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# Practical Model for Predicting Soil Salinity and Sodicity under Transient Conditions

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We present the preliminary development of the computer model tentatively named Soil Salinity. The model is intended as a management tool for predicting the **salinity** and sodium distribution with depth and time. The model couples variably saturated water flow to $CO_2$ production and transport, solute transport, a generic plant growth submodel and a major ion chemistry submodel. Since the solution chemistry in the unsaturated zone is significantly influenced by variations in water content, temperature and $CO_2$ concentrations in the soil gas, all these variables are calculated by the model. The $CO_2$ transport submodel includes both liquid and gas transport. The production submodel accounts for both microbial and root respiration of $CO_2$ which are dependent on water content, temperature, salinity and plant and soil characteristics. The model considers that adverse salinity or water stress conditions reduce water consumption and reduce biomass yield proportionally to the reduction in water consumption. The model accounts for equilibrium reactions such as complexation, cation exchange and precipitation-dissolution among the major chemical components. The example presented demonstrates the applicability of the model for evaluating the impact of water quality and irrigation management on soil salinity and ion composition. The model provides predictions of water content, dissolved ions and exchangeable cations with time and depth. It is anticipated that in many instances users will not have a complete input data set, thus default parameters are available for some functions. For functions, for example, hydraulic properties, where default parameters are not appropriate, we make available a small menu based on soil texture.

## Introduction

Modeling the transport of major soluble ions in the unsaturated zone is required for prediction of soil salinity and the plant response to the management of the system. Realistic modeling of root zone chemistry requires consideration of processes in the gas, liquid and solid phases. Many factors may influence the transport and reaction parameters of the chemical system. The most important factors influencing the soil chemical dynamics are water flow, heat transport, and the dynamic changes in $CO_2$ concentrations. Soil temperature affects thermodynamic equilibrium constants, reaction rates, production of $CO_2$ and most importantly, plant growth. The $CO_2$ concentration exerts a major control on the biological and chemical processes in the soil and has a direct effect on the solution chemistry of the entire subsurface. This is particularly important when considering the reclamation of sodic calcareous soils using organic mulches, where the elevated concentrations of $CO_2$ result in enhanced dissolution of calcium carbonate.

Many models have been developed over the past two decades to quantify the physical and chemical processes affecting the transport of major ions. The hydrological models for water flow, solute transport and aqueous equilibrium chemistry were developed independently, and only recently has there been a significant effort to couple these models. Most of the modeling effort has so far been concentrated on the saturated zone, where changes in water velocity, temperature and pH are relatively gradual and hence less important than in the unsaturated zone. Therefore, most models were based on one-dimensional steady-state saturated water flow with fixed water velocity, temperature and pH. Only recently several models were published which can be applied to problems that include multicomponent solute transport and variably saturated water flow (ROBBINS et al.,l980a,b; LIU & NARASIMHAN, 1989; YEH & TRIPATHI, 1991). Robbins' equilibrium chemistry model was also the basis for the numerical code LEACHM of WAGENET and HUTSON (1987). These chemical and multicomponent transport models use either the total inorganic carbon as a conservative property and/or fixed pH as an input variable. However, in a soil environment the $CO_2$ concentrations fluctuate, resulting in increases in dissolved inorganic carbon and soil pH when $CO_2$ increases. Use of the open system condition which allows for transfer of carbon into or out of the system and use of alkalinity as an input variable is preferable to the fixed pH or fixed $CO_2$ assumption (SIMUNEK & SUAREZ, 1994).

Since the assumption of time invariant $CO_2$ is often not realistic, there is also a need for coupling mutticomponent models not only to variably saturated water flow and solute transport models but also to a $CO_2$ transport model (SIMUNEK & SUAREZ, 1994]. SIMUNEK and SUAREZ. (1993a) developed the SOILC02 model, which considers variably saturated water flow, heat and $CO_2$ transport and biological $CO_2$ production. In a companion paper, SUAREZ and SIMUNEK (1993) presented a sensitivity analysis for the input parameters as well as a discussion on the selection of the parameter values. The model was able to accurately predict $CO_2$ with depth and time under dynamic conditions, as shown by SUAREZ and SIMUNEK (1993).

SIMUNEK and SUAREZ (1994) coupled the two-dimensional variably saturated water flow and solute transport model SWMS_2D of SIMUNEK et al. (1992) with an expanded version of the speciation model CARBCHEM of **SUAREZ** (1977) and the $CO_2$ transport and production model of **SIMUNEK** and **SUAREZ** (1993a). The resulting multicomponent transport model for variably saturated porous media, UNSATCHEM-2D (**SIMUNEK & SUAREZ,** 1993b), is applicable to nonacid environments with pH > 6. A new multicomponent transport model that is applicable to the full range of pH values and includes silicate weathering reactions has also been developed **(SUAREZ & SIMUNEK, 1995).**

In this paper we present only the basic equations and a brief discussion of the various sections of the model. At the end of the paper, an example is provided that demonstrates the applicability of the model for salinity control and irrigation management.

## Model development

### *Variably saturated water flow*

One-dimensional isothermal Darcian flow of water in a variably saturated rigid porous medium is described by a modified form of the Richards equation with the assumptions that the air phase plays a negligible role in the liquid flow process and that the compressibility of both soil matrix and fluid can be ignored

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[K(\frac{\partial h}{\partial z} + 1)] - S \qquad (1)$$

where $\theta$ is the volumetric water content $[L^3L^{-3}]$, $h$ is the pressure head [L], S is a sink term representing water uptake by plant roots $[T^{-1}]$, $z$ is the spatial coordinate [L] (positive upward), $t$ is time [T], and $K$ is the unsaturated hydraulic conductivity function $[LT^{-1}]$.

The sink term, S, in (1) represents the volume of water removed per unit time from a unit volume of soil due to plant water uptake. The expression proposed by FEDDES et al. (1978) and subsequently modified to include salinity stress (VAN GENUCHTEN, 1987) is

$$S(h) = a(h)\, a_\phi(h_\phi)\, S_p \qquad (2)$$

where the dimensionless water and salinity stress response functions $a(h)$ and $a_\phi(h_\phi)$ depend on the soil water pressure head, $h$, and osmotic head, $h_\phi$ $(0 \leq a \leq 1)$, respectively, and $S_p$ is the potential water uptake rate, which is equal to the water uptake rate during periods of no water and salinity stress when $a(h)=a_\phi(h_\phi)=1$. Values for the osmotic head are obtained using osmotic coefficients and a modified form of the van't Hoff equation (**Suarez & Šimůnek, 1995**). We provide a small library of salt tolerance information for major crops.

### *Multicomponent solute transport*

The partial differential equation governing onedimensional advectivedispersive chemical transport under transient water flow conditions in partially saturated porous media is taken as,

$$\frac{\partial(\theta \quad c_k)}{\partial t}+\rho\frac{\partial \bar{c}_k}{\mathrm{at}}+\rho\frac{\partial \hat{c}_k}{\mathrm{at}}=\frac{\partial}{}(\theta D\frac{\partial c_k}{\partial z}-q_w c_k) \quad k=1,2,\ldots,N_c \qquad (3)$$

where $c_k$ is the total dissolved concentration Of aqueous component $k$ $\bar{c}_k$ is the total sorbed concentration of component $k$, $\hat{c}_k$ is the total solid phase concentration of component $k$, $\rho$ is the bulk density of the medium, $D$ is the dispersion tensor, $q_w$ is the volumetric flux and $N_c$ is the number of aqueous components. Solute uptake by plant roots is not considered in (3) as plants take up a negligible fraction of the salts present in the soil water. The second and third terms on the left side of Eq. (3) are zero for components that do not undergo ion exchange or precipitation/dissolution.

### *Car-bon dioxide transport*

A detailed development of the onedimensional carbon dioxide transport model and justification of respective assumptions is given in Šimůnek and Suarez (1993a). Transport of $CO_2$ in the root zone occurs in both the liquid and gas phases. We consider two transport mechanisms (**Patwardhan** et al., 1988), convective transport in the aqueous phase and diffusive transport in both gas and aqueous phases, as well as $CO_2$ production and/or removal. Thus one-dimensional $CO_2$ transport is described by the following mass balance equation

$$\frac{\partial(c_a\theta_a+c_w\theta)}{\partial t}=\frac{\partial}{\partial x_i}(\theta_a D_{ij}^a\frac{\partial c_a}{\partial x_j})+\frac{\partial}{\partial x_i}(\theta D_{ij}^w\frac{\partial c_w}{\partial x_j})-\frac{\partial}{\partial x_i}(q_i c_w)-S c_w+P \qquad (4)$$

where $c_w$ and $c_a$ are the volumetric concentrations of $CO_2$ in the dissolved phase and gas phase, respectively, $D_{ij}^{a}$ is the effective soil matrix diffusion coefficient tensor of $CO_2$ in the gas phase, $D_{ij}^{w}$ is the effective soil matrix dispersion coefficient tensor of $CO_2$ in the dissolved phase, $q_i$ is the soil water flux, $\theta_a$ is the volumetric air content and $P$ is the $CO_2$ production rate. The term $Sc_w$ represents the dissolved $CO_2$ removed from the soil by root water uptake, i.e., when plants take up water the dissolved $CO_2$ is also taken up by the plant roots. The volumetric concentrations of $CO_2$ in the dissolved and gas phases are related by the following equation

$$c_w = K_c c_a \tag{5}$$

where $K_c$ is the distribution constant, which is strongly dependent on temperature. Šimůnek and Suarez (1993a) defined the total aqueous phase $CO_2$, $c_w$, as the sum of $CO_2(aq)$ and $H_2CO_3$, and related it to the $CO_2$ concentration in the gas phase with Henry's Law. However, aqueous carbon also exists in the form of $HCO_3^-$, $CO_3^{2-}$, and other complexed species, such as $CaCO_3^0$, and these species should be included in the expression for $c_w$. Determination of these species cannot be made without use of a complete chemical speciation program.

We consider two processes for $CO_2$ production, production by soil microbes and production by plant root respiration. We assume that the $CO_2$ production by these two processes is additive and that it is possible to superpose the effects of environmental variables that alter production from the reference value (Šimůnek & Suarez, 1993a). The production of $CO_2$ is then considered as the sum of the production rate by the soil microorganisms, $\gamma_s$, and the production rate by plant roots, $\gamma_p$

$$P = \gamma_s + \gamma_p = \gamma_{s0} \prod_i f_{si} + \gamma_{p0} \prod_i f_{pi} \tag{6}$$

where the subscript $s$ refers to soil microorganisms and the subscript $p$ refers to plant roots, $\prod f_i$ is the product of reduction coefficients dependent on depth, temperature, pressure head (the soil water content), $CO_2$ concentration, osmotic head and time. The parameters $\gamma_{s0}$ and $\gamma_{p0}$ represent, respectively, the optimal $CO_2$ production by the soil microorganisms or plant roots for the whole soil profile at 20 °C under optimal water, solute and soil $CO_2$ concentration conditions. The individual reduction functions are given in Šimůnek and **Suarez** (1993a) and a discussion of the selection of values for optimal production as well as coefficients for the reduction functions is given in Suaru and Šimůnek (1993). This section serves not only to predict $CO_2$ concentrations but is also required as input to the water uptake submodel, since excessive $CO_2$ concentrations result in oxygen deficiency, reduced water uptake yield loss.

### *Crop submodel*

The plant submodel is designed to be interactive with the water flow and chemical submodels. The interaction includes both the root development and uptake of water and nutrients as well as different aspects of plant growth. Although the submodel will provide yield estimates as an output, this is secondary to the primary focus of providing plant response to salinity, primarily water uptake. The plant submodel is organized into canopy, root and shoot modules. The canopy and shoot modules are affected by the atmospheric variables. These modules are connected to the root module which is also affected by the water and salinity stress parameters. The canopy module simulates a single layer canopy and calculates components of a simplified energy budget, as well as carbon assimilation and transpiration rates.

The input atmospheric data includes hourly weather data in the IBSNAT (International Benchmark Site Network for Agrotechnology Transfer) version 3.0 format. It is understood that in most instances such information is not available, thus it is necessary to estimate hourly meteorological data from daily maximum-minimum data or whatever other data is available. In the absence of sufficient data the dynamic simulation of plant growth is disabled. In this instance reference evapotranspiration from a hypothetical grass crop (well watered, 12 cm height, with a albedo of 0.23 and canopy resistance to vapor transport of 70 s/m) is utilized or estimated according to FAO methodology (Smith, 1992), as follows

$$ET_0 = \frac{0.408\Delta(R_n - G) + \gamma\left[\frac{900}{T+273}\right]U_2(e_a - e_d)}{\Delta + \gamma(1 + 0.34U_2)} \qquad (7)$$

where $ET_0$ is the reference crop evapotranspiration [mm d“], $R_n$ is net radiation on a crop surface [MJ $m^{-2}d^{-1}$], G is soil heat flux [MJ$m^{-2}d^{-1}$], $T$ is absolute temperature [K], $U_2$ is windspeed measured at 2 m height [m $s^{-1}$], $e_a$-$e_d$ is the vapor pressure deficit [kPa], as calculated in Smith (1992), $\Delta$ is the slope of the vapor pressure-temperature curve [kPa K] as calculated in Smith (1992), and $\gamma$ is the psychrometric constant [kPa $K^{-1}$], deficit, as calculated in Smith (1992). Using this approach the optimal crop water consumption is calculated by multiplying the $ET_0$ values by the crop coefficient. Actual crop ET is calculated from the optimal value and the crop water, salinity and oxygen stress factors, as described above for $CO_2$ production. The model includes a Table of response functions for various crops.

In the detailed simulation of plant growth, root and canopy function are coupled through the common variable of canopy water potential. The continuity equation for water flux results from equating the expressions for root uptake and canopy transpiration and solving for canopy water potential. (**Choudhury & Idso, 1984**). The value for canopy water potential is used to compute canopy stomatal resistance, which in turn is used for the calculation of the canopy photosynthesis rate. Root water uptake is simulated using an Ohm's law expression, as is commonly used by others (e.g. **Choudhury & Idso, 1984**). Transpiration is calculated using the following version of the Pennman-Monteith equation,

$$E = \frac{\Delta R_n + \rho C_p (e_a - e_d)}{r_a \lambda(\Delta + \gamma(1 + r_c / r_a))} \qquad (8)$$

where $\rho$ is the atmospheric density [kg m$^{-3}$], $C_p$ specific heat capacity of moist air [kJ kg$^{-1}$ °C$^{-1}$], $r_c$ is the canopy resistance to water vapor diffusion, expressed as a function of canopy water potential, $R_n$ is the net radiation absorbed at the crop surface, and $r_a$ is the boundary layer or aerodynamic resistance to water vapor diffusion. Photosynthesis and respiration are based on a single leaf model generalized to the canopy level, using the non-rectangular hyperbola relation, as given in **Thornley and Johnson (1991)**. The radiation intercepted by the crop canopy is calculated using a Beer's law relation,

$$I = (1.0 - \exp(-k * LAI))G \qquad (9)$$

where $I$ is the intercepted radiation, $k$ is a crop specific parameter (with default to a value for a grass crop), $LAI$ is the leaf area index, calculated by the models, and G is the radiation flux at the crop surface.

Root function, which controls the water uptake distribution is contrcled by several factors. The maximum advance of the root front is determined from a genotype specific extension rate expressed as cm/degree day (the grass default value being 1.0 cm/day). The root front will not advance against a positive water potential gradient, except if the available soil pore space in a layer becomes limiting and the water potential of the layer being entered is sufficiently high to support growth. The rooting front will also not advance into layers saturated with water, nor into layers with specified impediments (high bulk density). The absolute depth is related to the crop specific parameter of the exponential root distribution function. In the absence of stress

$$R = a * \exp(-fz) \qquad (10)$$

where *R* is the amount of new root length at each depth z, and *f* is a crop-specific constant. This new growth distribution is modified by the following exponential function of water potential that simulates the tendency of roots to proliferate in the most favorable soil layers,

$$F = (1 - \exp(- a x^{b})) \qquad (11)$$

where *F* is a multiplier to Eq.(10) (with a value from 0 to 1.0), and *b* are given exponential constants and x is the maximum of zero and the difference between the soil water potential and a crop specific minimum water and salinity potential.

*Solution chemistry*

The chemical species which are considered in the models are given in Table 1; species that are only considered under acid conditions are highlighted. The chemical system for predicting major ion solute chemistry of the unsaturated zone includes either 37 or 55 chemical species (depending on the pH range). These are divided into five groups as listed in Table 1: *10* chemical components (calcium, magnesium, sodium, potassium, sulfate, chloride, nitrate, aluminium, silica, and organic matter), 25 complex aqueous species, seven possible solid species (calcite, gypsum, nesquehonite, hydromagnesite, dolomite, sepiolite, and gibbsite), six sorbed species, and seven species constituting the $CO_2$-$H_2O$ system.

Mass balance equations for the major components in the first group of Table 1 are defined as the sum of the corresponding constituent species. In addition to ten mass balance equations for major components, two mass balance equations for the total analytical concentration of carbonate and bicarbonate are defined.

$$\begin{aligned} CO_{3_T} &= \left[CO_3^{2-}\right] + \left[CaCO_3^0\right] + \left[MgCO_3^0\right] + \left[NaCO_3^-\right] \\ HCO_{3_T} &= \left[HCO_3^-\right] + \left[CaHCO_3^+\right] + \left[MgHCO_3^+\right] + \left[NaHCO_3^0\right] \end{aligned} \qquad (12)$$

where variables with subscript *T* represent the total solution concentration of that particular variable, and brackets refer to molalities (mol kg-‘). The expressions given above are used to calculate carbonate alkalinity, *Alk* ($mol_c kg^{-1}$) as

$$Alk = 2\, CO_{3T} + HCO_{3T} + [OH^-] - [H^+] \qquad (13)$$

*Table 1.*

Species considered in the chemical submodel

| | | | |
|---|---|---|---|
| 1 | Aqueous components | 10 | $Ca^{2+}$, $Mg^{2+}$, $Na^+$, $K^+$, $SO_4^{2-}$, $Cl^-$, $NO_3^-$, $H_4SiO_4^0$,<br>$Al^{3+}$, $Org^{3-}$ |
| 2 | Complexed species | 25 | $CaCO_3^o$, $CaHCO_3^+$, $CaSO_4^o$, $MgCO_3^o$, $MgHCO_3^+$,<br>$MgSO_4^o$, $NaCO_3^-$, $NaHCO_3^o$, $NaSO_4^-$, $KSO_4^-$,<br>$AlSO_4^+$, $Al(SO_4)_2^-$, $AlHSO_4^{2+}$, $AlOH^{2+}$, $Al(OH)_2$ $Al(OH)_3^0$, $Al(OH)_4^-$, $AlOrg^0$, $AlHOrg^+$, $HOrg^{2-}$, $H_2Org$ , $H_3Org^0$, $HSO_4$<br>$H_2SiO_4^{2-}$, $H_3SiO_4^-$, |
| 3 | Precipitated species | 7 | $CaCO_3$ , $CaSO_4 \cdot 2H_2O$, $MgCO_3 \cdot 3H_2O$,<br>$CaMg(CO_3)_2$, $Al(OH)_3$<br>$Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O$, $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$, |
| 4 | Sorbed species | 6 | $\bar{Ca}$, $\bar{Mg}$, $\bar{Na}$, K. Al, $\bar{H}$ |
| 5 | Additional species | 7 | $P_{CO2}$, $H_2CO_3^*$, $CO_3^{2-}$, $HCO_3^-$, $H^+$, OH-, $H_2O$ |

In addition to the mass balance equations, the charge balance equation for the solution is

$$\begin{aligned}
&2[Ca^{2+}]+2[Mg^{2+}]+[Na^+]+[K^+]+[CaHCO_3^+]+[MgHCO_3^+]+[H^+]+3[Al^{3+}]\\
&+2[AlOH^{2+}]+2[AlHSO_4^{2+}]+[AlOH_2^+]+[AlHOrg^+]+[AlSO_4^+]-2[CO_3^{2-}]-[HSO_4^-]\\
&-[HCO_3^-]-2[SO_4^{2-}]-[Cl^-]-[NO_3^-]-[OH^-]-2[H_2SiO_4^{2-}]-[H_3SiO_4^-]-3[Org^{3-}]\\
&-[NaCO_3^-]-[NaSO_4^-]-[KSO_4^-]-[Al(SO_4)_2^-]-[Al(OH)_4^-]-2[HOrg^{2-}]-[H_2Org^-]=0
\end{aligned} \qquad (14)$$

The activities of the species present in solution at equilibrium are related by the mass-action equilibrium equations. The solubility of $CO_2(g)$ in water is governed by Henry's law

$$K_{CO_2} = \frac{(H_2CO_3^*)}{P_{CO_2}(H_2O)} \qquad (15)$$

where the activity of $CO_{2(g)}$ is expressed in terms of the partial pressure $P_{CO2}$, $K_{CO2}$ is Henry's Law constant and $H_2CO_3^*$ represents both aqueous $CO_2$ and $H_2CO_3$. The equilibrium expressions for the dissociation of carbonic acid are written as

$$K_{a1} = \frac{(H^+)(HCO_3^-)}{(H_2CO_3^*)} \qquad (16)$$

$$K_{a2} = \frac{(CO_3^{2-})(H^+)}{(HCO_3^-)} \qquad \textbf{(17)}$$

where $K_{a1}$ and $K_{a2}$ are the first and the second dissociation constants of carbonic acid.

The model includes calculation of complex species for the major ions. Each complexation reaction for species in the second group of Table 1 is represented by an equilibrium expression. For example, for calcium sulfate:

$$K_1 = \frac{(Ca^{2+})(SO_4^{2-})}{(CaSO_4^0)} \qquad (18)$$

where $K_1$ is the equilibrium constant of the complexed species.

Cation exchange is treated in the model using the Gapon equation **(WHITE & ZELAZNY, 1986)**

$$K_{ij} = \frac{\bar{c}_i^{y+} (c_j^{x+})^{1/x}}{\bar{c}_j^{x+} (c_i^{y+})^{1/y}} \qquad (19)$$

where y and x are the valences of species *i* and *j*, respectively, and $K_{ij}$ is the Gapon selectivity coefficient. Exchange concentrations are expressed in moles of charge per kg of dry soil ($mol_c kg^{-1}$). It is assumed that the cation exchange capacity, $c_T$

($mol_c kg^{-1}$), is constant and independent of the pH. The assumption of constant exchange capacity is not valid for soils containing large amounts of variable charge, such as oxisols, but is necessary in the present models to maintain conservation of mass.

Consideration of precipitation or. dissolution is particularly important for soils which precipitate or dissolve calcium carbonate or gypsum. We consider five solid phases that constrain the solution to equilibrium whenever the solids are specified or ap proached from over-saturation: gypsum, nesquehonite, hydromagnesite, sepiolite, and gibbsite. Precipitation-dissolution of calcite is treated with either an empirical apparent solubility value or with a simple kinetic expression. Dissolution of dolomite is always considered to be a kinetic process. Discussion on the selection and consideration of these solids is given in SUAREZ and SIMUNEK (1995).

As mentioned above, the option exists to treat calcite precipitation by use of a kinetic expression. The reaction rate of calcite precipitation-dissolution, $R^C$, in the absence of inhibitors such as “foreign ions” and dissolved organic matter, can be calculated with the rate equation of INSKEEP and BLOOM (1985),

$$R^C = -11.82[(\mathrm{Ca}^{2+})(\mathrm{CO}_3^{2-}) - K^C_{SP}] \qquad (20)$$

The precipitation or dissolution rate of calcite is reduced by the presence of various inhibitors. SIMUNEK and SUAREZ (1993b) developed a function for the reduction of the precipitation-dissolution rates due to surface poisoning by dissolved organic carbon, based on the experimental data of INSKEEP and BLOOM (1986). The reaction rates of dolomite dissolution, $R^D$ ($\mathrm{mmol\ cm^{-2} s^{-1}}$), are calculated with the rate equation of BUSENBERG and PLUMMER (1982). As mentioned earlier, we do not consider the precipitation of dolomite. Formation of protodolomite, which has been observed in hypersaline environments, is treated as a mixture of magnesium carbonate and calcium carbonate, both of which are considered in our chemical model.

Calculation of the single ion activity coefficient is specified by using an extended version of the Debye-Huckel equation (TRUESDELL & JONES, 1974). The extended version of the Debye-Huckel equation (TRUESDELL & JONES, 1974), which can be used in the dilute to moderately saline concentration range, is given by

$$\ln \gamma = -\frac{A z^2 \sqrt{I}}{1 + Ba\sqrt{I}} + bI \qquad (21)$$

where *A* and B are constants that depend only on the dielectric constant, density, and temperature; z is the ionic charge, a and b are two adjustable parameters, and I is the ionic strength

$$I = 0.5 \sum_{i=1}^{M} z_i^2 m_i \qquad (22)$$

where M is the number of species in the solution mixture, $m_i$ is molality and z, is valence. The adjustable parameters a and b for individual species are given by **TRUESDELL and JONES (1974).**

At high ionic strength, activity coefficients are no longer universal functions of ionic strength, but are also dependent on the relative concentration of the various ions present in solution **(FELMY & WEARE, 1986).** The activity coefficients can then be expressed in a virial-type expansion using the Pitzer equations **(PITZER, 1979).** This model is considered accurate even for solutions with very high ionic strength (up to 20 molal) and can be used down to infinite dilution. The option is available, however the user needs to be aware that it increases the model computation time several fold.

The GALERKIN finite element method with linear basis functions is used to obtain a solution of the water flow (1) and solute (3) and $CO_2$ (4) transport equations subject to the imposed initial and boundary conditions. A detailed description of the solution of Richards' equation was given in **SIMUNEK** et al. (1992). The finite element method is also used to solve the heat, $CO_2$, and mutticomponent solute transport equations. A detailed description of the numerical solution for these transport equations is given in **SIMUNEK and SUAREZ (1993b).**

The governing solute transport equation (3) contains time derivative terms for the total dissolved, sorbed and solid phase concentrations. Because of the second and third terms, the solute transport equation (3) is highly nonlinear and an iterative process must be applied to obtain its solution.

Coupling between the transport and chemical submodules was described by **WALSH et** al. (1984), **CEDERBERG et al. (1985), and BRYANT** et al. (1986) (also used **by YEH & TRIPATHI (1991)).**

## Example

The simulation of water content, soluble ions and solid phases changes is demonstrated with the following example. Drainage water from the Welton-Mohawk Irrigation District is used for a one year irrigation simulation. We assume high frequency irrigation of one cm/day and a plant water uptake of 0.9 cm/day. The unsaturated hydraulic conductivity-water content relationship was taken as that of a sandy loam.

Figure la shows the change in water content with depth and time. Starting from a relatively dry soil it took about 100 days to reach steady state water content. The tracer concentrations shown in Figure 1 b demonstrate the effects of plant water uptake on soil ion concentrations. Tracer concentrations increase with time and depth. The large concentration increase with depth is consistent with the efficient water use (leaching fraction of 0.1) and downward movement of water and salts. The calcium

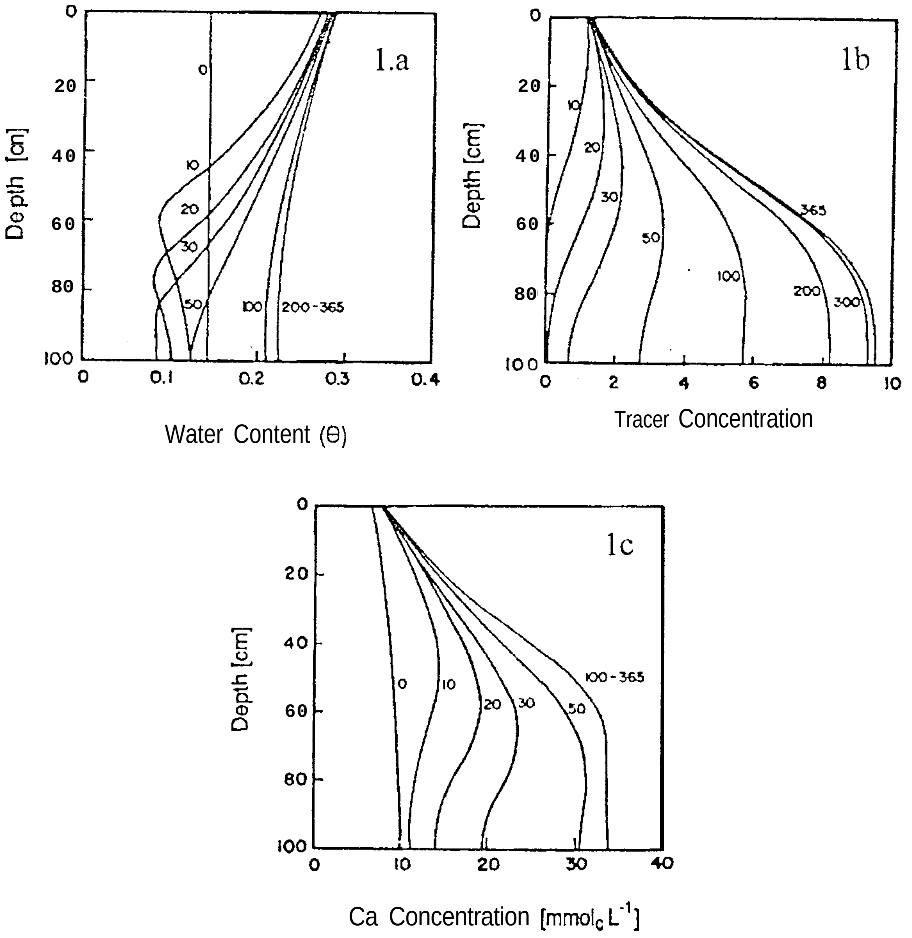

*Figure 1*

Depth versus concentration relations as a function of time (O-365 days) for water content (Fig. la), tracer concentration (Fig. lb) and Ca concentration (Fig Ic) for irrigation with Wellton-Mohawk drainage water at 1 cm/d and ET of 0.9 cm/d (leaching fraction of 0.1) concentrations, shown in Figure lc are similar to the tracer distributions except that calcium carbonate and gypsum precipitation limit the increase in concentration (a less than 4-fold increase at the bottom of the rootzone instead of a 10-fold increase).

## Summary and conclusion

The soil salinity model is intended as a practical model for the evaluation of salinity and sodicity problems. It includes the major ion chemical processes of cation exchange and solid phase dissolution and precipitation, water and solute movement under variably saturated conditions, plant growth and plant water uptake including the response to adverse environmental conditions such as salinity water stress and temperature. Because the model provides information about the reduction in yield due to stress it is suited for use as a management tool. The user can run multiple simulations with varying amounts of water, waters of different composition or addition of amendments and see the effects on soil salinity and plant yield. The model includes a Windows' based user friendly interface with both pre and post processors. The reclamation example demonstrates the importance of elevated $CO_2$ concentrations combined with ion exchange in enhancing the solubility of calcite. Use of the model for reclamation and soil water management should enable more efficient use of amendments and water resources.

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