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Use of TDR and Inverse Modelling to Determine Soil Water Concentration and Solute Transport Parameters

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Abstract: The upward movement of saltwater in soils through capillary rise poses a concern, given its potential to adversely affect soil structure and hydraulic properties. This underscores the critical necessity of real-time monitoring to accurately measure and assess the salt concentration in soil. Time-Domain Reflectometry (TDR) can be used to simultaneously measure the volumetric water content and bulk electrical conductivity of soil over time. Bulk electrical conductivity serves as a metric for estimating pore water electrical conductivity, providing a basis for establishing a correlation with the salt concentration in the soil. TDR instrumented capillary rise experiments were conducted to measure volumetric water content and bulk electrical conductivity of two distinct sand grades. These experiments encompassed trials involving varying salt concentrated solutions. Further testing was conducted using the same sands to establish empirical relationships between bulk and pore water electrical conductivity. The time series data, encompassing experimental volumetric water content and concentration was used for inverse modelling. Breakthrough curves of salt were fitted using an unsaturated flow and transport model to derive crucial solute transport parameters that are difficult to measure directly. The outcomes of this study offer insights into comprehending the intricate dynamics of water and salt within soil systems.

Introduction

The rise of saltwater due to capillary rise can lead to salt accumulation and soil salinization [1]. Consequently, the presence of salt (occurring from irrigation, weathering, use of deicing salts, etc.) at the soil surface can affect soil structure and strength and cause corrosion of steel reinforcement used in structures [2]. This emphasizes a necessity to monitor the salt concentration of soil due to capillary rise. Time-Domain Reflectometry (TDR) can be used to simultaneously measure the volumetric water content and bulk electrical conductivity of the soil in real-time. Capillary rise experiments coupled with TDR can allow for better understanding of water and saltwater dynamics in soil. The findings can be used to provide mitigation strategies in areas where saltwater rise is of concern.

This study investigates the capillary rise of saltwater at various concentrations for two distinct sand fractions (30/40 and 40/50) using TDR. Additional experiments were conducted to establish a relationship between bulk and pore water electrical conductivity [3]. This relationship was then used to convert the bulk electrical conductivity obtained from using TDR in the capillary rise experiments to pore water electrical conductivity and later salt concentration. The salt concentration data was then used in an unsaturated flow and transport model to determine solute transport parameters.

Theoretical Background

The section includes a brief description of the capillary rise phenomenon along with a brief review of the previous research related to capillary rise. The measurement principles used by TDR to measure water content and electrical conductivity are also summarized. Furthermore, the relationship between bulk and pore water electrical conductivity is explored.

Previous Research on Capillary Rise

Capillary rise, known as the rise of liquid, is affected by several factors such as the surface tension of the liquid, the density of the liquid, the contact angle between the solid-liquid interface, and the radius of the capillary. Jurin's Law for capillary rise is as follows:

$$h = (\sigma cos\gamma)/(\rho g r) \tag{1}$$

where h is the height of capillary rise, σ is the surface tension of the liquid, γ is the contact angle, ρ is the density of the liquid, g is the gravitational acceleration constant, and r is the radius of the capillary [4].

Researchers have investigated the effects of capillary rise in soils with the use of column experiments using a plexiglass column [1][5]. Consequently, the studies investigating saltwater rise did not consider the salt concentration changes within the soil column [1][5]. Quantifying the salt concentration changes in the soil profile are vital for understanding solute transport. TDR can be used to quantify salt concentration changes through measurement of bulk electrical conductivity.

Time-Domain Reflectometry

TDR employs an indirect method to measure the water content by relating it to the dielectric permittivity. The TDR system sends an electronic signal or pulse through a probe that is surrounded by soil [6]. The pulse travels along the length of the probe and is reflected back. The travel time of this signal is measured and related to the dielectric permittivity.

The bulk dielectric permittivity. is a combination of the soil, air, and water permittivity. Water is the dominant component in this as it has a dielectric permittivity of 79-82, thus it can be related to the water content. The following relationship for the apparent dielectric constant (ratio of dielectric permittivity to free space) denoted as K_a and the volumetric water content (θ) was used in the TDR system [7]:

$$\theta = 0.1138\sqrt{K_a} - 0.1758 \tag{2}$$

TDR measures the bulk electrical conductivity by using the reflected signals of the pulse sent through the probe. The reflected pulse can reveal electrical properties or conductance of the soil [6]. TDR uses the following relationship to obtain the bulk electrical conductivity:

$$EC_b = \left(\frac{K_p}{Z_c}\right) \cdot \frac{1-\rho}{1-\rho} \tag{3}$$

where EC_b is the bulk electrical conductivity, K_p is a constant for the probe in use, Z_c is the impedance of the cable, and ρ is the ratio of reflected to applied voltage [8].

Bulk Electrical Conductivity and Pore Water Electrical Conductivity

Bulk electrical conductivity (EC_b) is the conductivity of soil, water, and air in a given volume whereas pore water electrical conductivity (EC_w) is specific to the water in the soil pores. of the water phase in the soil pores. The EC_w can be related to the EC_b using relationships established in literature. The model used in this research to obtain EC_w from EC_b refers to Rhoades et al. [3], which accounts for the soil solid component electrical conductivity (EC_s), volumetric water content (θ), and calibration constants (a and b) as follows:

$$EC_b = \left(a\theta^2 + b\theta\right)EC_w + EC_s \tag{4}$$

Materials and Methods

Capillary rise experiments were performed using TDR, followed by a set of batch experiments to determine pore water electrical conductivity. The methods used in both sets of experiments are summarized below.

Capillary Rise Experiments

The soil used for the capillary rise experiments consisted of white silica sand. Two sand grades were tested, specifically 30/40 (grain size of 0.425 mm to 0.600 mm) and 40/50 (grain size of 0.300 mm to 0.425 mm). For the concentrated solutions, laboratory NaCl salt was used with a purity of 99%, supplied by Avantor VWR.

The experimental set up consists of the TDR measurement system manufactured by Campbell Scientific, a plexiglass column to hold the soil sample, a glass tray for holding the water solution, and a Mettler Toledo MS16000L scale for measuring mass of water entering the column. The TDR system consists of TDR100, a multiplexer (SDM8X50), a datalogger (CR800) and two

CS640 probes placed at 5 cm and 12 cm from the bottom of the column, respectively. Each probe has a length of 7.5 cm, and diameter of 0.16 cm. Pre-wetted soil to 1.5% gravimetric water content was compacted into the plexiglass column. The probes were inserted into the column post compaction. To prepare the concentrated solution, NaCl salt was mixed into deionized water. Experiments were conducted for each sand grade using 5 different testing solutions, including a control test (0, 2.5, 5, 7.5, and 10 g/L). Each experiment ran for 6 days and was stopped when the change in water entering the column was less than 5 g per day. The specific gravity was 2.65 for both sand grades. The average dry density and porosity for the 30/40 sand was 1.69 g/cm^3 and 0.365, whereas the 40/50 sand had an average dry density of 1.69 g/cm^3 and porosity of 0.363.

Pore Water Electrical Conductivity Experiments

Methods used to measure pore water electrical conductivity may include centrifugation or soil solution extraction methods. The approach used in this research was required extracting the pore water electrical conductivity of various soil columns at different electrical conductivities and saturation levels [9]. Upon preparation of the compacted soil column using sand pre-wetted with a salt solution, measurements of bulk electrical conductivity and volumetric water content were obtained using TDR. A soil suction extraction method may be used to extract the soil solution and assess for the pore water electrical conductivity.

Each sand was packed into columns with a height of 14 cm and diameter of 10 cm. Each sand was tested at 5 different saturation levels (40%, 50%, 60%, 80%, and 90%) and at 5 different concentrations using NaCl (0, 2.5, 5, 7.5, and 10 g/L). A TDR CS640 probe was then used to determine the bulk electrical conductivity and water content of each soil column.

To extract the pore water, a Büchner funnel setup was employed. This setup includes a funnel which is used to house the sample, a filter paper is placed under the sample, a clamp is used to secure the funnel, and a small bottle is placed inside the flask to collect water. A vacuum source was connected to the flask to extract the water out from the soil. Upon collecting the pore water, the electrical conductivity was measured using a lab electrical conductivity meter (TetraCon® 925). The results from this method were used to establish a relationship between bulk electrical conductivity and pore water electrical conductivity.

Results and Discussion

The results from the capillary rise experiments using TDR are presented in this section along with the method used to develop the empirical relationship relating bulk and pore water electrical conductivity. This relationship is used to convert the electrical conductivity from the capillary rise experiments to pore water electrical conductivity and estimate salt concentration.

TDR Results

Figure 1 shows the bulk electrical conductivity results for the 30/40 and 40/50 sand. The electrical conductivity increases with increasing concentration for both sands. The 30/40 sand shows the electrical conductivity to range from 0 dS/m to 2.4 dS/m with increasing salt concentration. For the 40/50 sand, the electrical conductivity increases from 0 dS/m to 2.8 dS/m as the salt concentration of the testing solution is increased.

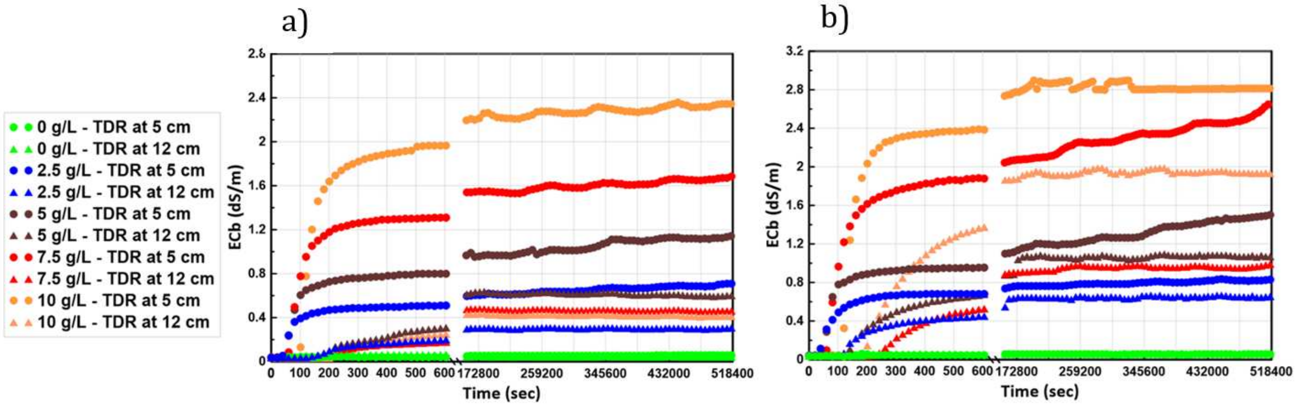

Figure 1: TDR bulk electrical conductivity versus time for the a) 30/40 and b) 40/50 sand [2].

Developing Empirical Relationship Relating Pore Water and Bulk Electrical Conductivity

Using the results from the batch experiments, an empirical relationship relating pore water and bulk electrical conductivity was developed following procedure from Rhoades et al. [3]. The procedure involves taking the soil surface electrical conductivity (EC_s) and subtracting that from the EC_b and dividing by the EC_w, as shown in Figure 2 for each sand grade. The EC_b is that measured using TDR in the batch experiments, whereas the EC_w is the electrical conductivity measured for the extracted soil solution. Note that the EC_s is the bulk electrical conductivity when the pore water electrical conductivity is approximately 0 dS/m [3]. This was measured to be 0.038 dS/m and 0.042 dS/m for the 30/40 and 40/50 sands, respectively.

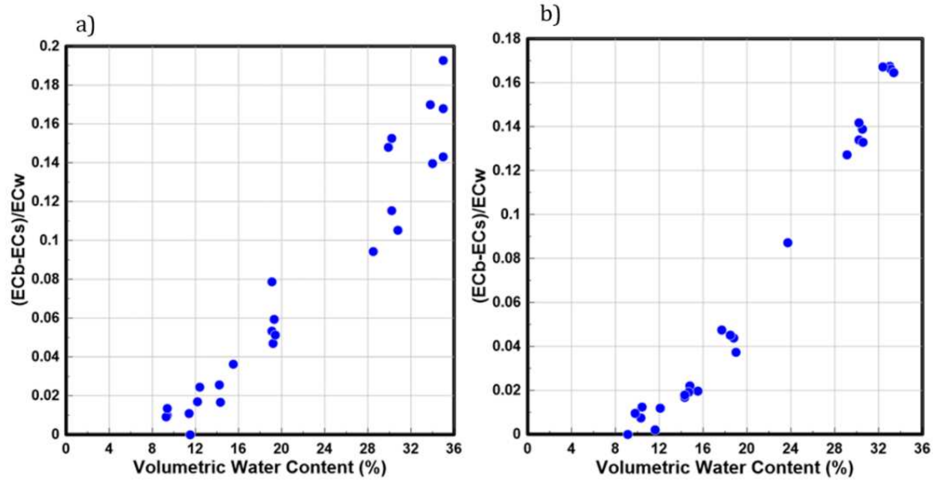

Figure 2: $(EC_b - EC_s)/EC_w$ versus volumetric water content for the a) 30/40 and b) 40/50 sand [2].

Note that Eq. 4 mentioned earlier can be rearranged as:

$$\frac{EC_b - EC_s}{\theta \cdot EC_w} = (a\theta + b) \tag{5}$$

The right side of the rearranged equation is a slope of a line (henceforth denoted as *T*) where a and b are calibration constants. The left side of the equation is the y-axis as shown in Figure 2, divided by the water content. Figure 3 shows the T versus the water content for each sand. A linear fit was used to obtain the calibration constants. The R^2 was estimated to be 0.83 for the 30/40 sand and 0.97 for the 40/50 sand.

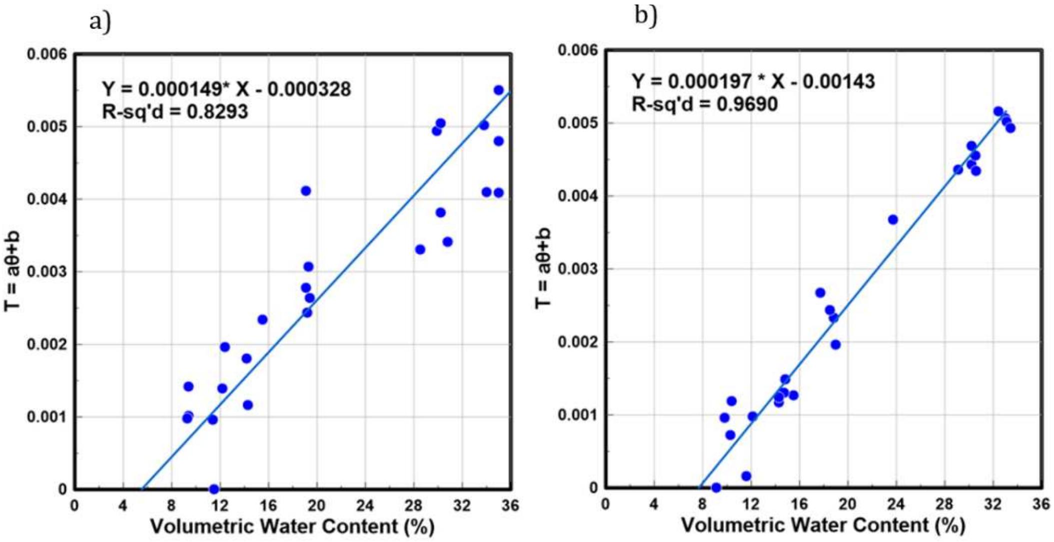

Figure 3: *T* versus volumetric water content for the a) 30/40 and b) 40/50 sand [2].

Using the calibration constants found using the linear fit and Eq. 4, the empirical equation for EC_w for 30/40 and 40/50 sand, respectively, is as follows:

$$EC_w = \frac{EC_b - EC_s}{0.000149\theta^2 - 0.0003328\theta} \tag{6}$$

$$EC_w = \frac{EC_b - EC_s}{0.000197\theta^2 - 0.00143\theta} \tag{7}$$

The EC_w obtained using these relationships can be converted to NaCl concentration using the relationship between molar mass of NaCl (58.4 g/mol) and electrical conductivity. Figure 4 shows the salt concentration estimated for each capillary rise experiment for the 30/40 and 40/50 sands. For the 30/40 sand, the concentration ranges from 0 g/L to 11 g/L whereas for the 40/50 sand, the concentration ranges from 0 g/L to 16 g/L. The concentration for the 40/50 sand maybe have been overestimated at higher electrical conductivity levels due to the intricacy associated with developing the empirical relationship from the batch experiments.

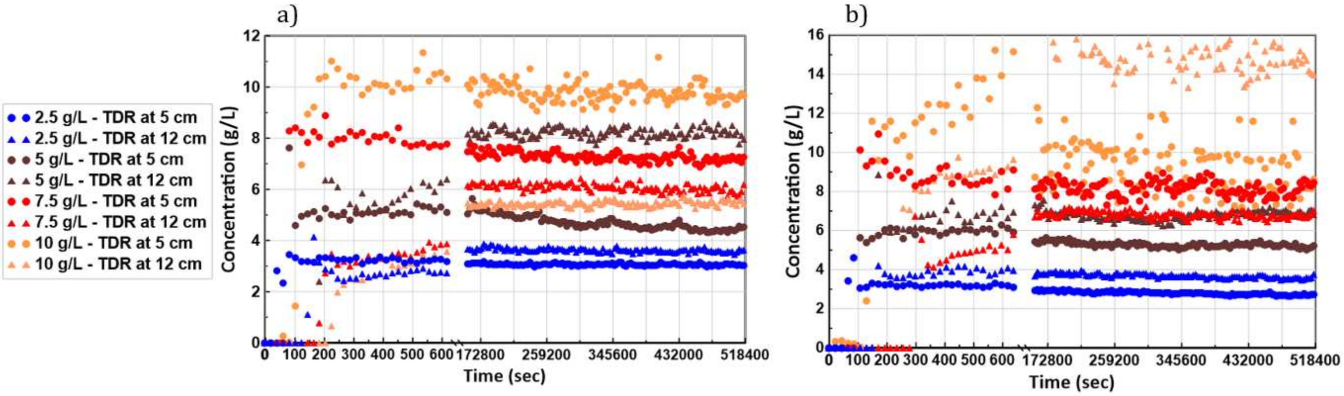

Figure 4: Concentration versus time for the a) 30/40 and b) 40/50 sand [2].

Inverse Modelling

HYDRUS-1D, an unsaturated flow and transport software, was used to determine solute transport properties for the sands used in this research using inverse modeling. Note that prior to determining solute transport properties, soil hydraulic parameters were also determined using an inverse model in HYDRUS-1D in which the water content data from TDR was used as the model input [2][10].

The first step in developing the inverse model requires entering water flow and solute transport boundary conditions. For the water flow conditions, a constant pressure head of 0 cm was set at the bottom of the column, and a constant flux of 0 cm/s was set at the top of the column. For the solute transport, the upper boundary was set as 0 g/L concentration flux and the lower boundary was set as the salt concentration that was used in the capillary rise experiments (2.5, 5, 7.5, and 10 g/L). The initial concentration for each sand was assumed to be 0.02 g/L. Observation data was added to the model (salt concentration and time). Observation nodes were added to the model at the location of the observed salt concentration i.e. location of the TDR probes. The solute transport model was then executed to determine dispersivity and diffusion coefficient. The soil hydraulic parameters using the van Genuchten (1980) model were determined inversely using HYDRUS-1D [2][10]. For the 30/40 sand, the residual and saturated water contents were estimated as 1.82%, and 28%, respectively, with a saturated hydraulic conductivity of 0.02 cm/s. The fitting parameters α and n were 0.14 and 2.81 respectively. For the 40/50 sand, the residual and saturated water contents were estimated as 2.56% and 28%, respectively, with a saturated hydraulic conductivity of 0.01 cm/s. The fitting parameters α and n were estimated as 0.10 and 2.60, respectively. Initial model inputs for dispersivity were taken as 3 cm for both sands whereas diffusion coefficient was 0.000011 cm/s for both sands.

Modelling Results

Figure 5 and Figure 6 show the results of the concentration versus time for each experiment along with the results obtained from modelling for each sand, at each of the TDR location. For both sands, the salt concentration obtained using the empirical relationship is shown to be higher than that estimated using the model. This may be due to experimental errors in obtaining the empirical relationship between bulk and pore water electrical conductivity. Furthermore, model limitations may add to the differences between the experimental and modelled concentration. TDR probes have a sensing range of 3 cm on all sides and the output results at a given location is the average along the sensing range. This means that the probe at 5 cm, can sense from 2 cm to 8 cm of the soil column height. However, the model uses observation nodes at specific locations only, which means that the estimated concentration from the model may not be comparable to the entire sensing range of the TDR. In addition, the model only allows the user to use observation data from one location only. This may also result in discrepancies between experimental and modelled results.

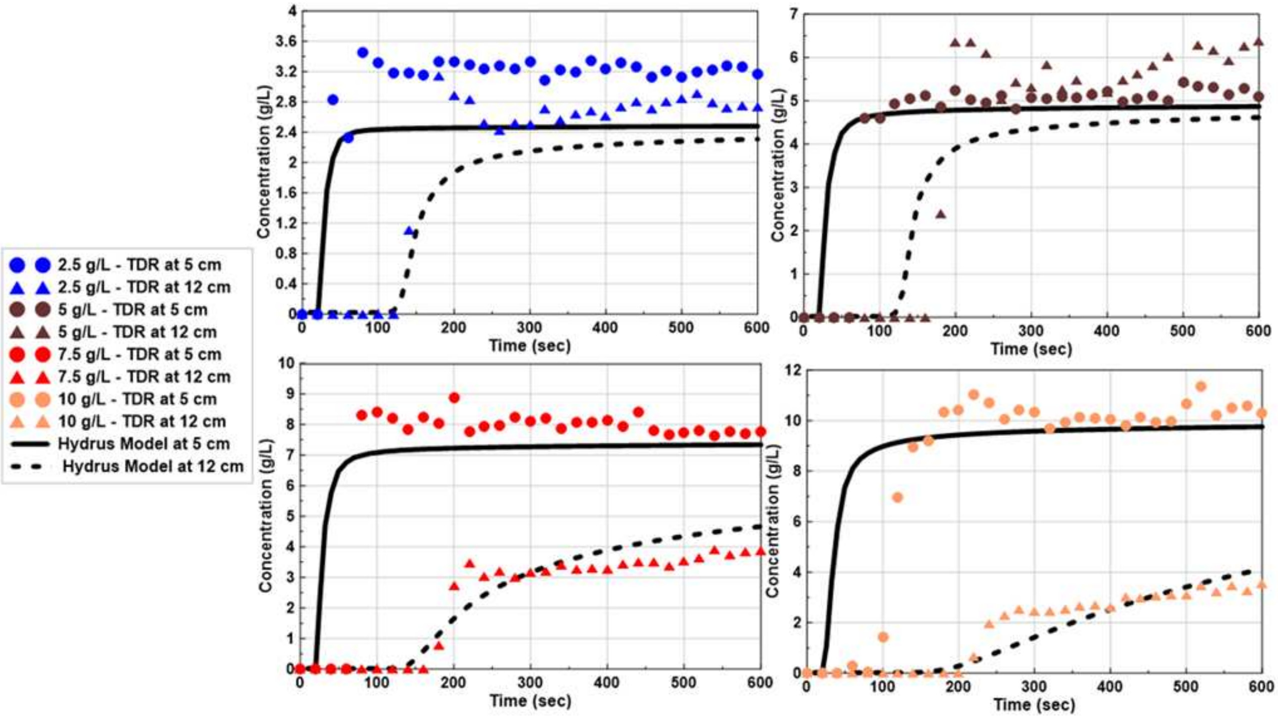

Figure 5: Concentration versus time predicted using HYDRUS-1D for the 30/40 sand [2].

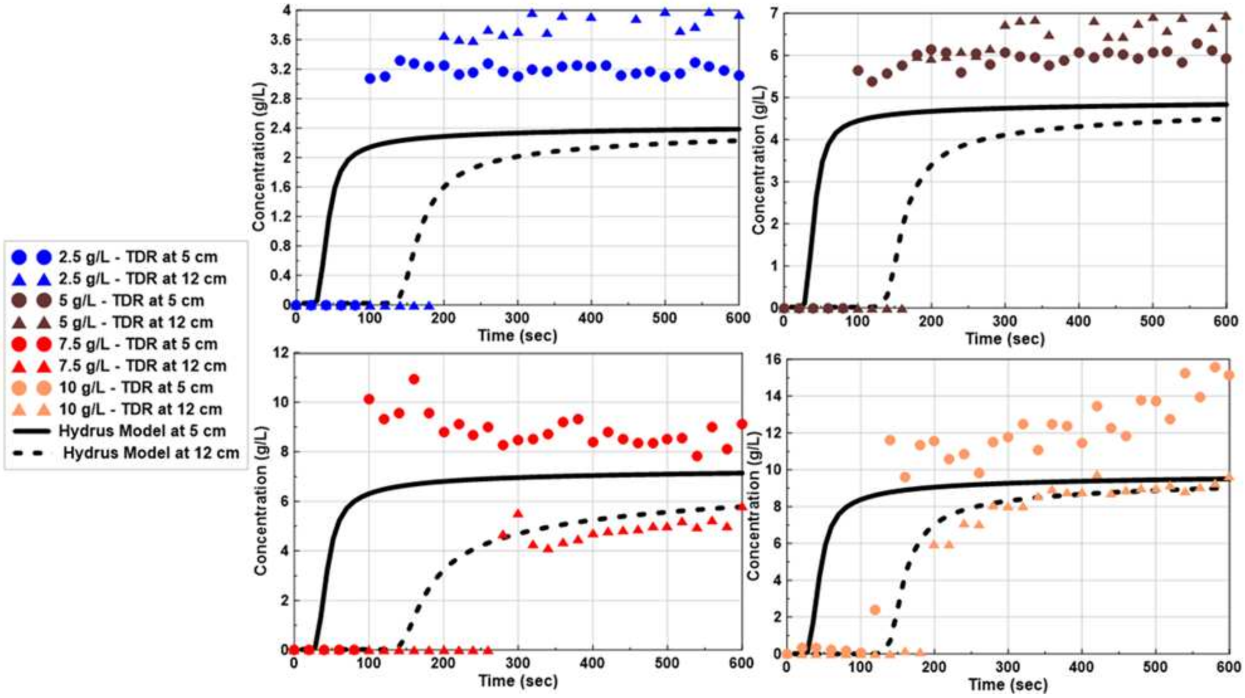

Figure 6: Concentration versus time predicted using HYDRUS-1D for the 40/50 sand [2].

The average dispersivity and diffusion coefficient for the 30/40 sand were estimated to be 1.3 cm and 0.094 cm^2/s. For the 40/50 sand, the average dispersivity and diffusion coefficient was 0.9 cm and 0.091 cm^2/s. The dispersivity for each sand falls within the range of 0.1 cm to 2.0 cm noted in literature whereas the diffusion coefficient falls in the range of 0.07 cm^2/s to 0.09 cm^2/s for sands [11][12].

Concluding Remarks

Capillary rise column experiments instrumented with TDR probes were used to assess the water content and electrical conductivity of two sand grades (30/40 and 40/50). In addition, a set of batch experiments were conducted to aid in estimating an empirical relationship between the pore water and bulk electrical conductivity. The following conclusions can be drawn from this research:

1. Instrumented capillary rise experiments provide valuable information on understanding the capillary rise of saltwater.
2. TDR works relatively well at lower salt concentrations whereas more noise is present in the measurements when the electrical conductivity is higher.
3. The technique used to convert the bulk electrical conductivity to pore water electrical conductivity performs reasonably well.
4. Inverse modelling combined with instrumented soil columns is a viable technique to estimate the solute transport parameters.

5. Solute transport parameters can be used to gain valuable insights on saltwater movement in areas where contamination is of concern.

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