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Simulating the Movement of a Reactive Solute Through a Soil Lysimeter Column Using a Functional Transport Model*

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Abstract

Trace Element Transport (TETTrans), a one-dimensional, functional model of solute transport introduced by Corwin and Waggoner [1, 2], is tested for its ability to simulate the movement of boron through soil lysimeter columns under varying irrigation management strategies, irrigation water qualities and cropping regimes. The test period covers three years (1100 days) and represents one of the most extensive controlled tests both in duration and variation in boundary conditions for the transport and simulation of boron through an unsaturated soil system. Simulations for four weighing soil lysimeters are presented. Each lysimeter differs in irrigation management strategy, quality of the irrigation water applied and cropping strategy.

The TETTrans model has the capability through a single parameter to account for deviations of water flow from strict piston displacement [1-3]. The parameter, termed the mobility coefficient, accounts for dispersion, diffusion and bypass, and is defined as the deviation of measured soil solution chloride concentrations from predicted chloride concentrations assuming piston-type displacement. By utilizing a temporally and

*This model was contributed by the U.S. Salinity Laboratory, USDA-Agricultural Research Service, 4500 Glenwood Drive, Riverside, CA 92501.
spatially varying mobility coefficient to improve TETrans' ability to simulate the movement of chloride, and thereby water flow, it is postulated that the simulation of an accompanying reactive solute (i.e., boron) will also be improved. Comparisons of predicted concentrations to measured soil solution concentrations of boron show that the simulations using a temporally and spatially varying mobility coefficient based on chloride data were significantly improved over assumptions of strict piston-type displacement. However, the ability to simulate the transport of boron was still not completely successful when the conventional Langmuir adsorption isotherm model was used. Even the use of several alternative equilibrium models of adsorption-desorption was not completely successful. The best fit to the data was with a modified Langmuir adsorption model which was "kinetically irreversible." The unquestionable confidence in the simulation of the water flow and plant water uptake aspects of the transport phenomenon, as evidenced by excellent chloride simulations, led to the conclusion that the knowledge of the chemistry of boron in soils from a modeling standpoint is not well-known, particularly if approached from a simplified, practical standpoint which tries to keep measured physicochemical-transport parameters to a minimum. The use of nonhysteretic, equilibrium models of adsorption-desorption are insufficient to describe the chemical behavior of boron in a transient-state soil system where dynamic changes in ion composition, ionic strength and pH are occurring; and where complexities of adsorption-desorption hysteresis are occurring.

A comparison of predicted soil solution boron concentrations using both TETrans and the Hanks' et al. [4] solute transport model to measured concentrations shows an improved ability of TETrans to simulate the movement of boron, particularly near the soil surface where preferential flow through cracks created from wetting and drying is a factor. The simulated results for both models were similar below 0.30 m.

Introduction

Because of the nation's growing concern over the protection of its groundwater supplies, the ability to model the migration of pollutants through the vadose zone is recognized as an essential tool in combating groundwater degradation. However, from a practical standpoint the soil data needed for most mechanistic approaches to transport modeling are well beyond the resources of most real-world users.

As defined by Addiscott and Wagenet [5], functional models of solute transport are "models that incorporate simplified treatments of solute and water flow and make no claim to fundamentality." Functional transport mod-
els fall into the management-oriented class of solute leaching models. More than ever, there is a need for simple, management-oriented models for interpreting and simulating solute movement through the vadose zone. The need for functional transport models arises from practicality and from limitations of more theoretically rigorous mechanistic approaches to transport. Aside from being mathematically simple, functional models have very modest input requirements. In addition, the required input parameters are all capacity factors which are less spatially variable than the rate parameters of mechanistic models. It is the spatially variable nature of typical soils which limits the accuracy of application of exact transport theory under field management situations. Stochastic transport models are usually not a practical alternative because the data from which they are derived are too labor and cost intensive.

An excellent review article by Addiscott and Wagenet [5] provides a concise, yet thorough, historical perspective for the development of functional models of solute transport. In short, deterministic functional models of solute leaching in soils first appeared in the literature around a third of a century ago [6–8]. These early solute transport models were an adaptation of chromatographic theory, and as a result, were mainly relevant to reactive solutes. As an offshoot of the earlier chromatographic approaches, simple layered models of solute transport appeared in the late sixties and early seventies [9–13]. These models were based upon the conservation of mass for both water and solute.

In the mass-conservation, layered models of Terkeltoub and Babcock [13] and Burns [10], water and solute entering a layer of soil mix with water and solute already present. If the new water content of the layer exceeds the field capacity of that layer, then any excess water and accompanying solute are passed to the next soil layer. This process is subsequently repeated for each layer of soil until a layer is reached which is either the bottom layer and drainage occurs, or the entering water is not great enough to bring the layer to field capacity. These simple models assumed that soil drains rapidly to field capacity and that the field capacity is the same for all layers. Burns [11] extended his model to include the effects of evaporation using the evaporative limit concept. These functional models were used to simulate salt movement [13]; and chloride, nitrate and water movement in soil columns [11, 14]. Subsequently, the model of Burns [10] was extended to predict the movement of a solute with no limiting assumptions about water content distributions [15], to include plant water uptake effects [16, 17] and to predict the transport of solutes that react with the soil either by anion exclusion [15], by adsorption [15, 18] or
by cation exchange [15, 19]. However, the models of Burns [10, 11, 14], Rose et al. [16, 17] and Bond and Smiles [15] assume that there is no preferential flow of water and solute through macropores and cracks. Corwin and Waggoner [1, 2] and Corwin et al. [3] addressed the problem of hydraulic bypass by introducing a single parameter, the mobility coefficient, which is based upon the deviation of measured soil solution chloride concentration from predicted chloride concentrations assuming piston-type displacement. The mobility coefficient accounts for the effects of diffusion, dispersion and bypass. Corwin and Waggoner [1, 2] and Corwin et al. [3] incorporated the mobility coefficient into a functional model, referred to as Trace Element Transport (TETrans), which was based upon the work of Burns [10, 11, 14], Rose et al. [16, 17] and Bond and Smiles [15]. Using a temporally and spatially varying mobility coefficient, TETrans was able to accurately predict the movement of chloride, and thereby water flow, through a soil lysimeter over an extensive 1100-day study period [3].

It is the intention of this study to build upon the work of Corwin and Waggoner [1, 2] and Corwin et al. [3] by demonstrating TETrans' ability to simulate the movement of a reactive solute, boron, through various soil lysimeter columns each differing in irrigation management strategy, irrigation water quality and cropping strategy. It is postulated that by utilizing the temporally and spatially variable mobility coefficient described by Corwin et al. [3] the simulation of a reactive solute will be significantly enhanced due to the ability to simulate water flow accurately.

Theory

The TETrans model is mass-balanced and layered and is driven by the amounts of water and solute added and lost rather than by rates of change. It models transport as a sequence of processes: (1) infiltration and drainage to field capacity, (2) instantaneous chemical equilibration for reactive solutes, (3) water uptake by the plant root resulting from transpiration and evaporative losses from the soil surface, and (4) instantaneous chemical reequilibration. The plant water uptake and water flow aspects of TETrans, including its mobility coefficient, have been described in detail by Corwin and Waggoner [1, 2] and Corwin et al. [3]. Because Corwin et al. [3] modeled the movement of chloride, a nonreactive solute, no adsorption chemistry model was discussed. In order to simulate the chemical behavior of boron, the Langmuir adsorption isotherm model is used because it requires only two parameters.
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The simplicity of the Langmuir adsorption model makes it compatible with the overall intent of TETrans which is to provide reasonably accurate predictions of solute transport with a minimum of input information required. Use of the Langmuir adsorption model assumes that the adsorption-desorption process is instantaneous and nonhysteretic. The same general approach that was taken by Burns and Collier [18] to model boron adsorption was also used in TETrans, except the Langmuir equation was kept in its original form.

Basically, TETrans divides the soil into a series of layers. Each layer is characterized by physical and chemical transport parameters which may be the same or different from those of other layers. These physical and chemical parameters include layer thickness, field capacity water content, minimum water content, adsorption coefficients, bulk density and initial conditions. After each irrigation or precipitation event, a portion of the resident soil water for a layer as defined by the mobility coefficient is displaced by the incoming water. The layer is brought to field capacity and the increment of water is completely mixed by a convective process with the undisplaced portion of the resident water. The layer is temporarily regarded as a closed system and a new equilibrium is established between the boron in solution and the boron adsorbed on the soil. If the field capacity is exceeded by the incoming water, the excess water is transferred to the second layer where the same process is repeated. Next, water is removed from each layer in accordance to a plant water uptake function which is either linear or exponential over the depth of the plant root system. The adsorbed and solution phases are again reequilibrated.

Model Description

The following model steps outline the sequence of events for the transport process within a defined depth interval, \( z_1 \) to \( z_2 \) (see the Notation section at end of text for any undefined terms):

1. Infiltration and Drainage

   A. Before an irrigation \((B_I)\) or precipitation,

\[
T_{BI} = T_{sw} + T_{ad} = V_t(\theta_{B_I}C_{BI} + \rho_bC_{ad}) \\
= VtC_{BI} + V_t\rho_bC_{ad}
\]

   \( T_{BI} \) is the total amount of solute in \( V_t \) immediately before an irrigation
(kg); \( T_w \) is the total amount of solute in the soil water of \( V_t \) (kg); \( T_{ad} \) is the total amount of adsorbed solute in \( V_t \) (kg); \( \theta_{BI} \) is the volumetric water content immediately before an irrigation (cm³/cm³); \( C_{BI} \) is the concentration of solute in the soil water immediately before an irrigation (kg/m³); \( \rho_b \) is the soil bulk density (kg/m³); \( C_{ad} \) is the adsorbed solute concentration (kg/m³); and \( V_{BI} \) is the volume of soil water in \( V_t \) immediately before an irrigation (m³).

B. After an irrigation and drainage to field capacity (\( AI \)),

\[
T_{AI} = T_{BI} + T_{in} - T_{out} = T_{BI} + V_{in}C_{in} - V_{out}C_{out}
\]  

(2)

i. where if \( 0 < \gamma < 1 \) and

a. if \( V_{in} > V_{fc} - (1.0 - \gamma)V_{BI} \), then

\[
V_{out} = V_{in} - V_{fc} + V_{BI}
\]  

(3)

\[
C_{out} = \frac{\gamma V_{BI}C_{BI} - V_{fc}C_{in} + V_{in}C_{in} + (1.0 - \gamma)V_{BI}C_{in}}{V_{out}}
\]  

(4)

\[
V_{AI} = V_{fc}
\]  

(5)

\[
C_{AI} = \frac{(1.0 - \gamma)V_{BI}C_{BI} + [V_{fc} - (1.0 - \gamma)V_{BI}]C_{in}}{V_{fc}}
\]  

(6)

b. else if \( V_{fc} - V_{BI} < V_{in} < V_{fc} - (1.0 - \gamma)V_{BI} \), then

\[
V_{out} = V_{in} - V_{fc} + V_{BI}
\]  

(7)

\[
C_{out} = C_{BI}
\]  

(8)

\[
V_{AI} = V_{fc}
\]  

(9)

\[
C_{AI} = \frac{(V_{fc} - V_{in})C_{BI} + V_{in}C_{in}}{V_{fc}}
\]  

(10)

c. else if \( V_{in} < V_{fc} - V_{BI} \), then

\[
V_{out} = 0
\]  

(11)

\[
C_{out} = 0
\]  

(12)

\[
V_{AI} = V_{BI} + V_{in}
\]  

(13)

\[
C_{AI} = \frac{V_{BI}C_{BI} + V_{in}C_{in}}{V_{BI} + V_{in}}
\]  

(14)

ii. otherwise if \( \gamma = 0 \) and
MOVEMENT OF A REACTIVE SOLUTE

a. if $V_{in} > V_{fc} - V_{BI}$, then eqs 3, 4, 5 and 6 are applied.

b. else if $V_{in} \leq V_{fc} - V_{BI}$, then eqs 11, 12, 13 and 14 are applied.

where: $T_{AI}$ represents the total amount of solute in a volume, $V_t$, of soil after an irrigation (kg); $T_{in}$ is the total amount of solute entering $V_t$ (kg); $T_{out}$ is the total amount of solute leaving $V_t$ (kg); $V_{in}$ is the volume of water entering $V_t$ ($m^3$); $C_{AI}$ is the concentration of solute in the soil water after an irrigation (kg/m$^3$); $C_{in}$ is the solute concentration of the entering water (kg/m$^3$); $V_{out}$ is the volume of water leaving $V_t$ ($m^3$); $C_{out}$ is the solute concentration of the exiting water (kg/m$^3$); $\gamma$ is the mobility coefficient, or more specifically, the fraction of $V_{BI}$ which is subject to piston-flow (where, $0 \leq \gamma \leq 1$, $\gamma = 0$ represents total bypass, $\gamma = 1$ represents complete piston-type flow); $1.0 - \gamma$ is the fraction of $V_{BI}$ which is subject to bypass; $V_{AI}$ is the volume of soil water in $V_t$ after an irrigation ($m^3$); and $V_{fc}$ is volume of water in $V_t$ at field capacity ($m^3$).

2. Chemical Equilibration

Chemical equilibration involves the partitioning of a reactive solute into the solution and adsorbed phases. Based on the conservation of mass, the total boron in a soil layer of thickness $z$ (total volume $V_t$) after an irrigation is equal to the boron present before the irrigation, plus the total boron entering the layer minus the total boron leaving the layer. This is represented in simple mathematical form as eq 15:

$$T_{AI} = T_{BI} + T_{in} - T_{out}$$

(15)

where, $T_{AI}$ represents the total amount of solute in a volume, $V_t$, of soil after an irrigation (kg), $T_{in}$ is the total amount of solute entering $V_t$ (kg) and $T_{out}$ is the total amount of solute leaving $V_t$ (kg). Equation 15 is more specifically represented in terms of the volume of water and solute concentration in the soil layer,

$$T_{AI} = T_{BI} + V_{in}C_{in} - V_{out}C_{out}$$

(16)

where, $V_{in}$ is the volume of water entering $V_t$ ($m^3$), $C_{in}$ is the solute concentration of the entering water (kg/m$^3$), $V_{out}$ is the volume of water leaving $V_t$ ($m^3$) and $C_{out}$ is the solute concentration of the exiting water (kg/m$^3$). After an irrigation the volume of water in $V_t$ equals either field capacity,

$$V_{AI} = V_{fc}$$

(17)
or  \( V_{AI} = V_{BI} + V_{in} \)  \( (18) \)

where \( V_{AI} \) is the volume of soil water in \( V_t \) after an irrigation (m\(^3\)), \( V_{fe} \) is the volume of soil water in \( V_t \) at field capacity (m\(^3\)) and \( V_{BI} \) is the volume of soil water in \( V_t \) immediately before an irrigation (m\(^3\)). Assuming instantaneous adsorption-desorption and assuming that boron obeys the Langmuir adsorption isotherm model, \( T_{AI} \) is partitioned into the adsorbed and the solution phases according to eq 19,

\[
T_{AI} = V_{AI}C_{AI} + V_t \rho_b \frac{kbC_{AI}}{1 + kC_{AI}} \quad (19)
\]

where, \( C_{AI} \) is the concentration of the solute in the soil water after an irrigation (kg/m\(^3\)), \( \rho_b \) is the bulk density (kg/m\(^3\)), \( k \) is the Langmuir affinity coefficient (m\(^3\)/kg) and \( b \) is the adsorption maximum (mg/kg). Using eqs 16 and 19 and solving for \( C_{AI} \), eq 20 is obtained,

\[
C_{AI} = \frac{-(V_{AI} + V_t \rho_b kb - T_{AI}k) \pm \sqrt{(V_{AI} + V_t \rho_b kb - T_{AI}k)^2 + 4V_{AI}kT_{AI}}}{2V_{AI}k} \quad (20)
\]

where the positive solution is the one needed. The total amount of boron in the adsorbed phase is represented by eq 21,

\[
T_{ad} = V_t C_{ad} = V_t \rho_b \frac{kbC_{AI}}{1 + kC_{AI}} \quad (21)
\]

and therefore, the adsorbed solute concentration, \( C_{ad} \), is,

\[
C_{ad} = \rho_b \frac{kbC_{AI}}{1 + kC_{AI}} \quad (22)
\]

Equations 20 and 22 determine the solution and adsorbed phase solute concentrations following an irrigation by using the value of \( T_{AI} \) from the mass-balance equation (eq 16) and the appropriate value for \( V_{AI} \) from either eq 17 or 18.

3. Plant Water Uptake

A knowledge of the total amount of evapotranspiration between irrigation events and the plant root distribution of a crop is needed for TETrans. The plant water uptake model simulates the net loss of water from each depth increment within the root zone of a maturing plant. Root growth is assumed
to occur linearly from the date of planting to the date of maturity. If the plant is harvested and the root system is terminated, all subsequent loss of water from the root zone occurs by a simulation of evaporative loss from the soil surface. TETTrans does not account for the upward movement of solute resulting from the processes of evaporation or transpiration. Evapotranspiration is only viewed as a sink for water loss which results in the concentration of the solute within the root zone. It is not viewed as creating a potential gradient which results in the net upward or downward movement of the solute between depth increments.

In TETTrans the distribution of the removal of water by the plant root is fitted with the option of two models: linear or exponential distribution. The linear distribution was used for the simulations in this paper. The linear root water uptake model is that of Perrochet [20] which is a synthesis of previous models and work presented by Molz and Remson [21], Feddes et al. [22], Hoagland et al. [23], Ritchie [24], Ritchie and Otter [25] and Prasad [26]. On a capacity basis, the volumetric root extraction function, $S$, is expressed by,

$$S(\psi, z) = r(\psi)g(z)T_p$$  \hspace{1cm} (23)

where, $\psi$ is the soil-water suction head (m), $z$ is the soil depth (m), $r(\psi)$ is the reducing factor, $g(z)$ is the root distribution function and $T_p$ is the potential volumetric transpiration (m$^3$). Perrochet [20] expresses the linear root distribution function by,

$$g(z) = \frac{\alpha_1(2z - L) + L}{L^2}$$  \hspace{1cm} (24)

where, $\alpha_1$ is the linear plant root distribution coefficient ($-1 < \alpha_1 < 1$), $z < L$ and $L$ is the plant root depth (m). The root distribution function must be normalized so that its integral over $L$ is unity. It is assumed in TETTrans that moisture conditions are optimal; consequently, the reducing factor, $r(\psi)$, is equal to 1. Since the actual volumetric transpiration, $T_a$, is the integral of the volumetric extraction function from the soil surface ($z = 0$) to the depth of root penetration ($z = L$), then the relative water uptake for a linear root distribution, $U_l(z)$, over the soil depth interval $z_1$ to $z_2$ (where, $0 < z_1 < z_2 < L$) becomes,

$$U_l(z) = (\alpha_1/L^2)(z_2^2 - z_1^2) - [(\alpha_1/L) - (1/L)](z_2 - z_1)$$  \hspace{1cm} (25)

Following the same logic, the relative water uptake for an exponential root
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distribution, \( U_e(z) \), over the soil depth interval \( z_1 \) to \( z_2 \) becomes,

\[
U_e(z) = \frac{e^{-\alpha z_1} - e^{-\alpha z_2}}{1 - e^{-\alpha L}}
\]  

(26)

where: \( a = \alpha z/L \), and \( \alpha_z \) is the exponential plant root distribution coefficient. Therefore, the water loss within the \( z_1 \) to \( z_2 \) depth interval is equal to the actual volumetric transpiration multiplied by the relative water uptake. \( V_{AI} \) is adjusted to \( V_{et} \) which represents the volume of soil water in \( V_t \) following the removal of water by root uptake to meet transpiration needs. So, the water withdrawn by plant roots for any given depth increment, \( z_1 \) to \( z_2 \), is removed in a manner which corresponds to the relative plant root water uptake expressed by either eq 25 or 26 which are a reflection of the plant root distribution. Within any given depth increment, the residing soil water cannot be withdrawn below a minimum volume of water, \( V_{min} \), by the plant root. \( V_{min} \) is an empirical value which lies above the water content at the wilting point and represents the lowest volume of water within \( V_t \) which is observed to occur after any evapotranspiration (ET) event.

Concomitant with the removal of water by the roots is the concentration of the solute. During the extraction of soil water, roots behave similar to a semipermeable membrane. Solutes remain behind as the water is extracted. Therefore, evapotranspiration results in the concentration of solutes within the root zone. For a nonreactive solute, the degree to which the solute is concentrated can be approximated by multiplying the solute concentration in the soil solution by \( V_{AI}/V_{et} \).

4. Chemical Reequilibration

Following the removal of water by the roots as described above, the volume of water in \( V_t \) just before the next irrigation becomes,

\[
V_{BI} = V_{AI} - V_{et}
\]  

(27)

where \( V_{et} \) is the volume of water in \( V_t \) removed by evapotranspiration (m³). Concomitantly, the solute is concentrated by the factor \( V_{AI}/V_{et} \) and another chemical equilibration occurs. Once again, eqs 20 and 22 are used to determine the solution and adsorbed phase solute concentrations except \( V_{BI} \) is used in place of \( V_{AI} \).
Methods and Materials

The details of the soil lysimeter experiment used to test TETrans have been described by Waggoner et al. [27] and again in an overview by Corwin et al. [3]. Basically, the study involved monitoring the movement of salts (major cations and anions, including chloride) and boron through the root zone for various irrigation management strategies, irrigation water qualities and crops. Because it is the focus of this paper to test TETrans' ability to simulate the movement of a reactive solute, specifically boron, through soil, a variety of irrigation management strategies and crops were deemed necessary to make the test sufficiently extensive to provide credibility to TETrans' simulation capabilities. As such, two different irrigation strategies, four different irrigation water qualities and two different crop strategies were used in varying combinations on 24 weighing soil lysimeter columns. The irrigation management strategies consisted of either conventional or cyclical irrigation. The conventional irrigation strategy involved using a single irrigation water from planting to harvesting date. In contrast, the cyclical irrigation strategy used a good quality irrigation water from preplant irrigation through the seedling stage of the plant. The good quality water was then followed by the application of a poor quality irrigation water from the time the plant was established as a healthy seedling until it was harvested. The cropping strategy consisted of either a single perennial crop (i.e., tall wheat grass) or the rotation of milo and wheat.

For this paper, four representative soils lysimeters were selected from the original group of 24 lysimeters. Each lysimeter differed either in irrigation management, cropping strategy or irrigation water quality. Table 1 outlines the general irrigation management and cropping strategy for each of the four lysimeters. Four different irrigation waters were synthesized. These waters ranged in quality from excellent (low salt and low boron content) to very poor (high salinity and high boron). The synthesized irrigation waters were designed to simulate California Aqueduct water, Colorado River water, Imperial Valley drainage water and San Joaquin Valley drainage water. Table 2 outlines the irrigation water compositions.

The soil columns were weighing lysimeters approximately 1.5 m in length. Each was filled with Arlington loam (Haplic Durixeralf). Soil solution extractors, time-domain reflectometry (TDR) rods and tensiometers were installed at depths of 0.075, 0.225, 0.375, 0.525, 0.675 and 0.825 m. These depths served as the midpoints of the depth increments arbitrarily selected for mod-
Table 1: General irrigation and crop management strategy for soil lysimeter columns (irrigation waters: CA = California Aqueduct water, CR = Colorado River water, IV = Imperial Valley drainage water and SJV = San Joaquin Valley drainage water).

<table>
<thead>
<tr>
<th>Lysimeter 6</th>
<th>Lysimeter 10</th>
<th>Lysimeter 39</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of irrigation:</td>
<td>Type of irrigation:</td>
<td>Irrigation water:</td>
</tr>
<tr>
<td>cyclical</td>
<td>cyclical</td>
<td>IV</td>
</tr>
<tr>
<td>Irrigation waters:</td>
<td>Irrigation waters:</td>
<td></td>
</tr>
<tr>
<td>CA and SJV</td>
<td>CR and IV</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Lysimeters 6, 10, and 39</th>
<th>Crop rotation: milo and wheat</th>
<th>Julian day</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Days to maturity</td>
<td></td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>45 days</td>
</tr>
<tr>
<td></td>
<td>wheat</td>
<td>45 days</td>
</tr>
<tr>
<td></td>
<td>Planting dates</td>
<td></td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>6/22/83</td>
</tr>
<tr>
<td></td>
<td>wheat</td>
<td>1/18/84</td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>7/3/84</td>
</tr>
<tr>
<td></td>
<td>wheat</td>
<td>12/21/84</td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>6/19/85</td>
</tr>
<tr>
<td></td>
<td>Harvesting dates</td>
<td></td>
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<td></td>
<td>milo</td>
<td>10/3/83</td>
</tr>
<tr>
<td></td>
<td>wheat</td>
<td>6/5/84</td>
</tr>
<tr>
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</tr>
<tr>
<td></td>
<td>milo</td>
<td>10/10/85</td>
</tr>
</tbody>
</table>

Table 2: Chemical composition of the synthesized irrigation waters.

<table>
<thead>
<tr>
<th>Water</th>
<th>Ca</th>
<th>Mg</th>
<th>Na</th>
<th>Ke</th>
<th>Cl</th>
<th>SO4</th>
<th>HCO3</th>
<th>B</th>
<th>EC</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA</td>
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<td>1.3</td>
<td>3.1</td>
<td>0.1</td>
<td>2.2</td>
<td>3.0</td>
<td>1.5</td>
<td>0.3</td>
<td>0.7</td>
</tr>
<tr>
<td>CR</td>
<td>4.6</td>
<td>2.6</td>
<td>5.7</td>
<td>0.1</td>
<td>3.4</td>
<td>7.2</td>
<td>2.6</td>
<td>0.7</td>
<td>1.3</td>
</tr>
<tr>
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<td>8.9</td>
<td>22.9</td>
<td>0.4</td>
<td>16.6</td>
<td>20.5</td>
<td>4.4</td>
<td>3.0</td>
<td>3.9</td>
</tr>
<tr>
<td>SJV</td>
<td>25.7</td>
<td>13.9</td>
<td>49.1</td>
<td>0.2</td>
<td>47.7</td>
<td>38.2</td>
<td>3.0</td>
<td>6.0</td>
<td>8.0</td>
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</table>

* In meq/L. † In kg/L. ‡ In dS/m.
§ California Aqueduct water. ‡ Colorado River water. ‡ Imperial Valley drainage water.
© San Joaquin Valley drainage water.
eling purposes to characterize the solute distribution through the root zone: 0–0.15, 0.15–0.30, 0.30–0.45, 0.45–0.60, 0.60–0.75 and 0.75–0.90 m. Soil solution from the extractors was taken at the beginning of the experiment and after each irrigation when the soil reached field capacity. The soil solution was analyzed for major cations and anions [28] and for boron [29]. The TDR measurements were taken to determine soil water content at regular time intervals [30–32]. In addition, the bulk density, field capacity and initial water content for each depth increment were established prior to the commencement of the experiment. The input data needed for TETTrans included: initial solute concentration in the soil water; initial water content of the soil; adsorption coefficients; dates and amounts of irrigation water applied; total evapotranspiration between irrigations; bulk density; water content at field capacity; water content at the wilting point; solute concentration of each irrigation water applied; and date of planting, days to maturity, date of harvest, maximum depth of root penetration and plant root distribution for each crop. Figures 1, 2, 3 and 4, and Tables 3 and 4 are a compilation of all the input data necessary for TETTrans.

The adsorption coefficients in Table 4 were determined using the batch adsorption technique. Ten grams of soil were brought to saturation with solutions of boron varying in concentration from 5 to 50 mg/L. The saturation pastes were regularly stirred and allowed to equilibrate under isothermal conditions (25 °C) for 1, 7 and 14 days. The solution extracted from the saturation paste using suction was analyzed for boron with the Azomethine-H technique [29]. The adsorption equilibrium data was used to calculate the affinity coefficient, $k$, and adsorption maximum, $b$, for the Langmuir equation,

$$\frac{x}{m} = \frac{kbC}{1 + kC}$$  \hspace{1cm} (28)

where $x/m$ is the adsorbed concentration (mg/kg) and $C$ is the soil solution concentration at equilibrium (mg/L).

After each irrigation, solution-extraction samples were taken when the soil-water content was at field capacity for that particular depth. The solution samples were analyzed for major salt cations and anions [28], and for boron [29]. The measured chloride concentrations were used, as described by Corwin et al. [3], to calculate both a constant and a temporally and spatially variable mobility coefficient for each lysimeter. The mobility coefficient adjusts water flow to fit the measured chloride concentration at each depth [3]. Subsequently, simulations of boron movement were generated from TETTrans and compared to the measured boron values obtained from the soil solution samples for the entire 1100 days of the transport study.
LYSIMETER 6

Figure 1: (a) Applied irrigation water and evapotranspiration amounts for Lysimeter 6. (b) Boron and chloride concentrations of the irrigation waters applied. (c) Measured and calculated leaching fraction for each irrigation event. The measured leaching fraction is determined from actual drainage and irrigation amounts. The calculated leaching fraction is determined from evapotranspiration and irrigation amounts.
Figure 2: (a) Applied irrigation water and evapotranspiration amounts for Lysimeter 9. (b) Boron and chloride concentrations of the irrigation water applied. (c) Measured and calculated leaching fraction for each irrigation event. The measured leaching fraction is determined from actual drainage and irrigation amounts. The calculated leaching fraction is determined from evapotranspiration and irrigation amounts.
Figure 3: (a) Applied irrigation water and evapotranspiration amounts for Lysimeter 10. (b) Boron and chloride concentrations of the irrigation waters applied. (c) Measured and calculated leaching fraction for each irrigation event. The measured leaching fraction is determined from actual drainage and irrigation amounts. The calculated leaching fraction is determined from evapotranspiration and irrigation amounts.
Figure 4: (a) Applied irrigation water and evapotranspiration amounts for Lysimeter 39. (b) Boron and chloride concentrations of the irrigation water applied. (c) Measured and calculated leaching fraction for each irrigation event. The measured leaching fraction is determined from actual drainage and irrigation amounts. The calculated leaching fraction is determined from evapotranspiration and irrigation amounts.
Table 3: Additional input parameters for all four lysimeters.

<table>
<thead>
<tr>
<th>Initial conditions (all depth increments)</th>
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<tr>
<td>soil solution chloride concentration (meq/L):</td>
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<td>soil water content (m³/m³):</td>
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<table>
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<tr>
<th>Physical properties (all depth increments)</th>
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<tr>
<td>bulk density (kg/m³):</td>
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<tr>
<td>water content at field capacity (m³/m³):</td>
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<td></td>
</tr>
<tr>
<td>water content at wilting point (m³/m³):</td>
<td>0.09</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Crop parameters</th>
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<tbody>
<tr>
<td>max root pen (m):</td>
<td>wheat</td>
<td>0.90</td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>0.90</td>
</tr>
<tr>
<td></td>
<td>grass</td>
<td>0.90</td>
</tr>
<tr>
<td>plant root dist:</td>
<td>wheat</td>
<td>40-30-20-10 [21]</td>
</tr>
<tr>
<td></td>
<td>milo</td>
<td>40-30-20-10 [21]</td>
</tr>
<tr>
<td></td>
<td>grass</td>
<td>40-30-20-10 [21]</td>
</tr>
<tr>
<td>α₀ = -0.8 or α₀⁺ = 1.5</td>
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</tr>
</tbody>
</table>

Table 4: Langmuir affinity coefficient, k, and adsorption maximum, b, at different equilibration times for an Arlington loam soil.

<table>
<thead>
<tr>
<th>Equilibration time (days)</th>
<th>k (L/mg)</th>
<th>b (mg/kg)</th>
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<tr>
<td>1</td>
<td>0.038</td>
<td>15.7</td>
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<tr>
<td>7</td>
<td>0.050</td>
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</tr>
<tr>
<td>14</td>
<td>0.056</td>
<td>18.7</td>
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Discussion of Results

The assemblage of measured and simulated data for the five depths of each of the four lysimeters is visually formidable. Nevertheless, results are presented for all depths of each lysimeter in order to demonstrate where the limitations of TETrans' simulation capabilities may exist and to evaluate its versatility and
general reliability. The differences in leaching fractions, water quality and crop for each of the presented lysimeters provide a wide range of boundary conditions upon which to test TETrans' ability to simulate boron movement under complex transient-state conditions.

Lysimeter 6 would be expected to be the most complex with regards to the physicochemical dynamics of boron transport because it was subject to cyclical irrigation using waters of extremely different quality and to a crop rotation of milo and wheat. The soil chemical environment would be expected to vary due to the cyclical irrigation of good and poor waters (see Figure 1b). The root environment would be constantly changing due to root growth over the maturity of the plant and to the rotation of the crop. A dynamic root system would pose difficulties in the simulation of water flow due to the fluctuation in the water uptake distribution by the plant. However, it was found that the plant root distribution as reflected by the root water uptake function was the same for both milo and wheat (see Table 3). Time-domain reflectometry (TDR) measurements of water content changes resulting from plant water uptake for all four lysimeters showed that each crop (milo, wheat or wheat grass) only reached a maximum root penetration depth of approximately 0.90 m and that plant root water uptake was best simulated by the 40-30-20-10 distribution suggested by Molz and Remson [21].

Figure 1c shows an additional feature of Lysimeter 6 which is characteristic of the general behavior of the other lysimeters (see also Figures 2c, 3c and 4c). The occasional lack of correspondence between the measured leaching fraction (LF), based on actual drainage and irrigation water amounts, and the calculated LF, based on evapotranspiration (ET) and irrigation water amounts, showed that on irregular occasions the columns tended to build up water in the lower portions of the profile over two, and sometimes three, irrigations before a breakthrough of drainage water would occur. This fact is corroborated by TDR measurements. The problem was remedied by the application of a vacuum at the bottom of the lysimeter to facilitate drainage. These factors would have some potential effect upon the chemistry of boron adsorption-desorption at the lower depths. Consequently, even though monitoring instruments were installed in the soil column at 0.825 m, the data collected for the 0.75-0.90-m interval was ignored because of the boundary effects of the lysimeter design.

The general fluctuations in ET for each lysimeter reflect seasonal effects (see Figures 1a, 2a, 3a and 4a). Naturally, the lysimeters with alternating crops of milo and wheat showed a similar ET pattern (see Figures 1a, 3a and
4a) which was distinctively different from the perennial wheat grass ET pattern (Figure 2a). For Lysimeter 6, the general fluctuations in the chloride concentration of the soil solution at the 0–0.15-m depth increment (see Figure 5) are the consequence of the changes in chloride concentration of the irrigation water (see Figure 1b). Similar fluctuations occurred for Lysimeter 10 because it was also subjected to an irrigation strategy which cycled between good and poor quality water. The fluctuations are dampened out with depth with no noticeable retardation shift in the dampened curves because chloride is not adsorbed. The simulation by TETrans of the chloride concentration in the soil solution for the five depth increments of Lysimeter 6 is remarkably accurate whether a constant mobility coefficient of 0.5 is used or whether a temporally and spatially variable mobility coefficient is used. However, since a temporally and spatially variable mobility coefficient is, in essence, a point-by-point adjustment to the measured data [3], it is a slightly better fit than a constant mobility coefficient. Nevertheless, the difference is so subtle that an overlay at the presented scale of Figure 5 showed no significant difference.

Figure 5 clearly shows the excellent ability of TETrans to simulate water flow using a temporally and spatially variable mobility coefficient (designated by gamma=variable in Figure 5) which accounts for diffusion, dispersion and bypass effects [3]. However, the strength of simulating water flow based on measured chloride concentrations of the soil solution can become a weakness in the simulation of an accompanying solute (e.g., boron) because erroneous measures of chloride result in the determination of spurious mobility coefficient values. Duplicate and possibly triplicate samples and measurements of chloride would increase accuracy.

In Lysimeters 9 and 39 the soil solution chloride concentration at each depth increment rose quickly after 3–4 irrigations to a stable level characteristic of the incoming irrigation water and the extent of root water uptake for that depth increment. The same excellent simulation of soil solution chloride concentration for each depth was found for Lysimeters 9, 10 and 39. Actually, the outlying points are more likely to be suspect of being errors in measurement or in collection of the sample than a weakness of the model because they represent values which are either exceeding a condition of complete bypass or complete piston flow. Both of these conditions are physical impossibilities. In essence, TETrans temporally and spatially calibrates the water flow to fit the measured chloride concentrations of the soil solution.

Figure 6 shows a comparison of the measured boron concentrations of the soil solution taken at field capacity and simulations assuming no adsorption
Figure 5: Predicted and measured chloride concentrations of the soil solution at field capacity for the top five depth increments of Lysimeter 6. (The gamma=variable designation indicates that a temporally and spatially variable mobility coefficient, $\gamma$, was used in TETrans.)
Figure 6: Predicted (assuming no adsorption) and measured boron concentrations of the soil solution at field capacity.
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of boron. Quite obviously, the simulations of boron assuming no adsorption will mimic those of chloride (compare Figures 5 and 6). The difference of magnitude results from the concentration of boron in the irrigation water. The most interesting feature of Figure 6 is how closely the simulations of the 0–0.15 and 0.15–0.30-m depth increments match the measured boron concentrations. This suggests boron may be behaving like a conservative ion for the top 0–0.30 m. The apparent discrepancy at day 913 is misleading as measured data for that day is absent and a sharp decrease would be expected to occur because of the application of irrigation water with a very low boron concentration (see day 913 of Figure 1b). The simulations for all subsequent depths are noticeably different from the measured boron concentrations. Obviously, some unexpected chemical behavior or lack of it is occurring in the top 0–0.30 m, because it is well-known that boron undergoes adsorption-desorption reactions on soil.

Figure 7 is the next piece to the puzzle of understanding the transport of boron. Figure 7 shows the simulations which result from the use of the conventional Langmuir adsorption isotherm model. Table 4 shows the Langmuir coefficients for the adsorption of boron on Arlington loam soil for equilibration times of 1, 7 and 14 days. The values for \( k \) and \( b \) for seven days were used in the simulations because the average time between irrigations was approximately 1–2 weeks. Though the boron concentrations are more closely simulated for the bottom three depths (i.e., 0.30–0.45, 0.45–0.60 and 0.60–0.75) than in Figure 6, the top two depth increments are significantly worse. Obviously, the conventional Langmuir model is not sufficient to describe the adsorption chemistry for the transient conditions existing over the duration of this study.

Subsequently, a variety of chemical models and scenarios were tested. These included (1) the Langmuir model except trying a variety of different \( k \) and \( b \) values, (2) the modified Langmuir model proposed by Burns and Collier [18], (3) the two-site Langmuir model, (4) the Keren-Mezuman phenomenological equation for boron adsorption [33, 34], and (5) the Langmuir model modified so that adsorption is irreversible beyond a specified adsorbed concentration. Conceptually, the last model is analogous to hysteretic adsorption-desorption where the desorption is “kinetically irreversible,” or more precisely, the desorption is so slow as to appear irreversible for the time frame of this study.

Of the various chemical models tested, only the hysteretic, or more appropriately, the “kinetically irreversible” model improved the boron simulation
Figure 7: Predicted (assuming Langmuir-type adsorption, where $k = 17.9 \text{ L/mg}$ and $b = 0.0503 \text{ mg/kg}$) and measured boron concentrations of the soil solution at field capacity.
capability of TETrans for all four lysimeters (see Figures 8, 9, 10 and 11). For Lysimeter 6, irreversible adsorption occurred once the adsorbed concentration, $x/m$, reached 5.5 mg/kg. This value was arbitrarily established as a consequence of noticing the calculated adsorbed concentration at the time when the measured solution concentration of boron began to decrease, approximately day 600 for each of the four lysimeters. Lysimeter 9 was found to have the same inflection point, $x/m = 5.5$ mg/kg, upon which to commence irreversible adsorption. For Lysimeter 10 and 39, irreversibility was set to occur at $x/m = 3.6$ and 4.5 mg/kg, respectively.

The Keren-Mezuman phenomenological equation for boron adsorption is able to account for the effects of pH upon boron adsorption. Unfortunately, aside from initial measures of soil pH there were no reliable temporal measures of pH for the five depth increments. Nevertheless, possible pH ranges were selected for each depth increment which were the minimum and maximum likely pH. These ranges were used in the Keren-Mezuman model with the result that none of the characteristic oscillations of the soil solution boron concentration for the four lysimeters could be produced. However, next to the "kinetically irreversible" model this model was the closest in its simulations.

Even though the "kinetically irreversible" adsorption model resulted in the best simulations of soil solution concentrations of boron with depth and over time, there is still considerable discrepancy between calculated and measured boron, particularly in the bottom three depth increments. This would suggest that the model does not represent a reliable facsimile of what is actually occurring chemically. Rather, it should be concluded that the current chemical models of boron adsorption are not sufficient in describing the chemical behavior of boron reactions in soil over long periods of time. If only the first 400 days had been simulated, then it would appear that a simple Langmuir model would have been sufficient (see Figure 7). This held true for all four lysimeters. The duration of the study proved important in identifying the limitation of several current chemical equilibrium models.

There appears to be roughly a yearly periodicity to the fluctuations, regardless of the type of irrigation management, irrigation water quality or crop. Potentially, all readily available adsorption sites have been filled at approximately day 600 and the desorption of boron from these sites is kinetically too slow to be significant. The soil solution boron would then behave like chloride and fluctuate according to the concentration of incoming irrigation water, assuming that the root water uptake for each lysimeter has been normalized.
Figure 8: Predicted (assuming irreversible adsorption occurs when the boron concentration of the adsorbed phase reaches 5.5 mg/kg) and measured boron concentrations of the soil solution at field capacity.
Figure 9: Predicted (assuming irreversible adsorption occurs when the boron concentration of the adsorbed phase reaches 5.5 mg/kg) and measured boron concentrations of the soil solution at field capacity for the top five depth increments of Lysimeter 9.
Figure 10: Predicted (assuming irreversible adsorption occurs when the boron concentration of the adsorbed phase reaches 3.6 mg/kg) and measured boron concentrations of the soil solution at field capacity for the top five depth increments of Lysimeter 10.
Figure 11: Predicted (assuming irreversible adsorption occurs when the boron concentration of the adsorbed phase reaches 4.5 mg/kg) and measured boron concentrations of the soil solution at field capacity for the top five depth increments of Lysimeter 39.
Figure 12: A comparison of predicted (assuming irreversible adsorption occurs when adsorbed phase boron concentration reaches 5.5 mg/kg) soil solution boron concentrations for TETrans (solid line with diamonds) and for the Hanks et al. model (solid line), and measured boron concentrations (squares) at field capacity for three depth increments (0-0.15 m, 0.30-0.45 m and 0.60-0.75 m) of Lysimeter 9.
since the various uptake distributions were found to be nearly equal. However, if this were true, then Lysimeters 9 and 39 would not have the observed fluctuations which, of course, are present. Ostensibly, a seasonal influence is having an effect. Since it appears the oscillations in soil solution boron concentration follow a year-long cycle with the peak boron concentration occurring in the fall and the lowest concentration occurring in the spring, maybe temperature has an effect. Even though the lysimeters stood above ground and were not insulated, it is not likely that temperature alone would have such pronounced effects. Nevertheless, a similar lysimeter experiment is currently underway to determine if the observed boron fluctuations are an artifact of the lysimeter design and construction.

A comparison of the simulated movement of boron using TETrans to the numerical transport model developed by Hanks et al. [4] shows that near the soil surface TETrans is able to simulate the movement of boron more precisely (see depth 0–0.15 m of Figure 12). At greater depths the models were similar in their simulation ability (see depths 0.30–0.45 m and 0.60–0.75 m of Figure 12). The inability of the Hanks’ et al. [4] model to simulate the movement of boron at the soil surface is likely due to its inability to handle preferential flow and to inaccuracies in the determination of hydraulic conductivity at the very low moisture contents present near the soil surface. In both TETrans and the Hanks et al. [4] model, the “kinetical irreversible” chemical adsorption model was used.

Conclusion

The bridge between basic and applied research regarding the modeling of boron transport through a soil clearly depends upon a knowledge of the major factors influencing the adsorption and desorption of boron and the ability to quantify their effects with a chemical model which is parsimonious. The effects of pH [35], ionic strength [36], exchangeable ions [36, 37], iron and aluminum oxides [38–42], temperature [43], organic matter [44–46], clay mineralogy [33,36,47–52], and wetting and drying [37] on the adsorption of boron have been well-documented for numerous laboratory studies. Similarly, the hysteresis of boron adsorption-desorption has been studied under laboratory conditions [53–56]. Until very recently, the modeling of the adsorption of an inorganic chemical by soil was done exclusively with adsorption isotherm equations, such as the van Bemmelen-Freundlich isotherm equation, the Langmuir isotherm equation or a modification (i.e., two-sited Lang-
muir equation). However, the limitations of the adsorption isotherm equations in relation to adsorption mechanisms have resulted in attempts to model surface phenomena. These surface phenomena approaches include surface complexation models, the constant capacitance model, the triple-layer model and the objective model [57]. Of these four surface phenomena models only the constant capacitance model has been applied to soil with some potential success [58]. The equilibrium adsorption models have the advantage of simplicity, but are of questionable reliability because they do not account for factors influencing adsorption (i.e., pH, ionic strength, exchangeable ions, iron and aluminum oxides, temperature, organic matter and wetting and drying). The surface chemistry models lack simplicity, but are able to account for some of the major factors influencing adsorptive behavior.

As shown in this and previous publications [1, 3], TETrans is capable of modeling the movement of a conservative ion, and thereby water flow, when a mobility coefficient is used to account for bypass. The ability to simulate the movement of a reactive solute using TETrans is less impressive though still acceptably close. In comparison to the numerical transport model of Hanks et al. [4], TETrans showed an increased ability to model the transport of boron through the upper portion of the soil profile because of its ability to account for preferential flow. Nevertheless, there is still ample room for improving the agreement between predicted and measured results. Because TETrans is capable of modeling water flow so closely, it appears that the inability to simulate a reactive solute just as precisely is due to insufficiencies in the chemical model. Even though several equilibrium models of adsorption were tested, with the "kinetically irreversible" model performing the best, no model was particularly outstanding. These equilibrium models were selected over the surface phenomena models because they are considered parsimonious by real-world standards which is in keeping with the real-world application philosophy behind the development of TETrans [2]. Ostensibly, the current practical models of boron adsorption are inadequate to simulate the complex chemical behavior of boron in a transient-state soil system. Even though the effects of pH, ionic strength, exchangeable ions, wetting and drying, clay mineralogy and hysteresis have been well-documented for laboratory studies, the need is for a model of boron adsorption-desorption which is sufficiently sophisticated to at least incorporate the influences of pH and hysteresis, yet be parsimonious so that it has real-world utility.

It can be concluded that a chemical model of boron adsorption-desorption sufficiently sophisticated, yet simple enough to be practical and to reliably
simulate the complex and dynamic chemical environment occurring in a transient-state soil system, does not exist.

**Summary**

TETrans is a simplified, one-dimensional transport model which can simulate the vertical movement of trace elements, nonvolatile organic chemicals and salts through the soil. It is specifically designed to be user-friendly in its operation and to be used for real-world transport applications where a minimum of transport parameters are available to the user.

TETrans was developed for two applications. The first application was the assessment of the movement of nonvolatile solutes under field conditions. This would meet the needs of agricultural, industrial and engineering applications. For field applications TETrans has definite appeal because it does not require information which can only be obtained from costly laboratory analyses such as the relationship between hydraulic conductivity, matric potential and water content; or the relationship between dispersion-diffusion and pore water velocity. The second application was as an educational tool for studying the interrelationship of the processes involved in solute transport through the vadose zone. As an educational tool, TETrans assists in understanding the basic physicochemical dynamics of a solute as it moves through the soil and into the groundwater. Aside from minimizing parameter requirements for its operation, TETrans reduces the complexities of input and output found in most transport models to interactive menu screens and dialogue boxes. The student's time is spent more in the analysis of output than in learning how to operate the software.

As a functional model, TETrans incorporates simplified treatments of solute and water flow with no claim to fundamentality; consequently, it has definite limits of application. Specifically, TETrans is not designed to meet the detailed requirements and scrutiny of laboratory applications which are more appropriately met with mechanistic transport models that are more theoretically robust. For instance, the affects of hydrodynamic dispersion and diffusion upon transport cannot be analyzed with TETrans. Nonetheless, the basic interrelationships between water movement, evapotranspiration and basic chemical processes of adsorption and exchange can be studied.

The ability of TETrans to simulate the transport of a reactive solute through soil has been tested. Though shown to be a simulation model with definite real-world utility, TETrans has limitations which are the consequence
of the current state of development of practical chemical models of adsorption. Because TETrans is able to adjust water flow to fit measured chloride concentrations in the soil solution over time and with depth, an evaluation of various chemical models' ability to determine partitioning between adsorbed and solution phases was possible for a transient-state soil system. It appears that the current level of development of simplified chemical equilibrium models of adsorption-desorption significantly limits the ability of TETrans to accurately predict the one-dimensional transport of boron in complex situations.

**Notation**

- $a_1$: linear plant root distribution coefficient ($-1 < a_1 < 1$)
- $a_2$: exponential plant root distribution coefficient ($a_2 > 0$)
- $g$: mobility coefficient, or more specifically, the fraction of $V_{BI}$ which is subject to piston-flow (where, $0 \leq \gamma \leq 1$, $\gamma = 0$ represents total bypass, $\gamma = 1$ represents complete piston-type flow)
- $1.0 - \gamma$: fraction of $V_{BI}$ which is bypassed
- $\rho_b$: soil bulk density (kg/m$^3$)
- $\psi$: soil-water suction head (m)
- $\theta_{BI}$: volumetric water content immediately before an irrigation (cm$^3$/cm$^3$)
- $\theta_{fc}$: volumetric water content at field capacity (cm$^3$/cm$^3$)
- $a$: $a_2/L$
- $b$: Langmuir adsorption maximum (mg/kg)
- CA: California Aqueduct water
- CR: Colorado River water
- $C_{ad}$: adsorbed solute concentration (kg/m$^3$)
- $C_{AI}$: concentration of solute in the soil water after an irrigation (kg/m$^3$)
- $C_{BI}$: concentration of solute in the soil water immediately before an irrigation (kg/m$^3$)
- $C_{fe}$: concentration of solute in the soil water at field capacity (kg/m$^3$)
- $C_{out}$: solute concentration of the exiting water (kg/m$^3$)
- ET: evapotranspiration
- $g(z)$: root distribution function
- IV: Imperial Valley drainage water
- $k$: Langmuir affinity adsorption coefficient (L/mg)
- $L$: plant root penetration depth (m)
- LF: leaching fraction
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\( r(\psi) \) reducing factor

SJIV San Joaquin Valley drainage water

\( S(\psi, z) \) volumetric root extraction function

\( T_a \) integral of the volumetric extraction function from the soil surface \((z = 0)\) to the depth of root penetration \((z = L)\)

\( T_aD \) total amount of adsorbed solute in \( V_t \) (kg)

\( T_{AI} \) total amount of solute in a volume, \( V_t \), of soil after an irrigation (kg)

\( T_{BI} \) total amount of solute in a volume, \( V_t \), of soil immediately before an irrigation (kg)

\( T_{in} \) total amount of solute entering \( V_t \) (kg)

\( T_{out} \) total amount of solute leaving \( V_t \) (kg)

\( T_p \) potential volumetric transpiration (m³).

\( T_{sw} \) total amount of solute in the soil water of \( V_t \) (kg)

\( U_l(z) \) relative water uptake over the soil depth interval \( z_1 \) to \( z_2 \) for a linear root distribution

\( U_e(z) \) relative water uptake over the soil depth interval \( z_1 \) to \( z_2 \) for an exponential root distribution

\( V_{AI} \) volume of soil water in \( V_t \) after an irrigation (m³)

\( V_{BI} \) volume of soil water in \( V_t \) immediately before an irrigation (m³) = \( \theta_{BI} V_t \)

\( V_{fc} \) volume of water in \( V_t \) at field capacity (m³) = \( \theta_{fc} V_t \)

\( V_{in} \) volume of water entering \( V_t \) (m³)

\( V_{min} \) minimum volume of soil water in \( V_t \) (m³)

\( V_{out} \) volume of water leaving \( V_t \) (m³)

\( V_t \) a unit volume of soil within the depth interval \( z_1 \) to \( z_2 \) (m³)

\( x/m \) adsorbed concentration of the Langmuir adsorption isotherm (mg/kg)

\( z \) soil depth with zero at the soil surface and positive downward (m)

References


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