

DYNAMIC SIMULATION OF VERTICAL NON-ADSORBED ANION TRANSPORT

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SUMMARY

A model for the simulation of leaching of non-adsorbed anions is described. The model can also be used to study the degree of salinization by evaporation.

The accent is laid on usefulness under practical conditions. In view of this it has been assumed that transport of ions is only caused by mass flow and hydrodynamic dispersion.

Data about soil and profile, initial water and salt conditions and ground-water level must be known. Given a precipitation and evaporation distribution the model can compute the leaching or accumulation of nitrate or chloride during a long period of *e.g.* 125 days.

The results of a number of computations are compared with theoretical expectations and actual measurements. There is a passably good agreement.

INTRODUCTION

Researchers (*e.g.* Köhnlein⁹, Van der Paauw¹¹) have found a relationship between amount of precipitation in winter and nitrogen response of the crop in the next spring. A negative correlation exists between winter precipitation and inorganic soil nitrogen content. Therefore leaching of nitrate has to be taken into account when nitrogen dressing is recommended. For this recommendation one meets the difficulty that for the same precipitation, differences in amount of leaching are caused by differences in soil characteristics, and in the level of the water table. Kolenbrander¹⁰ correlated the depth of leaching with the average air content of the profile. This empirical approach could not explain all differences satisfactorily. The question arises whether it is possible to find a solution by building a model based on soil-physical processes by which the leaching of nitrate can be simulated.

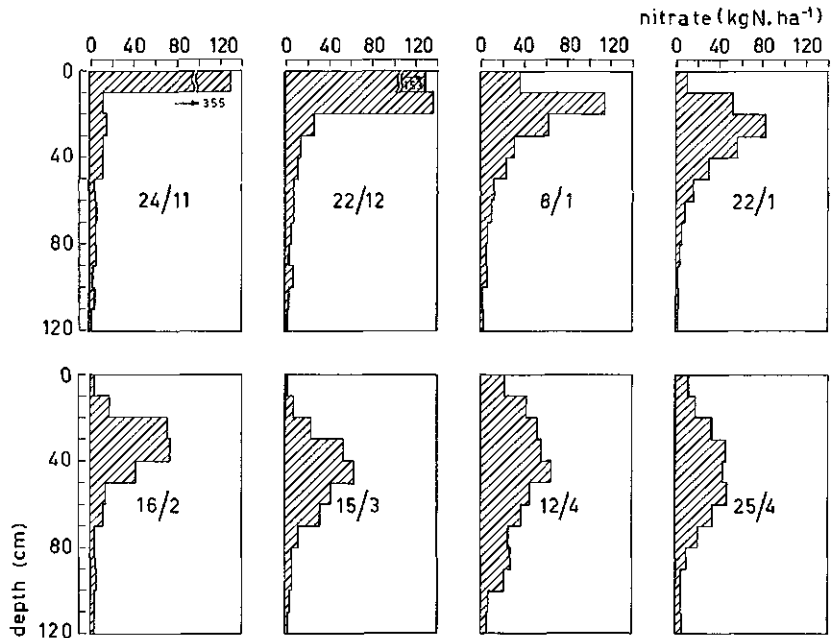


Fig. 1. Nitrate distribution in a soil with a shallow water table after a dressing of 250 kg N.ha⁻¹; 24/11 etc. indicate date of sampling.

The leaching of *e.g.* nitrate shows the characteristic distribution shown in Figure 1: a band of a dressing becomes dispersed. This dispersion is caused by diffusion, and in porous media by s.c. hydrodynamic dispersion or miscible displacement (Gardner³). The hydrodynamic dispersion results from the variations in flow velocities among soil pores, which cause the solute to be dispersed with respect to the average solution flow velocity (Hillel⁶, Kirkham and Powers⁸). It is evident that this dispersion has to be considered in the description of the leaching process.

Neglecting the influence of diffusion, permissible for practical purposes according to Kirkham and Powers⁸ and Frissel *et al.*², the transport of non-adsorbed anions is effected by the mass flow (the average flow velocity) and by the dispersion, which is also influenced by the average water velocity. Consequently, the mass flow is the most important factor in the leaching process.

As the differential equation describing the water velocity as a function of differences in potentials and gravity is not analytically

soluble, a numerical approach has been used comparable with the method described by Van Keulen and Van Beek ⁷. Using the computed water movements the associated changes in anion content can be calculated.

DESCRIPTION OF THE SIMULATION MODEL

The variations in soil-water content θ (in $\text{cm}^3 \cdot \text{cm}^{-3}$) in time t (in day) and depth x (in cm) can be expressed by the following partial differential equation in which Darcy's law and the continuity equation are combined and the separated matrix potential and gravitational potential are converted into water contents:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[D(\theta) \frac{\partial \theta}{\partial x} + K(\theta) \right] \quad [1]$$

in which:

$D(\theta)$ = $K(\theta)/C(\theta)$ is diffusivity in $\text{cm}^2 \cdot \text{day}^{-1}$,

$K(\theta)$ = hydraulic conductivity of the soil in $\text{cm} \cdot \text{day}^{-1}$,

$C(\theta)$ = $d\theta/dP_m$ is differential moisture capacity in $(\text{cm H}_2\text{O})^{-1}$,

P_m = soil matrix potential in $\text{cm H}_2\text{O}$ and

x = position in profile, positive in downward direction, in cm.

As $D(\theta)$ is a function of the soil-water content, Equation [1] is a non-linear differential equation which is not soluble by analytical methods. An approximate numerical solution can be achieved by altering Equation [1] into a finite difference equation by dividing

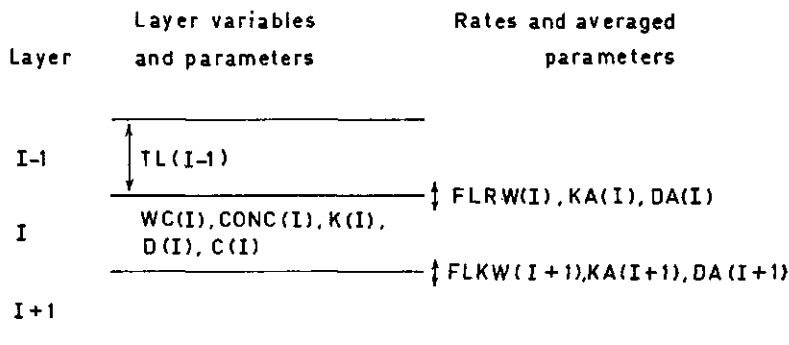


Fig. 2. Schematic description of the one-dimensional soil profile with layer subscript notation.

the non-uniform soil profile into a number of horizontal homogeneous layers, and by changing time discontinuously with finite time increments Δt (Kirkham and Powers⁸). Figure 2 gives a simplified diagram of the profile system. At a certain time the water content of each layer is calculated using the water content at a time step earlier and taking into account the amounts of water flowing into and from the layer during this time interval. After that the computation of the new flow rates for the following time step is performed. The corresponding equations using the terminology of Forrester¹ are:

$$\begin{aligned} WC(I).K = WC(I).J + DELT * (FLRW(I).JK - \\ - FLRW(I + 1).JK)/TL(I) \end{aligned} \quad [2]$$

and:

$$\begin{aligned} FLRW(I).KL = DA.K * (WC(I-1).K - \\ - WC(I).K)/(0.5 * (TL(I-1) + TL(I))) + KA.K \end{aligned} \quad [3]$$

in which WC (in $\text{cm}^3 \cdot \text{cm}^{-3}$), FLRW (in $\text{cm}^3 \cdot \text{cm}^{-2} \cdot \text{day}^{-1}$), and TL (in cm) represent respectively water content, flow rate and thickness layer, and DA and KA respectively average diffusivity and average conductivity of the two adjacent layers I-1 and I. FLRW(I) means the flow rate between layers I-1 and I. The indices J, K and L indicate the successive time points of computation; the indices JK and KL the intervals J till K and K till L, respectively. DELT equals the length of the time interval (in day).

Assuming no effect of diffusion, the transport of anions from a layer into an adjacent one is determined by the sum of the effects of mass flow and of dispersion. The first process FLRS (in $\text{kg} \cdot \text{ha}^{-1} \cdot \text{day}^{-1}$) is calculated by the Equations [4a] or [4b] (in these and following equations the time indices have been dropped):

$$FLRS(I) = 10.^8 * FLRW(I) * CONC(I - 1) \text{ if } FLRW(I) \geq 0 \quad [4a]$$

or:

$$FLRS(I) = 10.^8 * FLRW(I) * CONC(I) \text{ if } FLRW(I) \leq 0 \quad [4b]$$

The term CONC(I) means the concentration of the solute in the water in layer I (in $\text{kg} \cdot \text{cm}^{-3}$).

The partial effect of the dispersion DISPS (in $\text{kg} \cdot \text{ha}^{-1} \cdot \text{day}^{-1}$) to the total transport is described by the following equation with

DISP (in cm) as dispersion coefficient and ABS(FLRW(I)) as absolute value of FLRW(I) (Frissel *et al.*², Reiniger¹³):

$$\text{DISPS(I)} = 10.8 * \text{DISP} * \text{ABS(FLRW(I))} * \\ * (\text{CONC(I-1)} - \text{CONC(I)}) / (0.5 * (\text{TL(I-1)} + \text{TL(I)})) \quad [5]$$

The total transport of the salt TFLRS(I) (in kg.ha⁻¹.day⁻¹) equals the sum of FLRS(I) and DISPS(I).

However, the introduction of layers of finite thickness into the numerical solution causes an additional effect in the computed results which is called mathematical or pseudo-dispersion (Goudriaan⁴, Reiniger¹³). The corresponding dispersion coefficient SDISP equals the average layer thickness in cm divided by 2. The effect of this pseudo-dispersion SDISPS can also be calculated by Equation [5] using SDISP instead of DISP. The simulated transport of anions has to be corrected for this pseudo-dispersion effect and equals finally:

$$\text{TFLRS(I)} = \text{FLRS(I)} + \text{DISPS(I)} - \text{SDISPS(I)} \quad [6]$$

Using this equation and a parallel equation comparable with Equation [2], the ion contents of the layers at every time can be computed.

In these simulations it has been assumed that the soil-water flux streams from the middle of a layer to the middle of the adjacent layer and that the ions are distributed homogeneously in the layers.

The soil profile is bounded downwards by the water table, upwards by the soil surface. The water and salt variations in these boundary layers have to be calculated separately as follows.

Assuming no evaporation, the flow rate from the surface into the top layer is regulated by the amount of water on the surface supplied by precipitation. The hydraulic potential of it equals the sum of hydrostatic pressure on the top of the soil and the gravity potential. Therefore the gradient equals the difference between the hydraulic potential and the (negative) matrix potential in the top layer. In the model it is assumed that a thin layer at the surface of the top layer is always saturated with water. The salt applied as dressing on the surface is dissolved according to the solubility of this salt.

Precipitation raises the ground-water table, evaporation does the reverse. A layer is considered to belong to ground water if its water

content reaches saturation. Therefore, at every time step the program has to determine whether the top layer of the ground water has left the saturation point. In that case the water level falls by a layer thickness. In the other case it is determined next whether the water content of the first soil layer above the water table has reached the saturation content. The minimum water-table changes always equal the layer thickness.

PARAMETERS AND COMPUTING PROCEDURES

The conclusion from the preceding discussion is that starting from a certain initial situation the behaviour of water and ions can be computed in time and space. However, the always changing soil-parameter values must be known; and the parameters K , C and D are a function of the water content of the soil. For use of the model for practical circumstances the parameter values of the most common soil types must be available. The usefulness of the model decreases strongly if these values have to be determined separately in each case.

Rijtema¹⁵ studied the data available in the literature about the relationship between conductivity K and matrix suction for a number of soil types. He gives the following empirical functions:

$$K = a * \Psi^{-n} \quad \text{if } \Psi > \Psi_0 \quad [7a]$$

and:

$$K = K_{\text{sat}} * e^{-\alpha\Psi} \quad \text{if } \Psi \leq \Psi_0 \quad [7b]$$

in which Ψ is the matrix suction, K_{sat} is the conductivity at saturation and a and α are constants. The second equation is used in the low suction range, the point of transition to the first equation is indicated by Ψ_0 with $n = 1.4$. Rijtema classified the soil types into 20 groups for which the values of the constants (Table 1) and the suction-water content curves have been given. The differential moisture capacity C is the slope of these curves. Hysteresis effects have been neglected, and the omission will not be of practical importance in most cases (Rose¹⁴). For KA and DA , the arithmetical averages of the K - and D -values of the two layers in question are taken.

Data about the dispersion coefficient of Equation [5] are scarce;

TABLE 1
Values of K_{sat} , a , α and Ψ_0 of 20 soil type groups

Soil type	K_{sat} , cm. day ⁻¹	α , cm ⁻¹	a , cm ²⁻⁴ .day ⁻¹	Ψ_0 , cm
1. Coarse sand	1120	0.224	0.080	80
2. Medium coarse sand	300	0.138	0.63	90
3. Medium fine sand	110	0.0822	3.30	125
4. Fine sand	50	0.0500	10.9	175
5. Humous loamy medium coarse sand	1.0	0.0269	15.0	165
6. Light loamy medium coarse sand	2.3	0.0562	5.26	100
7. Loamy medium coarse sand	0.36	0.0378	2.10	135
8. Loamy fine sand	26.5	0.0398	16.4	200
9. Sandy loam	16.5	0.0737	0.24	150
10. Loess loam	14.5	0.0490	22.6	130
11. Fine sandy loam	12.0	0.0248	26.5	300
12. Silt loam	6.5	0.0200	47.3	300
13. Loam	5.0	0.0231	14.4	300
14. Sandy clay loam	23.5	0.0353	33.6	200
15. Silty clay loam	1.5	0.0237	36.0	300
16. Clay loam	0.98	0.0248	1.69	300
17. Light clay	3.5	0.0174	55.6	300
18. Silty clay	1.3	0.0480	28.2	50
19. Basin clay	0.22	0.0380	4.86	80
20. Peat	5.3	0.1045	6.82	50

an insight into the relationship between soil properties and the magnitude of this coefficient is lacking. It is impossible to determine these values for every soil type and for every soil profile (Frissel *et al.*²). For this reason the procedure to include this coefficient as such has been abandoned, since an accuracy could be suggested which this coefficient does not have. The solution has been found in another direction. It has already been mentioned that the introduction of layers causes a pseudo-dispersion for which a correction must be performed as given in Equation [6]. By neglecting the physical dispersion and by not correcting for this pseudo-dispersion the influence of the dispersion will be present in the computed results all the same. The influence of the magnitude of the dispersion coefficient is introduced by the size of the layer thickness. For every soil type or profile a thickness must be chosen corresponding with an estimated dispersion coefficient. The program used gives the possibility of choosing between thickness of 2.5, 5 and 10 cms.

In a numerical solution of a differential equation such as Equation [1] one always has to choose between the accuracy of the calculations

and the length of computational time related to the size of time step. It is apparent from Equations [2] and [3] that the integration over time is performed by the s.c. Euler method, in which a constant flow rate is assumed during every time interval. From this an inaccuracy arises which has a tendency to accumulate. However, this inaccuracy is decreased by using small time steps. The allowed maximum size of time step depends strongly on the expected flow rates. Concerning these rates the critical points are the flow rates between the layers with high water content, *e.g.* the layers in the neighbourhood of the ground-water level, with high *K*- and *D*-values (Equation [1] and Table 1). These rates are so high that the total computing times for the three most sandy soil types become too long owing to the necessary small time steps. Computations for profiles of *e.g.* the medium-fine sand type require steps of 0.0008 day or less; this means a total computing time of 30 minutes to simulate leaching during 6 days. For the less permeable soils time steps of 0.004 day or more are sufficient. As only fixed time steps are used protections against too much water transport into and from layers are incorporated in the program. The protections are permitted to work only rarely as the simulation results are influenced essentially by frequent occurrence of these.

Figure 3 gives a schematical flow diagram of the program. This program is written in Fortran IV and is available on application to the authors. The computations have been performed on the Telefunken TR 4.

RESULTS AND DISCUSSION

The correctness and the usefulness of the model are determined by the degree to which the computed results agree with general expectations and experience. A test can also be performed by comparing the results of the computation with results achieved by an analytical solution assuming certain boundary conditions. The best test will be achieved if results from the model agree with empirical data. The purpose of the model discussed is for use in practical situations. It is expected *e.g.* to predict the process of leaching in the field during a winter period of 125 days. Data usable for this kind of test are few in number; rarely do they meet the requirement that all initial conditions are known.

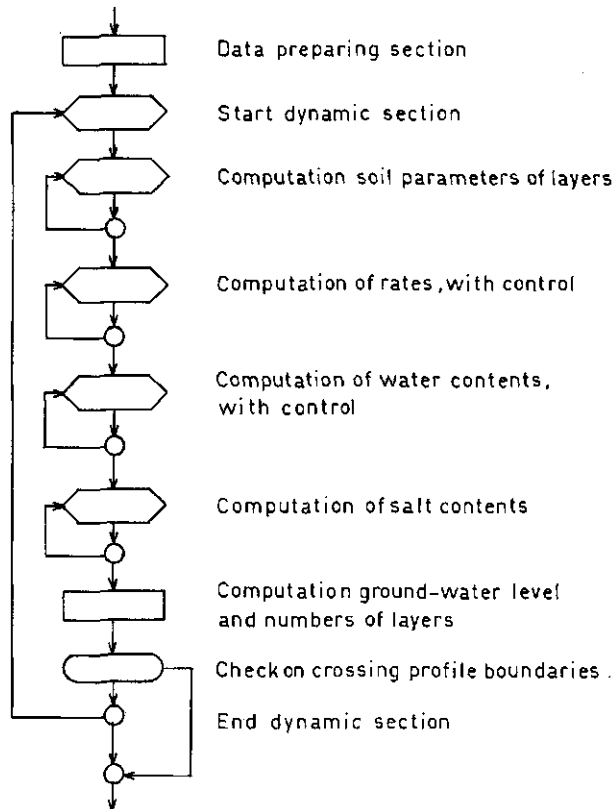


Fig. 3. Simplified flow chart of the simulation program.

One test is that the computed leaching distribution agrees with common experience as shown in Figure 1. The model should also demonstrate that the amount of precipitation and the soil profile influence the depth and distribution of leaching. The larger the precipitation the deeper and more spread out should be the distributions. At the same precipitation the leaching in a sandy soil should be faster than in a loamy soil. The results of the simulations do in fact agree with these expectations. In Figure 4 the leaching of nitrate after 125 days on a sandy and on a loamy soil type are compared. The results conform with the expected distribution, and the difference in depth of leaching between both soil types. In this way a number of simulation experiments have been performed.

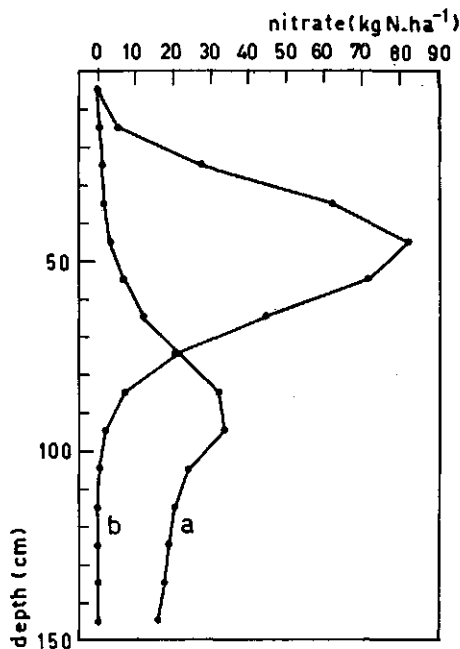


Fig. 4. Differences in simulated leaching distribution between a permeable (a) and a less permeable soil (b).

The next question could be whether the model describes reasonably the water movements. Testing this requirement with field data is also difficult. From soil-physical arguments it can be concluded that water in a soil with ground water but without precipitation and without evaporation will reach an equilibrium state after some time, in which there is a linear relationship between the height above ground-water level and the matrix suction. Figure 5 shows that the model meets this requirement. The initial moisture condition in this profile was too dry compared with the equilibrium state. After some time the linear relationship has been reached. The missing water had come from the ground water, whose level dropped some cms.

A test of predicted nitrate distribution gave a reasonable agreement with actual measurements. On a sandy soil with a very deep and therefore neglectable ground-water level a nitrate dressing of 300 kg.ha^{-1} was given in autumn. Samples of the profile were taken in winter after 125 days leaching. Figure 6 shows the agreement between the empirical and calculated distributions. In this and fol-

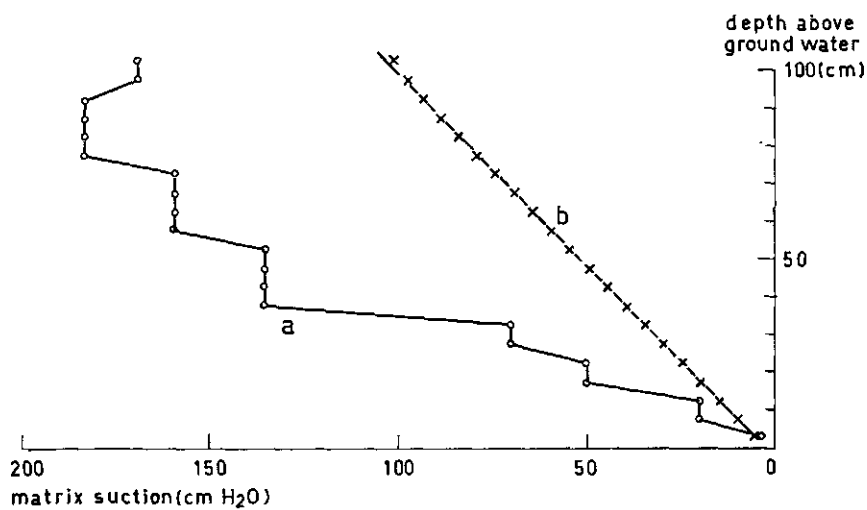


Fig. 5. Simulated shift in matrix suctions from initial (a) into equilibrium (b) state.

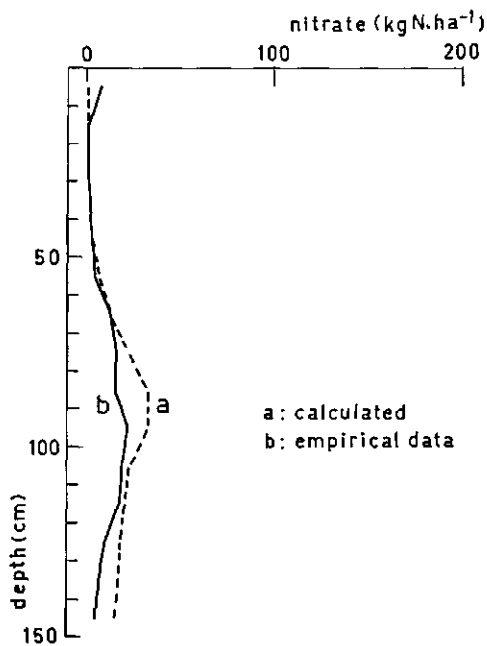


Fig. 6. Comparison between computed (a) and measured (b) leaching in a sandy soil, after 125 days; with a dressing of 300 kg N.ha^{-1} in November.

lowing calculations a layer thickness of 5 cm has been used. However for these soil types thickness of 2.5, 5 and 10 cms did not give essentially different distributions.

A difficulty is met in the computations of leaching in soils with a ground-water level. The precipitation is putting an amount of water into the soil which causes the level to raise after some time. In reality there is a natural or artificial drainage. In order to prevent a raise of the water table above the surface the model has been provided with an exponential pumping regulator which similar to practice tries to maintain the desired level. Figure 7 shows the effect of this pumping. The ground water in the simulation behaves as in a real polder district in which the capacity of the pumping-engine is not sufficient to pump out immediately the winter precipitation.

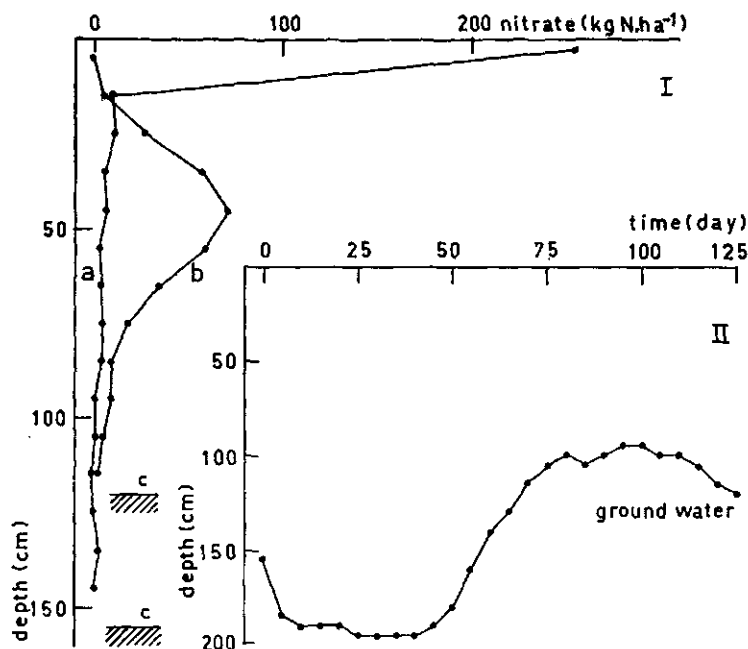


Fig. 7. I, Computed leaching distribution in a loamy soil; initial situation (a) and after 125 days (b) with different water tables (c). II, Movements of the groundwater table during this period.

Till now only downward transport by leaching has been discussed. However, we may assume that the same processes determine up-

ward transport of ions. In this case the simulation model can be used to describe the accumulation of salts in the top layer produced by evaporation. For this case an evaporation function has to be included in the model. A number of calculations has been performed demonstrating the effects of evaporation on salinization in relation to external evaporation rate, ground-water level and soil type.

The testing carried out is still insufficient. However, the results obtained till now are encouraging in spite of the neglect of such factors as diffusion, vapour transport, hysteresis etc. It is doubtful whether these simplifications effect substantially the usefulness of the computed results for field application. The heterogeneities of soil and region limit the necessity of accuracy (Philip¹²).

Simulation models have the big advantage that the influences of certain actions and of differences in conditions on the process can be studied easily. The desired changes have to be introduced into the model only and the results of the computations will demonstrate the effects. Such experiments under field conditions are usually very difficult to make. The structure of the profile gives no restriction since every combination of structural layer can be included. It is not necessary to assume steady-state conditions nor saturated situations (Hadas and Hillel⁵). As long as adsorption of ions is negligible their behaviour can be investigated by this simulation model. For this reason the model can also be used to study the leaching of chloride.

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