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Modelling of Solute Transport from Single Soil Aggregate

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Abstract: A numerical solution of solute transport from a single spherical aggregate when subject to different leaching techniques is presented in this paper. Theoretical calculations of leaching with different techniques showed that with *rest* periods (pure salt diffusion periods) equal to *on* periods (water application periods) water savings equal to 50% were possible with Intermittent Leaching (IL) when compared with Continuous Leaching (CL). However, water savings with IL increased with increasing *rest* periods such that during leaching by increasing duration of *rest* periods to twice of the *on* periods water savings up to 66% were calculated. Calculations revealed that saturated IL was more water use efficient than that of drained (empty macropores) IL.

Key words: Numerical, Leaching, Intermittent, Diffusion

Introduction

Saline soils cover about 10% of the total surface area of the dry land (Szabolcs, 1989) and about one third of all irrigated land (Yaron, 1981). These soils are usually reclaimed by leaching of salts from the soil surface. Two modes of water application, viz. continuous and intermittent are usually used during leaching process. Mathematical modelling of solute transport during leaching has been developed for macrospore level. In such models an average pore-water velocity and dispersion coefficient were used (Brenner, 1962 and Biggar and Nielsen, 1967). This convective-dispersive solute transport theory has been satisfactorily used for simulating non-sorbing solute transport under laboratory and field conditions (Nielsen and Biggar, 1962 and Kirda *et al.*, 1973). However, this approach has failed to describe solute transport through aggregated soils (Green *et al.*, 1972 and van Genuchten and Wierenga, 1977) and solute transport under unsaturated conditions (Gupta *et al.*, 1973 and Guadet *et al.*, 1977). A bimodal (dual porosity) pore size distribution exists in the aggregated soils. The flow and mixing of the solute occurs in large pores (macropores) while the small pores (micropores) within soil aggregates act as sinks or sources of the solute. Thus efficiency of any leaching technique depends on how quicker is solute removed from the aggregates. Hence solute transport at an individual aggregate level needs to be modelled.

The aim of this study is to provide simple model of the solute movement within aggregates. This paper describes numerical solutions of the solute movement in a single spherical aggregate, which is used to model continuous and intermittent leaching in soils with saturated and unsaturated conditions. Theoretical experiments of the leaching of a single aggregate by the various methods are conducted and the results are compared with each other in order to assess their suitability as water saving methods.

Numerical Solution of Solute Transport in a Single Spherical Aggregate: As the modelling of leaching of a column of aggregates is complicated due to the complex macropore geometry and increasing concentration in the macropores with depth, solute movement from individual single spherical aggregates is considered in assessing the various leaching techniques.

We consider the three-dimensional diffusion of solute in a spherical aggregate of uniform material of diameter 2*a*. To calculate how the distribution of solute changes with radial distance within the aggregate with time, the diffusion equation must be solved for the concentration *C*. The equation for radial diffusion with constant diffusion coefficient D_e is:

$$\frac{\partial C}{\partial t} = D_e\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right) \quad (1)$$

In dimensionless variables $R = r/a$ and $T = D_e\, t/a^2$ equation 6.1 can be written as:

$$\frac{\partial C}{\partial T} = \frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial C}{\partial R}\right) = \frac{\partial^2 C}{\partial R^2} + \frac{2}{R}\frac{\partial C}{\partial R} \quad (2)$$

To obtain a numerical solution to the diffusion equation under given condition the spherical aggregate is radially divided into *N* shells, each of thickness ΔR so that $N\Delta R = R$ and the concentration change in each layer is calculated after intervals of dimensionless time ΔT as shown in Fig. 1.

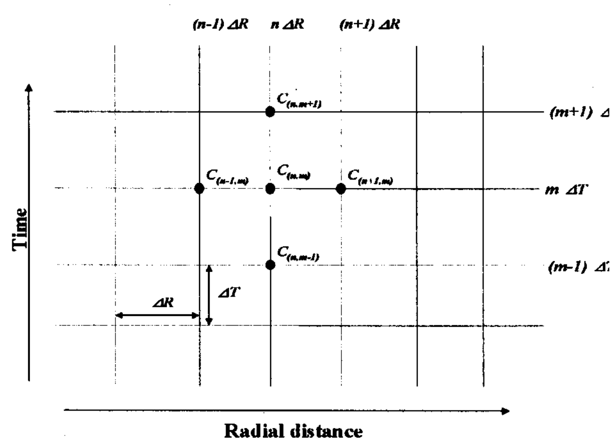

Fig. 1: Finite Difference Mesh for Radial Diffusion

The concentration at nodes $(n-1)\Delta R$, $n\Delta R$ and $(n+1)\Delta R$ after time $m\Delta T$ are $C_{n-1,m}$, $C_{n,m}$ and $C_{n+1,m}$ respectively. The concentrations at time $T = (m+1)\Delta T$, at these points are $C_{n-1,m+1}$, $C_{n,m+1}$ and $C_{n+1,m+1}$ respectively. Thus at time $T = (m+1/2)\Delta T$, we can write the rate of change of solute concentration at radial distance $R = n\Delta R$ as:

$$\left(\frac{\partial C}{\partial T}\right)_{n,m+1/2} = \frac{C_{n,m+1} - C_{n,m}}{\Delta T} \quad (3)$$

At time $T = m\Delta T$

$$\left(\frac{\partial^2 C}{\partial R^2}\right)_{n,m} = \frac{C_{n-1,m} + C_{n+1,m} - 2C_{n,m}}{\Delta R^2} \quad (4)$$

and also

$$\frac{2}{R}\frac{\partial C}{\partial R} = \frac{2}{n\Delta R}\left(\frac{C_{n+1,m} - C_{n-1,m}}{2\Delta R}\right) = \frac{1}{n\Delta R}\left(\frac{C_{n+1,m} - C_{n-1,m}}{\Delta R}\right) \quad (5)$$

By putting these values in equation 2

Or (6)

$$\frac{C_{n,m+1} - C_{n,m}}{\Delta T} = \left(\frac{C_{n+1,m} + C_{n-1,m} - 2C_{n,m}}{\Delta R^2} + \frac{1}{n\Delta R^2}\left(C_{n+1,m} - C_{n-1,m}\right)\right)$$

$$C_{n,m+1} = C_{n,m} + \frac{\Delta T}{\Delta R^2}\left(\left(C_{n+1,m} + C_{n-1,m} - 2C_{n,m}\right) + \frac{1}{n}\left(C_{n+1,m} - C_{n-1,m}\right)\right) \quad (7)$$

Leaching of Individual Aggregates by Different Leaching Methods: Individual aggregate is considered within a bed of aggregates and is theoretically leached with different leaching techniques.

Continuous Leaching: With the continuous leaching water is continuously ponded on the surface of the salt affected soil. Water thus continuously flows through the macropores around the aggregates carrying the solute with it. Hence, the aggregates can be assumed as if they were bathing in an infinite volume of well-stirred solution.

For continuous leaching the initial and boundary conditions for solute movement in a spherical aggregate are thus:

$C = C_o$ $0 < R < 1$ at $T = 0$

$\frac{\partial C}{\partial T} = 0,$ $R = 0$ at $T > 0$

and

$C = 0$ $R = 1$ at $T > 0$

For the finite difference calculations, we have

$C_{n,0} = C_o$ $0 < n < N$ $m = 0$

The water flowing through macropores is considered well-mixed so that the solute concentration at the surface of the aggregate is considered always 0, so that

$C_{N,m} = 0$ at $m > 0$

At the centre of the aggregate where there is no flow, the condition gives (Crank, 1975)

$$C_{0,m} = \frac{6}{\Delta R^2}\left(C_{1,m} - C_{0,m}\right) \quad \text{at } m>0 \quad (8)$$

Intermittent Leaching (Saturated Condition): To overcome the drawback of decreasing leaching efficiency with continuous leaching, the intermittent method of leaching is quite often used. This method of leaching is similar to the continuous leaching method except that the flow is regularly stopped after a predetermined period of time (*on* period) for a predetermined period of time (*rest* periods). Thus in this method water flows around the aggregates during *on* periods while it is stationary during the *rest* periods. The initial and boundary conditions needed in the numerical calculation for this method of leaching during first *on* period are:

$C_{n,0} = C_o$ $0 < n < N$ at $m = 0$

$C_{N,m} = 0$ at $0 < m < m1$

and

$$C_{0,m} = \frac{6}{\Delta R^2}\left(C_{1,m} - C_{0,m}\right) \quad \text{at } 0 < m < m1$$

Similarly initial and boundary conditions for the second *on* period are:

$C_{n,m3} = C_{n,m2}$ $0 < n < N$ at $m = m2$

$C_{N,m} = 0$ at $m2 < m < m3$

and

$$C_{0,m} = \frac{6}{\Delta R^2}\left(C_{1,m} - C_{0,m}\right) \quad \text{at } m2 < m < m3$$

where *m*1, *m*3, *m*5 etc are the time when water is flowing (*on* period). In the same way boundary conditions will change at the start of each *on* period.

The solute movement between the aggregate and the stagnant water during the *rest* periods is assumed to be only due to diffusion. The solute mass diffused from the aggregate increases the concentration of the bathing water. Hence the boundary conditions during first *rest* period are:

$$C_{0,m} = C_{n,m1}$$

and

$$\sum_{0}^{N}\left(C_{0,m1} - C_{n,m2}\right) = \beta C_{N,m} \quad \text{at } m1 < m < m2$$

Where β is the ratio of macropore volume and micropore volume around the aggregate. Boundary conditions for the second *rest* period are:

$$C_{0,m} = C_{n,m3}$$

and

$$\sum_{0}^{N}\left(C_{0,m3} - C_{n,m4}\right) = \beta C_{N,m} \quad \text{at } m3 < m < m4$$

where *m*2, *m*4, *m*6 etc are the time when the water is stagnant (*rest* period). In the same way boundary conditions will change for all *rest* periods.

Intermittent Leaching Under Drained Conditions: The solution for intermittent leaching was calculated for saturated conditions where during *rest* periods the macropores were kept saturated with water. However under field conditions this is rarely the case. During *rest* periods water continues to move downwards resulting in emptying of the macropores. Hence the soil changes from a saturated to an unsaturated condition in which the large macropores are air-filled. Therefore, under drained conditions when the macropores are empty during *rest* periods, the solute can only

redistribute within the aggregate. The boundary conditions for these numerical experiments are similar to those with saturated intermittent leaching except that during the *rest* periods the macropores are unsaturated.
The initial and boundary conditions for drained intermittent leaching during first *on* period are:

$C_{n,0} = C_o$ $\quad 0< n< N \quad$ at $m = 0$
$C_{N,m} = 0$ $\quad$ at $0< m < m1$
and

$$C_{0,m} = \frac{6}{\Delta R^2}\left(C_{1,m} - C_{0,m}\right) \quad \text{at } 0< m < m1$$

Similarly initial and boundary conditions for second *on* period
$C_{n,m3} = C_{n,m2}$ $\quad 0< n< N \quad$ at $m = m2$

$C_{N,m} = 0$ $\quad$ at $m2< m < m3$
and

$$C_{0.m} = \frac{6}{\Delta R^2}\left(C_{1,m} - C_{0,m}\right) \quad \text{at } m2< m < m3$$

In the same way boundary conditions will change at the start of each *on* period.
Since during the *rest* periods, macropores are unsaturated, so that there is only redistribution of salts within the aggregates. Thus the boundary condition during *rest* periods at the aggregate surface is

$$\frac{\partial C}{\partial T} = 0, \quad R = 1 \quad \text{at } m1< m < m2$$

giving
$C_{N,m} - C_{N-1,m} = 0$ $\quad$ at $m1< m < m2$
Similarly for second rest period
$C_{N,m} - C_{N-1,m} = 0$ $\quad$ at $m3< m < m4$
Thus each time during the *rest* periods there is only redistribution of solute within the aggregate.

Results and Discussion

Consider a single spherical aggregate of unit radius (R = 1) which is being leached by continuous leaching. The radius of the aggregate is divided into N+1 nodes with the node spacing equal to 0.05 (ΔR = 0.05) so that N = 20. Assuming unit effective diffusion coefficient and time increment equal to 0.0005 so that $T = D\ \Delta t / \Delta R^2$ = 0.2. The initial concentration (C_o) in the spherical aggregate is 1 while the bathing solution is initially salt free and is continuously flowing through the macropores. Thus the concentration at the interface after time T > 0 is assumed to be zero. The value of β was assumed equal to one because of simplicity in calculations and also because to consider the non-stirred bathing water during the *rest* periods as well-stirred. Using equations 7, 8 and the boundary condition at interface T > 0, the relative solute mass remaining in the aggregate with time was calculated in Excel spread sheets.
The results of the leaching expressed as relative solute mass remaining in the aggregate against dimensionless time compared with the results of continuous and saturated intermittent leaching are shown in Fig. 2.

The curve for the drained intermittent leaching shows the same decrease in the solute mass as for the continuous and saturated intermittent leaching during the first on period. However, during the *rest* periods there was no decrease in the solute mass of the aggregate for the drained intermittent leaching as the macropores were empty. During this period it was assumed that the solutes redistributed only within the aggregate. On the contrary, in the case of continuous and saturated intermittent leaching, solutes continued to diffuse out of the aggregate during the *rest* periods. Thus after time T = 0.2, 2.3% more solute mass was leached with the saturated intermittent leaching than with the drained intermittent leaching. These results show that in intermittent leaching there is an advantage in keeping the soil saturated during the *rest* period.

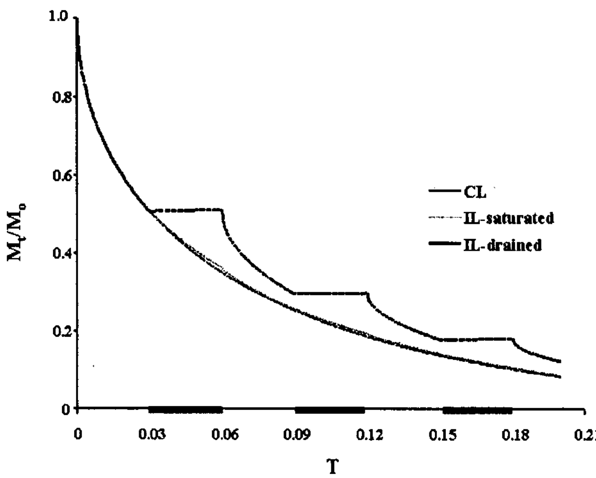

Fig. 2: Relative Solute Mass Remaining in the Aggregate Against Dimensionless Time T When Leached With Drained Intermittent Leaching, Compared With Results of Saturated Intermittent and Continuous Leaching. The on and Rest Periods are Equal To T = 0.03. Thick Lines on The X-Axis Represent Duration of The Rest Periods in Intermittent Leaching

The above results showed that by introducing a *rest* period equal to that of the *on* period in intermittent leaching 50% of water savings were possible. This suggests that for making more water savings during leaching the solute held in the aggregate should be given more time for diffusion by increasing the duration of the *rest* periods. Thus the duration of the *rest* periods was increased to twice that of the *on* periods (T = 0.06) and the results of the leaching were calculated. These are shown in Fig. 3.
Fig. 3 shows that the solute remaining in the aggregate at time T = 0.2 is approximately 9% when leached by continuous and saturated intermittent leaching but 17% when leached by drained intermittent leaching under these condition. Since during the *rest* periods in saturated intermittent leaching, there was no flow of water, saturated intermittent leaching utilised only 33% of the water used by continuous leaching. Drained

intermittent leaching also consumed 33% of the water but the aggregate still had 17% of solute mass remaining in it. This suggests that saturated intermittent leaching is more water use efficient than continuous and drained intermittent leaching.

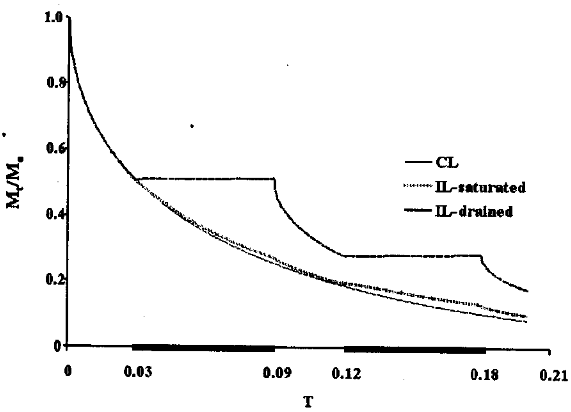

Fig 3: Relative Solute Mass Remaining in the Aggregate Against Dimensionless Time T When Leached with Drained Intermittent Leaching Along with Results of Saturated Intermittent and Continuous Leaching. The Rest Periods are Twice of the on Periods. Thick Lines on X-Axis Represent Duration of Rest Periods in Intermittent Leaching

During these theoretical experiments it was observed that the solute in the layers near to the surface of the aggregate washed out rapidly. However, the aggregate still had a high solute concentration at the centre. This suggests that after leaching although the average solute concentration within the aggregates is very low, even then the aggregates still have higher solute concentrations at their centres, which may affect the growth of early seedlings.

Conclusion

The comparison of various leaching techniques at micropore level with this simple numerical model showed that by providing time (*rest* period) for the solute to diffuse out from the micropores of aggregates into the flowing water in the macropores, more solute was leached using less water. Results showed that after time T = 0.2 approximately the same amount of salts were leached by intermittent leaching where the *on* periods were equal to the *rest* periods as that by continuous leaching. As there is no water flow during the *rest* periods, 50% less water was used with intermittent leaching compared with continuous leaching. Rest periods in intermittent leaching are actually providing time for solute to diffuse out into macropores without the application of any further water. The water requirement for leaching decreased with an increase in *rest* period. Laboratory experiments conducted in columns (Dahiya and Abrol, 1974, and Dahiya *et al.*, 1980) or in micro field plots (Miller *et al.*, 1965 and Dahiya *et al.*, 1981) have shown that leaching of salts was more water use efficient with intermittent leaching as compared with the continuous leaching.

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