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DESCRIPTION OF EQUILIBRIUM CHEMISTRY DURING

SOIL-WATER TRANSPORT

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Description of soluble salt leaching through soils and into groundwaters has been the focus of several research studies in recent years (Tanji et al. 1972; Dutt et al. 1972; Oster and Rhoades 1975; Melamed et al. 1977; Jury et al. 1978). The simulation models produced by these investigators have involved various levels of sophistication in the description of the constant processes of soil water transport and chemical reaction of solutes. Mechanistic water flow models (Melamed et al. 1977) often include empirical description of chemistry, while more complete soil chemistry description (Tanji et al. 1972; Dutt et al. 1972) has often been accompanied by a simple water flow model. The result of these facts has been the development of models limited in their transferability to other experimental cases, or models that sometimes produce questionable results when applied to situations for which they were not developed. With these considerations in mind, a detailed simulation model has been developed describing the one-dimensional soil water transport of several ionic species in the presence of chemical precipitation and dissolution and cation exchange. This paper describes the theoretical approaches taken, gives several examples of model validation, and then presents two hypothetical simulation cases that demonstrate model application. The specifics of structure, operation, and validation of this model with experimental data are explained elsewhere (Robbins 1979; Robbins et al. 1980a, b).

MODEL STRUCTURE

The model has been given the acronym SALTFL0, which will hereafter be used in this discussion. Before reviewing model equations and theoretical approaches, it is beneficial to get an overview of the variety of processes considered in the development of SALTFL0, and the organization of SALTFL0 operations.

The simulation program requires the following inputs:

- (1) The soil relationships between volumetric water content, matrix potential (cm) and hydraulic conductivity (cm/hr) at 0.01 increments of volumetric water content from saturation to zero water content.
- (2) Depth boundaries (cm)
- (3) Cation exchange capacity (me/100 g)
- (4) Soil bulk density (g/cm³) in each depth increment.
- (5) Initial soil profile volumetric water content, pH, and saturation extract values for Ca, Mg, K, Na, Cl and SO₄ (me/l), and the soil content on a weight basis of gypsum and lime. (The concentration of HCO₃ is calculated internally by the model using the pH.)
- (6) Soil surface boundary conditions for
 - a) Frequency, duration and rate of applied water (precipitation or irrigation).

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b) Potential evapotranspiration rates and durations.

c) Individual ion concentrations (listed above) in each increment of applied water

(7) Vanoslow selectivity coefficients describing cation exchange between the soil solid phase and paired combinations of the four cations listed above.

(8) Upper and lower allowable water contents for water extraction by plants.

(9) Crop factors, including days from planting to maturity, days to achieve a mature root profile, and percentage bare soil covered at maturity.

The simulation program output provides profiles of the following with time:

(1) Soil water contents and pressure heads.

(2) Ca, Mg, Na, K, Cl, SO₄, and HCO₃ in the soil solution.

(3) Calculation of electrical conductivity (EC) and sodium adsorption ratio (SAR) of the in-situ soil water.

(4) Exchangeable ion composition (me/100 g) for the four cations.

(5) Solid phase gypsum and lime content.

(6) Depth of water passing the bottom depth increment and depth of water extracted by plants (unless plants are assumed to be absent).

SALTFL0 involves the following sequence of operations:

(1) Values of soil physical properties, initial boundary conditions of soil water, soil chemical entities, evapotranspiration, and crop growth parameters are input.

(2) Roots are lengthened with time according to crop characteristics. A sigmoid growth rate is assumed and the mature root profile is scaled to fit intermediate growth stages.

(3) Evapotranspiration is partitioned between potential transpiration and potential evaporation. The surface flux rate is computed as a positive flux (rain, irrigation) or a negative flux (evaporation).

(4) Root extraction of water is calculated using the water potential gradient, soil water conductivity, osmotic potential, and plant flow resistance.

(5) Water flow is computed using a numerical solution of Darcy's water flow equation (Eq. 1 below).

(6) Each individual ion is transported by the combined mechanisms of mass flow, diffusion, and hydrodynamic dispersion, handled by numerical solution of the salt flow equation (Eq. 4 below).

(7) Concentrations of ions in solution, as well as precipitation and dissolution of lime (CaCO₃) and gypsum (CaSO₄) are calculated based upon chemical equilibrium relationships. Exchangeable ions are adjusted based on new solution concentrations.

(8) The time increment is calculated from the water flux. The program cycles back to the beginning for a new series of calculations, or exits depending on total time accumulated.

THEORY

Water Flow Model

Soil water flow was assumed to be isotropic, homogeneous, and one-dimensional. To include consideration of plant extraction of water during leaching, the basic water flow equation was assumed to be:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} K(\theta) \frac{\partial H}{\partial z} + A(z,t) \quad (1)$$

where θ = volumetric water content

$K(\theta)$ = hydraulic conductivity (cm/hr)

H = hydraulic head (cm)

z = depth (cm)

t = time (hr)

The root extraction term $A(z,t)$ was first used by Nimah and Hanks (1973). It may be defined as:

$$A(z,t) = \frac{[H_{\text{root}} + (\text{RRES} \cdot z) - h(z,t) - s(z,t)] \cdot \text{RDF}(z) \cdot K(\theta)}{\Delta x \cdot \Delta z} \quad (2)$$

where H_{root} = an effective water potential in the root at the soil surface (cm)

RRES = a root resistance term equal to $1 + R_c$, where R_c is a flow coefficient in the plant root system assumed to be 0.05. (When RRES is multiplied by z , the product will account for both the gravity term and the friction loss term in the root water potential. Thus, the root water potential at depth z is higher than the root water potential at the surface (H_{root}) by a

$h(z,t)$ = soil water pressure head (cm)

$s(z,t)$ = osmotic potential (cm)

RDF(z) = decimal proportion of total active roots in depth increment

Δz

Δx = distance between plant roots at the point in the soil where $h(z,t)$ and $s(z,t)$ are measured. Δx is arbitrarily assumed to be one (cm)

Δz = vertical distance over which root extraction of water is computed (cm)

Equation (1) was solved according to classical finite differencing techniques (Hanks and Bowers, 1962) to estimate hydraulic conductivities. At the upper boundary, conditions were subject to change over time as irrigation, rainfall, or evaporation was occurring. These surface water fluxes (EOR) were included as part of the water flow equation in the surface depth increment by approximating Darcy's law as

$$\text{EOR} = \frac{K_{i-1/2}^2 \left[\frac{(h_i^{i-1} + h_i^i)}{2} - \frac{(h_{i-1}^{i-1} + h_{i-1}^i)}{2} \right]}{\Delta z} \quad (3)$$

where $K_{i-1/2}$ is obtained by the method of Hanks and Bowers (1962). Recognizing that there is no (i-1) depth increment at the surface, Eq.(3) can be used to replace a portion of the approximated water flow equation for the first depth boundary (soil surface) by a single value, EOR. Values of EOR are input data, with positive values representing rainfall or irrigation and negative values indicating evaporation.

Lower boundary conditions of water that can be simulated by SALTFL0 include no flux ($\partial H/\partial z = 0$), a unit hydraulic gradient ($\partial H/\partial z = 1$), a constant soil-water pressure head or a water table.

Solute Flow Model

The diffusion-convection equation for the transport of a non-interacting solute under transient conditions is:

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta, q) \frac{\partial c}{\partial z} \right] - \frac{\partial}{\partial z} (qc) \quad (4)$$

where c = concentration of solute (mg/l)

q = volumetric water flux (cm/hr)

$D(\theta, q)$ = apparent diffusion coefficient (cm²/hr)

and the other terms are as defined above.

Equation (4) was used as the basis for transport of the four cations (Ca^{+2} , Mg^{+2} , Na^+ , K^+) and two anions (SO_4^{-2} , Cl^-) considered in the calculation of solute flux. The equation was solved by finite difference techniques (Wilson et al., 1980), with water contents and water fluxes provided by solution of Eq.(1). The value of $D(\theta, q)$ was approximated according to methods of Bresler (1973) as:

$$D_{i-1/2}^{j-1/2}(\theta, q) = D_0 a e^{b\theta} i_{i-1/2}^{j-1/2} + r \left| \frac{q_{i-1/2}^{j-1/2}}{\theta_{i-1/2}^{j-1/2}} \right| \quad (5)$$

where D_0 = diffusion coefficient in a free water system (cm²/hr)

a, b = empirical constants characterizing the soil

r = experimental constant depending on the characteristics of the porous medium

$\theta_{i-1/2}^{j-1/2}$ = average volumetric water content over the space and time

$i_{i-1/2}^{j-1/2}$ = increment

$q_{i-1/2}^{j-1/2}$ = average volumetric water flux over the space and time increment (cm/hr)

The solution to Eq.(4) was used six times to independently transport the four cations and two anions, after which the new ion concentrations were adjusted in each depth increment based on the chemical equilibrium and cation exchange subroutines detailed below. Mass balance and charge balance were maintained at all times. Sensitivity analysis showed that the water flow model used such small time increments that calculation of chemical equilibrium and cation exchange needed to be accomplished only once every 60 time steps. Precipitation or dissolution of gypsum and lime were calculated, and exchangeable ion concentrations altered at these times.

Equilibrium Chemistry Model

The chemical model used in SALTFL0 assumes that (1) the soil contains lime (CaCO_3), (2) the soil is sufficiently buffered that the pH of each depth increment is constant, and (3), each depth increment is an open system with respect to carbon dioxide (CO_2).

The soil solution electrical conductivity (EC, mmho/cm) was calculated from individual ion concentrations as:

$$\text{EC} = \sum K_i c_i^b \quad (6)$$

where c = ion concentration (me/l)

K_i, b = coefficients for each of the species Ca, Mg, Na, K, Cl, SO_4 , HCO_3 , CO_3 , NaSO_3 , CaSO_3 taken from McNeal et al. (1970).

Solution ionic strength (I, moles/l) was calculated from (Griffin and Jurinak, 1973)

$$I = 0.0127 \text{ EC} \quad (7)$$

Mono- and divalent ion activity coefficients (γ_1 and γ_2) were calculated from the Davies relationship (Stumm and Morgan, 1970)

$$\log \gamma_i = -0.509 Z_i^2 \left[\frac{\sqrt{I}}{1.0 + \sqrt{I}} - 0.31 \right] \quad (8)$$

where Z_i is the ionic charge.

The partial pressure of CO_2 (P_{CO_2}) was calculated from

with depth for Ca, Mg, Na, K, Cl and SO₄ as well as percent by weight gypsum and lime. Other input data required are bulk density, cation exchange capacity, pH and saturation percentage. These initial conditions do not need to be constant with depth.

Both the solute flow and chemical equilibrium models were organized such that the quality of the water applied as EOR (see Eq. (3)) could vary with each application. An additional piece of input data is therefore the activity of Ca, Mg, Na, K, Cl, and SO₄ in the applied water.

Cation Exchange Model

The cation exchange model developed for this study assumed that (1) the cation exchange capacity (CEC) was constant for a given depth, (2) the CEC was independent of pH, ion type and concentration, (3) the soil solution was a true solution, (4) cation exchange was a reversible process, (5) no anion exchange was occurring, and (6) the sum of exchangeable Ca, Mg, Na and K equalled the CEC. Using these assumptions,

$$CEC = X_{Ca} + X_{Mg} + X_{Na} + X_K \quad (15)$$

where X_{Ca}, X_{Mg}, X_{Na} and X_K are exchangeable ions (me/100 g).

A Vaneslow type selectivity coefficient was used to describe each paired combination of cations that might participate in exchange reactions. A total of six combinations was possible for the four cations considered in the model. Illustrating for calcium, it can be seen that three of the six possible expressions are:

$$\frac{(Ca)^{\frac{1}{2}} X_{Mg}}{(Mg)^{\frac{1}{2}} X_{Ca}} = K_1 \quad (16)$$

$$\frac{(Na) X_{Ca}}{(Ca)^{\frac{1}{2}} X_{Na}} = K_2 \quad (17)$$

$$\frac{(K) X_{Ca}}{(Ca)^{\frac{1}{2}} X_K} = K_3 \quad (18)$$

To calculate X_{Ca}, Eq. (16-18) were rewritten in terms of X_{Mg}, X_{Na}, and X_K, respectively and then were substituted into Eq. (15). X_{Ca} was isolated on the left hand side of the equation giving:

$$X_{Ca} = CEC + \left[\frac{(Mg)K_1}{(Ca)^{\frac{1}{2}}} + \frac{(Na)}{(Ca)^{\frac{1}{2}}K_2} + \frac{(K)}{(Ca)^{\frac{1}{2}}K_3} + 1 \right] \quad (19)$$

Using this procedure, equivalent expressions were developed for X_{Mg}, X_{Na}, and X_K. These equations are the basis of the cation exchange subroutine which equilibrates solution cation activities with exchangeable cation concentrations. Values of the selectivity coefficients are required by SALTFLD as input data. In principle, this approach can be expanded to any number of cations, provided the selectivity coefficient values are known or can be approximated for each paired combination.

$$P_{CO_2} = \frac{(H)^2 K_{sp}^2}{K_H K_{a1} K_{a2} (Ca)} \quad (9)$$

where (H) = hydrogen ion activity
 (Ca) = calcium ion activity
 K_{a1}, K_{a2} = first and second dissociation constants, respectively, for H₂CO₃,
 K_H = Henry's law constant for CO₂, and
 K_{sp2} = solubility product for CaCO₃.

Values of (CO₃) were calculated from

$$(CO_3) = \frac{K_{sp2}}{(Ca)} \quad (10)$$

while (HCO₃) was obtained from

$$(HCO_3) = \frac{P_{CO_2} K_H K_{a1}}{(H)} \quad (11)$$

Ion activities were corrected for ion pair formation, using activity coefficients and stability constants. The ion pairs considered significant were CaCO₃, CaHCO₃, CaSO₄, MgCO₃, MgHCO₃, MgOH⁺, MgSO₄, NaSO₄, and NaCO₃.

As an example, the correction of (Ca) for these ion pairs is shown below. The total calcium concentration in the system Ca_T (mole/l) is given by

$$Ca_T = \left[\frac{(Ca)}{\gamma_{Ca}} + \frac{(CaHCO_3)}{\gamma_{CaHCO_3}} + \frac{(CaOH^+)}{\gamma_{CaOH^+}} + \frac{(CaCO_3)}{\gamma_{CaCO_3}} + \frac{(CaSO_4)}{\gamma_{CaSO_4}} + \frac{(CaSO_4^+)}{\gamma_{CaSO_4^+}} \right] \quad (12)$$

Monovalent activity coefficients were assumed to be equal and are denoted below as γ₁. The divalent activity coefficient is denoted below as γ₂. By proper substitution and rearrangement Eq. (12) can be written (Hassett and Jurinak, 1971):

$$(Ca) = Ca_T \left[\frac{1}{\gamma_2} + \frac{K_{a1} K_H P_{CO_2}}{(H) K_{a2} \gamma_1} + \frac{K_{a1} K_H K_{sp}^2 (SO_4)}{(H) K_{a2} \gamma_1} + \frac{(H) K_{d1}}{K_{d4}} \right] \quad (13)$$

where K_{d1} represents the appropriate stability constant for a given ion pair, K_{d4} = (OH⁻) and all other terms have been previously defined. Expressions of a similar form were developed for (Mg), (Na), (K), (Cl), and (SO₄). Precipitation or dissolution of lime (CaCO₃) and gypsum (CaSO₄ · 2H₂O) can be determined using corrected values of (Ca), (CO₃), and (SO₄) and the appropriate stability constants in an equation of the form:

$$(Ca - X)(AN - X) = K_{sp} \quad (14)$$

where X is the moles of slightly soluble salt that must be added to or removed from the system to bring it to equilibrium and AN is the appropriate solution anion activity.

Cation activities developed from the above process were used in the calculations of the cation exchange model.

The chemical equilibrium model requires initial saturation extract values

EXPERIMENTAL METHODS

SALTFL0 has been validated in a series of leaching experiments that are described in detail elsewhere (Robbins et al., 1980a, b). These experiments were conducted in continuously weighing lysimeters, and involved the irrigation of two soils (one gypsiferous and one calcareous) with three different quality salty waters at 10% and 25% leaching fractions. The lysimeters (Robbins and Willardson, 1979) were 0.30 m in diameter and 1.18 m deep. Porous ceramic cups were inserted through the side of each lysimeter at soil depths of 0.25, 0.50 and 0.75 m. Drains were provided in the bottom of the lysimeters. The lysimeters were planted to alfalfa (day 1) and irrigated with distilled water until plants were established. On day 19 treatments with the salty waters were initiated, with irrigation scheduling determined by water use and desired leaching fraction. Each lysimeter treatment was replicated three times. Soil solution samples were taken on days 42, 140, 189, 227 and 248. Treatments were terminated on day 243. After 258 days soil samples were taken for selectivity coefficient determination.

For this study, no attempt was made to predict crop yield because of the unusual growing conditions. The crops were grown primarily to extract soil water, thereby concentrating the soil solution and causing chemical precipitation.

Only two treatments, called I and II, of the 12 treatments modeled will be discussed. Treatment I was the irrigation of Penoyer loam [coarse-silty, mixed (calcareous) mesic Typic Torriorthents] (0.7% gypsum by weight) with a low gypsum water (Table 1) at a 25% leaching fraction. This treatment produced the greatest gypsum dissolution rate of all treatments in the study. Treatment II consisted of irrigation of Hunting silty clay loam [fine-silty, mixed (calcareous), mesic Aquic Ustifluvents] (0% gypsum) with a high calcium sulfate water (Table 1) at a 10% leaching fraction. This treatment produced the greatest gypsum precipitation.

Table 1. Irrigation water compositions (lysimeter study)

	Ca	Mg	Na	K	Cl	SO ₄	HCO ₃	Total
	me/l							
Water 1	12.0	1.0	1.5	0.5	1.5	12.0	1.5	15.0
Water 2	5.0	3.5	6.0	0.5	13.0	0.5	1.5	15.0

RESULTS

Complete details of the agreement between measured cation and anion concentrations and SALTFL0 predictions are reported elsewhere (Robbins et al., 1980a, b). A summary of the data is presented in Fig. 1 for Case I and in Fig. 2 for Case II. Agreement in all cases between measured and calculated values was good. It is important to note that SAR (mmole/l)^{1/2}, defined as

$$\text{SAR} = \frac{\text{Na}}{\sqrt{\frac{\text{Ca} + \text{Mg}}{2}}} \quad (20)$$

where Na, Ca, Mg concentrations are in me/l, cannot be accurately calculated without reasonable simulation of the solution concentrations of these three cations. Similarly, the accurate prediction of all cations and anions was prerequisite to the calculation by SALTFL0 of EC using Eq. (6). The model predicted all ions with sufficient accuracy to produce the agreement of Fig. 1-2.

Calculated bicarbonate concentrations generally were slightly lower than measured (measured values 10-15 me/l, calculated 8-10 me/l). SALTFL0 used a pH of 6.9 for the Penoyer soil and 6.8 for the Hunting soil, because it was found by trial and error that these pH values gave the best overall results. The measured pH values of the saturation extracts for the Penoyer and Hunting soils were 7.3 and 7.5, respectively. It should be noted that a natural soil

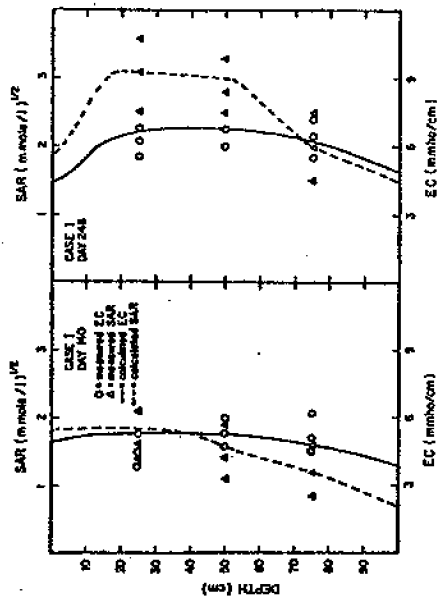


Fig. 1. Predicted and measured SAR and EC for Case I.

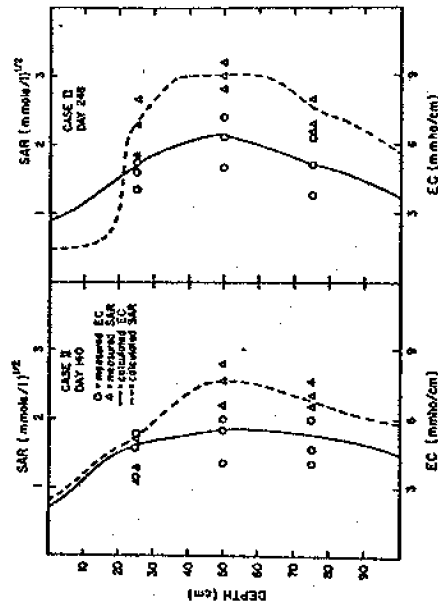


Fig. 2. Predicted and measured SAR and EC for Case II.

is in equilibrium with a much higher PCO₂ than is a laboratory saturation extract, hence a lower pH should be expected (Oster and Rhoades, 1975).

The ability to match measured data with SALTFL0 calculations provides confidence in the model's predictive capabilities. The following two cases are therefore presented as examples of the model's versatility and potential application.

A sandy loam soil was presumed irrigated with power plant blowdown water (Table 2). The soil profile was assumed homogeneous in physical and chemical properties to a depth of 240 cm (Table 3). In Case A, the blowdown water was applied once weekly for 10 hours at a rate of 0.4 cm/hr. In Case B, given the same initial soil conditions and water quality, blowdown water was applied at the same rate and frequency, but interspersed between these applications was the application of "good" quality water (Table 2). The purpose of these cases

Table 2. Applied water quality for demonstration simulation cases A and B

	me/l							mmho/cm	
	Ca	Mg	Na	K	Cl	SO ₄	HCO ₃		
Blowdown									
water only	18.00	9.10	13.50	0.30	1.44	37.70	1.80	40.94	4.21
Interspersed									
good quality									
water	1.00	1.00	1.00	1.00	1.50	1.50	0.50	4.00	0.43

Table 3. Initial soil conditions of physical and chemical properties for demonstration simulation exercises A and B

Depth (cm)	Volu- metric water content (%)	Gyp- sum (%)	Lime (%)	pH	Bulk den- sity (g/cm ³)							SO ₄
					Ca	Mg	Na	K	Cl	me/l		
2	0.15	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
10	0.18	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
25	0.20	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
50	0.25	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
75	0.25	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
100	0.28	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
150	0.25	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	5.7	15.0	
200	0.20	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	2.7	15.0	
240	0.20	0.5	0.01	7.7	1.52	3.6	2.6	12.5	2.0	2.7	15.0	

is to demonstrate the sensitivity of the model to transient cases of soil water movement and equilibrium chemistry. No plants were assumed to be present. The final application of water was at time 3400 hours, with redistribution then permitted for the final 240 hours.

As can be seen from Tables 4-6, substantially different water and solute concentrations were predicted for the two cases over the time of simulation. In particular, the columns listing EC, SAR, and the precipitated salts demonstrate the effects of the two water management cases on the soil profile. Case A exhibits increasingly saline soil solution concentrations in the upper 25 cm of the soil profile until at the end of the 160 day simulation the EC in the upper 2 cm is predicted to be 19 mmho/cm. The importance of simulating not just total salts (as indicated by EC) but also individual ions is evidenced by the predicted SAR values. Case B, with twice the quantity of water applied, is characterized by lower SAR values after 160 days at virtually all depths. Both parameters (EC and SAR) are often required by regulatory agencies interested in the environmental effects of waste water disposal. Also of interest are the total quantities of salt estimated delivered to the 240 cm depth (Table 7) as the result of the water and salt applications.

SALTFO shows substantial promise as a tool to be used in the description of the leaching of soluble salts under transient water flow conditions. It is also a reasonably economical model. The 3840 hours of simulation needed in Case A (including 88 irrigation and redistribution cycles) cost only \$14 worth of CPU time on a Burroughs 6700 computer. The program is in Fortran.

Table 4. SALTFO predictions for time 680 hr for Cases A and B

Depth (cm)	me/l							EC	SAR	Gypsum	Lime
	Ca	Mg	Na	K	Cl	TSO ₄	EC				
Case A, Time = 680 hr (28 days)											
2	0.26	25.8	8.0	23.9	1.8	2.3	54.4	4.5	5.8	0.59	0.01
10	0.28	29.9	6.7	28.7	2.2	4.3	60.4	5.3	6.7	0.53	0.01
25	0.23	28.2	3.8	17.5	2.1	4.7	44.9	4.1	4.4	0.49	0.01
50	0.18	26.9	2.9	13.6	2.1	4.7	39.3	3.7	3.5	0.48	0.01
75	0.19	26.7	2.8	12.8	2.1	5.1	38.1	3.6	3.4	0.47	0.01
100	0.20	27.0	2.7	12.6	2.1	5.6	37.1	3.6	3.3	0.47	0.01
150	0.20	27.0	2.7	12.6	2.1	5.7	37.0	3.6	3.3	0.48	0.01
200	0.20	26.7	2.7	12.6	2.1	5.7	37.3	3.6	3.3	0.48	0.01
240	0.20	26.7	2.7	12.6	2.1	5.7	37.3	3.6	3.3	0.48	0.01
Case B, Time = 680 hr (28 days)											
2	0.30	22.4	5.2	18.7	1.4	1.5	44.7	3.6	5.0	0.54	0.01
10	0.30	26.3	4.2	13.5	1.8	2.0	41.9	3.5	3.5	0.47	0.01
25	0.25	25.7	3.1	12.9	1.9	2.3	39.9	3.5	3.4	0.48	0.01
50	0.21	25.9	2.8	12.7	2.0	2.8	38.9	3.5	3.4	0.48	0.01
75	0.21	26.0	2.7	12.6	2.0	3.2	38.5	3.5	3.3	0.48	0.01
100	0.22	26.7	2.7	12.6	2.1	5.0	37.4	3.5	3.3	0.47	0.01
150	0.22	26.9	2.7	12.6	2.1	5.5	37.1	3.6	3.3	0.48	0.01
200	0.22	26.7	2.7	12.6	2.1	5.7	37.0	3.6	3.3	0.48	0.01
240	0.20	27.0	2.7	12.6	2.1	5.7	37.0	3.6	3.3	0.48	0.01

Table 5. SALTFO predictions for time 2720 hr for Cases A and B

Depth (cm)	me/l							EC	SAR	Gypsum	Lime
	Ca	Mg	Na	K	Cl	TSO ₄	EC				
Case A, Time = 2720 hr (113 days)											
2	0.14	28.4	32.2	53.4	2.3	5.8	105.8	8.6	9.7	0.99	0.01
10	0.20	26.0	15.1	49.4	2.2	4.5	84.7	7.2	10.9	0.63	0.01
25	0.22	26.6	6.8	41.6	2.1	4.5	69.3	6.2	10.2	0.54	0.01
50	0.21	26.0	4.0	31.4	2.1	4.4	56.7	5.2	8.1	0.50	0.01
75	0.19	25.9	3.1	25.0	2.0	4.4	49.5	4.6	6.4	0.49	0.01
100	0.20	26.3	2.7	15.3	2.1	4.4	40.5	3.8	4.0	0.48	0.01
150	0.20	26.4	2.7	13.2	2.1	4.8	38.3	3.6	3.5	0.48	0.01
200	0.20	26.6	2.7	12.7	2.1	5.3	37.7	3.6	3.3	0.48	0.01
240	0.20	27.0	2.7	12.6	2.1	5.7	37.1	3.6	3.3	0.48	0.01
Case B, Time = 2720 hr (113 days)											
2	0.12	37.4	25.0	36.9	1.7	4.6	92.6	7.5	6.6	0.68	0.01
10	0.19	24.8	7.2	17.4	1.5	1.7	47.3	3.9	4.4	0.45	0.01
25	0.22	25.5	4.6	16.3	1.7	1.7	44.4	3.8	4.2	0.48	0.01
50	0.23	25.1	3.4	16.1	1.9	1.7	43.2	3.7	4.3	0.49	0.01
75	0.22	24.9	2.8	16.1	1.9	1.7	42.6	3.7	4.3	0.49	0.01
100	0.22	25.2	2.6	13.7	2.0	1.7	40.4	3.5	3.7	0.48	0.01
150	0.22	25.3	2.5	12.9	2.0	1.7	39.2	3.4	3.5	0.48	0.01
200	0.22	25.5	2.7	12.7	2.1	2.1	39.2	3.4	3.3	0.48	0.01
240	0.20	26.8	2.7	12.6	2.1	5.7	37.3	3.6	3.3	0.48	0.01

Table 6. SALTFO predictions for time 3840 hr for Cases A and B

Depth (cm)	θ _v	TCa	Mg	Na	me/l	K	Cl	ISO ₄	EC	SAR	Cypsum	Lime
Case A, Time = 3840 hr (160 days)												
2	0.12	34.9	88.2	143.2	3.2	18.7	242.7	19.2	18.3	1.25	0.01	
10	0.13	24.0	16.9	45.7	2.1	4.9	80.6	6.9	10.1	0.65	0.01	
25	0.15	23.2	6.9	42.7	2.0	4.4	67.6	6.1	11.0	0.57	0.01	
50	0.16	23.4	4.1	38.6	2.0	4.6	61.4	5.6	10.4	0.52	0.01	
75	0.17	24.0	3.3	36.2	2.0	4.5	59.3	5.4	9.8	0.50	0.01	
100	0.18	25.3	2.8	20.9	2.0	4.4	44.9	4.2	5.6	0.48	0.01	
150	0.19	26.0	2.7	15.3	2.1	4.4	40.2	3.7	4.0	0.48	0.01	
200	0.20	26.3	2.7	13.3	2.1	4.7	38.4	3.6	3.5	0.48	0.01	
240	0.20	26.8	2.7	12.6	2.1	5.7	37.3	3.6	3.3	0.48	0.01	
Case B, Time = 3840 hr (160 days)												
2	0.12	30.7	19.4	25.5	1.4	3.1	71.3	5.9	5.1	0.70	0.01	
10	0.14	24.5	7.5	15.7	1.4	1.6	45.9	3.8	3.9	0.43	0.01	
25	0.16	24.7	4.9	15.6	1.6	1.6	43.7	3.7	4.1	0.48	0.01	
50	0.17	25.0	3.6	15.7	1.8	1.6	42.5	3.7	4.1	0.49	0.01	
75	0.19	24.5	2.8	16.5	1.9	1.6	42.7	3.7	4.5	0.49	0.01	
100	0.19	24.8	2.6	15.6	2.0	1.7	41.7	3.6	4.2	0.48	0.01	
150	0.21	25.0	2.5	14.4	2.0	1.7	40.8	3.5	3.9	0.48	0.01	
200	0.21	25.5	2.6	13.3	2.0	1.9	39.6	3.5	3.6	0.48	0.01	
240	0.20	27.0	2.7	12.6	2.1	5.7	37.0	3.6	3.3	0.48	0.01	

mmho/cm
+ mmole/l²

Table 7. Water and solute budget summary for demonstration simulation Cases A and B (leaching past 240 cm depth)

	Total water applied (cm)		Total good water (cm)		Total evaporation (cm)		Total drainage (cm)	
	Case A	Case B	Case A	Case B	Case A	Case B	Case A	Case B
blowdown	87.8	87.8	0	87.6	41.5	72.0	57.4	114.0
Total leaching (tons/ac)	Ca	Mg	Na	K	Cl	SO ₄		
Case A	2.59	2.50	5.68	0.52	2.20	24.34		
Case B	8.95	2.59	7.49	0.49	3.14	42.95		

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