

## Numerical Solution of the Salt Diffusion Equation for Non-Stirred Bathing Solutions

<sup>1</sup>A. A. Siyal, <sup>2</sup>P. B. Leeds-Harrison, <sup>2</sup>E. G. Youngs, <sup>3</sup>F.C. Oad and <sup>3</sup>Z.A. Abro  
<sup>1</sup>Z. A. Bhutto Agricultural College Dokri, Larkana, Pakistan  
<sup>2</sup>Cranfield University at Silsoe, MK45 4DT, United Kingdom  
<sup>3</sup>Sindh Agriculture University Tandojam, Pakistan

**Abstract:** A numerical solution of the salt diffusion equation for non-stirred bathing solution is presented. Theoretical calculations of the salt diffusion from a slab into a non-stirred bathing solution showed that there is no effect of non-stirred bathing solution on the rate of diffusion if the ratio of macro and micropore volumes ( $\beta$ ) is less than unity. Since under field conditions the value of  $\beta$  for aggregated soils is much less than one. Therefore it is suggested that the analytical solution of the diffusion equation for well-stirred bathing solution can be used under field conditions where bathing solution is non-stirred.

**Key Words:** Diffusion-Salts-Modelling-Macro and Micropores

### Introduction

Modelling of solute transport in aggregated soils is complicated due to their bi-modal pore size distribution (Biggar and Nielsen, 1967; Youngs and Leeds-Harrison, 1990). To model such systems a bi-continuum (or dual porosity) approach is often used, in which the porous medium is considered to comprise two pore regions: (i) macropore region around aggregates which provides passage for leaching water and (ii) the micropore region within aggregates (Deans, 1963; Coats and Smith, 1964). All the solute in the soil is considered to be held in the soil micropores. The micropores are therefore considered as a source or sink for the solute (Green *et al.*, 1972; De Smedt and Wierenga, 1979). The solute transport between two pore regions is only by diffusion (Passioura, 1971). Thus rate of diffusion of salts from micropores greatly affects the salt leaching efficiency during reclamation of the salt affected soils.

Many models have been suggested for modelling the solute transport under laboratory and field conditions. Most of these models are based on the salt diffusion equation for well-stirred bathing solutions suggested by Crank (1975). However, when aggregates are packed in a column, or in a real soil, the bathing water cannot be considered as being well-stirred. When a salt laden aggregate is placed in a non-stirred solution, the concentration in the bathing water near the aggregate rises quickly, while further away from the aggregate the concentration can still be very low. The rate of diffusion of the solute from the aggregate will therefore be different from that occurring if the bathing solution is well-stirred. Hence it is important to investigate this difference. This paper provides a numerical solution to the diffusion equation for aggregates in a non-stirred bathing solution. Due to the complex geometry of the macropores in packing of spherical aggregates, boundary conditions are not simply defined so that numerical analysis of the diffusion equation is difficult. However, boundary conditions are well defined for salt diffusion in a slab. Thus an analysis of the diffusion process in a slab for the non-stirred situations was used as an indication of the relative behaviour that

might be obtained in the spherical and other aggregate shapes.

**Theory:** Consider one-dimensional diffusion of solute in a slab. We wish to calculate how the distribution of solute changes with time in a slab of thickness  $2a$ . The slab is divided into  $2N$  layers each of thickness  $\Delta x$  so that  $N\Delta x = a$  and consider the changing concentration at intervals of time  $\Delta t$  (Fig. 1)

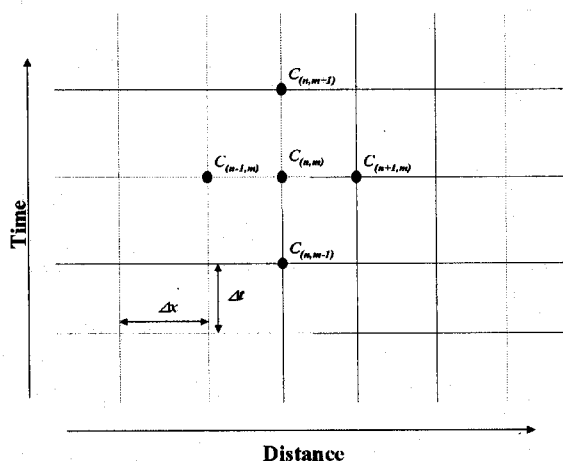


Fig. 1: Notation for the Concentration as a Function of Time in an Element of a Plane Sheet Plotted Against Time.

We consider the concentration  $C_{n,m}$  at node  $n,m$  where  $x = n\Delta x$  and  $t = m\Delta t$

The concentrations at points  $x = (n-1)\Delta x$ ,  $n\Delta x$  and  $(n+1)\Delta x$  at time  $t = m\Delta t$  are:

$C_{n-1,m}$ ,  $C_{n,m}$  and  $C_{n+1,m}$

The concentrations at time  $t = (m+1)\Delta t$ , at these points are:

$C_{n-1,m+1}$ ,  $C_{n,m+1}$  and  $C_{n+1,m+1}$

At time  $t = m\Delta t$ , we write the rate of change of solute concentration as:

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

and at time  $t = (m+1)\Delta t$

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

We also write:

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

If we suppose that:

$$\left(\frac{\partial C}{\partial t}\right)_{n,m+1/2} \cong \left(\frac{\partial C}{\partial t}\right)_{n,m} \quad (4)$$

then equation 3 can be written as:

$$\frac{C_{n,m+1} - C_{n,m}}{\Delta t} = D_e \frac{C_{n-1,m} + C_{n+1,m} - 2C_{n,m}}{\Delta x^2} \quad (5)$$

or

$$C_{n,m+1} = C_{n,m} + \frac{D_e \Delta t}{\Delta x^2} (C_{n-1,m} + C_{n+1,m} - 2C_{n,m}) \quad (6)$$

Suppose  $T = D_e \Delta t / \Delta x^2$ , then equation 6 can be written as:

$$C_{n,m+1} = C_{n,m} + T(C_{n-1,m} + C_{n+1,m} - 2C_{n,m}) \quad (7)$$

When making calculations with equation 7, instability occurs when  $D\Delta t / \Delta x^2 > 1/2$  resulting in negative concentrations at the nodes in the slab. Hence the value of  $D_e \Delta t / \Delta x^2$  is taken as  $1/2$  as an upper limit (Crank, 1975). Then equation 7 can be written as:

$$C_{n,m+1} = \frac{C_{n-1,m} + C_{n+1,m}}{2} \quad (8)$$

Thus we can calculate  $C_{n,m+1}$  at time  $(m+1)\Delta t$  when we know the solute distribution at time  $m\Delta t$ . This can be repeated at all nodes.

**Calculation For Diffusion In a Slab Immersed in a Non-Stirred Bathing Solution:** Suppose the slab is divided from its centre to its outer boundary (interface) by  $N_A$  nodes of width  $\Delta a$  and the bathing water by  $N_B$  nodes of width  $\Delta b$ . Thus  $a = N_A \Delta a$  and  $b = N_B \Delta b$ . The initial concentration in the slab at  $t = 0$  is  $C_0$  and that of the bathing solution is zero as shown in Fig. 2

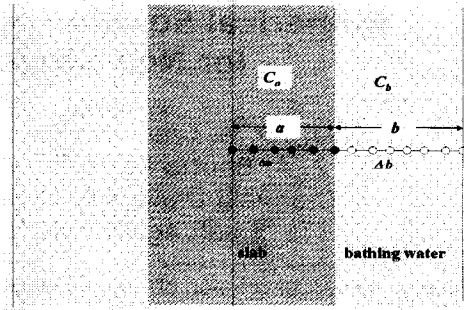


Fig. 2: Slab and Bathing Water Divided into Various Nodes for Determining the Solute Concentration at Each Node

The change in the concentration at any node in the slab after time  $(m+1)\Delta t$  can be written as:

$$C_{n,m+1} = C_{n,m} + \frac{D_A \Delta t}{(\Delta a)^2} (C_{n-1,m} + C_{n+1,m} - 2C_{n,m}) \quad (9)$$

But at the centre of slab  $\partial C / \partial x = 0$  so that  $C_{-1,m} = C_{1,m}$  and equation (9) can be written for node 0 as:

$$C_{0,m+1} = C_{0,m} + \frac{D_A \Delta t}{(\Delta a)^2} (2C_{1,m} - 2C_{0,m}) \quad (10)$$

At the interface (boundary between the slab and bathing water), the flux (per unit area) of salt  $F$  moving out of the slab and entering into the bathing water is given by Crank (1975):

$$\epsilon D_A \frac{\partial C_A}{\partial x} = D_B \frac{\partial C_B}{\partial x} = -F \quad (11)$$

where  $C_A$  is the solute concentration of the slab at  $x = a$ ,  $C_B$  is the solute concentration in the bathing water,  $D_A$  and  $D_B$  are the effective diffusion coefficients of the solute in the slab and bathing water respectively and  $\epsilon$  is the porosity of the slab. Equation 11 expresses the fact that solute enters one medium at the same rate as it leaves the other and takes into account the reduced volume of solute in the porous material.

We can also write for the change in the concentration of the slab at the interface:

$$\frac{\partial C_{N_A,m}}{\partial t} = \frac{2D_A}{\Delta a} \left( \frac{C_{N_A-1,m} - C_{N_A,m}}{\Delta a} - \frac{F}{\epsilon D_A} \right) \quad (12)$$

Similarly the change in concentration of the bathing water at the interface is given by:

$$\frac{\partial C_{N_B,m}}{\partial t} = \frac{2D_B}{\Delta b} \left( \frac{C_{N_B+1,m} - C_{N_B,m}}{\Delta b} + \frac{F}{D_B} \right) \quad (13)$$

Making  $F$  the subject of these equations then equating the results of  $F$  from equations 12 and 13, we have:

$$\frac{\partial C_{N_A,m}}{\partial t} \left( \frac{\epsilon \Delta a + \Delta b}{2} \right) = \frac{D_B}{\Delta b} (C_{N_B+1,m} - C_{N_B,m}) - \frac{\epsilon D_A}{\Delta a} (C_{N_A,m} - C_{N_A-1,m}) \quad (14)$$

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

and at time  $t = (m+1)\Delta t$

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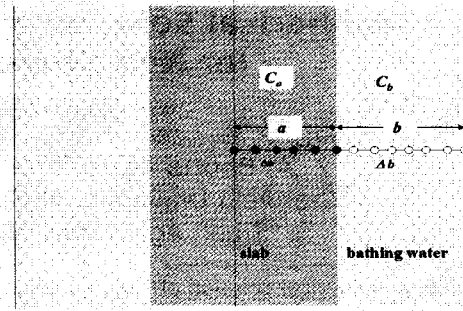


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Re-arranging the above equation

$$\frac{C_{N_i,m} - C_{N_i,m-1}}{\Delta t} = C_{N_i,m} + \frac{2D_B}{\Delta b(\varepsilon\Delta a + \Delta b)}(C_{N_i+1,m} - C_{N_i,m}) - \frac{2\varepsilon D_A}{\Delta a(\varepsilon\Delta a + \Delta b)}(C_{N_i,m} - C_{N_i-1,m}) \quad (15)$$

which is a finite difference form to use for the calculation of change in concentration at the interface.

The initial concentration at the interface at time  $t = 0$  can be calculated as:

$$C_{N_i,0} - C_{N_i+1,0} = \varepsilon(C_{N_i-1,0} - C_{N_i,0}) \quad (16)$$

Since  $C_{N_i+1,0} = 0$  and  $C_{N_i-1,0} = 1$  at  $t = 0$

$$C_{N_i,0} = \frac{\varepsilon}{1 + \varepsilon} \quad (17)$$

The change in concentration of the bathing water at the central node  $N_A + N_B$  is given by:

$$C_{N_A+N_B,m+1} = C_{N_A+N_B,m} + \frac{D_B \Delta t}{(\Delta b)^2} (2C_{N_A+N_B-1,m} - 2C_{N_A+N_B,m}) \quad (18)$$

**Example:** As an example of using these equations, consider a slab of unit cross sectional area ( $1 \text{ mm}^2$ ) and thickness of  $10 \text{ mm}$  having porosity of  $0.25$  being leached in bathing water having unit area and thickness of  $10 \text{ mm}$ . The diffusion coefficient of solute in the slab is  $0.035 \text{ mm}^2/\text{min}$  and that in the water is  $0.104 \text{ mm}^2/\text{min}$  (the values chosen are similar to those usually observed under field conditions). The initial solute concentration and mass in the slab are  $1 \text{ mg}/\text{mm}^3$  and  $2.5 \text{ mg}$  respectively, while the bathing solution is initially salt free. The total pore volume of the slab is  $2.5 \text{ mm}^3$ . The ratio between the bathing water to slab pore volume ( $\beta$ ) is therefore  $4$ . The numerical solution of the diffusion equation for non-stirred bathing solution was obtained using an Excel spreadsheet while Mathcad programme was used for well-stirred bathing solution.

The calculated change in mass of the solute in the slab is shown in Fig. 3

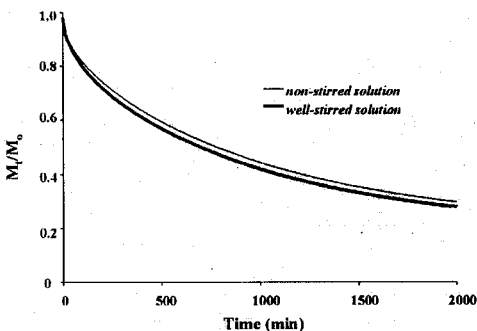


Fig. 3: Change in The Mass of Solute in the Slab With Time for Non-Stirred Bathing Water Compared With that for Well-Stirred Bathing Water ( $\beta = 4$ ,  $\varepsilon = 0.25$ ,  $A = 10 \text{ mm}$ ,  $B = 10 \text{ mm}$ ,  $D_A = 0.035 \text{ mm}^2/\text{min}$ ,  $D_B = 0.104 \text{ mm}^2/\text{min}$ )

where it is compared with that for a well-stirred bathing solution. Numerical results for the non-stirred

and well-stirred solutions showed only a small difference over the time period. When the bathing water is well-stirred,  $58\%$  of the solute mass diffused in  $1000$  minutes and  $72.5\%$  of the solute mass in  $2000$  minutes, whereas in the case of a non-stirred bathing solution,  $56\%$  of the solute mass diffused in  $1000$  minutes and  $70\%$  of the solute mass in  $2000$  minutes.

**Effect of  $\beta$  on the Rate of Diffusion in Well-Stirred and Non-Stirred Solutions:** The change in solute mass of a slab for different values of  $\beta$  (the ratio of macro and micropore volumes) was calculated by solving the diffusion equation numerically for well-stirred and non-stirred bathing water. The results are shown in Fig. 4

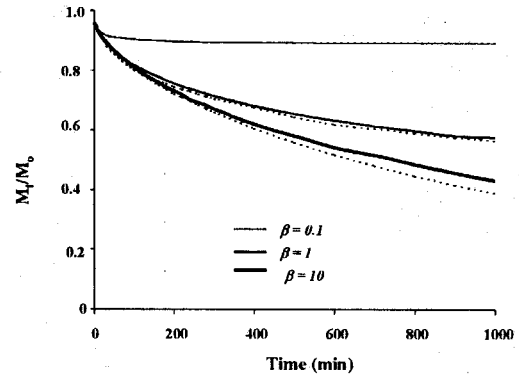


Fig. 4: Relative Solute Mass Remaining in the Slab Plotted Against Time Showing The Effect of Various  $\beta$  Values on the Rate Of Diffusion When a Slab Is Placed in Well-Stirred and Non-Stirred Solutions. ( $\varepsilon = 0.25$ ,  $A = 10 \text{ mm}$ ,  $D_A = 0.035 \text{ mm}^2/\text{min}$ ,  $D_B = 0.104 \text{ mm}^2/\text{min}$ ): The Broken Lines Represent When the Solution is Well-Stirred

The results for the mass remaining in the slab show that when  $\beta$  is greater than  $1$  there is only a small difference in the rate of diffusion for the two situations. When  $\beta$  is smaller than  $1$ , then they are effectively the same. Since in a real soil the micropore volume is usually much greater than the macropore volume, the value of  $\beta$  is therefore much less than  $1$ . Thus it can be inferred that the rate of diffusion in soil is not affected if the solution in macropores is non-stirred. Therefore the analytical solution of the diffusion equation for well-stirred solution suggested by Crank (1975) can be used under field conditions.

### Discussion and Conclusion

The results calculated theoretically in this paper for the diffusion of salts out of a slab showed that the mass of salt transferred to the bathing water is practically the same for well-stirred and non-stirred bathing water when the ratio of the volume of the bathing water to that of the pore space inside the aggregate ( $\beta$ ) is less than unity. We can tacitly assume that this is approximately the same for other aggregate geometries, in particular for spherical aggregates, when the packing makes calculations difficult because of the complex geometry of the macropore spaces. Theoretical calculations showed that the analytical solution of the diffusion equation for well-stirred solutions presented by Crank (1975), which is relatively simple, can be used for non-stirred bathing

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solutions when ratio of macro and micropores is less than unity as usually observed under field conditions.

### Symbols

$a$	distance from centre to the surface in slab
$b$	distance from the surface of slab to centre of the bathing water
$C_0$	initial solute concentration in the slab
$D_e$	effective diffusion coefficient
$D_A$	diffusion coefficient in the slab
$D_B$	diffusion coefficient in the bathing water
$F$	solute flux density.
$N_A$	number of nodes in slab
$N_B$	number of nodes in the bathing water
$n$	node number
$\Delta t$	time interval
$\Delta x$	thickness of layer in the slab
$T$	dimensionless time ( $D_e \Delta t / \Delta x^2$ )
$\epsilon$	volume of the bathing water / pore volume in the slab

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