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LEACHING OF AND SALINIZATION BY NON-ADSORBED ANIONS, A SIMULATION APPROACH

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Introduction

The leaching of e.g. nitrate in a soil profile shows a characteristic distribution: a band of a dressing becomes dispersed after some time (Gardner, 1965). This dispersion is caused by diffusion and by so called hydrodynamic dispersion. The hydrodynamic dispersion results from the variation in flow velocities among soil pores which cause the solute to be dispersed with respect to the average solution flow velocity (Kirkham and Powers, 1972). In this respect there is no difference between downward and upward water movements.

Neglecting the relatively small influence of diffusion (Frissel et al., 1970; Kirkham and Powers, 1972) the transport of non-adsorbed anions is effectuated 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 this transport.

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 (1971). Using the computed water movements the connected changes in anion content can be calculated. The ultimate construction of the leaching model has been determined largely by the requirement of usefulness in practical situations.

The simulation model

The variations in soil-water content θ (in $cm^3.cm^{-3}$) 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 seperated matrix potential and gravitational potential are converted into water contents:

(I)
$$\frac{\delta \theta}{\delta t} = \frac{\delta}{\delta x}\left(D(\theta)\frac{\delta \theta}{\delta x} + K(\theta)\right)$$

in which

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

$K(\theta)$ is hydraulic conductivity of the soil in $cm.day^{-1}$

$C(\theta) = d\theta/dP_m$ is differential moisture capacity in $(cm\ H_2O)^{-1}$

P_m is soil matrix potential in cm H_2O and

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

As the size $D(\theta)$ is a function of the soil-water content, equation 1 is a non-linear differential equation which is not soluble by analytical methods. A numerical approximative solution can be achieved by altering equation 1 into a finite difference equation by dividing the non-uniform soil profile into a number of horizontal homogeneous layers and by changing time discontinuously with finite time increments. At a certain time the water dontent of each layer is calculated using the water content at a time step earlier and taking into account the amounts of water flowed 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 level and rate equations using the terminology of Forrester (1961) are:

(2) WC(I).K = WC(I).J + DELT * (FLRW(I).JK - FLRW(I+I)/JK)/TL(I)

and

(3) FLRW(I).KL = DA.K*(WC(I-I).K - WC(I).K)/(0.5*(TL(I-I)+TL(I))) + KA.K

in which WC (in $cm^3.cm^{-3}$), FLRW (in $cm^3.cm^{-2}.day^{-1}$) and TL (in cm) represent respectively water content, flow rate water 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 the layer into an adjacent one is determined by the sum of the effects of mass flow and of dispersion. The first process FLRS (in $kg.ha^{-1}.day^{-1}$) is calculated by the equations 4a or 4b (in these and following equations the time indices have been dropped):

(4) FLRS(I) = $10.^{8}$ * FLRW(I)* CONC(I-I) if FLRW(I) $\geq$ 0

or

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

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

The partial effect of the dispersion DISPS (in $kg.ha^{-1}.day^{-1}$) 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) (Reiniger, 1970; Frissel et al., 1970);

(5) DISPS(I) = $10.^{8}$ * DIPS * ABS(FLRW(I)) * (CONC(I-1) - CONC(I))/ (0.5 * (TL(I-1) + TL(I)))

The total transport of the salt TELRS(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 (Reiniger, 1970; Goudriaan, 1972). The corresponding dispersion coefficient SDISP equals the average layer thickness in cm divided by 2. The effedt 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:

(6) TELRS(I) = FLRS(I) + DISPS(I) - SDISPS(I).

Starting at known initial conditions of soil-water contents, anion contents and water table, and using this equation and a level equation comparable with equation 2 the ion contents of the layers (in $kg.ha^{-1}$) at every time can be computed. 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.

Parameters and computing procedures

For use of the model for practical circumstances the parameter values of the most common soil types must be available by calculation. The significance of the model decreases strongly if these values should have to be determined separately in each case.

Rijtema (1969) studied the data available in literature about the relationship between conductivity K and matrix suction. From this study he derived empirical equations for K as a function of the matrix suction. Rijtema classified the soil types into 20 groups for which the values of the constants of the equations and the suction curves (pF-curves) have been given. With the aid of these curves and of the equations the conductivity values at every water content can be calculated. In these calculations the hysteresis effects have been neglected, which omission will not have a practical meaning in most cases (Rose, 1971). As KA and DA the arithmetical averages of resp. the K- and D-values of the two layers in question are taken (Van Keulen and Van Beek, 1971).

The dispersion coefficient as such has not been used in the model. It has already been mentioned that the introduction of layers causes a pseudodispersion for which a correction must be performed as given in equation 6. By neglecting the physical dispersion and by not correcting for this pseuso-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 written in Fortran IV is intended to simulate transport processes during long periods. In this respect the maximum allowable (fixed) time-step size is important and depends strongly on the expected top rates. In the neighbourhood of the water table the rates are so high that the total computing time for the 3 most sandy soil types becomes too long owing to the necessary small time steps. Computations (with a Telefunken TR 4) for profiles of e.g. the medium-fine sand type ask steps of 0.0008 day of less; this means a total computing time of 30 minutes to simulate the leaching during 6 days. For less permeable soils steps of 0.004 day or more are sufficient.

Results and discussion

The usefulness of a model is determined strongly by the degree in which the computational results do agree with general experience and with theoretical and empirical data. In this case we meet the difficulty that data for such testing of leaching and salinization results during a long period are scarce. Some tests of leaching will be discussed.

In figure I the leaching of a nitrate dressing (300 $kg.ha^{-1}$) after 125 days on a sandy and on a loamy soil type are compared. The results demonstrate the expected distribution and the difference in depth of leaching between a permeable and a less permeable soil. In this way a number of simulation experiments have been performed of which the results confirmed the general expectations.

Another 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 a water table but without precipitation and without evaporation will reach the equilibrium state after some time. In this state there is a linear relationship between the height above ground-water level and the matrix suction at this point. The water in the soil has to move into this equilibrium from any chosen moisture state. The model meets this requirement. If the initial moisture state in a profile is e.g. too dry compared with the equilibrium state, the water contents in the model are increased to those belonging to the equilibrium and after some time the linear relationship is reached. The missing water comes from the ground water of which the level will drop.

Tests with empirical data gave a reasonably good agreement. On a sandy soil with a very deep and therefore neglectable water table a nitrate dressing of 300 $kg.ha^{-1}$ was given in autumn. Samples of the profile were taken in winter in which nitrate was determined. The leaching over 125 days has been computed. Figure 2 shows the agreement between the empirical and calculated distributions.

Precipitation is putting an amount of water into the soil which causes the water table 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 3 shows the effect of this pumping. The water table in the simulation behaves as in a real polder district in which the capacity of the pumping-engine is not sufficient to pump out directly the winter precipitation.

Up till now only the downward transport by leaching has been discussed. However, we have already discussed that the same processes

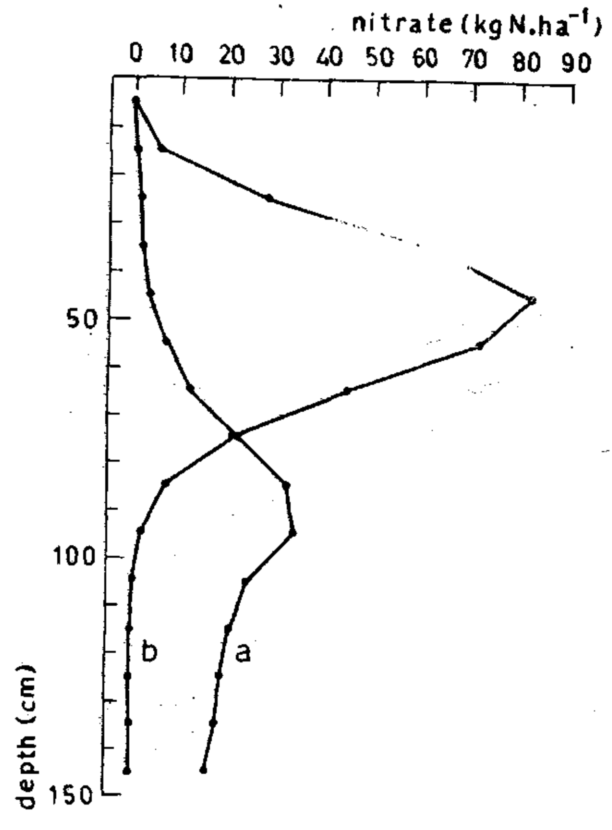

Fig. 1. Computed nitrate distributions in a permeable sandy (a) and in a less permeable (b) soil by leaching during 125 days (without water table)

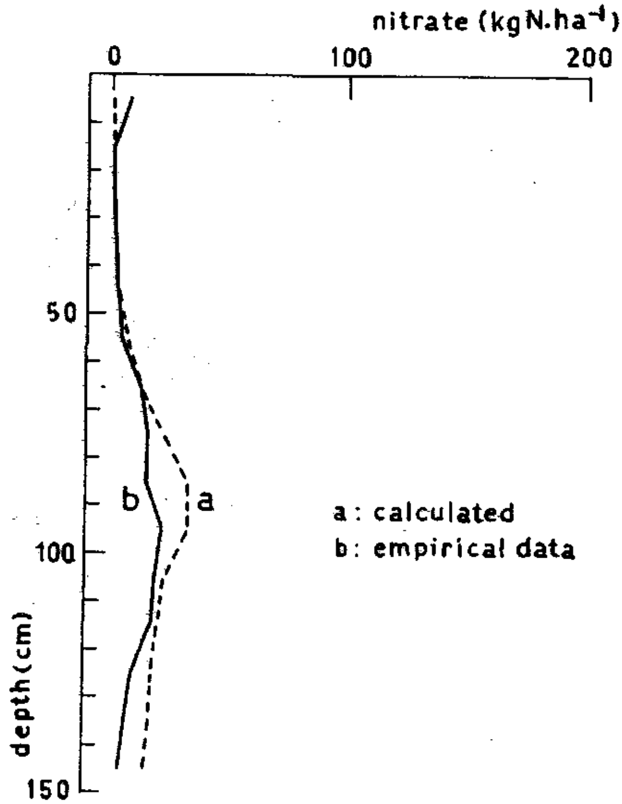

Fig. 2. Computed (a) and empirical (b) nitrate distributions by leaching during 125 days (without water table)

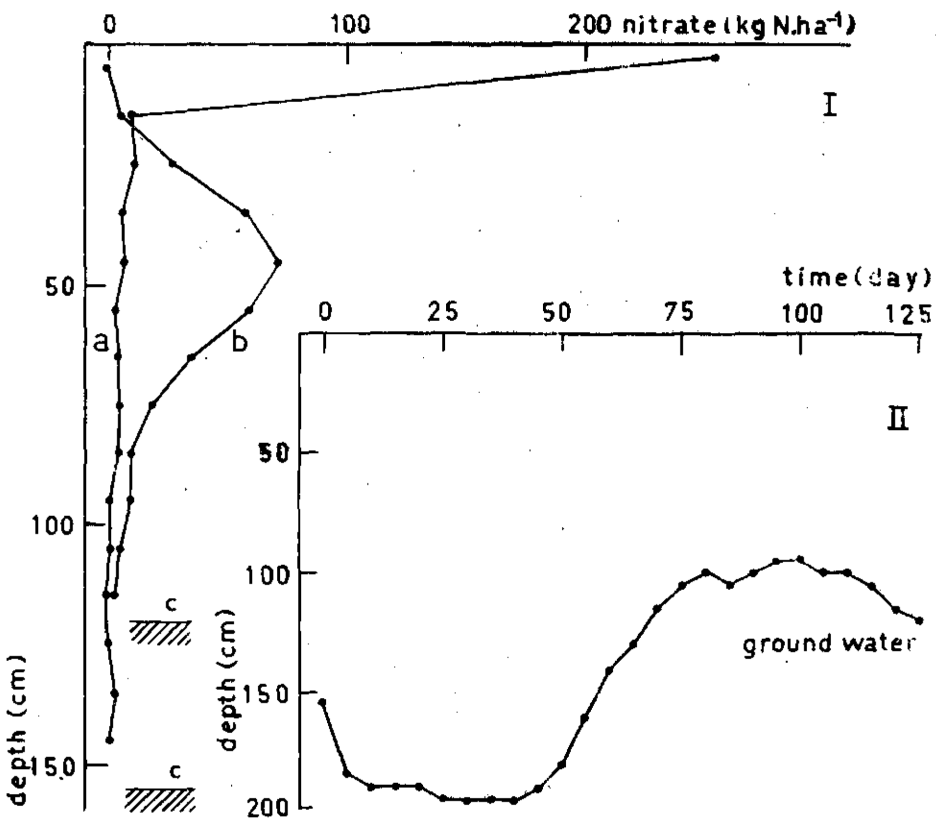

Fig.3. I, computed nitrate distributions at the beginning (a) and after 125 days (b) in a loamy soil with water tables (c).
II, computed water-table movements during this period (with pumping-out).

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

The testing carried out is still insufficient. However, the results obtained up till now are encouraging in spite of neglection of some factors as there are diffusion, damp transport, hysteresis, etc. It is doubtful whether these simplifications affect substantially the usefulness of the computed results for fiels application. The heterogeneities of soil and region limit the necessity of high accuracy (Philip, 1972). The acceptability of the model is enlarged by the fact that it is based on generally accepted soil-physical laws. The simulation approach has the advantage that one is not limited by unreal boundary steady-state and saturated conditions.

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Summary

Leaching and salinization are simulated by one model, regarding both phenomena as results of opposite directions of the same transport processes (mass flow and dispersion). The solution of the differential equations describing this transport can not be achieved analytically; a numerical approach has been used.

Knowing initial conditions of soil-water contents, anion contents and water table and using empirical relationships between water content and conductivity, accumulation and leaching of non-adsorbed anions during a long period (e.g. 125 days) can be simulated for every soil type and profile and for every precipitation and evaporation distribution.

Résumé

Le lessivage et l'accumulation d'anions non-adsorbés tels que le nitrate et le chlore furent simulés dans un modèle où les deux phénomènes furent considérés comme le résultat des mêmes transports mais en sens opposés (transport d'eau et dispersion). Les équations différentielles qui décrivent ces transports ne peuvent être résolues analytiquement. A cet effect une méthode numérique fut utilisée.

Sous condition que les teneurs initiales en l'eau et en sels soient connues ainsi que le niveau initial de la nappe phréatique et en utilisant les relations empiriques entre le degré d'humidité du sol et la conductivité de l'eau non-saturee, il devient possible de simuler le lessivage ou l'accumulation pour une période assez longue (par ex. 125 jours) pour des sols, profils, répartitions pluviométriques et évaporations quelconques.

Zusammenfassung

Auswaschung von und Versalzung mit nicht-adsorbierten Anionen wie Nitrat und Chlor sind in einem Model simuliert worden, wobei beide Erscheinungen als Resultanten derselben aber in entgegengesetzter Richtung fliessenden Transportprozesse (Wasserbewegung und Dispersion) betrachtet worden sind. Die Lösung der diesen Transport beschreibenden Differentialgleichungen sind analytisch nicht erreichbar, dazu ist ein numerischesVerfahren angewendet worden.

Mit der Voraussetzung dass die Anfangsgehalte von Wasser und Salze und der Anfangsgrundwasserspiegel gegeben worden sind, und mit Benutzung von empirischen Zusammenhängen zwischen Bodenwassergehalt und ungesättigter Wasserleitfähigkeit können die Auswaschung und die

Anreicherung während einer langen Periode (z.B.125 Tage) für beliebige Bodentypen, Profile und Niederschlags- und Verdunstungsverteilungen simuliert worden.

Резюме

На модели изучались вынос солей и засоление как противоположные по направлению явления одних и тех же процессов переноса (массопереноса и дисперсии). Решение дифференциальных уравнений, описывающих этот перенос, нельзя получить аналитическим путем, поэтому был использован численный метод.

Зная начальную влажность почвы, содержание анионов и уровень грунтовых вод, а также используя эмпирические зависимости между влажностью и водопроводимостью, можно изучить на модели накопление и вынос непоглощаемых анионов в течение длительного периода (например, 125 суток) для каждого типа почвы, почвенного профиля, количества атмосферных осадков и степени испарения.