Analytical solution to salt-water movement in soil and the determination of the hydrodynamic dispersion coefficient

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Modeling the coupled movement of salt and water in the soil profile is of great interest to soil scientists and agronomists when combating soil salinity and in maintaining the sustainable use of saline soils. The hydrodynamic dispersion coefficient is the most important parameter for simulating the salt movement process. In this study, an analytical solution to the 1-D convection-diffusion differential equation (CDE), formulated under appropriate initial and boundary conditions, was used to model the salt-water movement in the soil profile. Laboratory experiments, using a silt loam and a silty clay loam soil in short soil columns (10 cm), were conducted under the same conditions of leaching solution sodium absorption ratio (SAR) (2, 10, 20, 30) and concentration (80, 40, 20, 10, 2, 0 meq/L) as those used in the analytical solution of the CDE. Breakthrough curves, as functions of pore volume and salt concentration in the discharged solution were determined. The appropriate analytical solution was fitted to the breakthrough curves using the Golden-Section Search method to determine the hydrodynamic dispersion coefficient for salt movement in the different soil profiles under the various experimental conditions. The computed results indicated that the 1-D CDE well represented the salt leaching processes as indicated by the experimental data, except for the cases that resulted in extremely low hydraulic conductivity causing incomplete breakthrough curves. For a given SAR, higher salt concentrations in the leaching solution gave better fits of the analytical solution to the breakthrough curve. For a given salt concentration, solutions with lower SAR values were better fitted. The hydrodynamic dispersion coefficient generally increased with increased pore flow velocity. The increases were exponentially related to pore flow velocity for the silt loam but the relationship was more linear for the silty clay loam.

Key words: Soil salinity, convection-diffusion equation, analytical solution, diffusivity coefficient, breakthrough curve.

INTRODUCTION

Soil hydraulic conductivity (HC) decreases with increasing exchangeable sodium percentage (ESP) and decreasing electrical conductivity (EC) of the soil solution (Moutier et al., 1998, 2000). The HC of a soil is directly associated with the infiltration of irrigation water and salt leaching efficiency. When saline water is used for irrigating saline soils, salt movement in the soil profile is always of great concern, affecting the management objectives of maintaining soil sustainability and avoiding ground water pollution. Miscible displacement and/or the breakthrough curve, which describes the relationship between leachate pore volumes and salt concentrations in the effluent, have long been used for the study of...
solute movement in the soil profile (Hillel, 1998).

Solute movement in soil is a complex process. The movement of solute in soils involves two interrelated processes, namely convection and hydrodynamic dispersion (Lei et al., 1988). Convection conveys salts along with the mass flow of the soil solution within the mobile regions while dispersion allows salts to come to an equilibrium concentration within the soil solution and between regions where the soil solution is mobile or immobile. Numerous mathematic models have been developed to simulate the movement of solute in soils (Perfect et al., 2002). The convection-diffusion equation (CDE) is a widely used mathematical expression of the phenomenon. In the CDE, the hydrodynamic dispersion coefficient is considered to be the most important parameter to be determined (Zheng et al., 1995).

There are many methods to determine the hydrodynamic dispersion coefficient. Breakthrough curves, because of the simple calculation, have been widely used to obtain the hydrodynamic dispersion coefficient. Fitting the breakthrough curves with the analytical solution to the CDE gives an estimate of the hydrodynamic dispersion coefficient (Ren, 1999a; Zhu et al., 1998). In such cases, the average velocity of the pore flow is used in the CDE (Ren, 1999) but, practically, the velocity of pore flow would vary with time, especially under irrigation of saline soils with varying water quality. Little research has aimed to determine the effect of water quality on the hydrodynamic dispersion coefficient.

The objectives of this study were: 1) to formulate the mathematical model of convective and diffusive movement of salts in the soil profile as related to breakthrough curves; 2) to find the analytical solution of the salt transfer process; 3) to conduct laboratory experiments under different conditions to simulate the mathematical model using breakthrough curves; 4) to fit the breakthrough curves with the analytical solution to estimate the hydrodynamic dispersion coefficient for the given conditions; and 5) to quantify the hydrodynamic dispersion coefficient as a function of the velocity of pore flow.

One-D convection-diffusion equation and its analytical solution

Ignoring the absorption and reaction processes of salts in the soil, the horizontal (1-D) movement of salts in a saturated soil profile is given by the convection-diffusion (partial differential) equation as:

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}$$  \hspace{1cm} (1)

Where $c$ is the salt concentration, meq/l; $t$ is time, h; $x$ is coordinate, cm; and $v$ is the averaged velocity of pore flow, cm/h; and $D$ is the hydrodynamic dispersion coefficient, cm$^2$/h.

The initial and boundary conditions associated with Equation (1) are given as:

Initial condition:

$$c(x,0) = \begin{cases} c_0, & x = 0, \\ c_1, & x > 0, \end{cases}$$  \hspace{1cm} (1a)

Boundary conditions:

$$c(0,t) = c_0$$
$$c(\infty,t) = c_1$$  \hspace{1cm} (1b)

Where, $c_1$ is the initial salt concentration of the soil solution; $c_0$ is the concentration of the added leaching liquid, a constant value, at location $x = 0$.

Using Laplace’s transformation on both sides of Equation (1) changes Equation (1) into the following form:

$$sC(x,s) - c(x,0) + v \frac{dC}{dx} = D \frac{d^2C}{dx^2}$$

that is,

$$sC - c_1 + v \frac{dC}{dx} = D \frac{d^2C}{dx^2}$$
$$D \frac{d^2C}{dx^2} - v \frac{dC}{dx} - sC = -c_1$$  \hspace{1cm} (2)

in which $C = \{c(t)\} = C(x,s) = \int_0^\infty e^{-s}C(t)dt$, which is the Laplace’s transformation. $\{\}$ stands for Laplace’s transformation and $s$ in $C(s)$ means $C(s)$ is a spatially dependent function.

The boundary conditions as given by Equation (1b) are transformed into the following forms:

$$c(0,s) = \frac{c_0}{s}$$  \hspace{1cm} (2a)
$$c(\infty,s) = \frac{c_1}{s}$$  \hspace{1cm} (2b)

The homogeneous equation of Equation (2),

$$D \frac{d^2C}{dx^2} - v \frac{dC}{dx} - sC = 0, \hspace{1cm}$$

as an ordinary differential has the solution in the following form:

$$C(x,s) = A(s) \exp \left( \frac{vx}{2D} \cdot \sqrt{\frac{4D}{4D} + s} \right) + B(s) \exp \left( \frac{vx}{2D} \cdot \sqrt{\frac{4D}{4D} + s} \right)$$  \hspace{1cm} (2b)
while \( C = \frac{c_1}{s} \) is the particular solution to Equation (2).

Hence the final solution to Equation (2) is given as:

\[
C(x,s) = A(s)\exp\left(\frac{vx}{2D} - \frac{x}{\sqrt{4D}} \sqrt{v^2 + s}\right) + B(s)\exp\left(\frac{vx}{2D} + \frac{x}{\sqrt{4D}} \sqrt{v^2 + s}\right) + \frac{c_1}{s}.
\]  

(3)

Substituting \( x = 0 \), \( c = c_0 \), \( C = \frac{c_0}{s} \) and \( x = \infty \), \( c = c_1 \), \( C = \frac{c_1}{s} \) into Equation (3) gives:

\[
A(s) + B(s) + \frac{c_0}{s} = \frac{c_0}{s} \tag{3a}
\]

\[
B(s)\exp\left(\frac{vx}{2D} + \frac{x}{\sqrt{4D}} \sqrt{v^2 + s}\right) + \frac{c_1}{s} = \frac{c_1}{s} \tag{3b}
\]

\[
A(s) = \frac{c_0 - c_1}{s} \tag{3d}
\]

Substituting Equation (3c) and Equation (3d) into Equation (3) gives the following:

\[
C(x,s) = \frac{c_0 - c_1}{s} \exp\left(\frac{vx}{2D} - \frac{x}{\sqrt{4D}} \sqrt{v^2 + s}\right) + \frac{c_1}{s} \tag{4}
\]

Using the inverse Laplace’s transformation, the spatial dependent function, \( C(x,s) \) is transformed back into the time-dependent function as the solution to Equation (1) given as:

\[
\frac{c - c_1}{c_0 - c_1} = \frac{1}{2} \text{erfc}\left(\frac{x - vt}{2\sqrt{Dt}}\right) + \frac{1}{2} \exp\left(\frac{vx}{D}\right) \text{erfc}\left(\frac{x + vt}{2\sqrt{Dt}}\right) \tag{5}
\]

MATERIALS AND METHODS

Experimental device

The experimental system is shown in Figure 1. Perspex soil columns used in the experiments were 15 cm in height and 5 cm in diameter. Solutions were supplied from a Mariotte bottle to maintain a constant pressure head. The effluent was collected in a measuring cylinder.

Soil sample preparations

The two soils used in the experiments came from the Wunanwu Agro-meteorological Experimental Station of Xinjiang Autonomous Region in Western China. Physiochemical properties of the experimental soils are listed in Table 1. The two soils were selected to have different clay contents, since clay content affects the degree and consequences of clay swelling and dispersion affecting the soil HC. The soil samples, air-dried and passed through a 2 mm sieve before use, were packed, layer by 2 cm layer, into the columns to obtain a uniform bulk density of 1.3 g/cm³, similar to that found in the cultivated soil layer. At the bottom of the column, a 1 cm layer of coarse sand was used to facilitate drainage. The total height of the soil column was 10 cm using 255 g of soil. The packed soil columns were saturated with NaCl-CaCl₂ solutions with a concentration of 0.5 M and different SAR values (30, 20, 10 or 2) to reach the desired ESP values Between 2 and 30, since SAR and ESP values are considered to be equivalent at equilibrium (FAO, 2000).

EXPERIMENTAL TREATMENTS AND MEASUREMENTS

The experiments used two soil types (as described above), one hydraulic gradient (4.55), four SAR values (30, 20, 10, and 2) and six solution concentration levels (80, 40, 20, 10, and 2 mM; and distilled water-DW), in a completely randomized design. The experimental arrangements are listed in Table 2.

The 0.5M NaCl-CaCl₂ solutions (with SAR values equal to 30, 20, 10, or 2) were introduced at the bottom of the columns to saturate the soil samples from below. When the soils were saturated, the direction of flow was reversed to leach the samples from top to bottom, using the Mariotte bottle to maintain a constant head. For each given SAR value at the fixed hydraulic gradient (4.55), the soil samples were leached with about 20 pore volumes of the 0.5M Cl solution until the steady state saturated hydraulic conductivity, \( K_{ss} \), was reached, which was later used for a reference value.

Subsequently, the soil samples were leached with consecutive Cl solutions, with the designated SAR value, in concentrations of 80, 40, 20, 10 and 2 mM, and then finally with deionized water. Samples of the effluent were taken continuously at the outlet at 80, 40, 20, 10 and 2 mM, and then finally with deionized water. Samples of the effluent were taken continuously at the outlet at measured time intervals for determination of discharge rates and EC. Three replicates of each treatment were made. To reduce errors caused by uneven packing of the soil samples, relative hydraulic conductivity values were computed as the ratios of the actual conductivity values to the \( K_{ss} \) values for the solutions with given SAR values.

The saturated hydraulic conductivity was determined from Darcy’s law:

\[
K = -\nu / \nabla H \tag{6}
\]

Where \( \nu \) is the flow flux, the discharged volume per unit time per unit area (m³/(m²·s)); and \( \nabla H \) is the hydraulic gradient, dimensionless or m/m, which was constant in this study.

RESULTS AND DISCUSSION

Determination of the hydrodynamic dispersion coefficient

For a given experimental run, the pore volumes and the corresponding solution concentrations were recorded and plotted as a breakthrough curve, or equivalently the functional relationship of concentration with time was given as:
Figure 1. Schematic of the experimental equipment.

Table 1. Physiochemical properties of the experimental soils.

<table>
<thead>
<tr>
<th>Soil Type</th>
<th>EC (dS/m)</th>
<th>Cation exchange capacity (meq/100 g)</th>
<th>Exchangeable Na</th>
<th>Clay (&lt;2 µm)</th>
<th>Silt (2-20 µm)</th>
<th>Sand (20-200 µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silty clay</td>
<td>3.2</td>
<td>15.46</td>
<td>2.1</td>
<td>0.32</td>
<td>25</td>
<td>30</td>
</tr>
<tr>
<td>Silt loam</td>
<td>21</td>
<td>18.05</td>
<td>22.8</td>
<td>4.11</td>
<td>35</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 2. Experimental design.

| Hydraulic gradient, $\nabla H$ | 4.55 |
| Sodium absorption ratio (SAR) | 30   |
| Exchangeable sodium percentage ESP) | 30 |
| Concentration (meq/L) | 80 |
| Soil types | Silty clay loam | Silt loam |

The analytical solution given by Eq. (5), with $x$ being given as $x = X$, was fitted with the measured series given by Eq. (7). The sum of the squared errors ($\Delta$) was given as:

$$\Delta = \sum_{i=1}^{N} \left[ C(X, t_i) - \hat{C}_i \right]^2$$  \hspace{1cm} (8)

The Golden-Section Search method was used to find an optimal value of $D$ in Equation (5) to minimize the sum of the squared errors, $\Delta$. This optimal value of $D$ was the best fit hydrodynamic dispersion coefficient for any given breakthrough curve. The hydrodynamic dispersion coefficients for different solution concentrations are listed in Table 3. Figures 2 and 3 show the experimentally measured data series and the fitted curves using the determined optimal $D$, for the two different soils. Figures 2 and 3 indicated that for most cases, the
analytical solution using the determined $D$ values well fitted the measured data for the two different soils and for the different water qualities, with almost all the correlation coefficients being greater than 0.9. This indicated that the classic 1-D convection-diffusion equation effectively simulated the salt leaching processes. When the HC was extremely low so that the salt solutions could not "breakthrough" the soil column, (that is, when SAR = 30 and 20, $C_0 = 2$ and $C_1 = 10$; and when SAR = 10, $C_0 = DW$ and $C_1 = 2$), the analytical solution did not well fit the measured data. Figures 2 and 3 also indicated that, for a given SAR, the higher the solution concentration the better the analytical solution fitted the measured data. Furthermore, for a given salt concentration, the lower the SAR the better the analytical solution fitted the measured data.

Effects of flow velocity on hydrodynamic dispersion coefficients

The value of $D$ is dependent on the experimental conditions and the soil studied (Brusseau, 1993; De and Weirenga, 1984; Koch and Fluhler, 1993). Hydrodynamic dispersion is an effect that combines molecular diffusion and mechanical dispersion. Molecular diffusion of a solution is due to the random movement of molecules or Brownian motion. Solute molecules tend to move from places where the solution concentration is higher to places where the concentration is lower until a uniform concentration is reached.

The mechanical dispersion process involves the flow of the solute through the soil pore system at the micro-scale. Uneven distributions of soil particles of various sizes result in pore sizes of different sizes whereby a sandier soil which have larger pores than a clayier soil and flow velocities would be greater. Flow velocity might be expected to be greater in the silt loam than in the silty clay loam because of the higher clay content. But this seemed to depend on the SAR in our study. It was true of the cases where SAR was 20 or 10 but not where SAR was 30 or 2. Soil texture also determines the flow path length, which is directly related to the number of flow pathways, and is generally greater in clayier soils. A longer flow path would result in a greater number of pore volumes of solute required for total breakthrough to

Table 3. Optimized hydrodynamic dispersion coefficients ($D$) for solutions with different sodium absorption ratios (SAR) and initial ($C_1$) and final ($C_0$) concentrations or for deionized water (DW) for two soil types.

<table>
<thead>
<tr>
<th>SAR</th>
<th>$C_1$ meq/l</th>
<th>$C_0$ meq/l</th>
<th>Silty clay loam</th>
<th>Silt loam</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Average pore flow velocity cm/h</td>
<td>$D$ cm$^2$/h</td>
<td>Correlation coefficient, R</td>
<td>Average pore flow velocity cm/h</td>
</tr>
<tr>
<td>80</td>
<td>40</td>
<td>2.97</td>
<td>10.80</td>
<td>0.951</td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>1.84</td>
<td>3.60</td>
<td>0.961</td>
</tr>
<tr>
<td>30</td>
<td>20</td>
<td>0.66</td>
<td>0.65</td>
<td>0.928</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>0.17</td>
<td>0.01</td>
<td>0.964</td>
</tr>
<tr>
<td>2</td>
<td>DW</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>40</td>
<td>2.14</td>
<td>6.36</td>
<td>0.966</td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>1.64</td>
<td>4.98</td>
<td>0.954</td>
</tr>
<tr>
<td>20</td>
<td>10</td>
<td>0.76</td>
<td>0.45</td>
<td>0.960</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>0.19</td>
<td>0.40</td>
<td>0.818</td>
</tr>
<tr>
<td>2</td>
<td>DW</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>40</td>
<td>3.23</td>
<td>17.50</td>
<td>0.951</td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>2.84</td>
<td>17.50</td>
<td>0.969</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>2.32</td>
<td>15.40</td>
<td>0.947</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>0.99</td>
<td>1.17</td>
<td>0.954</td>
</tr>
<tr>
<td>2</td>
<td>DW</td>
<td>0.19</td>
<td>3.50</td>
<td>0.883</td>
</tr>
<tr>
<td>80</td>
<td>40</td>
<td>5.87</td>
<td>30.56</td>
<td>0.957</td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>6.41</td>
<td>36.40</td>
<td>0.948</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>6.13</td>
<td>15.80</td>
<td>0.969</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>4.19</td>
<td>8.06</td>
<td>0.968</td>
</tr>
<tr>
<td>2</td>
<td>DW</td>
<td>1.41</td>
<td>4.46</td>
<td>0.940</td>
</tr>
</tbody>
</table>
occur and effectively reduces the average flow velocity. Variations in flow friction, which is greater at the edges of the pore than in the center, and the occurrence of dead-end pores are also factors affecting the dispersion coefficient. All four factors affect the way in which the solutions disperse throughout the soil pore system, the pore flow velocity and the rate at which they equilibrate with the soil solution.

When flow velocity is high, the influence of mechanical dispersion tends to dominate the salt dispersion process. On the other hand, when pore flow is low or has ceased mechanical dispersion is low or negligible and molecular diffusion dominates the dispersion process. In most cases, the hydrodynamic dispersion coefficient increases with flow velocity. The relationship of $D$ with $v$ can be most commonly be represented by linear and exponential models (Perfect et al., 2001). Bruderer et al. (2001) suggested that Taylor's relationship ($D \propto v^2$) should be used for homogeneous porous media while linear relationships ($D \propto v$) should be used for non-homogeneous porous media. For the disturbed soil samples in our experiments, different functional relationships between $D$ and $v$ best fitted the results for the two different soils, as shown in Figure 4. An exponential function best fitted the data for the silt loam while a linear function was better for that of the silty clay loam.

When $v = 3.91$ cm/h, the $D$ values for the 2 soils were the same (16.5 cm$^2$/h) as calculated from the functional

Figure 2. Measured and fitted breakthrough curves for the silt clay loam using solutions with different sodium absorption ratios (SAR) and initial ($C_1$) and final ($C_0$) concentrations (meq/L) or deionized water (DW).
relationships (Figure 4). When \( v < 3.91 \text{ cm/h} \), the \( D \) value of silt loam was higher than that of silty clay loam whereas when \( v \) was between 3.91 and 30.91 cm/h, the \( D \) value of the silty clay loam was higher than that of the silt loam. The reasons for this behavior can be explained as follows: when the flow velocity was relatively small, that is with higher SAR values and lower solution concentrations, the pore system of the silt loam soil, having a higher clay content, tended to become more blocked by swollen and dispersed clay particles than that of the silty clay loam. The blockages and reduced pore sizes led to lower pore velocities in both soils but necessitated a higher degree of molecular solute dispersion resulting in higher \( D \) values in the case of the silt loam. When pore flow velocity was higher, which corresponded to conditions of higher solution concentration and lower SAR values, soil clay swelling was negligible. Mechanical dispersion was the dominant factor and possibly the soil with the higher content of clay particles had a more stable structure of with larger aggregates and pore sizes, which resulted in reduced molecular solution dispersion and a lower \( D \) value.

Effects of salt concentration and sodium adsorption ratio on the hydrodynamic dispersion coefficients

Using SAS software, the effects of \( C \) and SAR on \( D \) of two soils were analyzed using multiple linear regressions. The resulting regression equations were:
$D = 12.55 + 0.41C - 0.64SAR \quad R^2 = 0.67 \text{ (Silty clay loam)}$

$D = 9.80 + 0.41C - 0.51SAR \quad R^2 = 0.62 \text{ (Silt loam)}$

The two regression equations indicated that hydrodynamic dispersion coefficients increased with the increase in salt concentration and the decrease of the sodium adsorption ratio. The magnitude of the effect of salt concentration on the hydrodynamic dispersion coefficient was the same for the two soils, while the sodium adsorption ratio had a greater effect on the value of $D$ for the silty clay loam than for the silt loam soil. These two regression equations could be used to predict the hydrodynamic dispersion coefficients of saline soil irrigated with water of different salt concentrations and sodium adsorption ratios.

**Conclusions**

Hydrodynamic dispersion coefficients for the different conditions were determined from the fitted equations for the breakthrough curves. The analytical solution to the classic 1-D convection-dispersion equation (CDE) gave hydrodynamic dispersion coefficients ($D$) values that enabled accurate simulation of salt solution movement in soils. The determined hydrodynamic dispersion coefficients generally increased with pore flow velocity, indicating higher rates solute dispersion at higher flow velocities. Hydrodynamic dispersion coefficients ($D$) increased with the increase in salt concentration and the decrease of the sodium adsorption ratio.

The $D$ value was exponentially correlated with flow velocity for the silt loam soil and linearly correlated with...
Figure 3. Measured and fitted breakthrough curves for silt loam using solutions with different sodium absorption ratios (SAR) and initial ($C_1$) and final ($C_0$) concentrations (meq/L) or deionized water (DW) (continued).

Figure 4. Relationships between pore flow velocities and hydrodynamic dispersion coefficients.
flow velocity for the silty clay loam. Clay swelling and dispersion adversely affected the accuracy of the fitted equations to the data. The procedures for determining the D values and the D value themselves would be useful in simulating salt leaching processes.

The consequence of clay swelling and dispersion blocking the soil pores serves to emphasis the need to first reduce soil ESP before lowering irrigation water concentrations when attempting to efficiently improve saline soils.

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