J. of Ag. Eng. - Riv. di Ing. Agr. (2007), 3, 17-22

TRANSPORT OF SOLUTES IN THE FIELD AS AFFECTED BY IRRIGATION

Alessandro Comegna, Antonio Coppola, Gerardo Severino, Angelo Sommella¹

1. Introduction

In the last decade, many problems related to soil and groundwater conservation, tackled by recovering non-conventional resources and through rational, coordinated management of various resources, have led to increased awareness of processes involved in natural systems [6].

Particular attention has been focused on the hazards posed by widespread pollution of groundwater resources, which are especially vulnerable due to the extent of the surface area directly affected by land use [5].

Major progresses have been achieved through parallel studies in setting up experimental techniques for monitoring inorganic, organic and biological substances to be found in soils and aquifers [7], using mathematical tools and having widespread recourse to numerical calculations [17], as well as characterizing natural systems on a statistical basis [11].

From the theoretical point of view, there are insuperable difficulties in giving a detailed and thorough definition, by direct analytical means, of the salient properties of solute transport in the soil layer affected by the above phenomena, especially when there is the filtration of liquids that transport, in solution or in suspension, substances that interact with one another, with the liquid phase and with the soil matrix. These substances, whose toxicity renders them hazardous, penetrate the soil, with some remaining in the root zone and the rest moving towards deeper layers. The tortuosity and considerable irregularity of the very fine flow paths, the presence of channels biopores, dead end pores, cracks whose size and continuity depend on the geometry and management of the porous media within which the flow occurs, slows or increases the diffusion rate of the pollutant; precipitation and release of the transported parts is facilitated, as well as dispersion; exchange and mass reduction processes occur, caused by chemical and biochemical reaction [3].

The most commonly used research techniques currently involve setting up mathematical models for simulating flow, transformation and root adsorption [1]. Along these lines, Nielsen and Biggar [15] were the first to set up a straightforward convective–dispersive CD mathematical model to simulate the flow of Cl^{-} and Br^{-} ion tracers. Davidson et al. [8] also simulated one-dimensional flow, in the soil, of water containing nitrogen compounds similar to those normally found in run-off $(NH_{4}^{+}, NO_{3}^{-2})$ and the connected ion exchange processes; convection and dispersion processes, together with root adsorption and microbiological transformation of nitrogen have also been taken into consideration.

However, according to most recent studies, it is becoming increasingly clear that such models fail to exhaustively describe the phenomena in their totality and are also difficult to apply on a regional level because of the heterogeneity of natural porous media and the large number of chemical, physical and biological parameters to be considered [11].

At present, the parameters used in solute flow simulation models may be measured only by time-consuming laboratory or field experiments.

Miscible displacement techniques, imported from the petroleum industry, have gained widespread acceptance and use in soil science, laboratories since the 1960s. One of the best known introductions of such techniques, in the field of soil science, was made by Nielsen and Biggar [14]. The miscible displacement technique requires an apparatus to maintain steady flow and invariant soil water content conditions when the initial soil solution of concentration C_i is invaded and displaced by a second miscible solution of concentration C_0 . The next step is the collection of the outflowing solution at the column base using a fraction collector for monitoring the ionic concentration of the solute. The plots of the outflowing solution's solute content versus time are called breakthrough curves BTCs.

In field studies, ion concentrations in the medium

Paper received 21.07.2006; accepted 27.06.2007

Eng. ALESSANDRO COMEGNA, phD; Prof. ANGELO SOMMELLA, Full Professor; Eng. GERARDO SEVERINO, Assistant Professor, Department of Agricultural Engineering and Agronomy, University of Naples, ITALY; Prof. ANTONIO COPPOLA, Associate Professor, Department DI-TEC, University of Basilicata, ITALY.

18

are measured by sampling the solution circulating at various points of the soil profile by means of solution samplers. In the case of structured soils, which encompasses preferential flow paths in the matrix, it would appear more appropriate to take soil samples in order to analyse, in the laboratory, the interstitial solution. The taking of soil samples, though destructive, allows more accurate estimates of the spatio-temporal concentrations of the *resident solution* $C_r(z,t)$ [10]. In other field situations, such as in the presence of a drainage network, the concentration of the circulating solution $C_f(x,t)$ may be measured by sampling the run-off at the network main channel [16].

Recently the importance was underlined of monitoring soil solute concentration in arid and semiarid regions where sustainable agricultural productions is, increasingly, dependent on irrigation and fertilizers [12].

Many studies have made it clear that the fate of agricultural chemicals at field soils depends greatly on the imposed boundary conditions [13]. Following this argument we should expect the leaching of a tracer to depend on the method of irrigation. Under flood or high-rate sprinkler irrigation, when water is allowed to pond on the soil surface, transport down preferential pathways should be uninpeded and deep movement of solutes is expected. In contrast, if water is not allowed to pond on the soil surface, as under drip or low-level sprinkler irrigation movement, down preferential pathways should be limited by the application rate and less preferential flow observed. In addition, under ponded conditions, the inherent spatial variation of soil infiltration properties should increase the field scale dispersion of a leaching chemical in comparison to transport under the flux-controlled boundary condition of sprinkler irrigation [9].

Given the advantage of acquiring a suitable number of field observations, which are particularly useful in parallel basic research, field trials were designed to expand the data base for unsaturated zone solute transport on a scale of practical interest for agricultural and farm water management scenarios, as well as to study the growth of solute dispersion below the soil surface under flood and sprinkler irrigation.

In the following analysis of our experiment, we impose a number of simplifying assumptions to permit certain features of the transport process to be diagnosed.

2. Materials and methods

2.1 Interpretative model of chemical transport

To describe the transport of a conservative non-interacting tracer, e.g., chloride, at meso-scale (e.g., in a soil plot of some m^2 area and some meters depth), a one-dimensional numerical model based on the convection-dispersion equation (CDE, Eq.1) [12] may be used. Both parameters, *D* and *v* usually depend on soil properties as well as on initial and boundary conditions and vary with depth and time. For the situation of refilling soil during the summer in temperate climates with relatively saturated flow down to the moving front, due to irrigation regime, we here simply assume depth and time independent parameters D and v. So we get:

$$R\frac{\partial C_r}{\partial t} = D\frac{\partial^2 C_r}{\partial z^2} - v\frac{\partial C_r}{\partial z}$$
(1)

where C_r [ML⁻³] is the resident solute concentration, $v=q/\theta$ [LT⁻¹] is the average water velocities, q [LT⁻¹] is the Darcy velocity, θ [L³/L⁻³] the volumetric water content, D [L²T⁻¹] the coefficient of hydrodynamic dispersion, z [L] the distance in the direction of the flow, t [T] is the time and R the retardation factor equal to [2,18]:

$$R = 1 + \rho \frac{k}{\theta} \tag{2}$$

where ρ [ML⁻³] is the apparent soil bulk density and *k* [L³M⁻¹] is the distribution coefficient of the linear isotherm obtained at equilibrium.

For some simple initial and boundary conditions, analytical solution of Eq.1 are at hand (see for example van Genuchten and Wierenga [21]). For a single δ (Dirac) input at the soil surface the analytical solution for the resident concentration is:

$$C_r(z,t) = \frac{v}{\sqrt{\pi Dt}} \exp\left[-\frac{(z-vt)^2}{4Dt}\right] -\frac{v^2}{2D} \exp\left[\frac{zv}{D}\right] erfc\left\{\frac{z+vt}{\sqrt{4Dt}}\right\}$$
(3)

where *erfc* is the complementary error function.

2.2 Experimental site

The illustrated model has been calibrated taking into account an experiment carried out on a clay soil, pedologically classified as Vertic Usthortens and located near Potenza (Italy).

Two 4 m^2 plots (Fig. 1) were clipped of their native grass vegetation for the experiment. Each plot was splitted in 4 subplots perimetrically embanked and irrigated by means of a eight-nozzles sprinkler with a

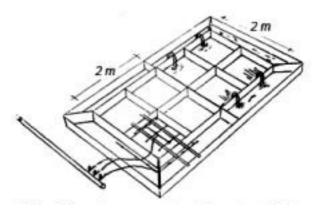


Fig. 1 - Schematic representation of experimental plot.

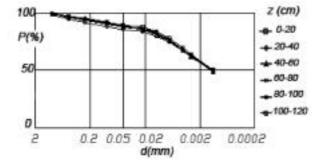


Fig. 2 - Grain-size particle distribution referred to different profiles depths.

discharge (q=4 l/s) able to deliver uniformly (C_u =85%) on the soil surface, during a short time interval, a chloride pulse (*Cl*⁻) as *KCl* salt at an areal density of 2 mole *Cl*⁻/m².

The Cl^{-} pulse was subsequently leached downward by irrigation water scheduled in terms of net water supply (I) in five increments (400 m³/ha) over two months as flood irrigation on the first plot and as sprinkler irrigation on the second one. The net water supply (I=irrigation+precipitation-evaporation) was similar for both plots, which allowed the comparison of Cl^{-} profiles for the two types of irrigation. Evaporation was determined by means of a weighting microlysimeter [4].

Soil samples were collected with an Edelman core sampler at every 0.10 m until a depth of 1.20 m at four different times (5, 20, 35, 60 days) after chemical application. At each sampling time and depths 4 different points are sampled (one for each plot).

Later, the soil samples were analyzed in laboratory in order to determine the main soil physical properties and to estimate water contents. In Fig. 2 we related the grain-size distribution curves obtained for the different soil profile depths.

To extract Cl^{-} from soil, 20 g of air-dry soil were mixed with 40 cm³ of distilled water in a polypropylene centrifuge tube and shaken for 10 h. The clear supernatant solution was analyzed for Cl^{-} using an ion-specific electrode setup (Mod 60502-120 electrode and Model 78 pHmeter, Methrom, Swiss).

Soil bulk density in the plots were used, along with soil moisture content, to calculate Cl^{-} concentration depth profiles $C_r(z,t)$.

2.3 Data analysis

In particular, for agricultural application from the water content and chloride concentration profiles we are interested in quantifying: i) the total resident chloride mass m_i (gm⁻²) (Eq.4), ii) the depth to the centre of mass X_i (cm) and iii) the spread around the centre of mass σ_i (cm²), respectively represented by the moments of the first (Eq.6) and the second order (Eq.7).

$$m_i = \int_{z=0}^{z} \theta(z,t_i) C(z,t_i) dz$$
(4)

$$X_i = \frac{1}{m} \int_{z=0}^{z} z \theta(z, t_i) C(z, t_i) dz$$
 (5)

$$\sigma_i^2 = \frac{1}{m_i} \int_{z=0}^{z} (z - X_i)^2 \theta(z, t_i) C(z, t_i) dz \qquad (6)$$

To test transport behaviour it is also necessary to evaluate the effective velocity of the liquid phase v_0 (cm d⁻¹) (Eq.7) and the transport velocity v_s (cm d⁻¹), (Eq.8):

$$v_{\theta} = \frac{1}{\Delta t} \frac{1}{\theta}$$
(7)

$$\mathbf{v}_s = \frac{X_{ini} - X_i}{\Delta t} \tag{8}$$

in which Δt is time existing between two sampling times $(\Delta t=t_i)$, θ is the mean volumetric water content estimated from the soil surface to the sampling maximum depth Z (cm) in time interval Δt , X_i and X_{i+1} the depths to centre of mass of Cl, respectively at sampling times t_i and t_{i+1} . Supporting a general thesis, it will be possible to obtain $v_s > v_0$ and this because of the mixing and the flow due to water and solute preferential ways.

Finally supposing that the examined soil can be considered homogeneous, as clearly shown in Fig. 2, and the flow of the liquid phase is steady, it was possible to model experimental chloride concentration profiles experimentally obtained by means of a two parameters convection-dispersion model (CDE).

In particular, considering the phenomena of anionic exclusion and adsorption negligible (R=1), we could obtain an estimation of dispersion coefficient Dand velocity v_0 , with a non linear optimisation algorithm which minimizes the sums of the squares of the residuals between measured and calculated values of resident concentrations by means of the analytical solution of the Eq.1, suggested by van Genuchten and Wierenga [18].

3. Results and discussion

The determinations of water content carried out in laboratory through gravimetric method allowed to obtain the moisture profiles $\theta(z)$ of Fig. 3.

As we can deduce from it, higher water content values are present in the plot irrigated by flood above all deeper in the profile; moreover, the irregularities in both water content distributions are probably ascribed to the preferential flows of the liquid phase which chiefly start up under flood irrigation.

In our experiment measurements are conducted at discrete time intervals, and constant averages water content and flux have to be assumed between these intervals. Thus quasi-steady assumption provide a description of flow conditions which is consistent with data collected in the field and consequently the CDE equation can be quite successful in predicting the average behaviour transport in soil.

The results of calculations carried out with the Eqs.

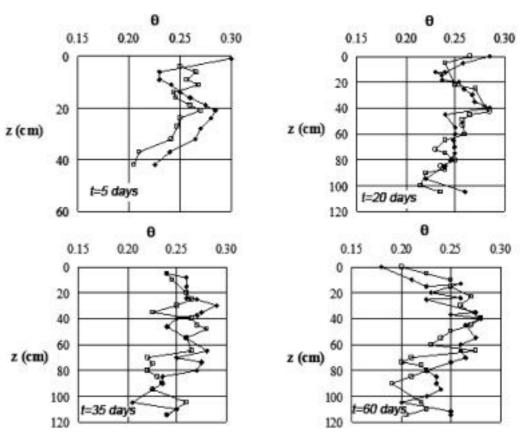


Fig. 3 - Comparison of water content profiles under flood (**■**) and sprinkler (**□**) irrigation at time: 5, 20, 35 and 60 days.

Sampling Time: days	FLOOD IRRIGATION				
	5.0	20.0	35.0	60.0	
X_i (cm)	3.5	36.0	27.1	50.0	
σ_{i}	5.0	20.2	35.0	43.2	
$m_i(\%) \ 0 \le z \le 10$	85.0	12.0	20.0	18.2	
m(%) z > 90	_	6.2	4.5	28.7	
$v_0 ({\rm cm} {\rm d}^{-1})$	_	1.9	-0.24	0.88	
v_{s} (cm d ⁻¹)	_	2.16	-0.59	0.92	
v_s/v_0	_	1.14	2.46	1.94	
$D (\rm cm^2 d^{-1})$	_	12.0	10.0	_	
r^2	_	0.86	0.88	_	

TABLE 1a - Mean transport parameters under flood irrigation.

Sampling Time: days	SPRINKLER IRRIGATION				
	5.0	20.0	35.0	60.0	
X_i (cm)	5.2	36.1	45.0	57.2	
σ_{i}	3.8	17.0	25.0	28.0	
$m_i(\%) \ 0 \le z \le 10$	74.0	8.9	11.0	5.5	
m(%) z > 90	_	2.6	3.5	15.6	
$v_0 ({\rm cm}{\rm d}^{-1})$	_	1.84	0.51	0.59	
$v_s (\mathrm{cm} \mathrm{d}^{-1})$	_	2.06	0.59	0.70	
v_s/v_0	_	1.12	1.15	1.18	
$D ({\rm cm}^2{\rm d}^{-1})$	_	10.0	9.8	_	
r ²	_	0.89	0.92	_	

TABLE 1b - Mean transport parameters under sprinkler irrigation.

20

4-8, have been related in Table 1a, b. In it, we can underline that the depths to the centre of mass are comparable for the two methods while the dispersion around the centre of mass appeared to be basically larger under flood than under sprinkler irrigation.

Owing to evaporation, we have upward solute transport in the first soil stratum (0<z<10cm); in fact, the fraction of chloride mass in this stratum is greater than under sprinkler irrigation; again in the case of flood irrigation, because of preferential flows, it has been observed a more significant chloride presence in profile higher depths (z>90 cm). In both cases, the velocity of the *Cl*⁻ center of mass v_s has been substantially higher of 10-20 % than the effective velocity of the liquid phase v_o , this denoting the presence of preferential flows into the examined soil.

The displacement of the centre of mass is surely controlled by the net water supply I: the centre of mass moves, at first, downward in the 2^{nd} sampling time and then upward within the 2^{nd} and 3^{rd} sampling time; indeed, chloride fraction, in the first 10 cm, increases from 12 to 20%; similarly, in the case of a splinkler irrigated plot, chloride mass increases from 8.9 to 11%. Therefore, evaporation and preferential flows contribute to the solute dispersion in the opposite directions, that means a smoothing of Cl anion concentration profile.

In Table 1, we have reported the conclusive evaluations of transport parameters with the coefficients of determination (r^2) , obtained employing the optimisation method suggested by van Genuchten and Wierenga [18].

In order to give a more meaningful comparison, in Fig. 4 we report the Cl profiles obtained from Eq.3, using the parameters given in Table 1: We can note a

good agreement between the measured and calculated chloride concentration profiles; in addition to this, we can observe how well CDE model predicts the depth to the centre of mass even if the concentration peak value is always underestimated.

4. Conclusions

Soil chloride transport analysis, in this note related, has been carried out on the basis of water content profiles and resident chloride concentrations measured during a wide time interval, with reference to the plots that were irrigated with different methods.

In this way, in the present analysis different factors play an essential role as they imply the effects due to irrigation, evaporation, hydrodynamic dispersion including the diffusive phenomena of anionic exclusion and adsorption.

In practice it is difficult to separate, during field measurements, the effect of a single factor on transport. However, in this study it has been possible to examine the effects, on transport processes, due to two different irrigation methods.

An accurate definition of transport parameters has been given with the use of convection-dispersion model, after having tested the hypothesis about the homogeneous medium and quasi steady-state regime of the liquid phase.

At other field scales, it is known, conditions of perfect homogeneity of the medium rarely happen and the study concerning solute transport is connected to spatial variability of hydraulic and hydro-dispersive properties of soil.

However, in order to get a more precise evaluation

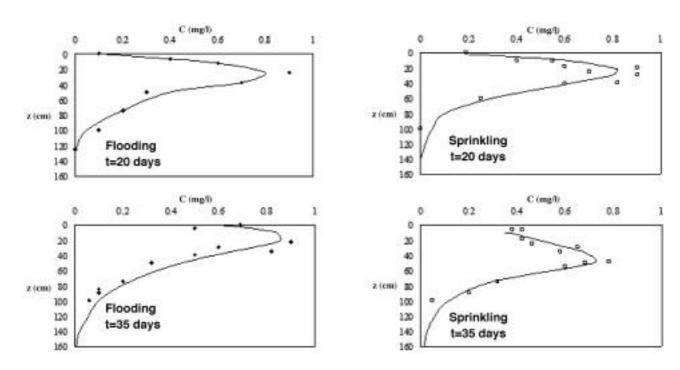


Fig. 4 - Measured (\bullet,\Box) and simulated (-) $C_r(Cl^-)$ profiles under flood and sprinkler irrigation.

22

of transport parameters, it is necessary a considerable progress in the researches about the new measurement technologies.

The achieved results, at the selected scale of our experiment, suggest a possible use of convection-dispersion models in reclamation of lands subjected to degradation phenomena due to intensive agronomic management as well as in the case of ecological incidents.

5. References

- ADDISCOTT T.M., WAGENET R.J., Concept of solute leaching in soils: a review of modeling approaches. J.Soil Sci., (1985) 36, 411-424.
- [2] BAHUER H., Simple derivation of the retardation equation and application to preferential flow and macrodispersion. Ground Water, (1991), 29, 41-46.
- [3] BEVEN K., GERMANN P., *Macropores and water flow in soils*. Water Resour. Res., (1982), 18, 1311-1325.
- [4] BOAST C.W., ROBERTSON T.M., A microlysimeter method for determining evaporation from bore soil: Description and laboratory evaluation. Soil Sci. Am. J., (1982), 6, 680-695.
- [5] CARRAVETTA R., Il degrado della circolazione sotterranea nel meridione d'Italia. Pubbl. Dpt. Ing. Civile, II Universita degli studi di Napoli, (1996).
- [6] CAVAZZA L., Agricoltura e Ambiente. L'aspetto tecnico del problema visto nel suo insieme. Genio Rurale, (1989), 11, 56-69.
- [7] COMEGNA V., COPPOLA A., SOMMELLA A., Nonreactive solute transport in variously structured soil materials as determined by laboratory-based time-domain reflectometry TDR. Geoderma, (1999), 92, 167-184.
- [8] DAVIDSON G.M., RAO P.S.C., SELIM H.M., Simulation of nitrogen movement, transformation and plant uptake in the root zone. Proc. of National Conference "Irrigation Return Flow Quality Management", Colorado St. University, (1977).
- [9] JURY W.A., STOLZY L.H., SHOUSE P., A field test of the transfer function model for predicting solute transport. Water Resour. Res., (1982), 18, 369-375.
- [10] JURY W.A., SPOSITO G., Field calibration and validation of solute transport models for the unsaturated zone. Soil Sci. Soc. Am. J., (1985), 49, 1331-1341.
- [11] JURY W.A., RUSSO D., SPOSITO G., *The spatial variability of water and solute transport properties in unsaturated soil*. Hilgardia, (1987), 55, 1-31.
- [12] JURY W.A., GARDNER W.R., GARDNER W.H., Soil Physics. 5th edn., (1991), Wiley, New York.
- [13] KLUITEMBERG G.J., HORTON R., Effect of solute appli-

cation method on preferential transport of solutes in soil. Geoderma (1990), 46, 283-297.

- [14] NIELSEN D.R., BIGGAR J.W., Miscible displacement: 1. Experimental information. Soil Sci.Soc. Am. Proc., (1961), 25, 1-5.
- [15] NIELSEN D.R., BIGGAR J.W., Miscible displacement in soils: theoretical considerations. Soil Sci. Soc. Am. Proc., (1962), 26, 216-221.
- [16] RICHARD T.L., STEENHUIS T.S., *Tile drain sampling of preferential flow on a field scale*. J. Contam. Hydrol. 3, 307-325. Soil Sci. Soc. Am. J., (1988), 57, 668-673.
- [17] SANTINI A., Modeling water dynamics in the soilplant-atmosphere system for irrigation problems. Excerpta, (1992), 6, 133-166.
- [18] VAN GENUCHTEN M.TH., WIERENGA P.J., Solute dispersion coefficients and retardation factors. In: Klute, A. Ed., Methods of Soil Analysis, Part I, 2nd edn. Agron. Monogr. 9, (1986). ASA and SSSA, Madison, WI.

SUMMARY

This study documents and compares the transport of a conservative solute in near saturated soil profiles under flood and sprinkler irrigation. The experiments were carried out on a clay Vertic-Usthortens soil located near Potenza (Italy). Two 2x2 m² plots were clipped of their native grass vegetation. After spraying on the surface a Cl⁻ pulse as KCl salt; water was applied in five increments over two months as flood irrigation on the first plot and as sprinkler irrigation on the second one. Chloride resident concentration C_r , was sampled by soil coring at four different days after chemical application. $C_r(z,t)$ profiles were analyzed by spatial moment method. The recovered mass of Cl and location of center of mass were comparable for the two types of irrigation. The spread around the center of mass, however, was higher for the flood-irrigated plot. In the flood-irrigated plot, more mass leached below the depth of 90 cm. The velocity of the center of mass was consistently 10-20% larger than the piston displacement velocity. To evaluate the nature of transport, the $C_{x}(z,t)$ distributions were modelled using quasi-steady solution of convection-dispersion equation(CDE). At the scale of our experiments the profiles of Cl⁻ resident concentration are well-simulated.

Key words: Solute transport, convection-dispersion model, irrigation methods.