) = \frac{A}{N} e^{-(A+B)t} \sum_{k=0}^n \frac{(At)^k}{k!} \quad (46)$$

Using eqs. (30), (31) and (32) it follows:

$$\bar{t} = \frac{N+1}{2(A+B)} \quad (47)$$

and

$$\sigma_t^2 = \frac{(N+1)(N+5)}{12(A+B)^2} \quad (48)$$

For a tracer ion like Cl^- combination of (47) and (48) gives for N:

$$N = \frac{5\bar{t}^2 - 3\sigma_t^2}{3\sigma_t^2 - \bar{t}^2} \quad (49)$$

The layer thickness then follows from eq. (15):

$$L_n = d_b \frac{2N-1}{N^2} \quad (50)$$

and for θ the solution of (49) and (50) has to be introduced into eq. (47):

$$\theta = \frac{\bar{t} f_d}{(N+1)L_n} \quad (51)$$

Considering next a solute involved in adsorption and chemical decomposition it follows from eq. (45) that for the constant final value of the breakthrough curve the following expression holds:

$$S_c = \lim_{t \rightarrow \infty} S(t) = \frac{1}{N} \sum_{m=0}^n \left(\frac{A}{A+B} \right)^{m+1} = \frac{1}{N} \frac{A}{B} \left\{ 1 - \left(\frac{A}{A+B} \right)^N \right\} \quad (52)$$

for $B \neq 0$, where S_c = constant, final, value of the breakthrough curve.

Solution of eq. (52) for α is not possible. The following relation is found:

$$\alpha = \frac{\frac{f_d}{\theta L} \left\{ 1 - \left\{ 1 - \frac{\alpha}{f_d} \theta N L_n S_c \right\}^{1/N} \right\}}{\left\{ 1 - \frac{\alpha}{f_d} \theta N L_n S_c \right\}^{1/N}} \quad (53)$$

By trial and error the proper value for α can be found. From eq. (47) it then follows for R :

$$R = \frac{2\bar{t}}{N+1} \left(\frac{f_d}{\theta L_n} + \alpha \right) - 1 \quad (54)$$

3. THE HP 97 PROGRAMME

The model described by eq. (10) for downward movement and eq. (24) for upward movement has been programmed for the HP 97 calculator. Memory space is sufficient to allow application of the model with a maximum of 20 soil layers. The programme has four entry possibilities that will be discussed below.

Under LBL A the basic data are stored in the calculator memory. In case of downward movement these basic data are the following:

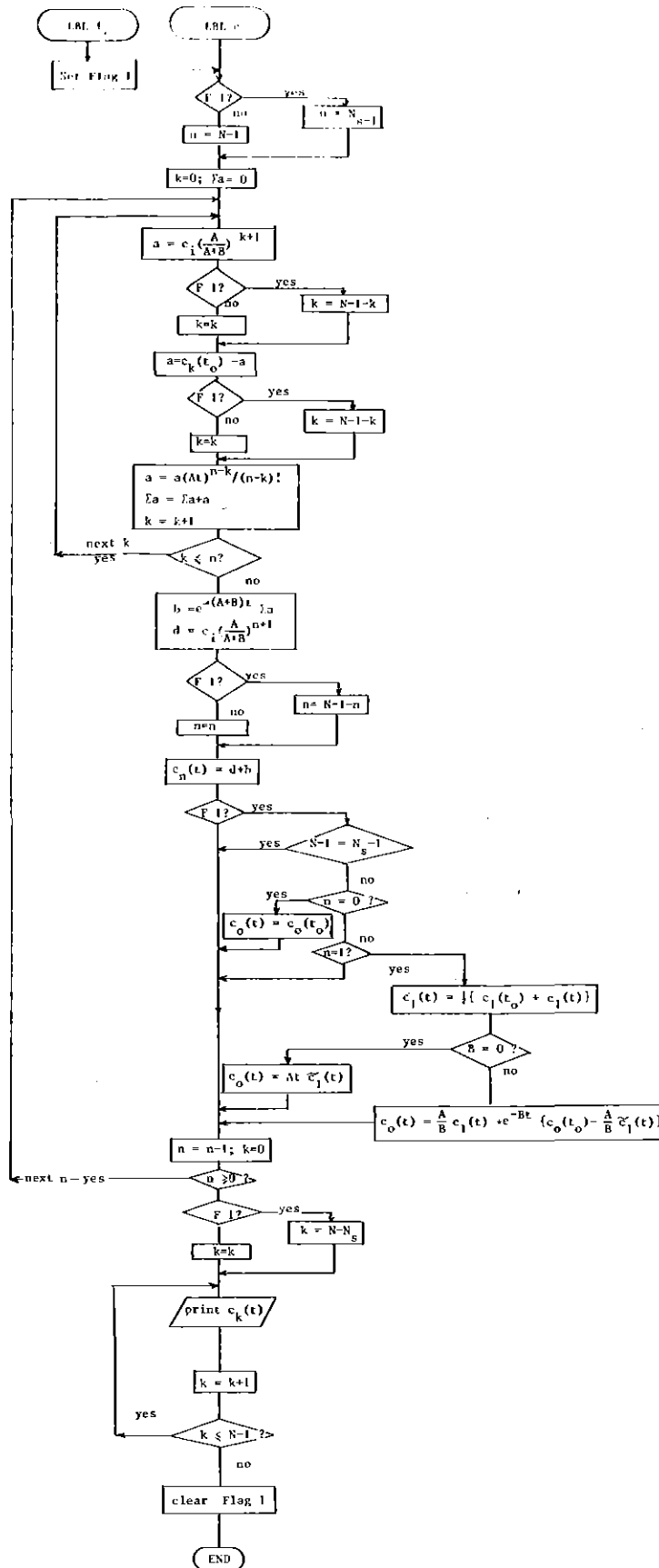


Fig. 5. Flow diagramme main programme

N_{l-1} = number of the lowest layer participating in the downward flux
 c_i = concentration of the influent flux
 At = parameter A multiplied with time step t
 Bt = parameter B multiplied with time step t

In case of upward movement these basic data are:

$N-1.N_{s-1}$ = where N is the total number of soil layers considered and
 $N-1$ defines the lowest soil layer in the model. N_s is the
number of layers participating in the seepage flux pattern.
 $N-1$ and N_{s-1} are separated by the decimal point. For N_{s-1}
two digits are reserved
 c_s = concentration of seepage influent flux
 At = defined as before
 Bt = defined as before

Under LBL C the main programme is executed for the downward movement case. For the seepage case LBL fc is the proper entry and flag 1 is set to indicate seepage. Execution is then transferred to the main programme under LBL C (see Fig. 5 for the flow diagramme). During the programme execution this flag is tested and if true the layer numbering transformation is performed. This flag testing procedure is also used if seepage reaches the root zone to calculate the concentration of the top layer with the adapted (simplified) equations (28a) and (28b). It is thus assumed in the model that if the seepage flux reaches the root zone evapotranspiration equals seepage.

Under LBL D the drainage water quality for the pseudo two-dimensional case is calculated (eq. 19.). Two data have to be entered: N_u - the number of stream tubes in the unsaturated zone not draining to the field drain, and N_d - the number of stream tubes actually draining. When entering $N_d + N_u$ instead of N_u and N_p , the number of stream tubes draining to the aquifer instead of N_d , the concentration of the deep percolation to the aquifer is calculated. The complete programme is given in the annex to this report.

4. OPERATION OF THE MODEL

The operation of the model can be characterized by the summation curves and impulse responses. In this chapter the influence of the parameters N , R and α on the shape of both curves will be explored. Finally, the operation of the two-dimensional approximation will be given, and compared with the one-dimensional results.

4.1. Effect of layer thickness

Considering a soil column of limited length, this column can be subdivided into a number of layers. In Fig. 6a the calculations of a breakthrough curve ($S(t)$) for a column with length 10, an effective moisture content $\theta = 0.5$ and a leaching flux $f_d = 1$ are presented for a layer thickness L_n of 10 ($N = 1$), 5 ($N = 2$), 2.5 ($N = 4$), 1.25 ($N = 8$) and 0.625 ($N = 16$).

It can be seen in the figure that the greatest amount of dispersion is simulated with $N = 1$ (L_n big) and that the simulated dispersion decreases with increasing N (decreasing L_n). The time scale has been multiplied with the factor A/N . When At/N equals 1 the soil moisture in the column has been refreshed once ($f_d t = \theta L_n$). For increasing N the breakthrough curve approaches the line $At/N = 1$, that represents the breakthrough curve for piston flow (no dispersion). In Fig. 6b the corresponding impulse responses are presented. It can be seen that with increasing N the impulse response reaches its maximum later and that attenuation is less.

In Fig. 7 the salt profiles at different times are presented. Upon increasing N the salt front is steepened (less dispersion).

4.2. Effect of adsorption

In Fig. 8a the breakthrough curves for four values of R , the distribution ratio are presented. The curve for $R = 0$ is identical to the curve from Fig. 6a with $N = 8$. It can be seen from the curves that the effect of (linear) adsorption is a delay of the breakthrough curve. The dimensionless time scale used in Fig. 6a cannot be used here because the parameter A changes for different values of R . For $R = 0$ the

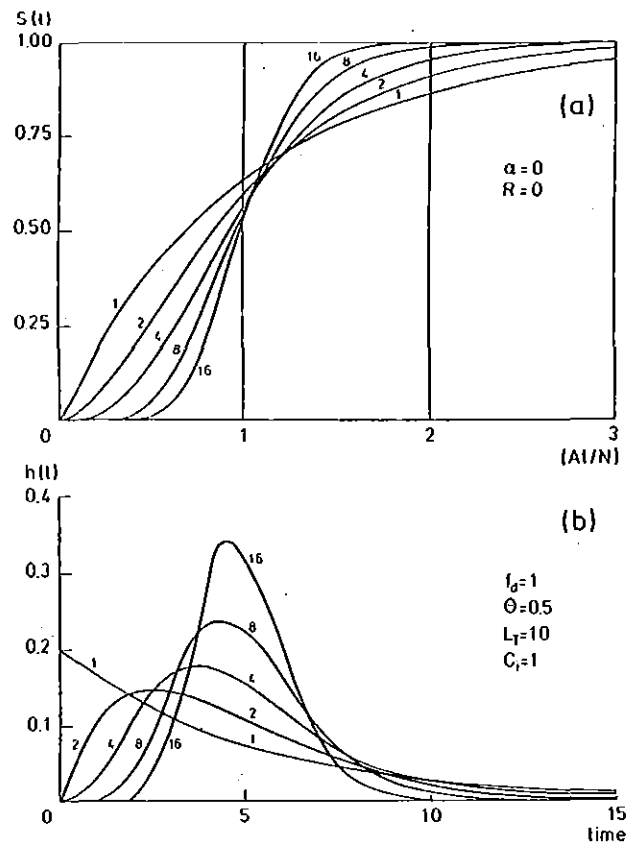


Fig. 6. Effect of layer thickness on summation curve (a) and unit salinograph (b). The number refers to the number of layers considered, N , and $L_n = L_T/N$

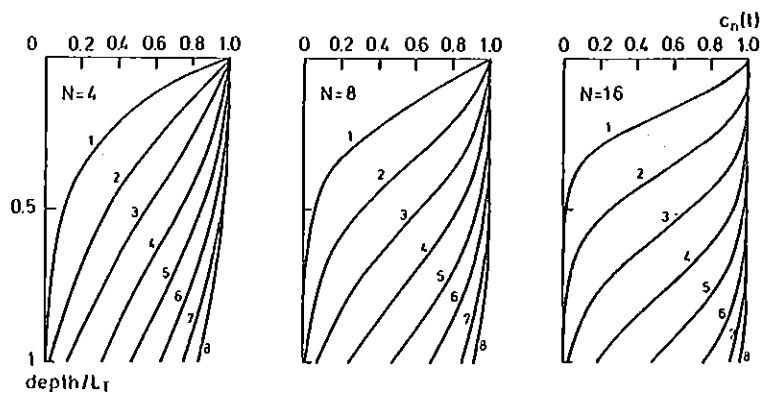


Fig. 7. Effect of layer thickness on salt profile. The number refers to the time elapsed. At $t = 5$ the influent volume equals the volume of the column ($At/N = 1$)

dimensionless time $tA/N = 1$ at $t = 5$. For $R = 1$ $tA/N = 1$ at $t = 10$; for $R = 2$ at $t = 15$ and for $R = 4$ at $t = 25$. The coefficient of delay therefore equals $1+R$.

In Fig. 8b the corresponding impulse responses are given. It can be seen that for increasing R the maximum is reached later and that attenuation increases.

In Fig. 9 the salt profiles for different t values are given. It can be seen that the salt front in the soil is delayed, but not remarkably changed by increasing (linear) adsorption, indicating that the dispersion remains unchanged. The attenuation of the impulse responses should therefore not be attributed to increased dispersion.

4.3. Effect of decomposition

In Fig. 10a the breakthrough curves for different α values are presented. The curve for $\alpha = 0$ is identical to the curve from Fig. 6a with $N = 8$. The effect of increased decomposition is a lower final concentration in the effluent. In Fig. 10b the corresponding impulse responses are given. It clearly shows that the effect of a higher value of α is a lower maximum, but the maximum appears earlier in time.

In Fig. 11 the salt profiles are given.

4.4. Effect of two-dimensional approximation

In Fig. 12a the two-dimensional formulation is compared with the one-dimensional (column), for the breakthrough curves. It can be seen that for all the cases considered the pseudo two-dimensional model gives a faster reaction. In Fig. 12b the impulse responses are given. For the two-dimensional cases the maximum of the curves is at $t = 0$. In Fig. 13 the solute distribution for the three cases ($\alpha = 0$ and $R = 0$; $\alpha = 0$ and $R = 1$; and $\alpha = 0.16$ and $R = 0$) are given.

In Fig. 13a the relative solute distribution for $t = 2, 4$ and 6 is given for the case without adsorption and decomposition. In Fig. 13b adsorption ($R = 1$) is considered and the same distribution is noticed with a certain delay (the distribution at $t = 4$ is identical to that for $R = 0$, Fig. 13a at $t = 2$). In Fig. 13c decomposition is considered and the relative solute distribution changes with respect

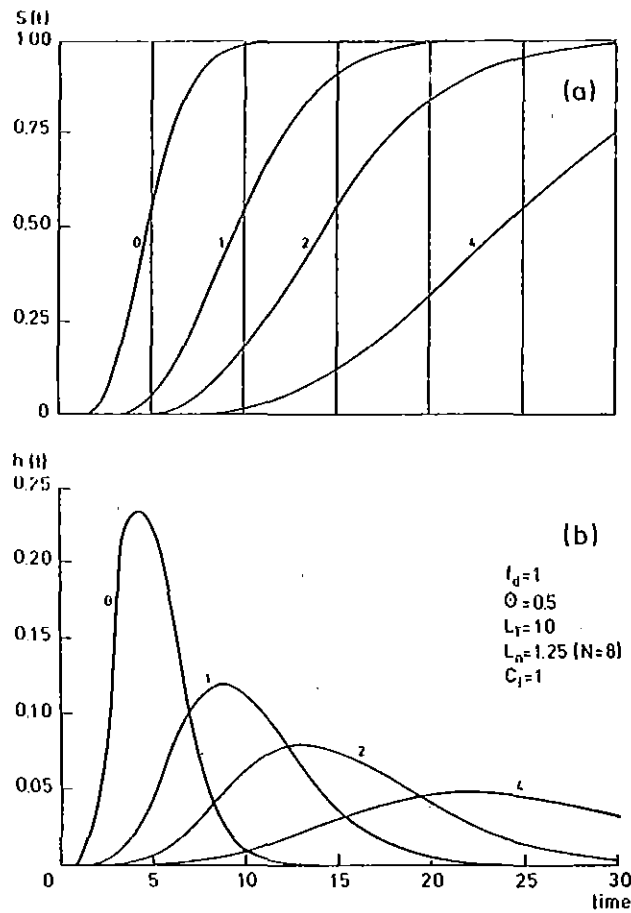


Fig. 8. Effect of adsorption on summation curves (a) and unit salinographs (b). The number refers to the value of R used

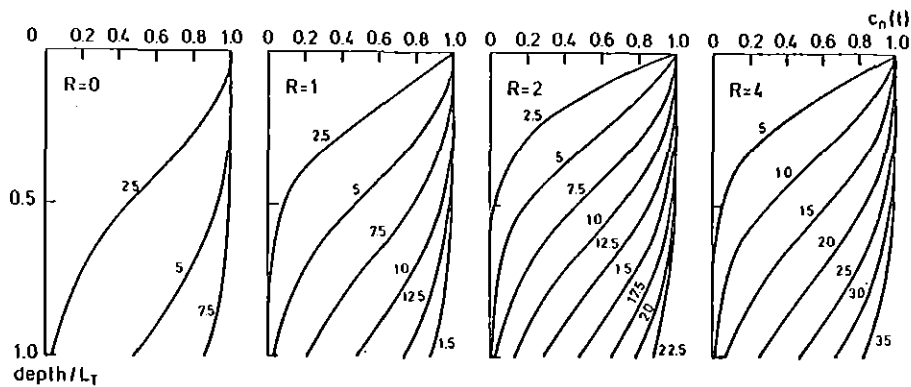


Fig. 9. Effect of adsorption on salt profile. The numbers refer to the time elapsed. At $t = 5$ the influent volume equals the volume of the column

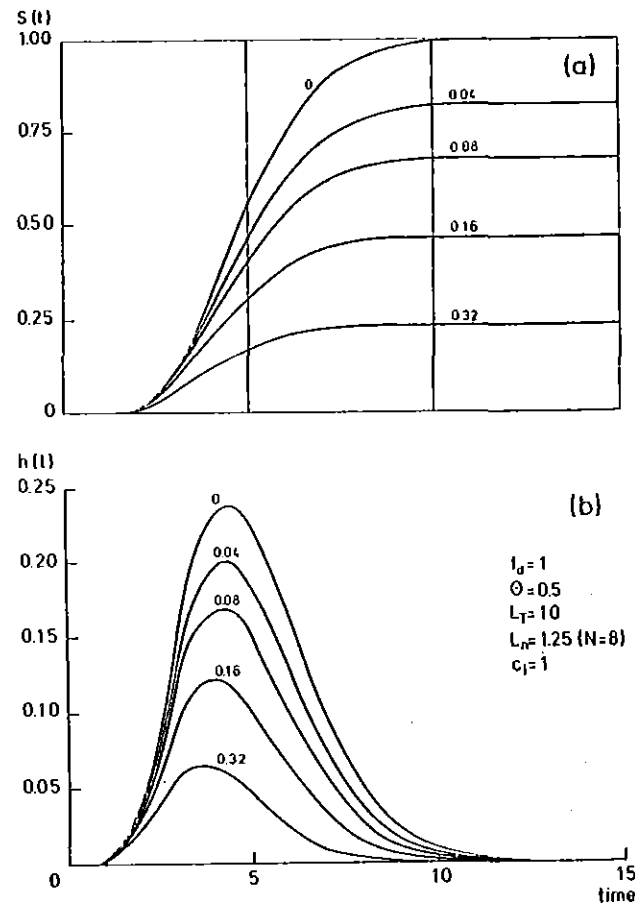


Fig. 10. Effect of decomposition on summation curves and unit salinographs. The numbers refer to the value of α used

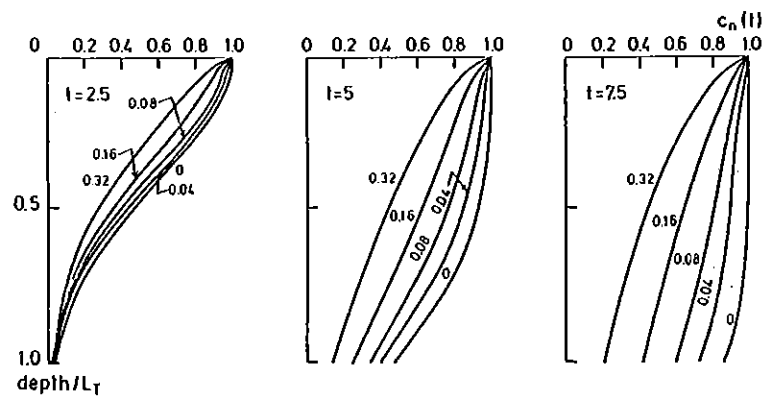


Fig. 11. Effect of decomposition on salt profile. The numbers refer to the value of α used

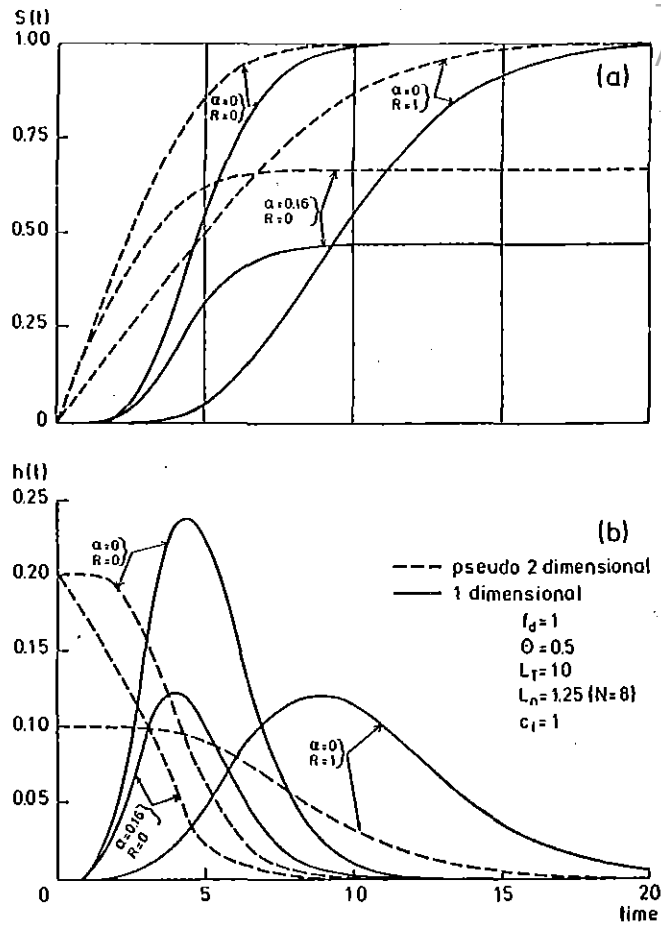


Fig. 12. Effect of pseudo two-dimensional formulation on summation curves and unit salinographs

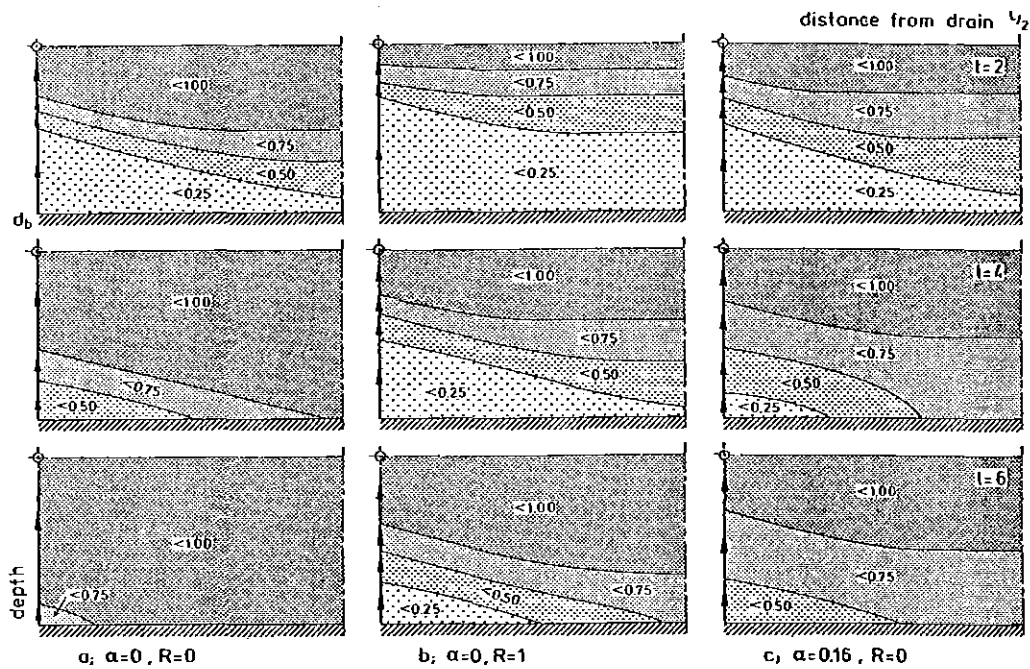


Fig. 13. Relative solute distribution for the pseudo two-dimensional model

to the previous two cases. It can be seen from this figure that a relative high concentration of the solute is drained from the area just beside the drain and a relative low concentration from the area far from the drain (longer pathway).

5. RESULTS

The model formulation and the use of the moments to find the system parameters have been tested with data of some column experiments reported by HOEKS et al. (1979) in chapter 5.1. In chapter 5.2 an application of the pseudo two-dimensional formulation with seepage data reported by ABDEL NASSER (1983) will be discussed.

5.1. Column experiments

The experiment used for simulation has been performed with a sandy loam soil. The column, 40 cm long, has been filled with air-dry soil. Next the soil was wetted by adding oxygen-free distilled water until saturation. The total porosity was 0.415. The column was percolated with a leachate from a waste tip under anaerobic conditions (N_2/CO_2 atmosphere with 30-35 volume % CO_2 in the gas mixture). The leachate was added to the column by means of a pump at an average rate of 9.06 mm/day (varying from 9.86 during the first period of the experiment to 8.76 mm/day during the last period). The effluent of the column was collected under anaerobic conditions (N_2/CO_2 gas mixture) to avoid oxidation. The breakthrough curves for Cl^- (influent concentration 506 mg/l), Na^+ (influent concentration 363 mg/l) and NH_4^+ (influent concentration 135 mg/l) are presented in Fig. 14. On the vertical scale the relative effluent concentration is given (concentration of the effluent divided by the influent concentration) and on the horizontal scale the time (corrected for the small variations in the average leaching rate).

Through these measurements, the breakthrough curves (summation curves) were approximated by hand-fitting. Next the impulse responses have been constructed (Fig. 15) by plotting the slope of the - hand fitted - breakthrough curves. For the three impulse response curves

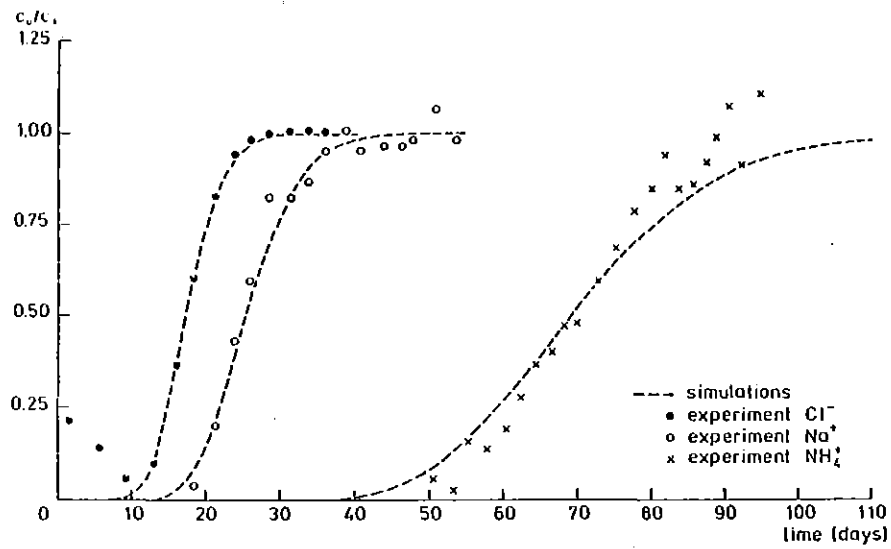


Fig. 14. Measured and simulated breakthrough curves experiment II-6
(experimental data after Hoeks et al., 1979)

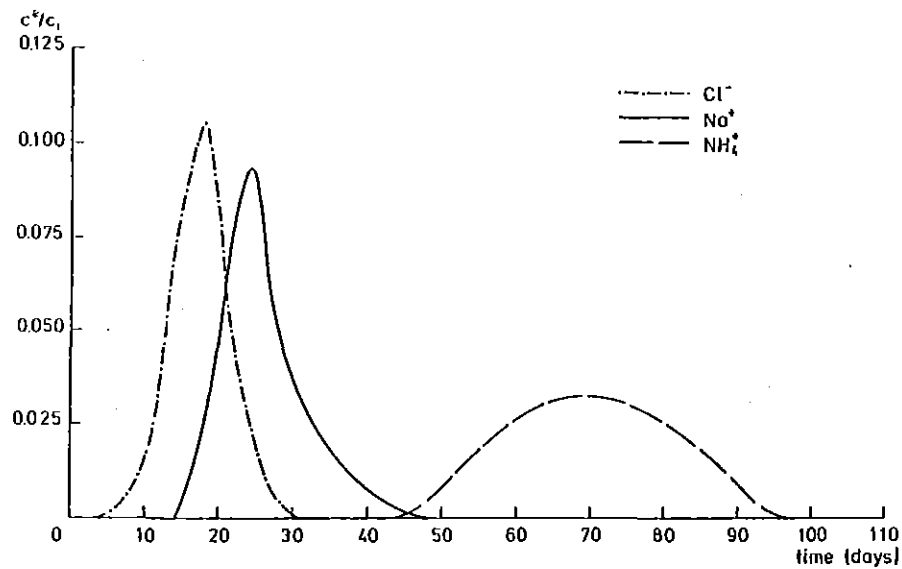


Fig. 15. Experimental impulse responses for Cl^- , Na^+ and NH_4^+ experiment II-6

the average and the standard deviation have been determined.

	\bar{t} (days)	σ_t^2 (days) ²
Cl ⁻	17.72	14.24
Na ⁺	26.08	32.84
NH ₄ ⁺	70.71	128.75

Applying eq. (40) for the Cl⁻ example gives for the effective moisture content $\theta = 0.401$. This indicates that about 3.5% of the soil solution is immobile and not involved in the transport of solutes.

Application of eq. (41) for the Cl⁻ example gives for the optimum layer thickness $L_n = 18.14$ mm. The optimum number of soil layers would thus be 22. Twenty layers being the maximum for the HP 97 programme, calculations have been performed with $N = 20$, $L_n = 20$ mm and $\theta = 0.401$. The results are included in Fig. 14.

Using eq. (44) and taking $\alpha = 0$ gives for the distribution ratio for the Na⁺ example $R = 0.47$ and for the NH₄⁺ example $R = 2.99$. The resulting simulations for Na⁺ and NH₄⁺ are included in Fig. 14.

The results for Cl⁻ and Na⁺ are quite satisfactory: the simulation agrees very well with the experimental results. For NH₄⁺ the simulation is less accurate. It must be concluded therefore that the adsorption mechanism for NH₄⁺ cannot be described properly by the linear adsorption formula. In other words: the NH₄⁺ concentration used exceeds the limitation posed in the formulation of the model.

GOUDRIAAN (1973) and later HAMAKER (1975) showed that the apparent diffusion coefficient can be calculated with:

$$D_{app} = \frac{f_d L_n}{2\theta} \quad (55)$$

The apparent diffusion coefficient calculated with eq. (55) and the distribution ratios found here can be compared with the values found by Hoeks:

	D_{app}	R	Hoeks (1979)
Cl^-	2.6×10^{-5}		$1.5 \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$
Na^+		0.46	0.47
NH_4^+		2.99	2.9

In Fig. 16 the breakthrough curve of the Chemical Oxygen Demand (COD) that is considered a measure for the organic load is presented. The concentration of the influent was 6.640 mg/l. In the same figure the curve for Cl^- is included for comparison. Two facts can be remarked: first the organic matter seems to be slightly adsorbed by the soil. Second, decomposition seems to start only after about 25 days. The reason for this may be that the methane gas formation which is the process responsible for the organic matter decomposition is initiated by bacteria. This means that the bacteria growth itself has to be considered and that the approach proposed in chapter 2.9 for a solute involved in both adsorption and decomposition (eqs. 43 and 44) for finding the α and R parameter cannot be used. An alternative approach has therefore been used here.

Through the COD data in Fig. 16 for $0 < t < 25$ a curve has been draughted by hand-fitting. This curve has been extrapolated for the period after $t = 25$, neglecting the decomposition effects. In Fig. 17 the slope of this COD* summation curve has been plotted giving the impulse response for COD* (the asterix indicates that decomposition is neglected). For this COD* impulse response curve the average and standard deviation have been calculated: $\bar{t} = 19.40$ days and $\sigma_t^2 = 19.11 \text{ days}^2$. With eq. (44), taking $\alpha = 0$, the distribution ratio R is found: $R = 0.096$. The equilibrium value for α , which is the value when the bacteria population reaches its maximum size can be found with the use of eq. (42). Applying this equation and taking $R = 0.096$ the final value for α is found: $\alpha = 0.156$.

Sigmoid curves describing bacterial population growth can be given on basis of the logistic differential equation:

$$\frac{dP_t}{dt} = r P_t (P_{max} - P_t) P_{max}^{-1} \quad (56)$$

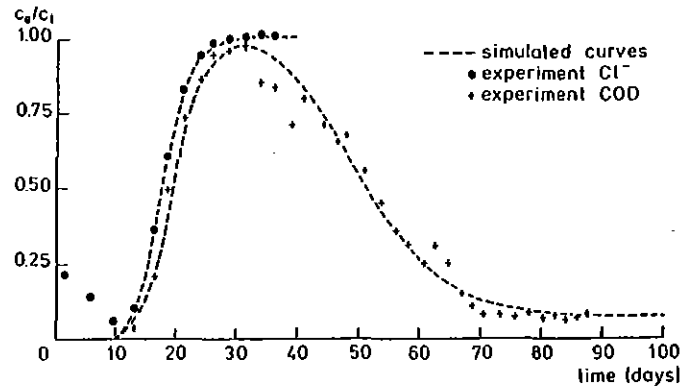


Fig. 16. Measured and simulated breakthrough curve for COD experiment II-6 (experimental data after Hoeks et al., 1979). The curve and data for Cl^- are included for comparison

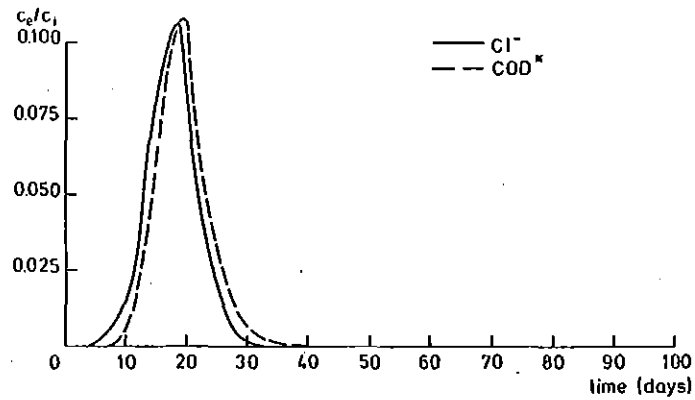


Fig. 17. Experimental impulse response for COD* (neglecting decomposition effects) experiment II-6. The impulse response for Cl^- is included for comparison

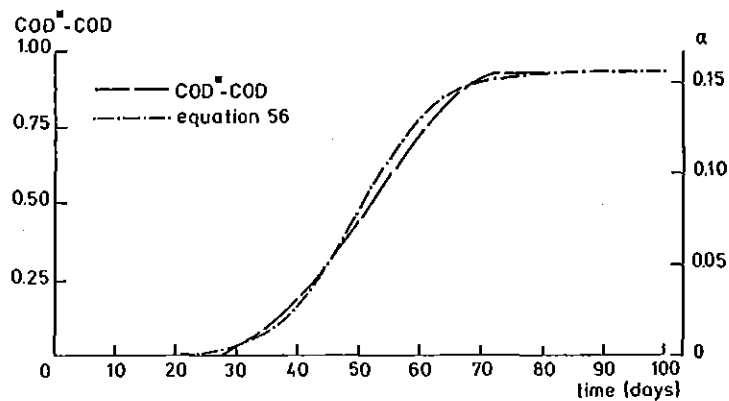


Fig. 18. Bacteria population growth curve experiment II-6

in which r is the coefficient of increase which a population would have if ample food is available, P_{\max} is the maximum or equilibrium population density under the conditions of the food supply present and P_t is the population density at time t .

Integration of the equation yields:

$$\frac{P_{\max} - P_t}{P_t} = \frac{P_{\max} - P_0}{P_0} e^{-rt} \quad (57)$$

where P_0 is the population density at time t equals 0.

Assuming that α is proportional to the bacteria population, the activity coefficient can be given as a function of time as:

$$\frac{\alpha_{\max} - \alpha_t}{\alpha_t} = \frac{\alpha_{\max} - \alpha_0}{\alpha_0} e^{-rt} \quad (58)$$

and can be found by subtracting the COD curve from the extrapolated COD* curve (Fig. 18). On the right vertical axis the scale for α is given. The activity curve is calculated with $\alpha_{\max} = 0.156$, $\alpha_0 = 6.510^{-5}$ and $r = 0.157$. The resulting simulation curve with varying α values (assumed constant for intervals of 5 days in the calculations) according to Fig. 18 is presented in Fig. 16. The good agreement between the simulated curve and the experimental data indicates that the methane gas formation process may be properly described by a first order decomposition equation (4) of organic matter.

5.2. A field experiment

ABDEL NASSER (1983) studied the water and salt balance of a small area (appr. 30 acres) in the northern part of the Nile Delta in Egypt. The study area is close to the Manzala lake and is subject to heavily saline seepage. No fresh irrigation water is available to the farmers in this region; they irrigate their crops with the moderately saline water from the Bahr Hadus drain. The study area is irrigated by the use of a diesel engine; drainage is by sakkia, a buffalo draughted water wheel. The field drains are spaced approximately 20 m apart and are roughly 50 cm deep. During the winter season 1980/81,

the area was planted with berseem, a fodder crop giving 3 to 5 cuttings per season. Data were collected on irrigation water supply and drainage water discharge (both quantity and salinity), on precipitation and on the vertical soil salinity distribution midway between the field drains at the beginning and at the end of the winter season.

Using meteorological data from the nearby stations Port Said and Mansura Abdel Nasser used the data on irrigation and drainage water quantity and the approach for calculating the actual evapotranspiration proposed by RIJTEMA (1981) to find the most probable actual seepage inflow from deeper layers. He arrived at a value of 0.46 mm/day.

For the solute movement simulation Abdel Nasser used eq. (10) for downward flow and eq. (24) for upward (seepage) flow. Because these two equations are derived for constant fluxes and a separation depth between the leaching and the seepage flow pattern, the interval must be subdivided in a number of subintervals based on the number of layers involved in both flux patterns. This will be elaborated below.

The layer thickness was conveniently chosen as 50 cm, the depth of the unsaturated zone. By this choice of layer thickness eq. (28b) is validated for the case of seepage into the unsaturated zone, be it that a correction has to be applied if evapotranspiration exceeds upward seepage.

Considering an irrigation of I mm at time $t = 0$, the groundwater table will rise. The drainable volume of water stored above the groundwater table is given by the expression:

$$V(o) = I + V(t-1) - M_{RZ} \quad (59)$$

where $V(o)$ = quantity of water stored in the unsaturated zone above field capacity (mm)

I = irrigation (mm)

$V(t-1)$ = quantity of water still stored in the unsaturated zone above field capacity at the end of the previous time step (mm)

M_{RZ} = moisture deficit (below field capacity) at the end of the previous time step (mm)

It should be noted that M_{RZ} is zero when $V(t-1)$ is positive and $V(t-1)$ is zero when M_{RZ} is positive.

It has been assumed that during that part of the time step that $V(t)$ is positive, evapotranspiration takes place from this 'reservoir' and that moisture depletion of the root zone takes place only after this reservoir has been depleted. Simultaneously with the withdrawal of water for evapotranspiration, drainage takes place. Drainage has been assumed to be proportional to the quantity stored. The continuity equation for this reservoir can be formulated:

$$\frac{dV(t)}{dt} = - \{E_a + aV(t)\} \quad \text{for } V(t) \geq 0 \quad (60)$$

where E_a = actual evapotranspiration in mm/day

$$a = \frac{\pi^2 k d}{\mu L^2} = \text{reaction factor of the reservoir day}^{-1}$$

k = permeability in m day⁻¹

d = thickness water bearing layer below draindepth in m

μ = drainable pore space

L = drain distance in m

Equation (60) can be solved for the boundary condition $V(t) = V_0$ for $t = 0$:

$$V(t) = (V_0 + \frac{1}{a} E_a) e^{-at} - \frac{1}{a} E_a \quad (61)$$

The drainage flux leaving the unsaturated zone results:

$$fd = aV(t) = (aV_0 + E_a) e^{-at} - E_a \quad \text{for } V(t) \geq 0 \quad \text{and } fd = 0 \quad \text{for } V(t)=0 \quad (62)$$

The upward seepage flux being considered constant (0.46 mm/day) it is clear that upon depletion of the 'reservoir' (\equiv upon lowering the water table) the separation depth between leaching and seepage flux patterns is moving upward. Because the soil is divided into a limited number of layers the non:steady state equation (62) can be approximated by a succession of steady states for which the mass balances can be drafted. To this purpose the calculation interval which has been taken conveniently as the irrigation interval has to be subdivided into a number of sub periods, during which the number of participating layers

for the leaching and for the seepage flux pattern remains constant.

Using the ratio between the (downward) leaching flux and the total (drainage + seepage) flux γ , the number of layers participating in the leaching flux pattern at the start of the irrigation interval can be calculated:

$$\begin{aligned} N_{\ell}(t_o) &= \text{Int} \{Nu + \gamma (N - Nu) + 0.5\} \text{ for } f_d(t_o) > 0 \\ N_{\ell} &= 0 \text{ for } f_d = 0 \end{aligned} \quad (63)$$

where $N_{\ell}(t_o)$ = number of layers to be considered for the leaching pattern for the longest streamtube (midway between drains) at the beginning of the irrigation interval

Int () = integer function, takes the integer of the expression between brackets

$$\gamma = \frac{aV_o}{f_s + aV_o} \text{ for } t = t_o$$

The time steps Δt_i during which the number of layers participating in the leaching pattern is $N_{\ell}(t_o)$, $N_{\ell}(t_o)-1$, $N_{\ell}(t_o)-2$,, 0 can be calculated with:

$$\Delta t_i = \frac{1}{a} \ln \left\{ \frac{a V(t_i) + Ea}{a V(t_{i+1}) + Ea} \right\} \quad (64)$$

where $V(t_i) = \frac{1}{a} \frac{\beta}{1-\beta} f_s$ = the volume $V(t)$ after i intervals Δt_i , for which the number of layers involved in the leaching flux pattern decreases with one

$$\text{and } \beta = \frac{N_{\ell}(t_o) - Nu - i - 0.5}{N - Nu}$$

for $i = 0, 1, 2, \dots, N_{\ell}(t_o) - Nu - 1$

with $V(t_i) = V_o$ at $t = 0$

The volume of drainage water during each time step Δt_i can be calculated:

$$f_d \Delta t_i = V(t_{i+1}) - V(t_i) - E_a \Delta t_i \quad (65)$$

For each time step Δt_i the number of participating layers in

the leaching and seepage pattern and the volumes of leaching and seepage water are known and equation (10) for leaching and (24) for seepage can be used.

For the calculation of the salinity of the top layer (unsaturated zone) one more simplification has been made. During leaching the moisture content of the top layer is held constant (at field capacity). During each time step Δt_i the quantity $f_d \Delta t_i$ (equation 65) is leached and afterwards the concentration of the top layer is corrected for actual evapotranspiration according to:

$$c_o(t) = \frac{c'_o(t) \theta L_n + E_a \Delta t_i c_i}{\theta L_n} \quad (66)$$

During periods with seepage into the unsaturated zone the same procedure has been followed. Equation (28b) was used in this case, however, giving rise to a smaller correction for the evatranspiration:

$$c_o(t) = \frac{c'_o(t) \theta L_n}{\theta L_n - \Delta t_i (E_a - f_s)} \quad (67)$$

where $c_o(t)$ = soil salinity after correction
 $c'_o(t)$ = soil salinity before correction
 $\Delta t_i (E_a - f_s)$ = moisture depletion due to evapotranspiration
in mm (= M_{RZ})

Whenever seepage into the root zone has been the case, the moisture depletion will be remedied during the first successive irrigation (see equation 59) and another correction for refilling the moisture deficit has to be applied:

$$c_o(t+1) = \frac{c_o(t) \{ \theta L_n - M_{RZ} \} + c_i M_{RZ}}{\theta L_n} \quad (68)$$

where $c_o(t+1)$ = initial soil salinity after irrigation

The flow diagramme of the calculation scheme used for the Bahr Hadus study is presented in fig. 19.

In this study 5 soil layers with $L_n = 50$ cm have been used. The drainage barrier is therefore found at 1.90 m depth and for the reaction

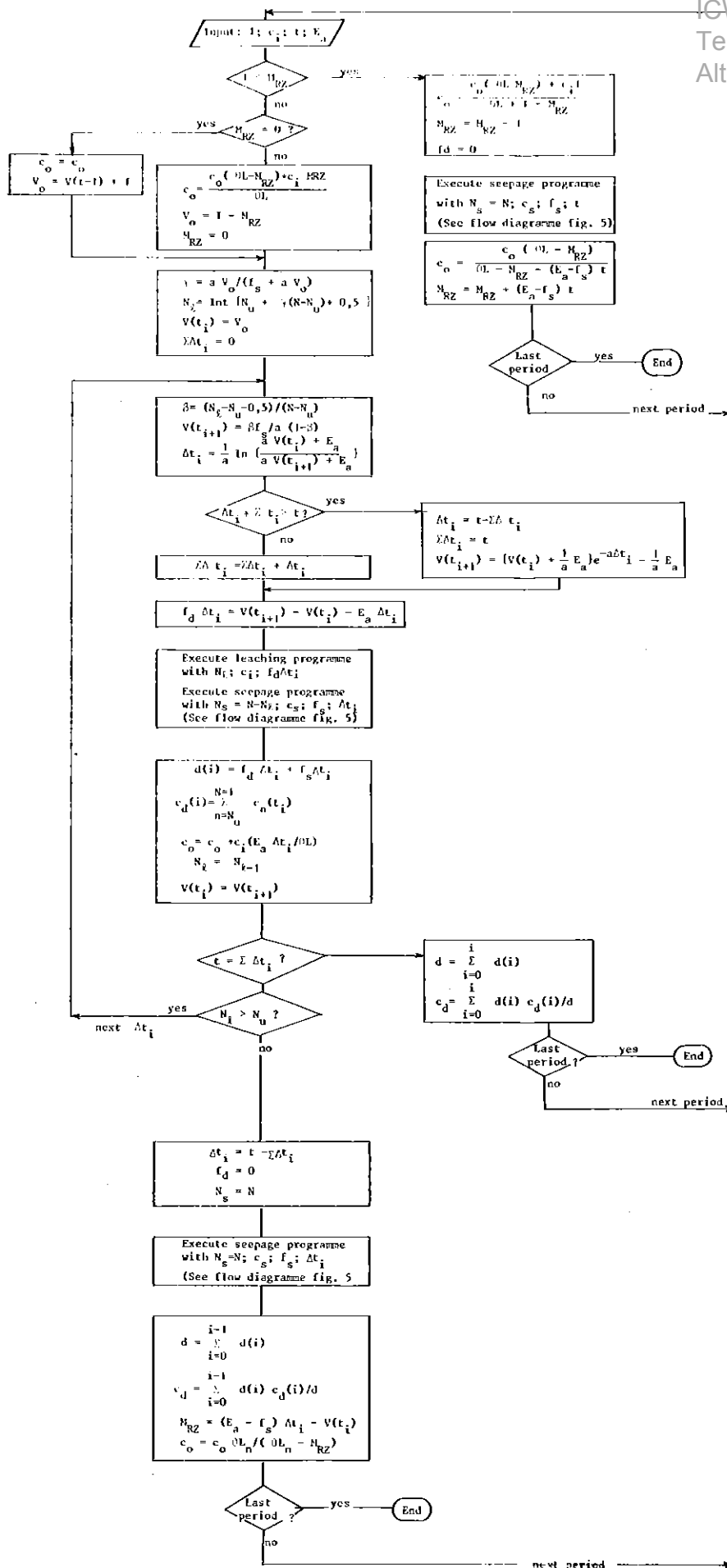


Fig. 19. Flow diagramme of the calculation scheme used for the Bahr Hadus study area

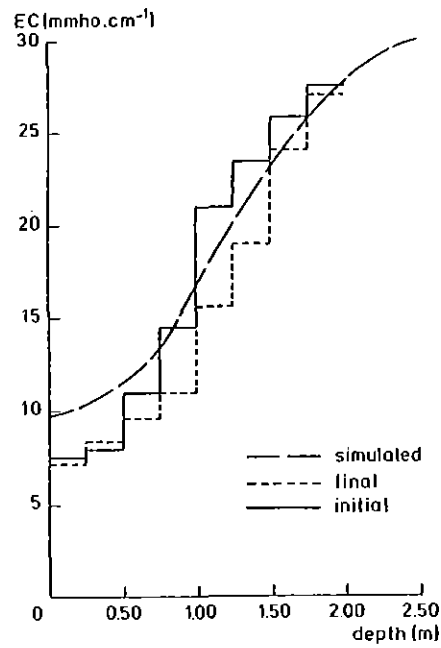


Fig. 20. Observed initial and final salt profile and simulated final salt profile, Bahr Hadus study area

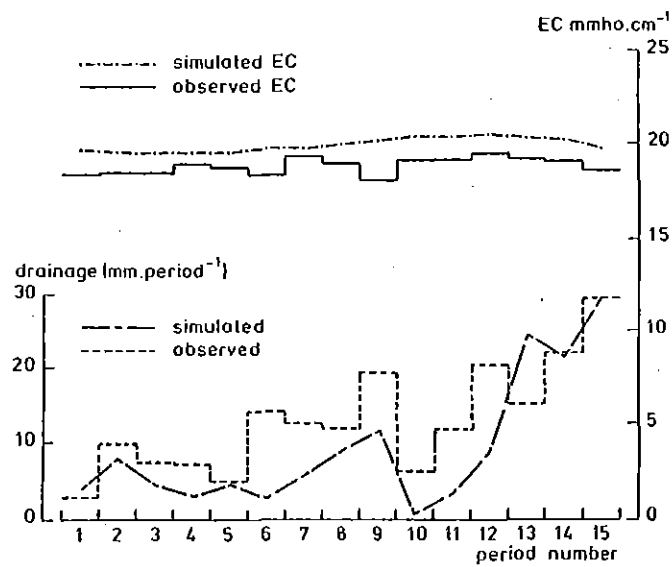


Fig. 21. Observed and calculated drain discharge and drainage water salinities, Bahr Hadus study area

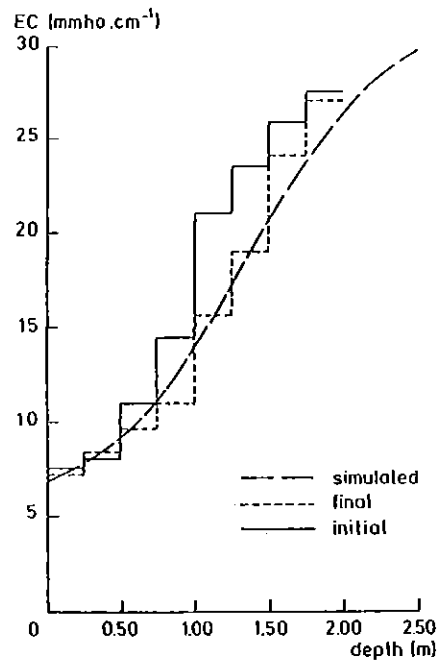


Fig. 22. Simulated salt profile Bahr Hadus study area. Input data slightly adjusted

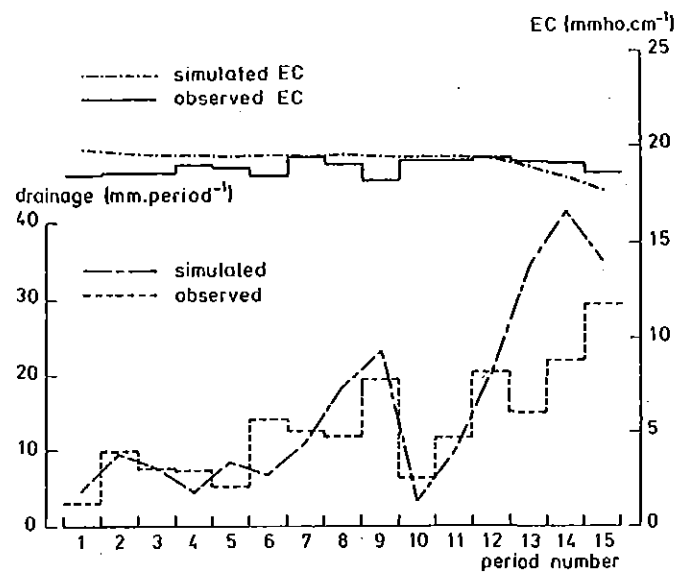


Fig. 23. Simulated drain discharge and drainage water salinity Bahr Hadus study area. Input data slightly adjusted

factor a a value of 0.05 day^{-1} can be calculated. The seepage flux was considered constant 0.46 mm/day and the salinity of the seepage water at 30 mmho/cm .

The results of the calculations are presented in fig. 20 where the calculated final salinity profile is compared with the observed initial and final salt profiles (average of 16 measuring points) and in fig. 21 where the calculated drain discharge and drainage water salinity are compared with the observed quantities for the 15 irrigation intervals during which data were collected.

The results not being very convincing Abdel Nasser performed a sensitivity analyses to the accuracy of his input data. He argued that a 10% deviation in the irrigation water measurements would not be very surprising. If a systematic deviation would occur he expected the measurements to be on the low side. Also for the irrigation water salinity a 10% deviation due to sampling difficulties can be expected. A systematic deviation would increase the irrigation water salinity; and the measurements would then be on the high side.

For the calculation of the actual evapotranspiration a full soil cover for the berseem crop has been assumed. The soil salinity of the top soil being around 7.5 mmho.cm^{-1} and the threshold value* for the berseem crop being app 1.5 mmho.cm^{-1} , Abdel Nasser argued that a 10% lower evapotranspiration due to growth retardation and a less than full ground cover can very well be expected.

In figs. 22 and 23 the results with a 10% higher irrigation water supply; a 10% lower irrigation water salinity; and a 10% lower evapotranspiration is presented. A much better agreement between observation and simulation is obtained.

* The threshold value of salinity indicates the salinity at which the crop yield starts to decline.

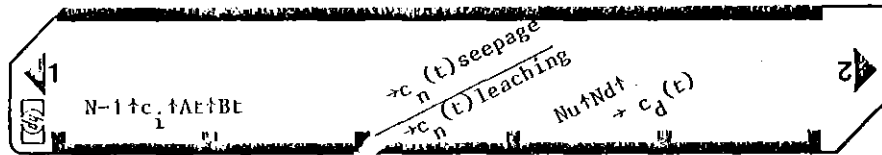
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ANNEX: HP 97 Programme

User Instructions

i



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Read programme card		<input type="text"/> <input type="text"/>	
2	Store the initial concentrations $c_n(t_0)$ in the calculator memory	$c_o(t_0)$ $c_i(t_0)$ etc.	STO <input type="text"/> 0 STO <input type="text"/> 1	
3	Read data N_s-1 or $N-1.N_s-1$; c_i or c_s At** and Bt***	$N_s-1/N-1$ c_i/c_s At Bt	<input type="text"/> <input type="text"/> <input type="text"/> <input type="text"/> <input type="text"/> <input type="text"/> A <input type="text"/>	$N_s-1/N-1.N_s-1$ c_i/c_s At Bt
4	Leaching; or seepage		C <input type="text"/> f <input type="text"/> c <input type="text"/>	$c_o(t)$ $c_i(t)$...
5	Read Nu, number of layers not draining; Nd, number of streamtubes draining; and calculate drainage water salinity	Nu Nd	<input type="text"/> <input type="text"/> D <input type="text"/>	$c_n(t)$ $c_d(t)$
6	Repeat steps 3 and 4 or 3, 4 and 5 for all time periods		<input type="text"/> <input type="text"/>	
	* the format of $N-1.N_s-1$ is dd.dd		<input type="text"/> <input type="text"/>	
	** $At = \frac{fd t}{\theta L(1+R)}$ fd = drainage flux t = time step θ = moisture content L = layer thickness R = distribution ratio		<input type="text"/> <input type="text"/>	
	*** $Bt = \frac{\alpha t}{\theta L(1+R)}$ α = decomposition coefficient		<input type="text"/> <input type="text"/>	

STEP	KEY ENTRY	KEY CODE	COMMENTS	
001	* LBLA	21 11	Leaching	Seepage
002	SPC	16-11		
003	STOE	35 15	Bt	
004	PRTX	-14		
005	R↓	-31		
006	STOB	35-12	At	
007	PRTX	-14		
008	R↓	-31		
009	STOC	35 13	c_i	c_s
010	PRTX	-14		
011	R↓	-31		
012	STOA	35 11	$N_{\ell}-1$	$N-1, N_s-1$
013	PRTX	-14		
014	SPC	16-11		
015	RTN	24	End of 'input' programme	
016	* LBLC	21 13	Main programme	
017	RCLA	36 11	$N_{\ell}-1$	$N-1, N_s-1$
018	F1?	16 23 01	no	yes
019	GSBO	23 00	Skip this step	GoSub 0(calc N_{s-1})
020	STOD	35 14	$n = N_{\ell}-1$	$n = N_s-1$
021	0	00		
022	ENT↑	-21		
023	ENT↑	-21	$\Sigma a = 0$	$\Sigma a = 0$
024	STOI	35 46	$k = 0$	$k = 0$
025	* LBLI	21 01		
026	R↓	-31		
027	R↓	-31	Σa	Σa
028	GSB6	23 06	GoSub 6{ $a=c_i(\frac{A}{A+B})^{k+1}$ }	GoSub 6{ $a=c_s(\frac{A}{A+B})^{k+1}$ }
029	CHS	-22	-a	-a
030	F1?	16 23 01	no	yes
031	GSB2	23 02	Skip this step	GoSub 2(transform layer number)

REGISTERS

0 RE	1 SE	2 RV	3 ED	4	5 FO	6 R	7 S	8 O I	9 L
S0 WA	S1 TE	S2 R	S3 C	S4 ON	S5 CE	S6 NT	S7 RA	S8 TIO	S9 NS
A $\frac{N_{\ell}-1}{N-1, N_s-1}$		B At		C $\frac{c_i}{c_s}$		D n		E Bt	
								I $k/N-1-k$	

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Σ→←ℓ	KEY ENTRY	KEY CODE	COMMENTS			
094	RTN	24	End of main programme			
095	*LBLO	21 00	Supporting subroutine, executed for seepage only			
096	RCLA	36 11	N-1.Ns-1			
097	FRC	16 44	0.Ns-1			
098	EEX	-23				
099	2	02				
100	x	-35	Ns-1			
101	RTN	24	End of subroutine			
102	*LBL2	21 02	LAYER NO TRANSFORMAT		RETRANSFORMATION	
103	RCLA	36 11	N-1.Ns-1		N-1.Ns-1	
104	INT	16 34	N-1		N-1	
105	RCLI	36 46	k		N-1-k	
106	-	-45	N-1-k		k	
107	STOI	35 46	Step 31	Step 66		
108	R↓	-31	-a	b+d		
109	RTN	24	End of subroutine			
110	*LBL5	21 05	Determines first layer for printing(seepage)			
111	GSBO	23 00	GoSub 0 (calculate Ns-1)			
112	STOD	35 14	Ns-1			
113	RCLA	36 11	N-1.Ns-1			
114	INT	16 34	N-1			
115	RCLD	36 14	Ns-1			
116	-	-45	N-Ns			
117	STOI	35 46				
118	RTN	24	End of subroutine			
119	*LBL6	21 06	Leaching		Seepage	
120	RCLB	36 12	Step 28	Step 63	Step 28	Step 63
121	RCLE	36 15	At	At	At	At
122	+	-55	Bt	Bt	Bt	Bt
123	RCLB	36 12	(A+B)t	(A+B)t	(A+B)t	(A+B)t
124	÷	-24	At	At	At	At
			(A+B)/A	(A+B)/A	(A+B)/A	(A+B)/A

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A		B		C		D		E	
								I	

For the register contents during execution of the main programme subroutines reference is made to the location in the main programme where the subroutines are called

STEP	KEY ENTRY	KEY CODE	COMMENTS	
032	RCLi	36 45	$c_k(t-1)$	$c_{n-k}(t-1)$
033	+	-55	$a = c_k(t-1) - a$	$a = c_{n-k}(t-1) - a$
034	RCLD	36 14	n	n
035	F 1?	16 23 01	no	yes
036	GSB2	23 04	Skip this step	GoSub 2(retransform) layernumber
037	RCLi	36 46	k	
038	-	-45	n-k	
039	RCLB	36 12	At	
040	$X \leftarrow Y$	-41	n-k	
041	Y^x	31	$(At)^{n-k}$	
042	X	-35	$a = a(At)^{n-k}$	
043	RCLD	36 14	n	
044	RCLi	36 46	k	
045	-	-45	n-k	
046	N!	16 52	$(n-k)!$	
047	\div	-24	$a = a / (n-k)!$	
048	+	-55	$\Sigma a = \Sigma a + a$	
049	ISZI	16 26 46	$k = k+1$	
050	RCLD	36 14	n	
051	RCLi	36 36	k	
052	$X \leq Y?$	16-35	If $k \leq n$ return	
053	GTO1	22 01	to label 1 for calculation of next a	
054	R+	-31	n	
055	STOI	35 46		
056	R+	-31	Σa	
057	RCLB	36 12	At	
058	RCLE	36 15	Bt	
059	+	-55	$(A+B)t$	
060	CHS	-22	$e^{-(A+B)t}$	
061	e^x	33		
062	x	-35	$b = e^{-(A+B)t} \Sigma a$	

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A $\frac{N_\ell - 1}{N-1 \cdot N_\ell - 1}$	B At		C $\frac{c_i}{c_s}$	D n		E Bt		I $k/N-1-k \mid n$	

STEP	KEY ENTRY	KEY CODE	COMMENTS	
063	GSB6	23 06	GoSub 6($d=c_i \left(\frac{A}{A+B}\right)^{n+1}$)	GoSub 6($d=c_s \left(\frac{A}{A+B}\right)^{n+1}$)
064	+	-55	b+d	b+d
065	F1?	16 23 01	no	yes
066	GSB2	23 02	skip this step	GoSub 2 (transform layer number)
067	RCLi	36 45	$c_n(t-1)$	$c_{N-1-n}(t-1)$
068	$X \leftarrow Y$	-41	$c_n(t) = b+d$	$c_{N-1-n}(t) = b+d$
069	STOi	35 45		
070	R↓	-31	$c_n(t-1)$	$c_{N-1-n}(t-1)$
071	F1?	16 23 01	no	yes
072	GSB9	23 09	Skip this step	GoSub 9 (calculation c_o) if $N_s = N$
073	0	00		
074	RCLD	36 14	n	
075	1	01		
076	-	-45		
077	STOD	35 14	n=n-1	
078	0	00		
079	STOI	35 46	k = 0	
080	$X \leq Y?$	16-35	If $n \geq 0$ return to Label 1 for	
081	GT01	22 01	calculation of next $c_n(t)$	
082	F1?	16 23 01	no	yes
083	GSB5	23 05	Skip this step	GoSub 5(calc.N- N_s)
084	*LBL7	21 07		
085	RCLi	36 45	$c_k(t)$	$c_{N-Ns+k}(t)$
086	PRTX	-14		
087	ISZI	16 26 46	k = k+1	$N-Ns+k = N-Ns+k+1$
088	RCLA	36 11	$N_\ell - 1$	$N-1.Ns-1$
089	INT	16 34	$N_\ell - 1$	N-1
090	RCLI	36 46	k	$N-Ns+k$
091	$X \leq Y?$	16-35	If $k \leq N_\ell - 1$ return to	If $N-Ns+k \leq N-1$ return
092	GT07	22 07	Label 7 for printing	to Label 7 for printing
093	CF1	16 22 01	next c_k	next c_{N-Ns-k} Clear flag 1

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A $N_\ell - 1$ $N-1.Ns-1$	B At		C $\frac{c_i}{c_o}$	D n		E Bt		I $n/N-1-n$ $\frac{k}{N-Ns+k}$	

STEP	KEY ENTRY	KEY CODE	COMMENTS			
125	1/X	52	$A/(A+B)$	$A/(A+B)$	$A/(A+B)$	$A/(A+B)$
126	RCLI	36 46	k	n	k	n
127	1	01				
128	+	-55	k+1	n+1	k+1	n+1
129	y^x	31	$(\frac{A}{A+B})^{k+1}$	$(\frac{A}{A+B})^{k+1}$	$(\frac{A}{A+B})^{k+1}$	$(\frac{A}{A+B})^{k+1}$
130	RCLC	36 13	c_i	c_i	c_s	c_s
131	x	-35	$c_i (\frac{A}{A+B})^{k+1}$	$c_i (\frac{A}{A+B})^{k+1}$	$c_s (\frac{A}{A+B})^{k+1}$	$c_s (\frac{A}{A+B})^{k+1}$
132	RTN	24	End of subroutine			
133	*LBL9	21 09	Subroutine for seepage into rootzone			
134	RCLA	36 11	N-1.Ns-1			
135	INT	16 34	N-1			
136	GSBO	23 00	GoSub 0 for calculation of Ns-1			
137	X≠Y?	16-32	If Ns-1 not equal to N-1 (seepage not reaching layers 0) return execution back to main programme			
138	RTN	24				
139	R↓	-31				
140	R↓	-31	$C_{N-1-n}(t-1)$			
141	RCLI	36 46	N-1-n			
142	x=0?	16-43	If the layer calculated is layer 0			
143	GTOa	22 16 11	Go to LBL a for restoring $c_0(t-1)$ in Register 0			
144	1	01				
145	x=y?	16-33	If the layer calculated is layer 1 Go to LBLE for calculating $c_0(t)$			
146	GTOE	22 15				
147	RTN	24	If N-1-n>1 return execution back to main programme			
148	*LBLa	21 16 11				
149	R↓	-31	$C_0(t-1)$			
150	STOi	35 45	Restore $c_0(t-1)$ in Register 0			
151	RTN	24	Return execution back to main programme			
152	*LBLE	21 15				
153	R↓	-31				
154	R↓	-31	$c_1(t-1)$			

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A		B		C		D		E	

For the register contents during execution of the main programme subroutines reference is made to the location in the main programme where the subroutines are called

STEP	KEY ENTRY	KEY CODE	COMMENTS
155	RCL1	36 45	$c_1(t)$
156	+	-55	$c_1(t) + c_1(t-1)$
157	2	02	
158	\div	-24	$\tilde{c}_1(t) = \{c_1(t) + c_1(t-1)\} / 2$
159	RCLE	36 15	Bt
160	X=0?	16-43	If no decomposition (Bt=0) continue calculations at Label 3
161	GT03	22-03	
162	CHS	-22	
163	e^x	33	e^{-Bt}
164	$X \leftrightarrow Y$	-41	$\tilde{c}_1(t)$
165	RCLB	36 12	At
166	RCLE	36 15	Bt
167	\div	-24	A/B
168	x	-35	$\tilde{c}_1(t) A/B$
169	ENT↑	-21	
170	CHS	-22	$-\tilde{c}_1(t) A/B$
171	RCLO	36 00	$c_o(t-1)$
172	+	-55	$c_o(t-1) - \tilde{c}_1(t) A/B$
173	$X \leftrightarrow Y$	-41	$\tilde{c}_1(t) A/B$
174	R↓	-31	
175	x	-35	$e^{-Bt} \{c_o(t-1) - A/B c_1(t)\}$
176	R↑	16-31	$\tilde{c}_1(t) A/B$
177	GT0e	22 16 15	Continue calculations at Label e
178	*LBL3	21 03	
179	R↓	-31	$\tilde{c}_1(t)$
180	RCLB	36 12	At
181	x	-35	At $\tilde{c}_1(t)$
182	RCLO	36 00	$c_o(t-1)$
183	*LBL e	21 16 15	Bt = 0 Bt ≠ 0
184	+	-55	$c_o(t) = c_o(t-1) + At \tilde{c}_1(t)$ $c_o(t) = A/B \tilde{c}_1(t) + e^{-Bt}$
185	ST00	35 00	$\{c_o(t-1) - A/B \tilde{c}_1(t)\}$
186	RTN		Return to main programme

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A		B		C		D		E	I

For the register contents during execution of the main programme subroutines reference is made to the location in the main programme where the subroutines are called

STEP	KEY ENTRY	KEY CODE	COMMENTS
187	* LBLC	21 16 13	Main programme for leaching
188	SF1	16 21 01	Set flag 1
189	GTOC	22 13	Execute main programme under LBLC
190	* LBLD	21 14	Calculate drainage water concentration (pseudo
191	STOD	35 14	2 - dimensional)
192	$X \leftarrow Y$	-41	Nd
193	STOI	35 46	Nu
194	+	-55	Nu + k (k=0)
195	1	01	Nd + Nu
196	-	-55	
197	STOA	35 11	Nd + Nu - 1
198	0	00	
199	STOE	35 15	$\Sigma c_{Nu+k}(t) = 0$
200	* LBL8	21 08	
201	RCLi	36 45	$c_{Nu+k}(t)$
202	RCLE	36 15	Σc
203	+	-55	$\Sigma c = \Sigma c + c_{Nu+k}(t)$
204	STOE	35 15	
205	ISZI	16 26 46	Nu+k = Nu + k+1
206	RCLA	36 11	Nu + Nd-1
207	RCLI	36 46	Nu+k
208	$X \leq Y?$	16-35	If k < Nd return to Label 8 to add one more
209	GTO8	22 08	layer
210	SPC	16-11	
211	RCLE	36 15	Σc
212	RCLD	36 14	Nd
213	\div	-24	$c_d(t) = \Sigma c / Nd$
214	PRTX	-14	
215	RTN	24	End of programme

REGISTERS

0	1	2	3	4	5	6	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A $\frac{N_{\ell}-1}{N-1, Ns-1}$	$\frac{Nd+Nu}{-1}$	B At	C $\frac{c_i}{c_s}$	D n Nd	E Bt ΣC	I $\frac{k}{N-Ns+k}$	Nu+k		