

A Convective Model Conm That Simulates Solute Redistribution Caused by Water Table Fluctuations

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Abstract

A study of the solute redistribution caused by water-table fluctuations in experimental packed columns of fine sand and a sandy clay loam soil using potassium chloride as a non-reactive tracer is modelled. With the water table initially at the soil surface, the redistribution of surface applied chloride down the profile was measured after the water table was lowered, then after it was raised again to the soil surface, and then after it was again lowered. In each case, sufficient time was allowed before measurements of chloride were made for the soil-water profile in the column to approach equilibrium conditions with the water table. A simple convection model (CONM) was developed and used to simulate the chloride redistribution. This was compared with the LEACHM model of Wagenet and Hutson based on the convection-dispersion equation, and the physical basis of each critically discussed. It was found that the experimental results in general agreed better with simulated results using CONM than with those using LEACHM. It was concluded that the chloride movement observed in the experimental columns was dominantly convective. The application of this work to optimise fertiliser requirements when subirrigation-drainage systems are employed is discussed.

Keywords: solute redistribution, convective transport, water table fluctuation

1. Introduction

The redistribution of applied fertilisers and pesticides down the soil profile takes place in the soil water and hence is affected by any irrigation and drainage of the area. Irrigation water applied to the surface can leach out salts from the soil profile to drains, and this is often the intention in order to avoid soil salinisation. However, there can also be leaching of applied agrochemicals that become unavailable to crops and can cause pollution of water resources. Such loss can be minimised by employing subirrigation-drainage systems in which the drainage and irrigation are controlled from the same subsurface drain tubes that can act either as sinks or sources of soil water (Skaggs, 1981; Oster et al., 1994; Oster, 1999).

Solutes are transported in the soil by convection with the moving soil water and by diffusion when there is a concentration gradient. These two processes are combined in the hydrodynamic dispersion equation (Hutson & Wagenet, 1995) which allows the simulation of the redistribution of solutes for given boundary conditions, using known or estimated values of soil hydraulic properties. This is the physical basis of the LEACHM model of Wagenet and Hutson (1986; 1987). However, in this model the soil hydraulic properties are included through the use of approximations (Rázuri et al., 2005). Furthermore, no account is taken of hysteresis in these properties that is important when there are cycles of draining and wetting such as those that occur with subirrigation-drainage systems. Results of simulation using LEACHM may therefore be unreliable in such situations and a simpler model of the solute behaviour might provide just as good or even better results. Such a model is possible if the diffusion component of the transport were neglected and the movement of solutes were assumed to be entirely convective, as in the model used by Burns (1974; 1976). In this paper the model CONM was developed in which the diffusion component was neglected. Its fit with results of laboratory experiments, using columns of soil materials and potassium chloride as a conservative tracer described elsewhere (Landeros, 1995), was compared with the fit given by LEACHM when there were consecutive cycles of falling and rising water table as experienced in subirrigation-drainage systems. The use of the simulation studies to provide guidance in the efficient use of agrochemicals in such systems is discussed.

2. Soil-water Regimes with Subirrigation-Drainage Systems

Subirrigation-drainage systems provide a means of controlling soil-water regimes that are both simple and efficient with subirrigation and drainage being effected from the same subsurface channels through the control of the head of water in them. During periods of subirrigation, the water table is maintained high, while during periods of drainage it is kept low. The cycles of wetting and draining produce periods when the soil above the water table is sometimes in a state of wetting and at others in a state of drainage. Hysteresis is thus exhibited in the soil-water relationships and the soil-water behaviour is hysteretic. The soil-water profiles show in particular a smaller capillary fringe when the soil is wetting during subirrigation cycles and larger one during drainage cycles (Skaggs et al., 2009).

The redistribution of solutes within the soil profile depends on the soil-water behaviour. Surface applied agrochemicals diffuse slowly into the soil during periods of unchanging water-table level when the soil-water movement is slow. When, however, the water table moves down, there is downward flow of soil water and the chemicals move downwards in the moving soil water. If, then, the water table moves upwards as a result of subirrigation, the chemical convective flow is also in an upward direction. Thus, salts are not leached out of the soil and there is a conservation of salts within the soil profile. The efficiency of this is dependent on the magnitude of the convection relative to the diffusion (Belder et al., 2005).

3. Laboratory Simulations

The redistribution of solutes in the soil profile during the fluctuating water-table regime experienced with subirrigation-drainage systems was simulated in the laboratory in packed columns of a fine sand and of a sandy clay loam. The physical properties of these soil materials are given elsewhere (Landeros, 1995). The soil materials were contained in prospect cylinders of length 0.6 m and of internal diameter 94 mm, made up of six sections, over a 30 mm gravel filter containing a perforated pipe that could either feed water to the column or drain water from it via a flexible pipe to a given constant head. Soil sampling for water content and solute content of the column when the soil was unsaturated was done by detaching each section using a cheese cutting wire and separating the section with a thin metal plate and then extruding the soil using a jack on the base of each section of the column. In the saturated soil, soil samples were taken using a spatula as well as extracting soil solution at the end of a simulation with a hypodermic needle entering the side of the column through small holes that were sealed during the simulation runs.

4. Modelling Solute Transport with Fluctuating Water Tables

Two models were used in this study to predict the experimental data of chloride redistribution caused by water table fluctuations in the fine sand and sandy clay loam columns used in the laboratory column experiments described in the previous section. The first model was a convection model (referred to here as CONM) developed on the basis of a principle similar to that used by Burns (1974; 1976) in his model that predicted the redistribution of soluble unadsorbed anions under field conditions. The second one was the LEACHM model (version LEACHP) described elsewhere (Wagenet & Hutson, 1986; 1987). The chloride redistribution profiles predicted with CONM and LEACHM are presented in the section of results and compared with those observed at the end of stages 1, 2 and 3 for the fine sand and the sandy clay loam columns.

5. The Convection Model CONM

The convection model CONM considers the convective transport of soluble unadsorbed anions such as chloride caused by one-dimensional vertical water table fluctuations. The soil is assumed to be homogeneous and solute uptake by plants or any other possible sink is not taken into account but could easily be included. The diffusive transport due to solute concentration gradients is assumed negligible in comparison with the mass movement with the soil water flow. Thus, solute is assumed to remain in the same parcel of water throughout. Preferential flow through macropores is assumed not to exist.

The model CONM divides the soil column into n layers of equal thickness. It considers that the soil-water profile is allowed to come into equilibrium with the water table after a given change, at which time the solute concentration profile is calculated by estimating the mass of solute that has travelled in a given parcel of soil water. This entails tracing the parcel of water from one layer to the next, the mixing of the solute with the solution already in the latter, and then the similar transference of solute to and from subsequent layers.

The model thus requires the equilibrium soil-water profile above the water table to be known at the beginning and end of the water table change, i.e., the soil moisture characteristic curves for the soil materials used. Also the initial solute concentration distribution is required. In modelling the experimental data, the solute was assumed to be concentrated all in the surface layer at the start of stage 1 and to be that calculated from the previous stage

for stages 2 and 3.

With a uniform soil column divided into a number n of discrete layers of equal thickness in each of which an equilibrium condition develops before the soil solution moves from layer i into layer $i+1$, the fraction of the solute that is transported from layer i into layer $i+1$ may be equated to the fraction of water moving from layer i into layer $i+1$, assuming that no chemical interaction takes place between the solute and the liquid and porous medium. A separate description of CONM is presented below for each of the three stages of the water table fluctuations.

5.1 Stage 1

Figure 1 shows the principle of the calculation procedure by which CONM predicted the redistribution of chloride that occurred at the end of stage 1 (i.e., when the water table was dropped from the surface down to a given depth) in the fine sand and sandy clay loam columns. θ_i is the fractional volumetric water content of layer i at the end of stage 1 (i.e. the equilibrium condition) for $i=1, \dots, n$, where n is the number of discrete layers in the column; θ_s is the fractional saturated moisture content; m_0 is the mass of chloride contained in the tracer solution volume (i.e., 45 mg) used in the experimental work; and m_i is the initial mass of chloride in layer i . In order to describe the application of CONM to stage 1, one can consider layers 1 and 2 (Figure 2).

The mass of chloride in layer 1 is the mass of chloride contained in the tracer solution (m_0) plus the background chloride in layer 1 (i.e., m_1). As the water moved down into layer 2 caused by the water table drop, a fraction of the total amount of water contained in layer 1 moved into layer 2 and simultaneously the bottom layer of the column drained out the same fraction of water. Thus with the assumption that the soil solution of layer 1 is in equilibrium with the fraction of water moving into layer 2, the fraction of chloride transported from layer 1 into layer 2 may be equated with the fraction of water moving into layer 2. Hence the mass of chloride being transported from layer 1 into layer 2 can be calculated by multiplying the mass of chloride in layer 1 (i.e., the mass of Cl⁻ as indicated in figure 2) by the fraction of water leaving layer 1. This fraction of water was expressed as the ratio of the fraction of water leaving layer 1 (i.e., $\theta_s - \theta_1$) to the saturated water content (θ_s), i.e., $(1 - \theta_1/\theta_s)$ since, with the water table at the soil surface, the soil material was initially saturated. For the purpose of this study, $(1 - \theta_1/\theta_s) = (1 - f_1)$ will be referred to as the “relative fraction”, which in a general form may be written as $(1 - f_i)$ for $i=1, 2, \dots, n$. The mass of chloride remaining in layer 1 at the end of stage 1 is therefore calculated by subtracting the mass of chloride transported into layer 2 (i.e., $(m_0 + m_1)(1 - f_1)$) from the mass of chloride initially in layer 1 (i.e., $(m_0 + m_1)$). Consequently, the mass of chloride in layer 2 was increased by $(m_0 + m_1)(1 - f_1)$ but at the same time it was decreased by an amount equal to $m_2(1 - f_2)$ because when the fraction of water leaving layer 1 entered into layer 2, it displaced a fraction of water equal to $(1 - f_2)$. This, in turn, resulted in a displacement of chloride from layer 2 equal to $m_2(1 - f_2)$, which was transported into layer 3. The principle used in the prediction of the transport of chloride between layers 1 and 2 was applied in the same way to layers 2 and 3, and in general to layers i and $i+1$.

5.2 Stage 2

In this case, the water table was raised from a given depth to the soil surface. With the convective transport of chloride now occurring as a result of subirrigation at the end of stage 2, the calculation procedure used by CONM is similar to that described in figure 1. $\theta_1, \theta_2, \dots, \theta_n$ are in the case the fractional volumetric water content of the soil column layers at the end of stage 1 which were given by the soil water characteristic. m_1, m_2, \dots, m_n are now the masses of chloride predicted by CONM at the end of stage 1. The prediction of the transport of chloride occurring between two adjacent layers at the end of stage 2 was similar to that used in stage 1. However, in this case the soil water within the soil column moved from its base towards the top layer as did the chloride. The calculation of the transport of chloride was therefore carried out from layer n upwards towards layer 1. In order to illustrate the procedure, layers n and $n-1$ were chosen. The amount of water entering into layer $n-1$ was assumed to be the amount of water that drained out of it during stage 1. Thus the mass of chloride transported from layer n into layer $n-1$ is equal to the product of the mass of chloride in layer n (m_n) and the relative fraction of layer $n-1$, i.e., $(1 - f_{n-1})$. Hence, the mass of chloride in layer $n-1$ became $(1 - f_{n-1})m_n + m_{n-1}$ and its new water content was considered to be θ_s . The mass of chloride remaining in layer n was then obtained by subtracting the mass of chloride transported into layer $n-1$ from the mass of chloride in layer n , i.e., $m_n - (1 - f_{n-1})m_n$. The procedure used in the prediction of the chloride transport between layers n and $n-1$ was applied in the same way to the other layers.

5.3 Stage 3

In this case, the water table was lowered after stage 2. The transport of chloride occurring at the end of stage 3 as a result of a further cycle of drainage was predicted with CONM in the same way as in stage 1, but with the

initial chloride distribution given by that calculated by CONM at the end of stage 2. $\theta_1, \theta_2, \dots, \theta_n$ are the fractional volumetric water content of the soil column layers at the end of stage 3 known from the soil moisture characteristic.

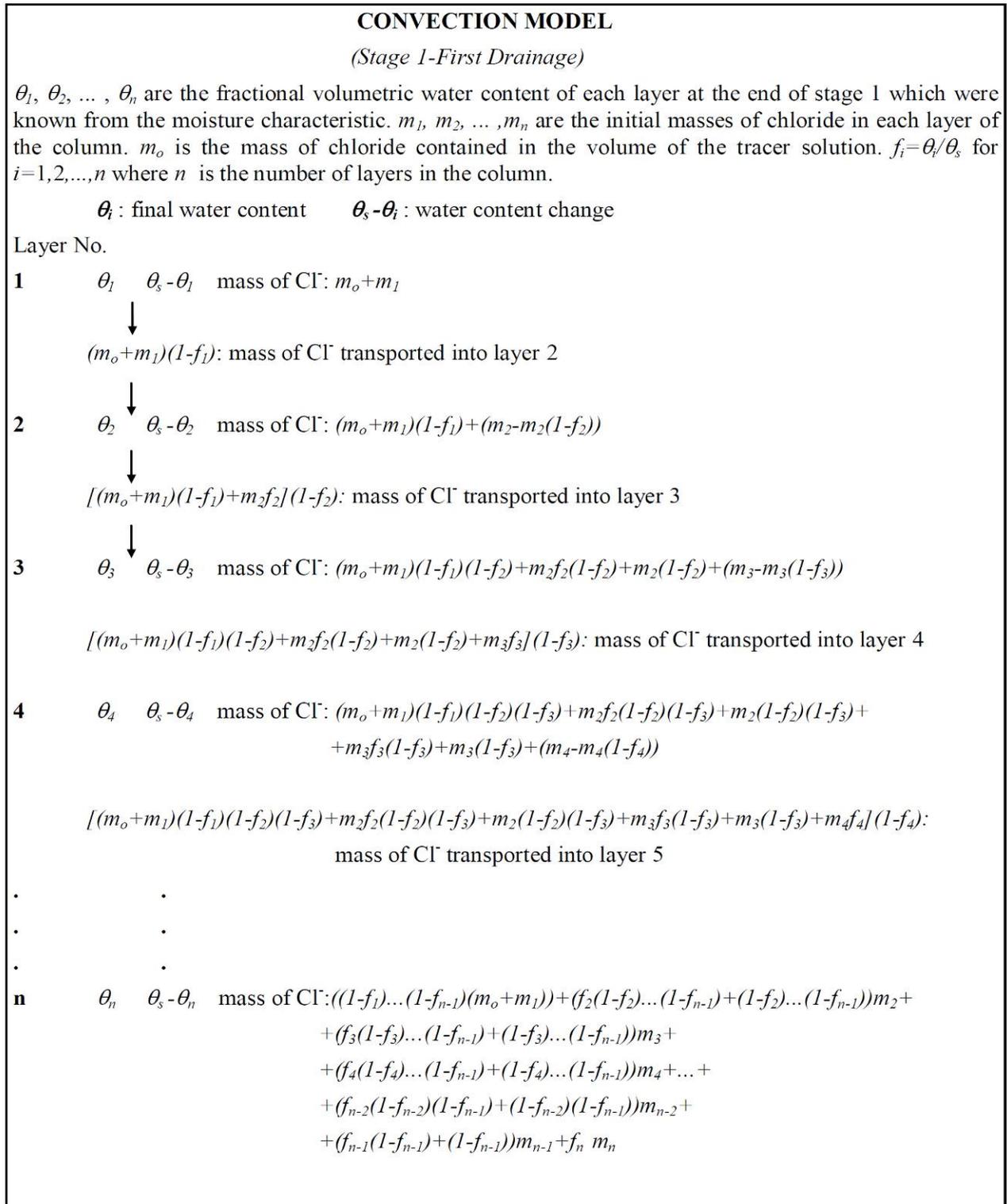


Figure 1. Procedure for computing the chloride redistribution at the end of stage 1 using CONM

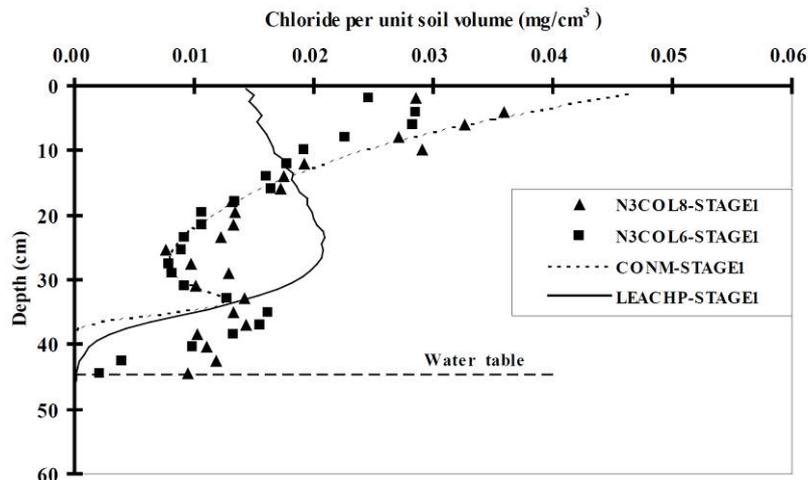


Figure 2. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 1 (columns 8 and 6), and those predicted with CONM and LEACHP (dispersivity = 0.5 cm) for the *fine sand* and draining water level 44.5 cm below the soil surface

6. Comparison of Models with Experiment

6.1 CONM

For the fine sand columns with a draining water level at depth 44.5 cm below the soil surface, CONM predicted reasonably well the mass of chloride per unit volume of soil observed at the end of stage 1 (Figure 2). The model overestimated the mass of chloride redistributed near the top surface, and underestimated the mass near the water table. This situation may be explained from the fact that CONM did not include in its predictions any preferential transport of chloride that could have taken place through large sized pores in the fine sand, for example at the walls of the PVC cylinder. For stage 2, it was found that CONM underestimated the redistribution of chloride occurring near the surface. Near the water table, the predicted chloride redistribution was close to the measured one (Figure 3). In the case of stage 3, the redistribution of chloride predicted with CONM underestimated that measured near the top surface, overestimated it at intermediate depths and underestimated it near the water table (Figure 4).

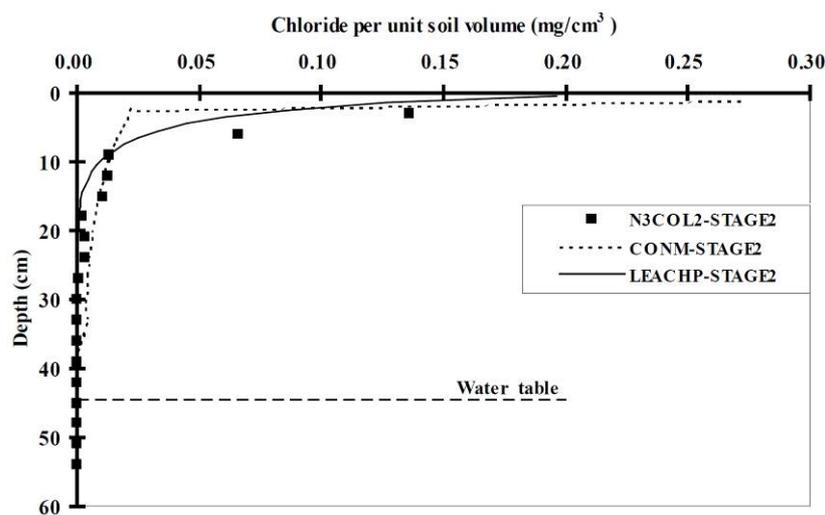


Figure 3. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 2 (column 2), and those predicted with CONM and LEACHP (dispersivity = 0.5 cm) for the *fine sand* after wetting from a water level 44.5 cm below the soil surface

For the sandy clay loam columns with a draining water level at depth 44.5 cm below the soil surface, CONM appeared to predict, in general, reasonably well the redistribution of chloride occurring at the end of stage 1 (see Figure 5). It is seen in figure 6 that CONM underestimated the chloride redistribution measured at intermediate depths, which could have been caused by preferential flow through large sized pores and possibly to anion exclusion. In the case of stage 2, the predicted chloride redistribution appeared to be in good agreement with that measured at the end of this stage (Figure 6). Concerning stage 3, CONM appeared to underestimate the chloride redistribution measured at the end of this stage for intermediate depths (Figure 7).

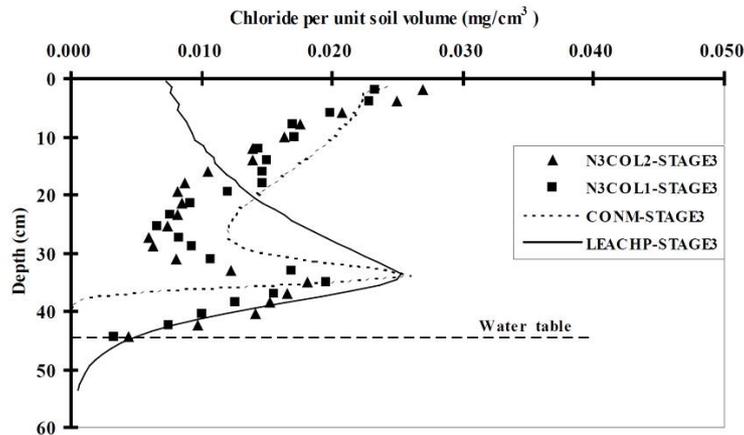


Figure 4. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 3 (column 2 and 1), and those predicted with CONM and LEACHP (dispersivity = 0.5 cm) for the *fine sand* and a draining water level 44.5 cm below the soil surface

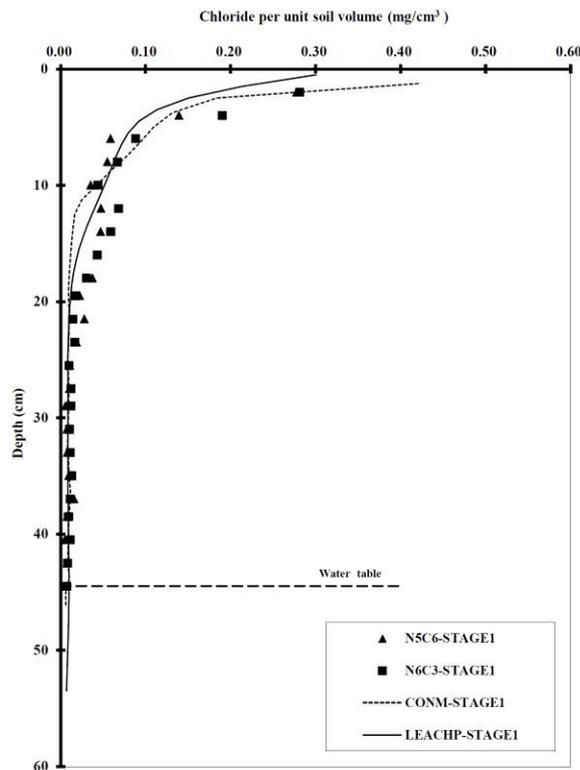


Figure 5. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 1 (columns 6 and 3), and those predicted with CONM and LEACHP (dispersivity=0.5 cm) for the sandy clay loam soil and a draining water level 44.5 cm below the soil surface

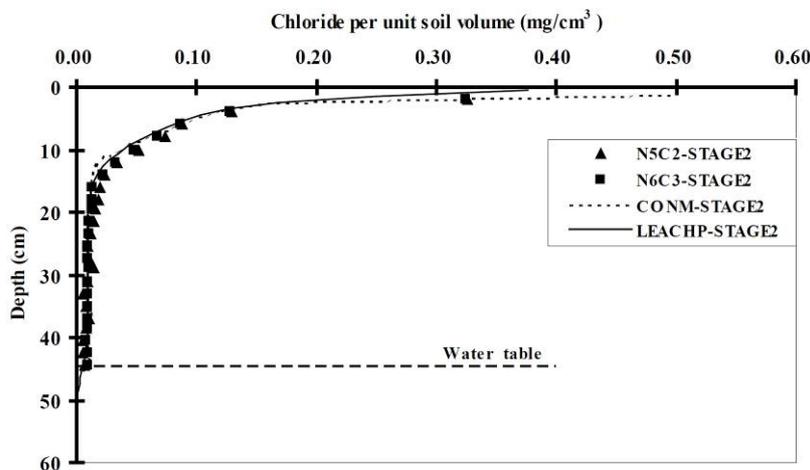


Figure 6. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 2 (column 2 and 3), and those predicted with CONM and LEACHP (dispersivity = 0.5 cm) for the *sandy clay loam* soil after wetting from a water level 44.5 cm below the soil surface

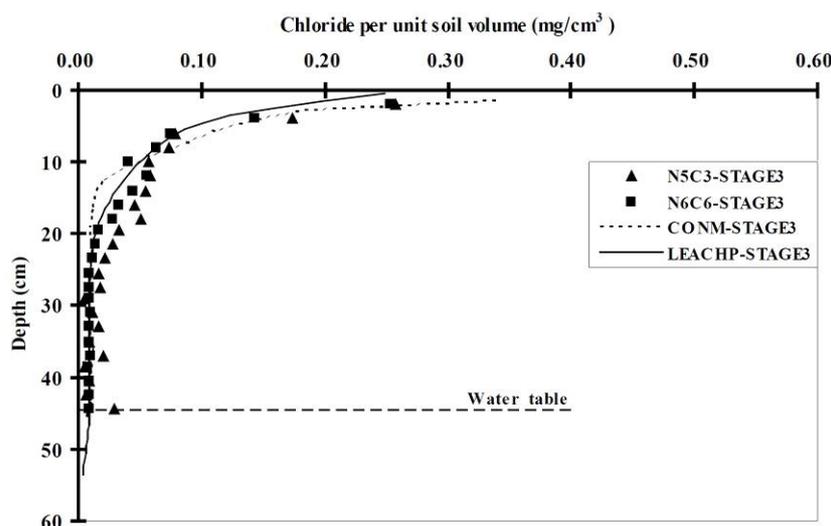


Figure 7. Profiles of mass of chloride per unit soil volume as a function of depth at the end of stage 3 (column 3 and 6), and those predicted with CONM and LEACHP (dispersivity = 0.5 cm) for the *sandy clay loam* soil and a draining water level 44.5 cm below the soil surface

6.2 LEACHP

As to the fine sand columns with a draining water level at depth 44.5 cm, the trend of the chloride redistribution profile predicted with LEACHP for stage 1 appeared to be different from that of the measured ones. The predicted profile followed the trend of the measured ones only near the water table, although LEACHP underestimated the masses of chloride per unit volume measured (Figure 2). Concerning stage 2, LEACHP underestimated the mass of chloride per unit soil volume measured near the top of the soil column. The trend of the predicted profile followed that of the measured one (Figure 3). In the case of stage 3, it appeared that LEACHP underestimated the mass of chloride per unit soil volume measured near the top surface, overestimated it at intermediate depths, and predicted it reasonably well near the water table (Figure 4).

For the sandy clay loam columns with a draining water level at depth 44.5 cm below the soil surface, the chloride redistribution profile predicted with LEACHP appeared to be in good agreement with the one measured at the end of stage 1 (Figure 5). Similarly, the redistribution of chloride predicted with LEACHP was also in

good agreement with those measured at the end of stage 2 (Figure 6). The same situation was observed for stage 3, i.e., the chloride redistribution profile predicted with LEACHP in general was in good agreement with the measured ones (Figure 7).

7. Conclusions

An assumption in using CONM is that diffusive transport is negligible in comparison with that due to convection. This was validated by calculating the diffusion transport in static conditions using the diffusion equation solution (Crank, 1956). The column experiments confirm that the effect of diffusion on the redistribution of chloride occurring at the end of stages 1, 2 and 3 in the fine sand and sandy clay loam columns was not significant, and that convection was the dominant mechanism by which chloride was redistributed as a result of drainage (stages 1 and 3) and sub-irrigation (stage 2). Thus the application of CONM to predict the redistribution of chloride occurring under the experimental conditions considered in this study is justified. However, it has to be mentioned that this is a very simple model that does not take into account other physical factors such as the variation of soil water flow velocities in the pore system of the soil, and the possibility of preferential flow along water-connected large sized pore sequences.

The differences between the mass of chloride per unit soil volume predicted with LEACHP and those measured at the end of stages 1, 2 and 3 for the fine sand and sandy clay loam columns may be due to:

- a) The soil water retention function used in LEACHP not predicting reasonably well the soil moisture characteristic of these soil materials. It does not deal with hysteresis, and the fluctuating water table produces hysteretic conditions;
- b) Preferential water flow which could have taken place through large sized pores not being simulated by LEACHP;
- c) The assumption that the dispersivity $\lambda=0.5$ cm, which was selected as the best value through a sensitivity analysis using values in the range of 0.3 to 15 cm and was used generally with the model;
- d) The variation of soil water flow velocities in different sized pores of these soil materials not fully being taken into account; and
- e) Anion exclusion not being considered.

In this particular study, it was in general observed that the experimental results agreed better with simulated results using CONM than with those using LEACHM.

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