

A Functional Model of Solute Transport that Accounts for Bypass

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ABSTRACT

Public awareness of groundwater contamination has created renewed interest in solute transport models that can be practically applied as groundwater quality management tools. Because of their simplicity with regard to input requirements, functional models of solute transport are excellent groundwater quality management tools. A functional model of one-dimensional solute transport that accounts for hydraulic bypass is presented. The transport model, TETrans, simulates the vertical movement of nonvolatile solutes (i.e., trace elements and nonvolatile organic chemicals) through the vadose zone. Plant water uptake is taken into account assuming no solute uptake by the plant. TETrans requires minimal input data for its operation. Since TETrans uses a mass-balance approach to solute transport, it offers the speed of an analytical solution and the versatility of a numerical approach without the need for input parameters, which are difficult to measure. TETrans is able to account for bypass with a single term, the mobility coefficient. The mobility coefficient, γ , represents the fraction of the soil liquid phase, which is subject to piston-type displacement; therefore, $1 - \gamma$ represents the fraction of the liquid phase that is bypassed. The mobility coefficient is a temporally and spatially variable parameter (within a range of 0 to 1), which is calculated from the deviation of the measured chloride concentration from the predicted concentration assuming piston displacement and assuming complete mixing of the resident soil solution and incoming water for a given irrigation and volume of soil. A constant mobility coefficient for a given depth or entire profile can be determined by averaging temporally varying mobility coefficients or averaging spatially and temporally varying mobility coefficients, respectively. In essence, the mobility coefficient simplistically accounts for three physical transport phenomena in a single term. On a microscopic level there is flow through cracks and macropores that bypasses small and dead-end pores. On a macroscopic level there is the flow of a mobile water phase independent of stagnant immobile phase of water, and the phenomenon of dispersion-diffusion. Simulations of chloride movement through a soil lysimeter column for an 1100-d period were compared to measured chloride concentrations in the soil solution at field capacity. A constant mobility coefficient significantly improved the capability of TETrans to describe the data when compared to simulations performed assuming complete piston-type displacement. However, the best simulation to the measured chloride data was for the use of a spatially and temporally variable mobility coefficient.

GROUNDWATER has become a major source of drinking, industrial, and agricultural water. Groundwater supplies will become an even more important natural resource as the world continues its ef-

fort to resolve the dilemma of meeting ever-growing demands for water with rapidly depleted and, at times, polluted surface water supplies. The growing concern over acute and chronic health affects resulting from contaminants in drinking water has brought the degradation of groundwater to the forefront of public attention. Groundwater quality is a primary environmental concern not only for health reasons, but because of the decrease in crop productivity, which can often accompany the use of poor quality irrigation water. The ability to model the migration of pollutants through the vadose zone is an essential tool in combating the degradation of our groundwater.

Over the past three decades numerous conceptual models for the movement of solutes through the unsaturated zone have been developed. Several reviews of these transport models have recently appeared in the literature (Addiscott and Wagenet, 1985; Nielsen et al., 1986; van Genuchten and Jury, 1987; Engesgaard and Christensen, 1988; Feddes et al., 1988). Basically two groups of transport models are recognized: deterministic and stochastic. Within these two categories there are additional subcategories of models. Functional models are a group of deterministic models that utilize simplified treatments of solute and water flow while making no claim to a fundamental description of the mechanisms involved in the transport process. As such, functional models require less input data and computer expertise for their application. Several functional models have been presented in the literature (Bressler, 1967; Tanji et al., 1972; Burns, 1975, 1976; Addiscott, 1977; Rose et al., 1982; Bond and Smiles, 1988).

More than ever before, there is a need for simple, management-oriented models for interpreting and simulating solute movement by leaching. This need for functional transport models arises from two limitations found in more theoretically rigorous mechanistic models of transport. First, the soil data needed for sophisticated analytical and numerical models are typically well beyond the capacity of most real-world users, such as the USEPA, Soil Conservation Service or Agricultural Extension Service. Second, the spatial variability typical of field soils limits the accuracy of application of exact transport theory under field management situations. As pointed out by Bond and Smiles (1988), "... the assumptions used to derive most flow equations presented in the literature are not satisfied in field soils, and analytical solutions of these equations are appropriate only to a very restricted set of initial and boundary conditions." Stochastic transport models do not provide a viable alternative for

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most real-world applications since again the data upon which they are derived are too labor and cost intensive to be practical.

In many well-drained soils, water movement responsible for solute transport can be approximately and simply calculated using water-balance accounting and a knowledge of field capacity. Using this simplified approach, no quantitative knowledge of the soil's hydraulic conductivity and of soil moisture retention curves is required. Previous models have been developed on this premise by Burns (1975), Rose et al. (1982), and Bond and Smiles (1988). However, in each of these models it was assumed that no bypass flow of water and solute through large pores had occurred. In aggregated soil or soil high in clay, bypass flow paths through macropores and cracks has a definite effect on the flow of solutes. In this case, flow can deviate significantly from the near piston-type flow exhibited in some well-drained soils. In addition, soil water is believed to be composed of two phases: an immobile water phase and a mobile water phase (Turner, 1958; Coats and Smith, 1964; Deans, 1963). It is only the mobile water phase that is miscibly displaced by incoming precipitation or irrigation water. The immobile water phase is bypassed. Developed on the premise of mass-balance applied by Burns (1975) and on a consideration of bypass flow, a simplified mathematical model of one-dimensional transport is presented, which simulates the vertical movement of trace elements and nonvolatile organic chemicals through the vadose zone. The model, subsequently referred to as TETrans (*Trace Element Transport*), is specifically designed for real-world transport applications where a minimum of transport parameters are available for the user.¹

THEORY

TETrans is a capacity model that defines changes in amounts of solute and water content rather than rates of change. As such, it is driven by the amounts of rainfall, irrigation, or evapotranspiration (ET) and only considers time indirectly by using the time from one irrigation or precipitation event to another. From a knowledge of water inputs and losses, and of soil-solute chemical interactions, TETrans predicts the average movement of reactive or nonreactive solutes in the unsaturated zone of the soil. Transport through the soil profile is modeled as a series of events or processes for a finite collection of discrete depth intervals. These sequential events or processes include: (i) infiltration and drainage to field capacity (i.e., field capacity represents the water content of a soil after free drainage has stopped, which, in most cases, is approximately 2 to 3 d after an irrigation), (ii) instantaneous chemical equilibration for reactive solutes, (iii) water uptake by the plant root resulting from transpiration and evaporative losses from the soil surface, and (iv) instantaneous chemical reequilibration. Each

process is assumed to occur in sequence within a given depth interval as opposed to reality where transport is a collection of simultaneous processes.

Aside from conceptualizing transport as a sequence of processes, five major theoretical assumptions are made in TETrans. First, drainage occurs through the soil profile to a depth-variable field capacity. Second, for a given depth interval, the depletion of stored water by evaporation and transpiration processes does not go below a field-observable minimum water content that lies above the water content associated with the wilting point of the crop. Third, dispersion is assumed to be either negligible or part of the phenomenon of bypass. Fourth, the chemical processes of adsorption-desorption are nonhysteretic and instantaneous. Fifth, the soil profile can be divided into a finite series of discrete depth intervals with each interval having homogeneous physical and chemical characteristics.

TETrans is a functional, deterministic model of solute transport in the unsaturated zone under transient-state conditions. TETrans accounts for the problem of bypass which in certain soils can have a very profound effect upon the movement and distribution of a solute. Several nonmechanistic transport models have previously addressed the problem of bypass (Addiscott, 1977, 1981; van Ommen, 1985a,b; White, 1985a,b). White (1985a,b) used a transfer function model that is actually a nonmechanistic, stochastic model and is not specifically regarded as a functional, deterministic model. The model of van Ommen (1985b) is a steady-state model. Only the models of Addiscott (1977, 1981) and van Ommen (1985a) are transient-state, functional models similar to TETrans. Addiscott (1977, 1981) used mobile-immobile phases to account for bypass, but was not able to simulate field data well. van Ommen (1985a) dealt with bypass by assuming that a fraction of the applied irrigation or precipitation water flowed directly to the groundwater through cracks and/or macropores, whereas the remainder flowed through the soil matrix. In contrast, TETrans assumes that a fraction of the incoming water entering each and every depth increment or layer is subject to bypass rather than bypassing the complete soil profile to enter the groundwater. Bypass occurs in TETrans from one layer to the next and not for the entire soil profile. Furthermore, previous models have used a fixed water content for the immobile phase, whereas TETrans defines the immobile phase as a fraction of the current residual water content (greater than or equal to the minimum allowable water content) just prior to an irrigation. This subtle difference permits greater latitude in the explicit fit of the mobility coefficient to measured chloride data as described in the subsequent subsection titled Bypass Considerations. In addition, this difference in the definition of the immobile phase allows for the displacement of water and solutes at all water contents above the minimum water content; consequently, even light irrigations will result in a displacement of the solutes. This allows for the modeling of light irrigations or low intensity rainfalls over extended time periods with subsequent downward movement of solute.

On a microscopic scale, bypass can result when water moves through pores where stagnant areas of

¹ The TETrans applications software package is available to interested users. The software package includes the TETrans object code, a software tutorial demo, and a user's manual. Please address requests to the senior author and include a 3.5 or 5.25 inch disk. Specify whether the IBM-compatible or Apple Macintosh version of TETrans is desired.

immobile water exist. This immobile soil water can exist as either a thin film around soil particles resulting from adhesive and cohesive forces, or as stagnant water in dead-end pores (Turner, 1958; Coats and Smith, 1964; Deans, 1963). Adjacent to the immobile film of water around a soil particle lies a mobile water phase. During an irrigation (or precipitation) event the incoming water miscibly displaces the mobile water while the immobile layer is bypassed. On a macroscopic scale, bypass can result from the movement of water through large cracks and channels, thereby bypassing entire aggregates of soil. The net effect of bypass is that some resident soil water containing a solute is not miscibly displaced by incoming water. This subsequently affects the amount of solute within a soil-depth increment.

Bypass flow in flux-based transport models (i.e., mechanistic models) is distinguished by differences in pore-water velocity from one point to the next. In contrast, bypass flow in capacity-based models, such as a simple mass-balance approach, can be approximated by the spatial variation in the quantity of the resident pore-water that is not involved in piston-type displacement following an irrigation or precipitation event. The quantity, or more specifically, the fraction of the total resident soil solution that is not miscibly displaced by incoming irrigation or precipitation water is subject to bypass. In order to address the problem posed by bypass in the most simplistic manner, a single term, the mobility coefficient (γ), which accounts for the effects of bypass due to the presence of immobile water and preferential flow through large pores and cracks, is used in TETrans. The mobility coefficient is defined as the fraction of the resident soil water that is subject to displacement; therefore, $1 - \gamma$ represents the fraction of soil water that is bypassed. The mobility coefficient is analogous to the volume of water theoretically and experimentally shown by Wierenga (1977) to be responsible for solute movement under transient water flow. Because bypass is influenced by the upper boundary condition, the mobility coefficient is very much dependent upon upper boundary conditions as well. For instance, the ponding of irrigation water on the surface will result in a different degree of bypass than lightly sprinkling, even though the same amount of water may have been applied. In TETrans, the mobility coefficient(s) can be constant over time and depth, constant over time and variable with depth, or variable over time and with depth. To determine temporally and spatially variable mobility coefficients, the deviation of the measured chloride concentration in the soil solution from the predicted chloride concentration assuming complete piston-type displacement is used for each irrigation/precipitation event and each depth increment.

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 Appendix for any undefined terms):

A. Infiltration and drainage

1. Before an irrigation (BI) or precipitation,

$$T_{BI} = T_{sw} + T_{ad} = V_i[\theta_{BI}C_{BI} + \rho_b C_{ad}] = V_{BI}C_{BI} + V_i\rho_b C_{ad} \quad [1]$$

where V_i is a unit volume of soil within the depth interval z_1 to z_1 (m^3); T_{BI} is the total amount of solute in V_i immediately before an irrigation (kg); T_{sw} is the total amount of solute in the soil water of V_i (kg); T_{ad} is the total amount of adsorbed solute in V_i (kg); θ_{BI} is the volumetric water content immediately before an irrigation (cm^3/cm^3); C_{BI} is the concentration of solute in the soil water immediately before an irrigation (kg/m^3); ρ_b is the soil bulk density (kg/m^3); C_{ad} is the adsorbed solute concentration (kg/m^3); and V_{BI} is the volume of soil water in V_i immediately before an irrigation (m^3).

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

$$T_{AI} = T_{BI} + T_{in} - T_{out} = T_{BI} + V_{in}C_{in} - V_{out}C_{out} \quad [2]$$

- a. where if $0 < \gamma \leq 1$ and

- (1) if $V_{in} > V_{fc} - (1.0 - \gamma)V_{BI}$ (see Fig. 1a for a schematic of this situation), then

$$V_{out} = V_{in} - V_{fc} + V_{BI} \quad [3]$$

$$C_{out} = [\gamma V_{BI}C_{BI} - V_{fc}C_{in} + V_{in}C_{in} + (1.0 - \gamma)V_{BI}C_{in}] / V_{out} \quad [4]$$

$$V_{AI} = V_{fc} \quad [5]$$

$$C_{AI} = [(1.0 - \gamma)V_{BI}C_{BI} + (V_{fc} - (1.0 - \gamma)V_{BI})C_{in}] / V_{fc} \quad [6]$$

- (2) else if $V_{fc} - V_{BI} < V_{in} \leq V_{fc} - (1.0 - \gamma)V_{BI}$, then

$$V_{out} = V_{in} - V_{fc} + V_{BI} \quad [7]$$

$$C_{out} = C_{BI} \quad [8]$$

$$V_{AI} = V_{fc} \quad [9]$$

$$C_{AI} = [(V_{fc} - V_{in})C_{BI} + V_{in}C_{in}] / V_{fc} \quad [10]$$

- (3) else if $V_{in} \leq V_{fc} - V_{BI}$, then

$$V_{out} = 0 \quad [11]$$

$$C_{out} = 0 \quad [12]$$

$$V_{AI} = V_{BI} + V_{in} \quad [13]$$

$$C_{AI} = (V_{BI}C_{BI} + V_{in}C_{in}) / (V_{BI} + V_{in}) \quad [14]$$

- b. otherwise if $\gamma = 0$ and

- (1) if $V_{in} > V_{fc} - V_{BI}$ (see Fig. 1b for a schematic of this situation), then Eq. [3], [4], [5], and [6] are applied.

- (2) else if $V_{in} \leq V_{fc} - V_{BI}$, then Eq. [11], [12], [13], and [14] are applied.

where T_{AI} represents the total amount of solute in a volume, V_b , of soil after an irrigation (kg); T_{in} is the total amount of solute entering V_i (kg); T_{out} is the total amount of solute leaving V_i (kg); V_{in} is the volume of water entering V_i (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_i (m^3); C_{out} is the

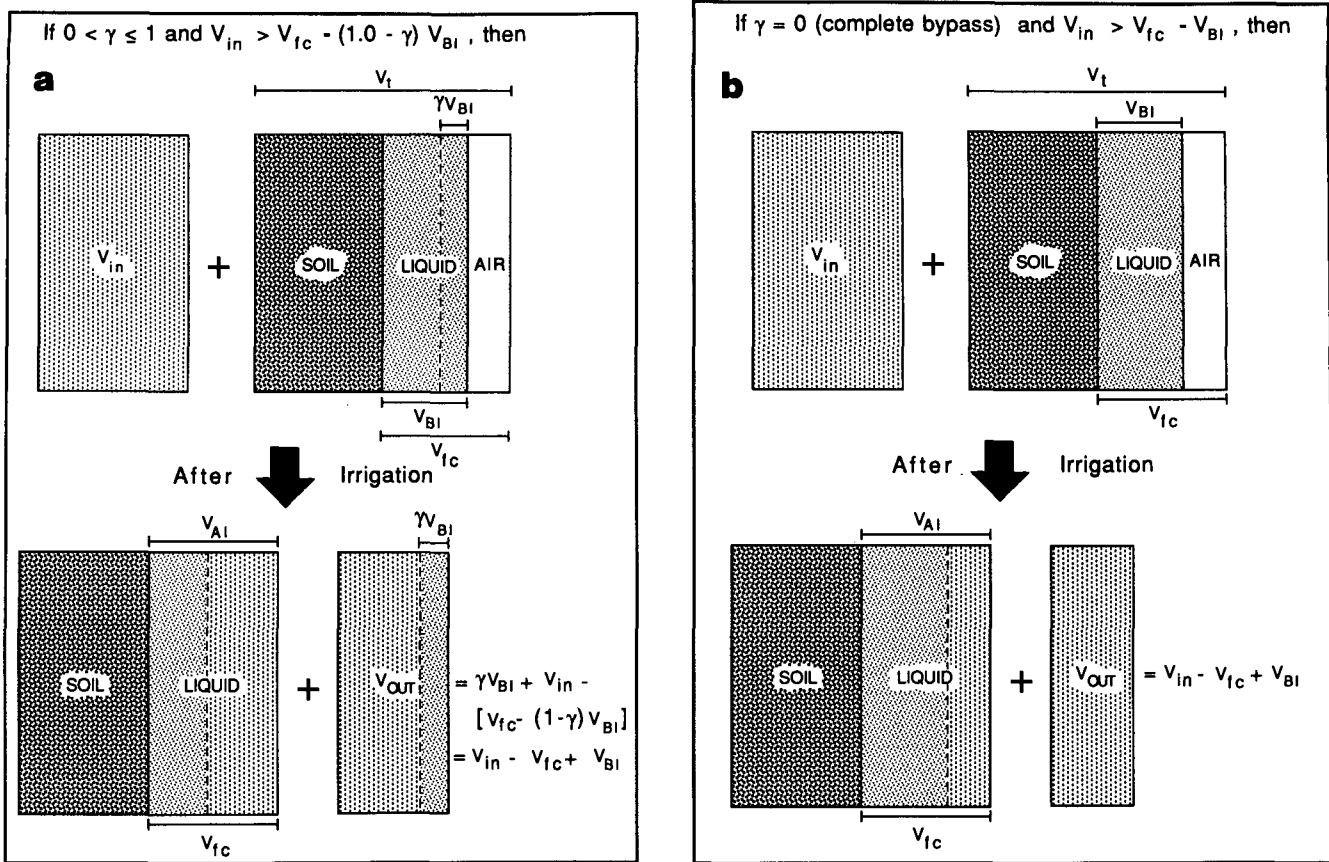


Fig. 1. (a) Conceptual schematic illustrating the influx of irrigation water into a unit volume of soil, V_n , under the conditions of $0 < \gamma \leq 1$ and $V_{in} > V_{fc} - (1.0 - \gamma)V_{BI}$. (b) Conceptual schematic illustrating the influx of irrigation water into a unit volume of soil, V_n , under the conditions of $\gamma = 0$ and $V_{in} > V_{fc} - V_{BI}$.

solute concentration of the exiting water (kg/m^3); γ is the mobility coefficient, or more specifically, the fraction of V_{BI} that 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} that is subject to bypass; V_{AI} is the volume of soil water in V_i after an irrigation (m^3); and V_{fc} is the volume of water in V_i at field capacity (m^3).

B. Chemical equilibration

Chemical equilibration involves the partitioning of a reactive solute into the solution and adsorbed phases. Since chloride is a nonreactive solute, no partitioning into solution and adsorbed phases is described herein (see Corwin et al., 1991, unpublished data, for a complete discussion of the partitioning of a reactive solute).

C. 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. TETrans does not account for the up-

ward movement of solute resulting from the processes of evaporation or transpiration. Evapotranspiration is only viewed as a sink for water loss that results in the concentration of the solute within the root zone. It is not viewed as creating a potential gradient that results in the net upward or downward movement of the solute between depth increments.

In TETrans 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 (1987), which is a synthesis of previous models and work presented by Molz and Remson (1970), Feddes et al. (1978), Hoagland et al. (1981), Ritchie (1984), Ritchie and Otter (1984), and Prasad (1988). On a capacity basis, the volumetric root extraction function, S , is expressed by,

$$S(\Psi, z) = r(\Psi)g(z)T_p \quad [15]$$

where Ψ 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 (1987) expresses the linear root distribution function by,

$$g(z) = [\alpha_1(2z - L) + L]/L^2 \quad [16]$$

where, α_1 is the linear plant root distribution coeffi-

cient ($-1 \leq \alpha_1 \leq 1$), $z \leq L$ 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 TETrans 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, $U(z)$, over the soil depth interval z_1 to z_2 (where, $0 \leq z_1 < z_2 \leq L$) becomes,

$$U(z) = (\alpha_1/L^2)(z_2^2 - z_1^2) - [(\alpha_1/L) - (1/L)](z_2 - z_1) \quad [17]$$

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

$$U_e(z) = (e^{-az_1} - e^{-az_2})/(1 - e^{-aL}) \quad [18]$$

where $a = \alpha_2/L$, and α_2 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 that corresponds to the relative plant root water uptake expressed by either Eq. [17] or [18], 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 that 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 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} .

D. Chemical reequilibration

No reequilibration is required for a nonreactive solute (see Corwin et al., 1991, unpublished data, for a discussion of the reequilibration of reactive solutes).

Bypass Considerations

The determination of temporally and spatially variable mobility coefficients is based upon the deviation of measured soil solution chloride concentrations from calculated concentrations assuming complete piston-type displacement of solute. In TETrans this deviation is assumed to be attributed in large part to bypass resulting from preferential movement through macropores and from the movement of a mobile water phase, thereby bypassing small dead end pores and a stagnant immobile phase of water. Though dispersion

and anion exclusion would also account for the deviation of chloride transport from strict piston flow, these effects are assumed to be negligible. If dispersion is a significant factor, then its effects are assumed to be inclusive within the bypass phenomenon, and compensated for in the mobility coefficient. To calculate the mobility coefficient, γ , for each irrigation and for each depth increment, Eq. [2] and [4] are used. Eq. [2] can be rearranged to give Eq. [19]

$$C_{out} = (T_{BI} + V_{in}C_{in} - T_{AI})/V_{out} \quad [19]$$

and Eq. [4] can be rearranged to give Eq. [20]

$$\gamma = (V_{out}C_{out} - V_{out}C_{in})/(V_{BI}C_{BI} - V_{BI}C_{in}) \quad [20]$$

Since T_{AI} can be calculated from the measurement of the chloride concentration of the soil solution at field capacity (for a nonreactive solute, $T_{AI} = V_{fc}C_{fc}$), then γ can be determined by substituting Eq. [19] into Eq. [20]

$$\gamma = (V_{in}C_{in} + T_{BI} - V_{fc}C_{fc} - V_{out}C_{in})/(V_{BI}C_{BI} - V_{BI}C_{in}) \quad [21]$$

which is the same as multiplying Eq. [5] and [6] and solving for γ . Equation [21] holds for the situation where $V_{in} > V_{fc} - (1.0 - \gamma)V_{BI}$ for $0 < \gamma \leq 1$. However, since γ is precisely the term that is being determined, then Eq. [21] can only explicitly be used when $V_{in} > V_{fc}$. If it is found that the total chloride, T_{AI} , measured for a depth increment is equal to Eq. [9] multiplied by Eq. [10] (i.e., $T_{AI} = (V_{fc} - V_{in})C_{BI} + V_{in}C_{in}$), then it is known that the condition $V_{fc} - V_{BI} < V_{in} < V_{fc} - (1.0 - \gamma)V_{BI}$ for $0 < \gamma \leq 1$ is the case; consequently, it is assumed that

$$\gamma = (V_{in} - V_{fc} + V_{BI})/V_{BI} \quad [22]$$

since it is impossible to determine γ explicitly and this represents the closest logical approximation. If the total measured chloride is equal to Eq. [13] multiplied by Eq. [14] (i.e., $T_{AI} = V_{BI}C_{BI} + V_{in}C_{in}$), then it is known that the condition $V_{in} \leq V_{fc} - V_{BI}$ exists; consequently, $\gamma = 0$ is assumed. If $T_{AI} = V_{BI}C_{BI} + (V_{fc} - V_{BI})C_{in}$ (i.e., T_{AI} equals Eq. [5] multiplied by Eq. [6] for $\gamma = 0$) when $V_{in} > V_{fc} - V_{BI}$, then $\gamma = 0$. The only condition for which γ has not been determined is when $V_{fc} - (1.0 - \gamma)V_{BI} \leq V_{in} \leq V_{fc}$ for $0 < \gamma \leq 1$. If all other conditions are not met, then this condition is assumed to be the case and Eq. [21] is invoked. Anomalous situations could arise where γ is calculated by Eq. [21] to be outside its defined range. By definition $0 \leq \gamma \leq 1$, so if γ is calculated to be less than 0, then γ is set equal to 0. Similarly, if γ is calculated to be greater than 1, then γ is set equal to 1. The possible reasons for γ extending beyond the range of 0 to 1 are discussed in the results section.

METHODS AND MATERIALS

A transport experiment which extended over an 1100-d time period was conducted to test TETrans' ability to account for bypass. The study used weighing soil lysimeter columns. The columns were constructed of PVC and stood 1.52 m tall with a radius of 0.227 m. The columns were filled with Arlington loam (Haplic Durixeralf). Soil solution extractors, TDR probes, and tensiometers were installed hor-

izontally along the side of the soil column at depths of 0.075, 0.225, 0.375, 0.525, and 0.675 m. A free-flow drain was at the bottom of the column. The lysimeter column design and strategy have been previously described in detail by Waggoner et al. (1990, unpublished data). Basically, the study involved monitoring the movement of salts (major cation and anions, including chloride) and boron through the root zone for various irrigation management strategies.

The water flow (including bypass) and the plant water uptake of TETrans were tested by a comparison of predicted to measured concentration distributions of chloride in the soil solution. Soil solution extracts were taken at every depth following each irrigation. The solution samples were taken when a given depth reached field capacity as measured with TDR.

Out of 24 columns used in the study, one representative column was chosen. Its selection was based on the fact that varying irrigation water qualities were used, that unexpected anomalous water flow behavior (presumed to be bypass) also occurring in several other columns was present and that a complete set of data existed for the 1100 d of their study. The irrigation waters used in the study were synthesized to approximate the chemical composition of California Aqueduct water and San Joaquin Valley drainage water. Good quality irrigation water (i.e., California Aqueduct water, which is low in salts and boron) was initially applied prior to planting and continued through the germination stage of each crop. This was followed by irrigating with a poor quality water (i.e., San Joaquin Valley drainage water, which is higher in salts and boron) through the crop's maturity and up until harvest. The rotation of good quality water with a poor quality water provided a more dynamic system to test TETrans' simulation capabilities (see Corwin et al., 1991, unpublished data). Along with the cyclical application of irrigation waters of sharply contrasting qualities, the crop was also rotated. A general treatment management description and the general chemical composition of the synthesized irrigation waters are provided in Tables 1 and 2, respectively.

The data needed to test the hydraulic aspect of TETrans' simulation capability included; initial chloride concentration in the soil water; initial water content of the soil; dates and amounts of irrigation water applied; total evapotranspiration

lost between irrigations; horizonization of the soil with the associated bulk density, water content at field capacity, and water content at the wilting point for each horizon depth increment; chloride concentration of each irrigation water applied; chloride concentration of the soil solution (at field capacity) after selected irrigations; and date of planting, days of maturity, date of harvest, maximum depth of root penetration, and plant root distribution for each crop. Figures 2, 3 and 4, and Table 3 are a compilation of all the input data for TETrans. Figure 2 shows the amount of irrigation water and when it was applied to the soil column. The fluctuating chloride concentration (approximately 2 and 50 meq/L) shown in Fig. 3 demonstrates how the different irrigation water qualities were cycled. The total evapotranspiration between irrigations is determined from Fig. 4 (i.e., ET rate multiplied by time). Table 3 shows miscellaneous input data for TETrans.

Though seemingly formidable in its input requirements, TETrans is far less parameter intensive than most other transport models, especially previous numerical deterministic models. In addition, the input parameters are more readily obtained than those needed for most other transport models that require a knowledge of hydraulic conductivities, water content-matric potential relationships, and dispersion-pore water velocity relations.

RESULTS

The measured chloride concentrations in the soil solution for each of the five depth increments under observation are shown in Fig. 5. The soil solution samples were taken at the midpoint (i.e., 0.075, 0.225, 0.375, 0.525, and 0.675 m) of each depth increment: 0 to 0.15, 0.15 to 0.30, 0.30 to 0.45, 0.45 to 0.60, and 0.60 to 0.75 m. Because TETrans determines the average movement of solute from one depth increment to another, comparisons with measured chloride concentrations are done on a depth increment basis. In order to minimize

Table 1. General treatment description of the soil lysimeter column.

Type of irrigation: cyclical			
Irrigation waters: California Aqueduct water and San Joaquin Valley drainage water.			
Crop rotation: milo [<i>Sorghum bicolor</i> (L.) Moench] and wheat (<i>Triticum aestivum</i> L.)			
Days to crop maturity:	milo	45 d	
	wheat	45 d	
Crop planting dates:	milo	22 June 1983	173
		(calendar) =	(day of experiment)
	wheat	18 Jan. 1984	393
	milo	3 July 1984	550
	wheat	21 Dec. 1984	721
	milo	19 June 1985	901
Crop harvesting dates:	milo	3 Oct. 1983	276
	wheat	5 June 1984	522
	milo	27 Nov. 1984	695
	wheat	7 June 1985	889
	milo	10 Oct. 1985	1014

Table 2. Chemical composition of the synthesized irrigation waters.

Irrigation water	Ca	Mg	Na	K	Cl	SO ₄	HCO ₃	B	EC
				meq/L				kg/L	dS/m
California aqueduct water	2.2	1.3	3.1	0.1	2.2	3.0	1.5	0.3	0.7
San Joaquin Valley drainage water	25.7	13.9	49.1	0.2	47.7	38.2	3.0	6.0	8.0

Table 3. Additional input parameters for TETrans.

Depth increments (m):	0.0 -0.15
	0.15-0.30
	0.30-0.45
	0.45-0.60
	0.60-0.75
Initial conditions (all depth increments)	
soil solution chloride concentration (meq/L):	0.0
soil water content (m ³ /m ³):	0.29
Physical properties (all depth increment)	
bulk density (kg/m ³):	1600.0
water content at field capacity (m ³ /m ³):	0.29
water content at wilting point (m ³ /m ³):	0.09
Crop parameters	
maximum root penetration (m):	wheat 0.90
	milo 0.90
plant root distribution:	wheat 40-30-20-10 (Molz & Remson, 1970)
	$\alpha_1 = -0.8$ or $\alpha_2 = 1.5$
	milo 40-30-20-10 (Molz & Remson, 1970)
	$\alpha_1 = -0.8$ or $\alpha_2 = 1.5$

redundancy, any future discussion will be restricted for the most part to the shallowest and deepest increments: 0.0 to 0.15 and 0.60 to 0.75 m.

Figures 6, 7, and 8 show a gradual improvement in the predictive quality of TETrans to simulate chloride movement using different mobility coefficients. Each figure compares the measured chloride concentration in the soil solution to the predicted concentration for a given depth over the 1100 d of the study. Figure 8a-c shows the best simulation to the measured chloride soil solution data using temporally and spatially variable mobility coefficients. However, the use of a single

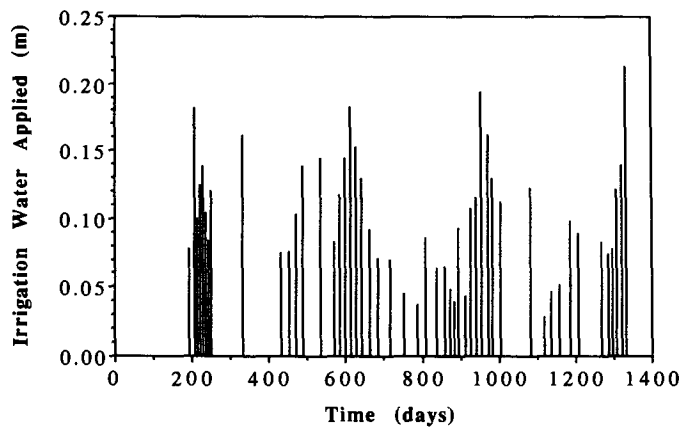


Fig. 2. Irrigation times (days) and amounts (m).

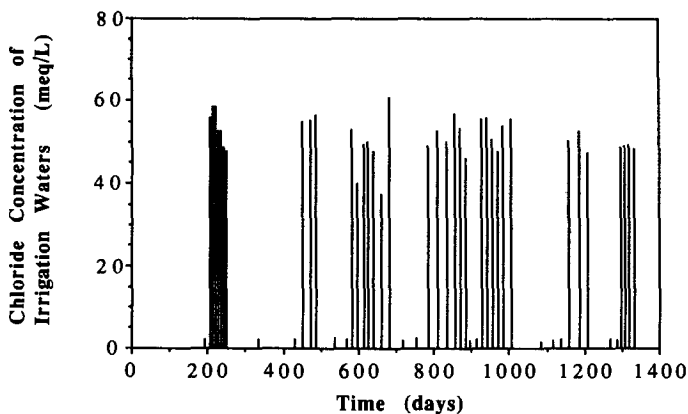


Fig. 3. Chloride concentration (meq/L) of the applied irrigation waters.

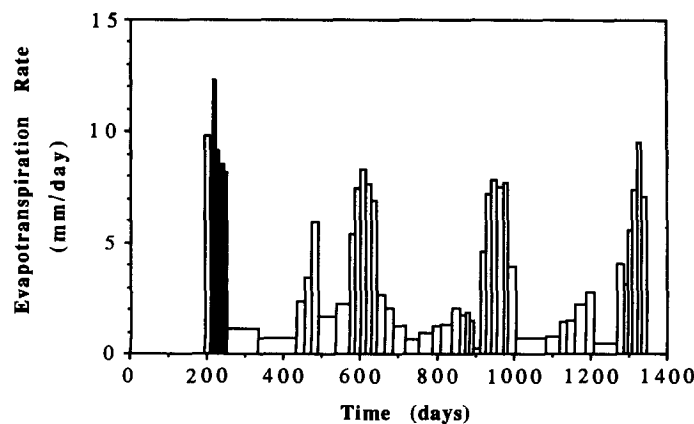


Fig. 4. Average evapotranspiration rate (mm/day) between irrigations.

mobility coefficient, $\gamma = 0.498$, which is an average of all the temporally and spatially variable mobility coefficients used in Fig. 8 likewise shows an extremely close simulation to the measured data (see Fig. 7a-c).

The mobility coefficient provides useful information regarding temporal and spatial changes in bypass. Ta-

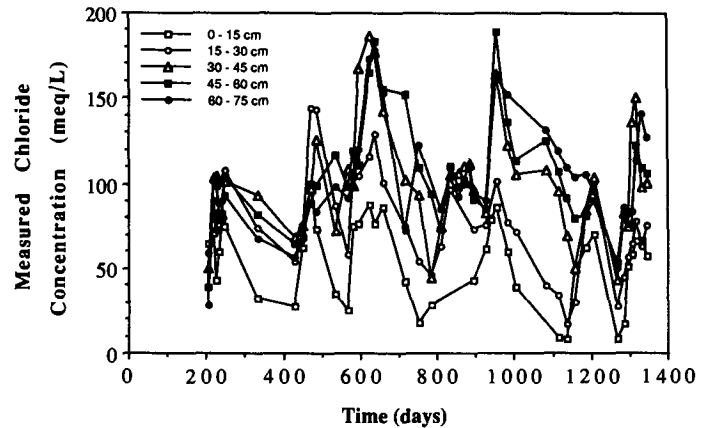


Fig. 5. Measured chloride concentration (meq/L) in the soil extract taken at depths of 0.075, 0.225, 0.375, 0.525 and 0.675 m.

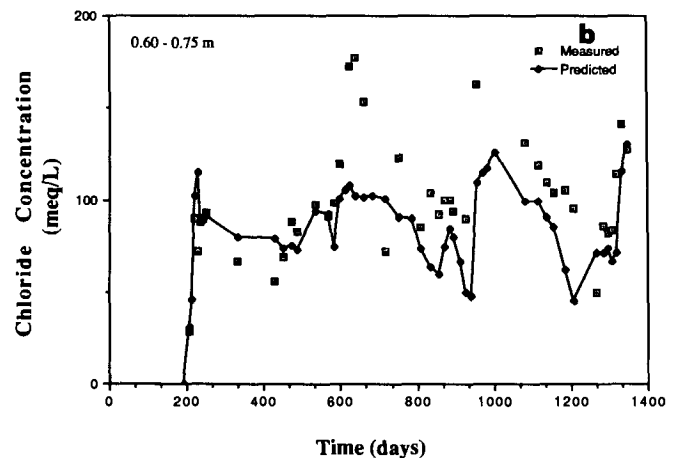
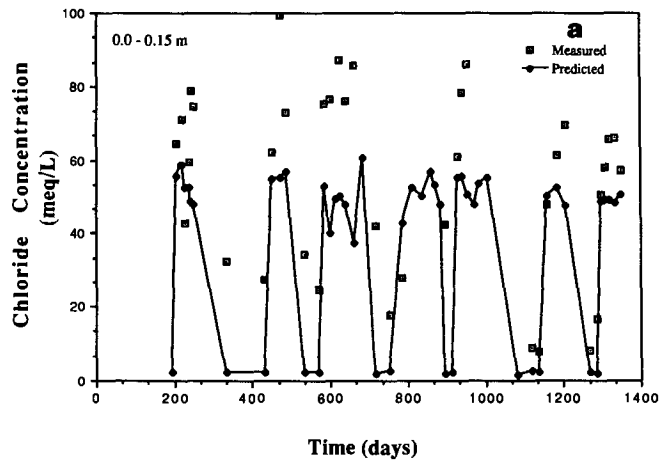


Fig. 6. (a) Comparison of measured chloride concentrations and predicted concentrations assuming complete piston-type displacement ($\gamma = 1.0$) for the depth increment 0-0.15 m. (b) Comparison of measured chloride concentrations and predicted concentrations assuming complete piston-type displacement ($\gamma = 1.0$) for the depth increment 0.60-0.75 m.

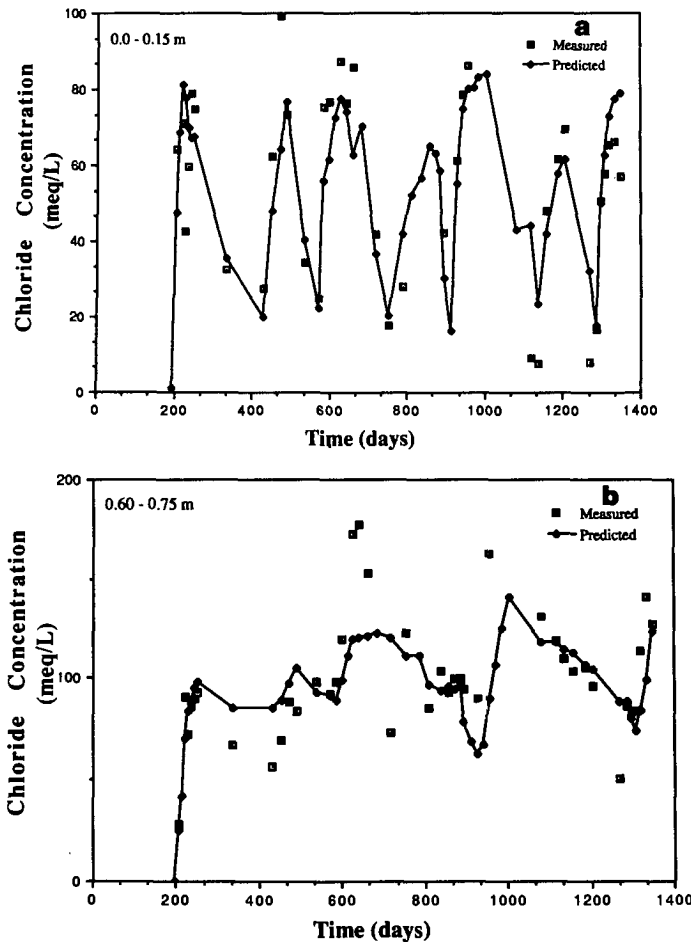


Fig. 7. (a) Comparison of measured chloride concentrations and predicted concentrations assuming $\gamma = 0.5$ for the depth increment 0–0.15 m. (b) Comparison of measured chloride concentrations and predicted concentrations assuming $\gamma = 0.5$ for the depth increment 0.60–0.75 m.

ble 4 shows a summary of the effects of seasonal change upon bypass. Specifically, Table 4 indicates the temporal and spatial variation in the mobility coefficient as a result of seasonal change.

DISCUSSION OF RESULTS

Figure 5 shows the measured chloride concentration in the soil extract taken at field capacity at depth increments of 0.30 m starting with a depth of 0.15 m. A general cyclical trend in chloride is seen that roughly follows the trend of evapotranspiration (see Fig. 4). As the evapotranspiration increases during the summer months, so does the chloride concentration particularly at the shallower depths. This could be a consequence of extracting soil solution samples at a water content drier than field capacity or due to a cyclical change in bypass. Because particular caution was taken to obtain soil solution extracts at field capacity by taking continuous TDR measurements, it is unlikely that soil solution extraction error was significant. However, a cyclical trend in bypass does seem likely. High temperatures and low humidity in the summer months produced a noticeably drier soil surface for the top few centimeters (0–0.075 m) of soil, which produced sur-

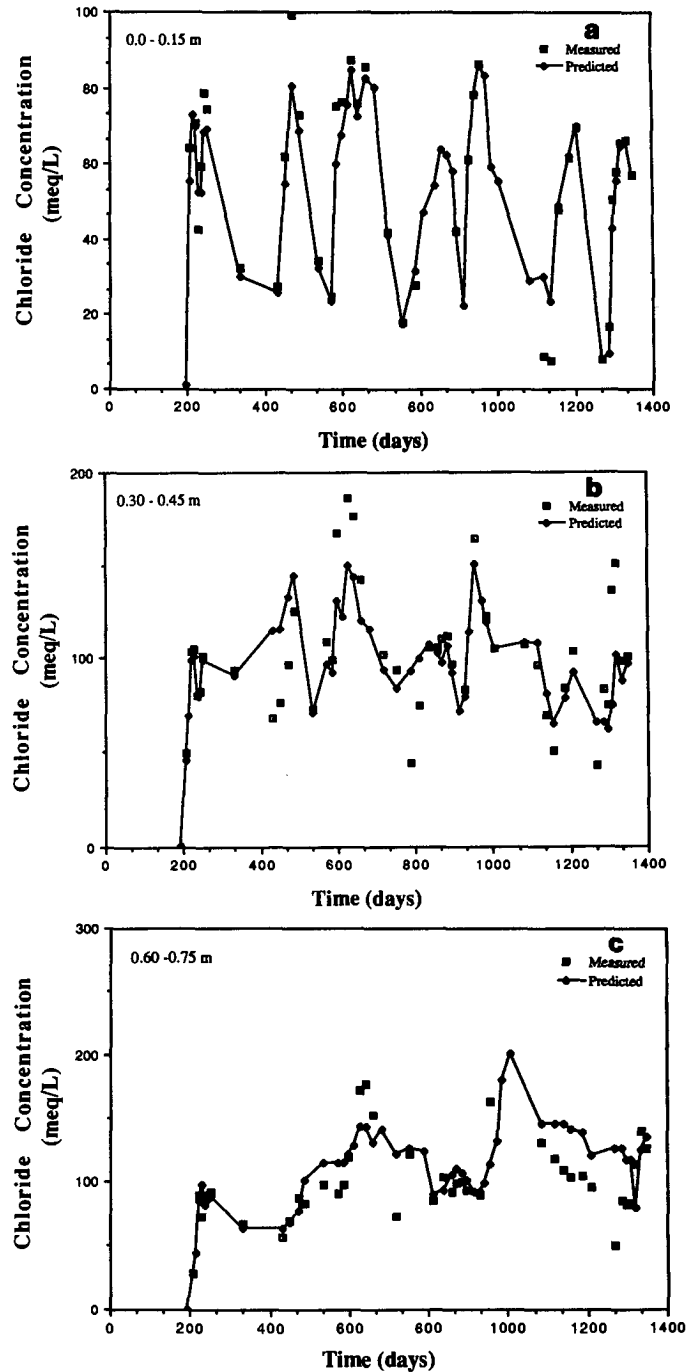


Fig. 8. (a) Comparison of measured chloride concentrations and predicted concentrations using temporally and spatially varying mobility coefficients for the depth increment 0–0.15 m. (b) Comparison of measured chloride concentrations and predicted concentrations using temporally and spatially varying mobility coefficients for the depth increment 0.30–0.45 m. (c) Comparison of measured chloride concentrations and predicted concentrations using temporally and spatially varying mobility coefficients for the depth increment 0.60–0.75 m.

faces cracks not noticeable during the winter months. The dry soil surface due in large part to surface evaporation resulted in increased cracking at the surface as compared with the winter months. Furthermore, an analysis of the seasonal-average mobility coefficient for each depth increment shows greater bypass to oc-

Table 4. Average mobility coefficients and associated standard deviations (in parenthesis) for the summer (July–August–September) and winter (January–February–March) months over the 1100 d of the study.

Year	Depth increment, m	Average mobility coefficient (γ)	
		July–August–September	January–February–March
1983	0.00–0.15	0.310 ± 0.097	0.468 ± 0.071
	0.15–0.30	0.399 ± 0.080	0.517 ± 0.065
	0.30–0.45	0.507 ± 0.111	0.573 ± 0.091
	0.45–0.60	0.540 ± 0.065	0.581 ± 0.054
	0.60–0.75	0.541 ± 0.021	0.582 ± 0.033
1984	0.00–0.15	0.362 ± 0.163	0.471 ± 0.173
	0.15–0.30	0.425 ± 0.161	0.526 ± 0.144
	0.30–0.45	0.466 ± 0.011	0.631 ± 0.044
	0.45–0.60	0.571 ± 0.077	0.581 ± 0.081
	0.60–0.75	0.550 ± 0.053	0.588 ± 0.054
1985	0.00–0.15	0.391 ± 0.102	0.454 ± 0.086
	0.15–0.30	0.463 ± 0.083	0.522 ± 0.055
	0.30–0.45	0.583 ± 0.076	0.565 ± 0.054
	0.45–0.60	0.513 ± 0.024	0.509 ± 0.011
	0.60–0.75	0.522 ± 0.065	0.531 ± 0.037
1986	0.00–0.15	0.403 ± 0.101	—
	0.15–0.30	0.458 ± 0.131	—
	0.30–0.45	0.452 ± 0.054	—
	0.45–0.60	0.503 ± 0.041	—
	0.60–0.75	0.511 ± 0.042	—

cur in the summer months than in the winter months (see Table 4). The fact that less bypass occurred during the winter resulted in a greater displacement of the resident soil solution, which lowered the chloride in the profile. In contrast, the increased bypass that occurred in the summer as reflected by the lower mobility coefficients resulted in the concentration of the chloride within the bypassed soil aggregates due to evapotranspiration.

Table 4 shows a comparison of the average mobility coefficient for summer (July–August–September) and winter months (January–February–March). The table substantiates the temporal and spatial change in bypass as a consequence of the formation of surface cracks caused by the extreme surface temperatures and low humidity of the summer months. In general, bypass was greater during the summer months, and regardless of the season was greatest for the top two depth increments, 0 to 0.15 and 0.15 to 0.30 m. Below 0.30 to 0.45 m the level of bypass was fairly constant and the variation as reflected by the standard deviation was less. In general, the standard deviation was less at each depth for the winter months than the summer months, indicating less variability in the mobility coefficient from July through September for the 1100 d of the study.

Comparisons of measured chloride concentrations in the soil solution and of simulated chloride concentrations assuming complete piston-type displacement (i.e., $\gamma = 1$) for the two depth increments are shown in Fig. 6a and 6b. It is quite obvious from these figures that the transport of chloride is not by strict piston displacement alone. It has been well known for decades that the movement of chloride through soil does not exhibit a behavior that is strictly piston-type in nature since several processes will influence its movement including bypass, dispersion, diffusion and anion exclusion. By the physical and chemical nature of the soil used in the lysimeter (i.e., loam), diffusion and

anion exclusion would not seem to cause the major discrepancies that are seen in Fig. 6a and 6b. However, an artifact of the design of the lysimeter, the problem of bypass down the side of a soil column, as well as additional bypass through cracks and large pores, may be an extremely significant factor.

Using a constant mobility coefficient of 0.5 for all depths and all irrigations resulted in a significantly improved fit of the calculated chloride concentrations to the measured chloride data (see Fig. 7a and 7b). A mobility coefficient of 0.5 was used because the average of all temporally and spatially variable mobility coefficients was $\gamma = 0.498 \pm 0.056^{**}$ (**represents the 99% confidence level). Though all of the factors of diffusion, dispersion, and anion exclusion would cause a departure from the solute movement and distribution, which is characteristic of piston displacement, bypass is probably the predominant cause in this particular study. This notion is indicated by the improved fit of the simulations to measured values using a mobility coefficient of 0.5 and by measures of water content changes that were recorded for the lysimeter using time domain reflectometry (TDR). The TDR probes installed at each of the soil solution sampler depths (0.075, 0.225, 0.375, 0.525, 0.675, and 0.825 m) indicated a rapid initial movement of water along the sides of the column just after irrigation water was applied. This was noticeable in the upper half of the lysimeter. However, the movement of water down the side of the lysimeter is probably not the predominant means of bypass since an effort was made before each irrigation to fill these cracks as best as possible. Several cracks crisscrossing the soil surface were usually present at the time of irrigation, particularly in the summer months when the soil surface would dry out to a greater extent than during the winter months. These cracks would visibly extend 0.15 m to as much as 0.30 m into the soil. So, not only did the flow of irrigation water down the sides of the column occur, but flow through surface cracks, root channels, and macropores that bypass entire soil aggregates, smaller pores, and dead end pores were likely.

The best overall fit of predicted to measured chloride data for all depth increments was for the use of temporally and spatially variable mobility coefficients. Simulated and measured results for 3 of the 5 depth increments are shown in Fig. 8a, 8b, and 8c. There are several potential reasons why the mobility coefficient would vary over time and depth. First is the lysimeter design. As mentioned, bypass down the column sides was at times noticeable from TDR measurements made just following the application of irrigation water. Because the columns were not insulated and were constructed of PVC, it is reasonable to believe that the PVC would heat up during the hotter months and expand away from the soil, thereby causing greater bypass. From TDR measurements it could be seen that the cracks extended as far down as 0.5 m and may have even gone deeper. However, an effort was made to minimize bypass down the side of the lysimeter by filling those cracks adjacent to the column with soil. Cracks that occurred elsewhere on the soil surface were not filled since these were considered to represent fissures that would naturally occur as a result of wetting

and drying processes. These naturally occurring cracks are probably responsible for the majority of bypass, particularly near the soil surface. Another reason is the channeling of water along plant roots and through root channels. As the root system increases over the maturation of the plant, the channeling of water would become more pronounced. Harvesting the plant would result in root death and shrinkage leaving an open channel. With time, these channels would fill with fine soil particles that filter through the soil and diminish channeling effects. Finally, deficiencies in the underlying assumptions of the model would be a factor. All of these factors would result in a changing level of bypass as indicated by changing mobility coefficients, both over time and with depth.

An indication of the general behavior of water flow may be deduced from the average of the temporally and spatially varying mobility coefficients for each depth increment. The depth-averaged mobility coefficients are 0.406 ± 0.135 , 0.470 ± 0.134 , 0.55 ± 0.120 , 0.520 ± 0.117 , and 0.540 ± 0.106 for depths 0 to 0.15, 0.15 to 0.30, 0.30 to 0.45, 0.45 to 0.60, and 0.60 to 0.75 m, respectively. The depth-averaged mobility coefficients sharply increase for the top two increments and then level off for the bottom three depths. This would indicate that greater bypass is occurring in the upper portion of the profile, which is probably the result of larger and greater numbers of cracks. The cracks at the surface are expected because of the drying out of the soil by evaporation and transpiration. The gradual decrease in the standard deviation with increased depth shows less temporal variation in the mobility coefficient at the lower depths. Ostensibly, seasonal changes in evaporation and transpiration are influencing the variation in bypass over the top 0.45 m of soil.

In several instances the calculated temporally and spatially variable mobility coefficients were either less than 0 or greater than 1, and thereby, had to be set to 0 and 1, respectively. The reason for this occurring would be the result of processes such as dispersion-diffusion and anion exclusion, as well as from experimental errors in obtaining a true measure of the average chloride concentration for a depth increment. Experimental error would be the result of samples taken at something other than field capacity, errors in chemical analysis, faulty sampling technique (i.e., not discarding solution present in the extractor that corresponded to a previous irrigation), or solute bypassing the solution extractor. Any one or a combination of these factors could have resulted in the determination of anomalous mobility coefficients.

SUMMARY

A functional model of solute transport through the unsaturated zone is presented. TETrans simplistically accounts for hydraulic bypass in its treatment of water flow. Using a weighing lysimeter the model was tested for its ability to simulate the movement of a non-reactive solute, chloride, in order to verify the water flow and plant water uptake portions of the model. Results showed that the use of a single adjustable pa-

rameter, the mobility coefficient, improved the predictive quality of the model.

The mobility coefficient represents the fraction of the resident soil water at the time of an irrigation, which is miscibly displaced by incoming water. The bypassed water includes both immobile water that is tightly held to soil particles by adhesive and cohesive forces, and water that is bypassed by incoming water moving preferentially through macropores or cracks in the soil. Other factors such as the effects of dispersion and diffusion would also be included, since they also represent a deviation from piston flow.

TETrans provides a practical means of modeling water movement under transient-state conditions since the input parameters needed for its operation are minimal and easily obtained in comparison to previous analytical and numerical mechanistic models of water flow. The only laboratory analysis required is the routine and quick measurement of chloride in soil solution extracts for the determination of the temporally and spatially varying mobility coefficient. The only essential parameter that is difficult to determine is the total evapotranspiration. Currently, subroutines of various ET models are being incorporated into TETrans source code to provide an estimation of evapotranspiration from more readily available meteorological data. A lysimeter experiment for various reactive solutes is being conducted to test the performance of TETrans using these ET models. All other input parameters required for the operation of TETrans are either easily estimated (e.g., plant root water uptake distribution, maximum plant root penetration) or available from quick and routine methods of measurement (e.g., bulk density; amount of applied water; field capacity water content; water content at the wilting point; initial conditions; horizon thicknesses; dates of planting, maturation, harvesting, and irrigation). Only for reactive solutes do additional analytical parameters become necessary. For trace elements and organic chemicals, adsorption coefficients are needed.

For field applications, the degree of bypass occurring at a location can be determined from temporal and spatial measurements of chloride concentration in the soil solution. Soil solution extractors installed at selected depths (preferably at the center of different soil horizons) are used to take soil solution extracts 2 to 3 d after each irrigation when the soil is at field capacity. The soil solution extracts are measured for chloride concentration. Using a subroutine within TETrans, the deviation of the measured chloride concentrations from the predicted concentrations assuming piston displacement is used to calculate temporally and spatially variable mobility coefficients. For texturally similar depth increments, the temporally and spatially variable mobility coefficients can be averaged to determine a constant mobility coefficient. As seen in Fig. 7, a constant mobility coefficient can still render excellent simulations of water flow (i.e., as demonstrated by the close fit of chloride data). In addition, a constant mobility coefficient can then be projected forward in time and TETrans can be used for predictive purposes without the need for the continuous measurement of chlorides. This approach for determining bypass is relatively quick, easy, and cost ef-

fective since the measurement of soil solution chloride is one of the most routine and inexpensive soil chemical analysis to perform.

Presumably the use of a mobility coefficient(s) determined from chloride data should improve TE-Trans' ability to model the movement and distribution of a reactive solute because of the improved accuracy in simulating the water flow and plant water uptake aspects of transport. Corwin et al. (1991, unpublished data) test this hypothesis with a lysimeter experiment that evaluates the performance of TE-Trans' solute transport simulation capabilities for the movement of boron with the use of both constant and variable mobility coefficients.

APPENDIX

Terms Used in this Article with Definitions

Abbreviation	Definition
α_1	Linear plant root distribution coefficient ($-1 \leq \alpha_1 \leq 1$)
α_2	Exponential plant root distribution coefficient ($\alpha_2 > 0$)
γ	Mobility coefficient, or more specifically, the fraction of V_{BI} that 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} that is bypassed
ρ_b	Soil bulk density (kg/m^3)
Ψ	Soil-water suction head (m)
θ_{BI}	Volumetric water content immediately before an irrigation (cm^3/cm^3)
θ_{fc}	Volumetric water content at field capacity (cm^3/cm^3)
a	α_2/L
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_{fc}	Concentration of solute in the soil water at field capacity (kg/m^3)
C_{in}	Solute concentration of the entering water (kg/m^3)
C_{out}	Solute concentration of the exiting water (kg/m^3)
$g(z)$	Root distribution function
L	Plant root penetration depth (m)
$r(\Psi)$	Reducing factor
$S(\Psi, z)$	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_i (kg)
T_{AI}	Total amount of solute in a volume, V_i , of soil after an irrigation (kg)
T_{BI}	Total amount of solute in a volume, V_i , of soil immediately before an irrigation (kg)
T_{in}	Total amount of solute entering V_i (kg)
T_{out}	Total amount of solute leaving V_i (kg)
T_p	Potential volumetric transpiration (m^3)
T_{sw}	Total amount of solute in the soil water of V_i (kg)
$U(z)$	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_i after an irrigation (m^3)
V_{BI}	Volume of soil water in V_i immediately before an irrigation (m^3) = $\theta_{BI}V_i$
V_{fc}	Volume of water in V_i at field capacity (m^3) = $\theta_{fc}V_i$
V_{fc}	Volume of water in V_i at field capacity (m^3) = $\theta_{fc}V_i$
V_{in}	Volume of water entering V_i (m^3)
V_{min}	Minimum volume of soil water in V_i (m^3)
V_{out}	Volume of water leaving V_i (m^3)
V_i	A unit volume of soil within the depth interval z_1 to z_2 (m^3)
z	Soil depth with zero at the soil surface and positive downward (m)

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