FAO-Salinity Laboratory SWS Model

Research Report No. 147

Version 1.1

Donald L. Suarez and Peter J. Vaughan

George E. Brown Jr. Salinity Laboratory, USDA-ARS

450 W. Big Springs Road

Riverside, CA

September, 2001

INTRODUCTION

The FAO-Salinity Laboratory SWS (soil-water-salinity) model described in this manual is intended to evaluate the suitability of a water for irrigation, primarily in arid and semiarid regions with emphasis on the effects of salinity and sodicity. The suitability of a water is evaluated in terms of its utility for crop growth. Thus the criteria is not only water salinity but the existing soil chemical and physical properties, the water requirements of the crop and its salt tolerance, adequacy of drainage and amount of water that can be infiltrated into the soil with consideration of the chemical factors that affect infiltration. The model is also suitable to evaluate the need for reclamation and to evaluate the effectiveness of different reclamation strategies, such as application of various amounts of gypsum. The model considers water flow, carbon dioxide production and transport, transport and chemistry of major dissolved ion species including cation exchange and mineral dissolution and precipitation and plant water extraction with consideration of water and salt stress. It is assumed that all nutrient levels are adequate for optimum plant growth.

Water flow is simulated with a variably saturated water flow model which considers the effects of salinity, sodicity and pH on hydraulic conductivity. The consideration of chemical factors on hydraulic conductivity is based on the response of arid zone soils from California. The quantitative response to these chemical factors is different for different soils but the simulation will nonetheless provide information about potential hazards associated with specific water and soil conditions.

The model allows for calculation of ET_0 using the FAO Penman-Monteith approach. Growth stages and crop coefficients are provided for selected crops, enabling calculation of ET_c. Plant water uptake takes into consideration the dynamic water and salt stress occurring in the root zone. This calculation requires the input of crop-specific salt tolerance information. This information is provided for major crops. The relative yield of a crop is calculated as the ratio of the water uptake to the optimum water uptake of the crop in the absence of water or salt stress.. The output from this plant model must be regarded as a representation, since it has not been optimized for each crop, planting regime and soil fertility, and locality. Until further testing the model should be used as a guide to specific management decisions rather than an absolute predictor of future conditions.

The user friendly interface utilizes default parameters and pull down menus. Additional options are available by changing the input file after initially creating the files with the interface. These options are explained in the help files. The help files provide information for the preparation of the input files.

The FAO-Salinity Lab SWS model is a modification of the fortran code in the UNSATCHEM model (Suarez and Simunek, 1992, Simunek and Suarez, 1996, Suarez and Simunek, 1997) with addition of a plant growth module, upgraded to 32 bit double precision code and with a Windows 95 user interface (developed in Visual Basic). The UNSATCHEM model in turn is based on the SOILCO2 model (Simunek and Suarez, 1993, Suarez and Simunek, 1993) with addition of a chemical speciation routine (Suarez, 1977), calculation of

cation exchange (from a routine in Robbins et al.,1980), and calculation of osmotic activity coefficients using the Pitzer routines of GMIN (Felmy, 1990). The plant response to salinity is calculated from salt tolerance tables.

The model includes prediction of carbon dioxide production and transport in both the liquid and gas phases. This information can be used to evaluate the potential for aeration problems but its primary function is for use in the chemical routines for prediction of pH and Ca and alkalinity concentrations. Heat transport is also considered. Accurate prediction of water movement, carbon dioxide concentration and heat transport may require detailed soil information, however for the objectives of this model default criteria can be readily utilized.

The model has provision for considering several water types, such as rain, irrigation water, ground water etc., as well as allowing for several soil layers with different chemical and physical properties. When used as a reclamation model, gypsum, calcite or acid can be mixed at any concentration to any depth selected by the user. The effects of chemistry on hydraulic conductivity can also be represented.

Since it is a dynamic model the irrigation inputs should be enter as specific time events of specified duration and intensity with corresponding entry of ET_0. The plant submodel can be utilized in either of two ways; either for a perennial crop, such as a grass with a fixed root distribution or an annual crop with a growing root distribution. In the case of a perennial crop the crop yield is expressed as a relative yield-meaning the ratio of the crop biomass under the simulated conditions to the crop biomass under unstressed conditions. In this instance we assume that the relative yield is equal to the actual water consumed divided by the optimum (unstressed water consumption).

PART 1: INSTALL

INSTALLATION

1.01   Installing the FAO-SWS Program

The directions given below describe how to install the FAO-SWS program. <u>Please read these directions carefully before attempting to install the FAO-SWS program!</u> You should refer to section 1.2 if you encounter any problems. <u>Additionally, please also be sure to read section 1.3 before you attempt to install the test case files.</u>

1.1   Standard Installing Instructions

The install the FAO-SWS program, run the setup.exe program, and then follow the on-screen setup instructions.

Note: we recommend that you install the FAO-SWS program in the following sub-directory: C:\Program Files\FAOSWS

1.2   Trouble Shooting any Installation Problems

1.2.1   Files needed during setup

In order for the FAO-SWS program to install properly, the setup.exe program must be able to access two support files: Fao-sws.cab and Setup.1st. These two files must be present on your installation media (i.e., on the CD or floppy disks). Additionally, they must be located in the same sub-directory as setup.exe.

1.2.2   File "out-of-date" or "older version" warnings

Some of the Microsoft Windows support *.ocx and/or *.dll files used by the FAO-SWS program uses may be older than the identical *.ocx and/or *.dll files already installed on your operating system. If you receive an "out-of-date" or "older verison" warning during the setup procedure, you should follow the suggested on-screen recommendation and retain your current files.

1.2.3   File Access Violation Errors

The setup.exe program will generate an access violation error if it attempts to install any *.ocx or *.dll file already in use by another program. *You should attempt to minimize these errors by shutting down all other programs before running the setup.exe program.* However, sometimes hidden background programs can still cause these errors to occur (this is especially true if your computer is part of a LAN [Local Area Network]; the network communication software running in the background can often cause these errors).

If you receive a "file access violation error" (particularly one associated with the installation of a program called MSVCRT.dll), select the "Ignore" option shown in the Windows message box and continue on with the installation procedure. (Note: Windows will warn you that the program you are installing may not function properly when you select this option. This warning can be ignored.)

1.3   Installing the Test Case Files

Two sets of demonstration test case file are automatically installed with the FAO-SWS program. These files are archived in the following two self extracting ZIP files:

FAOTest1files.exe
FAOTest2files.exe

These two self extracting ZIP files are stored in the test1 and test2 subdirectories, respectively. Under a standard installation, the locations of these two sub-directories will be:
C:\Program Files\FAOSWS\test1
and
C:\Program Files\FAOSWS\test2

(Note: the location of the FAOSWS sub-directory will be different if you did not install the program off the C:\Program Files sub-directory.)

To extract these test case files, locate and display the FAOTest1files.exe and/or

FAOTest2files.exe program using either My Computer or Windows Explorer, run the extraction program (by double-clicking on the file name), and then follow the on-screen extraction instructions.

WARNING! These self extraction program may attempt to incorrectly extract and install your test case files to the "C:\" root directory. IN ORDER FOR THE FAO-SWS PROGRAM TO LOCATE THESE FILES, you MUST adjust the destination option so that the test case files are extracted into the same sub-directory as the FAOTest1files.exe or FAOTest2files.exe program files (i.e., into the test1 or test2 subdirectories, respectively).

Note: We recommend that you retain these self extracting ZIP files in the test1 and test2 sub-directories. This will allow you to always recover a clean (i.e., uncorrupted) set of test case demonstration files in the future, should your extracted test case files ever become inadvertently corrupted or deleted.

PART 2: DESCRIPTION OF THE MODEL

This chapter provides theoretical background and description of the processes simulated in the model and equations used. The discussion is organized into various sections describing water flow, chemical processes in soil and water, calculation of optimal water consumption by a crop and plant responses to water and salinity stress.

WATER FLOW

Hydraulic functions

The model uses a modified version of the one-dimensional Richards= equation (Richards, 1952)

$$\frac{\partial \theta_w}{\partial t} = \frac{\partial}{\partial z}[K(\frac{\partial h}{\partial z} - 1)] - S \tag{1}$$

where h is the water pressure head, θ_w is the volumetric water content, K is the hydraulic conductivity function, t is time, z is the spatial coordinate, and S is the sink/source term, which in our case represents removal of water from the soil by plant roots. By use of this equation, effects of thermal and density gradients are neglected and it is assumed that the gas phase dynamics do not affect water flow. These simplifications are not justified in all instances but consideration of these processes is beyond the scope of this program.

The unsaturated soil hydraulic properties are described by a modified version of those proposed by van Genuchten (1980). The water retention and hydraulic conductivity functions are given by

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \tag{2}$$

and

$$K(h) = K_s K_r r = K_s r S_e^{1/2}\left[1 - (1 - S_e^{1/m})^m\right]^2 \tag{3}$$

respectively, where

$$m = 1 - 1/n \quad n > 1 \tag{4}$$

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \textbf{(5)}$$

and where θ_r and θ_s denote residual and saturated water content, (expressed as $cm^3cm^{-3)}$, respectively, K_s is the saturated conductivity [cm d^{-1}], K_r is the relative hydraulic conductivity, S_e is relative saturation and m, n, and α [cm^{-1}] are the empirical parameters of the hydraulic characteristics. In order to increase numerical stability in the range of h from 0 to -2 cm, we have specified a constant θ (θ_s) for that interval. Hydraulic characteristics are determined by a set of 6 parameters, θ_r, θ_s, α, n, K_s and the variable r, representing the effect of soil chemistry on hydraulic properties. Use of the model requires optimizing the first 5 parameters from the experimental water retention, pressure head, and saturated conductivity data. This parametrization can be performed using the RETC code (van Genuchten et al., 1991).

In keeping with the objectives of this model we do not expect users to conduct detailed studies on the water retention curve and unsaturated hydraulic conductivity of each soil used. It is considered that for water suitability, reclamation and prediction of crop stress due to salinity, the water retention vs pressure head curve is reasonably represented by the functions obtained from soil texture by Carsel and Parrish (1988). The major error for our applications is likely the saturated hydraulic conductivity, as water applied at a rate in excess of infiltration results in runoff. In some instances the values presented appear greater than what we observe- for example K_s for a loam soil. A user with more detailed hydraulic information may want to use the advanced option and input their own hydraulic parameters. In the absence of detailed hydraulic characteristics the advanced option can still be used to modify only the saturated hydraulic conductivity, maintaining the parameters relating to the water retention curve.

Chemical effects on hydraulic conductivity

Equation 3 differs uniquely from previous relations in that it includes a reduction term, r, which scales the hydraulic conductivity in relation to the chemical conditions in the soil. Optimal soil chemical conditions for infiltration are represented by values where r=1. Elevated levels of exchangeable sodium result in swelling of smectitic clays. Detachment of clay particles, dispersion, and subsequent clay migration and redeposition results in blocking of pores at low salinity and in the presence of exchangeable sodium (McNeal, 1968, Shainberg and Levy, 1992). This process is readily observed in the natural development of clay pan layers in soils and most dramatically in sodic, nonsaline soils. This process has also been related to the distribution of divalent cations, with Mg^{2+} being more susceptible to dispersion than Ca^{2+}. In addition, it has been determined that elevated levels of pH adversely impact saturated hydraulic conductivity, separate from the sodicity and salinity interactions (Suarez et al., 1984).

Suarez and Simunek (1997) represented the chemical effects on hydraulic properties by the use of a reduction function, r, given by

$$r = r_1\, r_2 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \textbf{(6)}$$

where r_1 is the reduction due to the adverse effects of low salinity and high exchangeable sodium fractions on the clay and r_2 is the adverse effect of pH. The r_1 term is given by McNeal (1968) as

$$r_1 = 1 - \frac{cx^n}{1 + cx^n} \tag{7}$$

where c and n are empirical factors, and x is defined by

$$x = f_m \; 3.6 * 10^{-4} \; ESP^* \; d^* \tag{8}$$

where f_m is the mass fraction of smectite (montmorillonite and beidellite) in the soil, d^* is an adjusted interlayer spacing and ESP^* is an adjusted exchangeable sodium percentage (percentage of the total cation exchange charge of the soil that is neutralized by Na^+). The term d^* is defined by

$$\begin{aligned}
d^* &= 0 & C_0 &> 300 \; \text{mmol}_c \, L^1 \\
d^* &= 356.4 \; (C_0)^{-0.5} + 1.2 & C_0 &\leq 300 \; \text{mmol}_c \, L^1
\end{aligned} \tag{9}$$

where C_o is the total salt concentration of the solution, and the term ESP^* is given by

$$ESP^* = ESP_{soil} - (1.24 + 11.63 \log C_0) \tag{10}$$

The reduction factor r_2, for the adverse effect of pH on hydraulic conductivity, was calculated from the SAR-pH hydraulic conductivity experimental data of Suarez et al. (1984), after first correcting for the adverse effects of low salinity and high exchangeable sodium using the r_1 values. Based on this limited data

$$\begin{aligned}
r_2 &= 1 & &\text{for pH} < 6.83 \\[1em]
r_2 &= 3.46 - 0.36 \, \text{pH} & &\text{for } 6.83 \leq \text{pH} \leq 9.3 \\[1em]
r_2 &= 0.1 & &\text{for pH} > 9.3
\end{aligned} \tag{11}$$

In view of the differences among soils, these specific values may not be generalized predictors of soil hydraulic conductivity. Soils differ in their reaction to these factors, in ways that are not yet completely understood. Thus although the above equations may not be generalized predictors, they do represent conditions of arid land soils examined at the U.S. Salinity Laboratory and they illustrate the changes in K that affect infiltration and solute movement under various chemical conditions. This option in the model should *not* be considered as a

quantitative prediction of what will occur at a specific site but is useful to evaluate the relative importance of the chemical effects under different soil and water conditions. Many other factors in addition to sodicity and pH affect soil aggregate stability, such as organic matter, soil texture, tillage etc., and it is reasonable to assume that there is an interaction between these factors and the chemical factors considered here.

PLANT MODELING

There are two options in the model relating to plant water uptake and root modeling, a fixed root distribution and root growth. In the case of a fixed rooting distribution, the root distribution is input by the user and remains constant throughout the simulation. This option is suited for use when simulating perennial crops such as alfalfa and pasture grasses. In this instance, water uptake depends only on input ET, and water and salt stress simulated by the model. The model predicts relative yield based on the ratio of predicted ET_a, to optimum ET_c, where the predicted ET_a takes into consideration the response to stress.

The root growth option is suitable for simulation of annual crops. In this case the user inputs an initial root distribution from which the roots will develop. This option requires additional inputs such as initial rooting depth maximum rooting depth, growing degree days etc.

Water uptake by plant roots-fixed root distribution

The sink term in Eq. 1 is defined as the volume of water removed from a unit volume of soil per unit of time as a result of plant water uptake. In the case of a fixed rooting distribution, the root water uptake in response to water and salinity stress is expressed as

$$ S = S_p \, \alpha_s(h) \, \alpha_\varphi(h_\varphi) \tag{12} $$

where S_p is the potential water uptake [$cm^3 cm^{-3} d^{-1}$] and $\alpha_\varphi(h_\varphi)$ is the osmotic stress function for water uptake and h_φ is the osmotic head [m]. The water stress response function, $\alpha_s(h)$, is a dimensionless function of the soil water pressure head ($0 \le \alpha \le 1$) described by van Genuchten (1987) as

$$ \alpha_s(h) = \frac{1}{1 + (\frac{h}{h_{50}})^p} \tag{13} $$

where h_{50} [m] and p are empirical constants. The default parameter of the model is set at h_{50} equal to -50 m and p is equal to 3. The parameter h_{50} represents the pressure head at which the water extraction rate is reduced by 50%. Specific values of the h_{50} and p parameters for salinity are presented in Table 1 for selected crops. If other crops are selected it is suggested

that in the absence of detailed information, the h_{50} value be calculated from the more traditional Maas-Hoffman relationship (Maas and Hoffman, 1977). They presented data in terms of an intercept electrical conductivity (EC) or osmotic pressure above which there was yield decline and an intercept that describes the yield decline with increasing salinity (expressed in terms of electrical conductivity). From the salt response slope intercept information the h_{50} can be readily calculated and p can be set to 3.0. This water stress response function, $\alpha_s(h)$, does not consider transpiration reduction near saturation. The decrease in water uptake that is sometimes observed at saturation is related to oxygen stress and is more properly treated based on prediction of the gas phase composition (for models such as this that include CO_2 production and transport).

The potential water uptake rate in the root zone is expressed as the product of the potential transpiration rate, T_c [LT^{-1}], and the normalized water uptake distribution function, β (z) [L^{-1}], which describes the spatial variation of the potential water uptake rate, S_p, over the root zone, as follows

$$S_p = \beta(z)T_c \tag{14}$$

For a fixed root distribution the function $\beta(z)$ is specified by the user in the input file.   The actual transpiration T_a is given by

$$T_a = \int_{L-L_r}^{L} S(h, h_\varphi, z)dz = T_c \int_{L-L_r}^{L} \alpha_s(h)\alpha_\varphi(h_\varphi)\beta(z)dz \tag{15}$$

The terms L and L_r are respectively the height at the soil surface (0) and the height (or depth) of the lowest root. The total actual transpiration at each time step is calculated by summation of the transpiration amounts for each of the root zone depth intervals. The transpiration in each of the depth intervals is based on the root distribution function and the stress calculated in that depth interval. There is no compensation at other depths for reduced water uptake within any depth interval. The total transpiration for the simulation is the sum of the actual transpiration time steps. The ratio of actual transpiration to optimal transpiration is taken as the relative yield. The stress reduction function given in equation (15) is obtained by multiplication of the product of the water and osmotic stress functions.

The fixed root option is always selected for a perennial crop. It is also possible to use the fixed root option for predicting the water uptake and relative crop yield for an annual crop. In this instance the input values are ET_0 multiply by the crop coefficient. Values for these coefficients are crop and locally specific as well as varying with time during growth, thus are ideally provided by the model user. Use of this option requires more detailed information but may provide more accurate prediction of water requirements and use if the crop factors are known for the crop and locality to be simulated. Table 2 presents data on selected crops.

Water uptake by plant roots-root growth option

A specification of the root growth option enables use of a simplified crop-root growth model. In this instance the input is still ET_c and this value must be input or calculated by the model. Additional plant specific information is required, including planting date, heat units to maturity and harvest date. The plant is divided into various stages of development, and the initial rooting depth must be specified. If the shallow initial root zone dries out there will be water stress. It is suggested that the user insure that the initial conditions are reasonable, with regard to the initial root distribution and the total amount of water extracted.

Root growth

The root depth, L_r, can be either constant or variable during the simulation. For annual vegetation the plant submodel is required to simulate the change in rooting depth with time. In UNSATCHEM (Simunek and Suarez, 1996 and Suarez and Simunek, 1997) the root depth is the product of the maximum rooting depth, L_m [cm], and the root growth coefficient, $f_r(t)$:

$$L_r(t) = L_m f_r(t) \tag{16}$$

To calculate the root growth coefficient, $f_r(t)$, Simunek and Suarez (1993) combined the Verhulst-Pearl logistic growth function with the growth degree day (*GDD*) or heat unit concept (Gilmore and Rogers, 1958). The logistic growth function is generally used to describe the biological growth at constant temperature, and the *GDD* model is utilized for determining the time between planting and maturity of the plant. The heat unit model cannot be used directly to predict biomass during the growth stage since it would predict a linear growth with time at constant temperature. Combining the heat unit concept with the logistic growth function, incorporates both time and temperature dependence on growth.

For the growth degree day function a suitable option is a modified version of the relation developed by Logan and Boyland (1983), who assumed that this function is fully defined by the temperature, T [K], expressed by a sine function to approximate the behavior of temperature during the day, and by the three temperature limits, T_1, T_2, and T_3 [K]. When the actual temperature is below the base value T_1, plants register little or no net growth. The plant growth is at a maximum level at temperature T_2, which remains unchanged for some interval up to a maximum temperature T_3, above which increased temperature has an adverse effect on growth.

Based on this information, Simunek and Suarez (1993) proposed the following dimensionless growth function

$$g(t)=0 \qquad\qquad t \leq t_p\,; t \geq t_h$$

$$g(t)=\begin{cases} \dfrac{1}{T_{Bas}} \left[\int \delta(T\text{-}T_1)dt - \int \delta(T\text{-}T_2)dt - \int \delta(T\text{-}T_3)dt \right] & t\varepsilon\,(t_p,t_m) \\ \\ g(t)=1 & t\varepsilon\,(t_m,t_h) \end{cases} \qquad \textbf{(17)}$$

where T_{Bas} are the heat units [KT] necessary for the plant to mature and the roots to reach the maximum rooting depth, t_p, t_m, and t_h represent time of planting, time at which the maximum rooting depth is reached and time of harvesting, respectively; and parameter δ introduces into the heat unit concept the reduction in optimal growth due to the water and osmotic stress. The expression inside the parenthesis of equation (17) reaches value T_{Bas} at time t_m when roots reach the maximum rooting depth. The individual integrals in equation (17) are evaluated only when the particular arguments are positive. Parameter δ is defined as the ratio of the actual to potential transpiration rates:

$$\delta = \frac{T_a}{T_p} \qquad\qquad \textbf{(18)}$$

Biomass or root development during the growth stage can also be expressed by the Verhulst-Pearl logistic growth function

$$f_r(t) = \frac{L_0}{L_0 + (L_m - L_0)e^{-rt}} \qquad\qquad \textbf{(19)}$$

where L_0 is the initial value of the rooting depth at the beginning of the growth period [cm] and r is the growth rate [T^{-1}].

Both growth functions (17) and (19) can be used directly to model the root growth. However, to avoid the drawbacks of each of the concepts, as discussed above, the equations can be combined (Simunek and Suarez, 1993), substituting the growth function calculated from the heat unit concept (17) for the time factor in the logistic growth function (19):

$$t = t_m\, g(t) \qquad\qquad \textbf{(20)}$$

where t_m is the time when GDD reaches the required value for the specific plant species (T_{Bas}). This value is not known a priori; only the product rt_m must be known and that can be selected, for example, so that $f_r(t)$ equals 0.99 for $g(t)=1$.

HEAT TRANSPORT

Prediction of temperature in the unsaturated zone is required for prediction of chemical speciation, mineral equilibria and plant root growth as well as for prediction of CO_2 production. Simunek and Suarez (1994) include a heat transport routine which is used for prediction of the factors discussed above. The one dimensional equation for heat transport is

$$C_p(\theta_w)\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta_w)\frac{\partial T}{\partial z}\right] - C_w q_w \frac{\partial T}{\partial z} \tag{21}$$

Where $\lambda(\theta_w)$ is the apparent thermal conductivity coefficient of the soil and $C_p(\theta_w)$ and C_w, are the volumetric heat capacities of the soil solid and liquid phases, respectively. The volumetric heat capacity is expressed as

$$C_p(\theta_w) = C_n\theta_n + C_o\theta_o + C_w\theta_w + C_a\theta_a \approx (1.92\theta_n + 2.51\theta_o + 4.18\theta_w)10^6 \quad (Jm^{-3}\ {}^oC^{-1}) \tag{22}$$

where θ is the volumetric fraction , C is the heat capacity and the subscripts n, o, a and w represent the mineral phase, organic matter phase , gas phase and water phase respectively. The thermal conductivity is calculated using the empirical equation developed by Chung and Horton (1987) as follows,

$$\lambda_0(\theta_w) = b_1 + b_2\theta_w + b_3\theta_w^{0.5} \tag{23}$$

where $\lambda_s(\theta_w)$ is the thermal conductivity of the soil and water and b_1, b_2, and b_3 are the fitting parameters. Default parameters are provided by the model.

CALCULATION OF CROP ET

Water consumption at any time step is calculated based on ET_c and the stress reduction factor. In the absence of input ET_c information the model will predict ET_c using the FAO version of the Penman Monteith equation (Allen et al., 1998), given as

$$ET_0 = \frac{0.408\Delta(R_n - G) + \gamma(\frac{900}{t+273})U_2(e_s - e_a)}{10(\Delta + \lambda(1 + 0.34U_2))} \tag{24}$$

where ET_0 is expressed in cm/d, Δ is the slope of the saturation vapor pressure curve (kPa ${}^0C^{-1}$), R_n is the net radiation at the crop surface (MJ m^{-2}d^{-1}), G is the soil heat flux density (MJ m^{-2}d^{-1}), γ is the psychrometric constant (kPa ${}^0C^{-1}$), t is the mean daily air temperature (${}^0C$), e_s is the saturation vapor pressure (kPa) at the specified temperature, e_a is the measured or calculated vapor pressure, and U_2 is the wind speed at a height of 2 m above the surface (ms^{-1}).

The slope of the saturation vapor pressure versus temperature, Δ, is calculated from the relationship,

$$\Delta = \frac{4098 \, (0.611 \exp(\frac{17.27t}{t+237.3}))}{(t+237.3)^2} \tag{25}$$

where t is the mean daily air temperature (^{0}C). The psychrometric constant is calculated from

$$\gamma = 0.665 10^{-3} P \tag{26}$$

where P is the atmospheric pressure (kPa). The constant 0.665 is the product of the specific heat at constant pressure, c_p (0.001013 MJ kg^{-1} ^{0}C) divided by the product of the latent heat of vaporization (2.45 MJ kg^{-1}) and the ratio of the molecular weight of water vapor to dry air (0.622). For these purposes it is sufficient to neglect barometric changes and calculate the pressure from the mean pressure at sea level and the elevation of the site. At 20 ^{0}C

$$P = 101.3 \left[\frac{293 - 0.0065z}{293} \right]^{5.26} \tag{27}$$

R_n, the net radiation is the difference between the value of incoming net shortwave radiation (R_{ns}) and net outgoing longwave radiation R_{nl},

$$R_n = R_{ns} - R_{nl} \tag{28}$$

R_{ns} is ideally measured but when not available can be calculated with the following equation (Allen et al., 1998),

$$R_{ns} = 0.77 \, (0.25 + 0.50 \frac{n}{N}) R_a \tag{29}$$

where n/N is the ration of the actual hours of sunshine to the maximum possible hours of sunshine for that day. This value is input by estimating the fraction of daylight hours in where there is direct sunlight on the field. The recommended value of 0.25 represents the fraction of extraterrestrial radiation reaching the surface on overcast days and the value of 0.5 represents the difference between the fraction of extraterrestrial radiation reaching the surface on overcast and clear days (Allen et al., 1998). The term R_a, depends on the solar constant, latitude, and date and time of the day. Since we are not calculating daily ET$_0$ then R_a can be calculated daily by,

$$R_a = 37.6 \, G_{SC} d_r (\omega_s \sin\psi \sin\delta + \cos\psi \cos\delta \sin\omega_s) \tag{30}$$

where R_a = extraterrestrial radiation [MJ m^{-2} day $^{-1}$], G_{SC} is the solar constant equal to 0.0820 MJ m^{-2} min^{-1}, d_r is the inverse of the relative distance between the Earth and Sun, ω_s is the sunset hour angle, [rad], ψ is the latitude at the location [rad], and δ the solar declination [rad]. The inverse relative distance is calculated as

$$d_r = 1 + 0.033 \cos (0.0172 J) \tag{31}$$

where J is the calendar date of the year. The latitude in degrees, L_a is converted to latitude in radians ψ by

$$\psi = 0.01745 (L_a) \tag{32}$$

The solar declination δ, is calculated from

$$\delta = 0.409 \sin (0.0172 J - 1.39) \tag{33}$$

where J is again the calendar date of the year. The sunset hour angle is given by

$$\omega_s = arc \cos (-\tan \psi \tan \delta) \tag{34}$$

Calculation of R_{nl} in Equation (28) requires calculation of R_s and R_{so}, the solar radiation and the clear sky solar radiation. R_s is given by

$$R_s = (0.25 + 0.5 \tfrac{n}{N}) \tag{35}$$

and R_{so} by

$$R_{so} = (0.75 + 2 \times 10^{-5} z) R_a \tag{36}$$

where z is the elevation in meters above sea level and the value of 0.75 is the sum of the fraction of extraterrestrial radiation reaching the earth on a clear day. R_{nl} can then be calculated from R_s and R_{s0} using

$$R_{nl} = 4.903 \times 10^{-9} \left[\frac{T_{\max k}^4 + T_{\min k}^4}{2} \right] (0.34 - 0.14(e_a)^{0.5}) \left(1.35 \frac{R_s}{R_{SO}} - 0.35 \right) \tag{37}$$

where T_{max} is the maximum absolute temperature during the day and T_{min} the minimum absolute temperature.

The mean saturation vapor pressure e_s is approximated by
where e^0_{min}, the saturation vapor pressure at the daily minimum temperature(t_{min}) in ^{o} C is

$$e_s = \frac{e^0_{max} + e^0_{min}}{2} \qquad \textbf{(38)}$$

given by

$$e^o_{t\,min} = 0.611\exp\left(\frac{17.27t_{min}}{t_{min} + 237.3}\right) \quad t_{min} = t - 0.5\Delta t \qquad \textbf{(39)}$$

and e^0_{max} is given by

$$e^o_{t\,max} = 0.611\exp\left(\frac{17.27t_{max}}{t_{max} + 237.3}\right) \quad t_{max} = t + 0.5\Delta t \qquad \textbf{(40)}$$

The actual vapor pressure e_a can be estimated from

$$e_a = e^0_{min} \cdot \frac{RH_{max}}{100} \qquad \textbf{(41)}$$

where RH_{max} is the maximum relative humidity. ET_0 can now be calculated by equation 24, using equation 25 through 41 and with input of wind speed, latitude, elevation, calendar date, mean daily temperature, daily temperature fluctuation, fraction of the day that is clear, and maximum relative humidity, all factors that should be readily available.

Crop coefficients and calculation of ET_c

Crop coefficients serve to convert the ET_0 values into ET_c for the crops of interest. The reference ET_0 is for a hypothetical crop with an assumed height of 0.12 m having a surface resistance of 70 s m^{-1} and an albedo of 0.23, resembling a grass crop of uniform height, well watered and growing actively. For annual crops stage of growth as well as crop characteristics affect the coefficients thus they must be stage dependent. In the absence of a coupled crop specific growth model the transition to various stages depends on climatic factors, thus the crop coefficients vary according to location as well as time. Shown in Table 1 are the length of crop stages for use in calculation of crop coefficients. Table 2 presents the crop coefficients for major crops and selected locations and planting dates, taken from FAO Irrigation and Drainage Paper 56 (Allen et al., 1998). These values are utilized to calculate the

ET$_c$ values used in the model.
CONCENTRATION/PRODUCTION OF CARBON DIOXIDE

Unsaturated zone models typically either consider a closed system with constant inorganic carbon, as is also commonly considered for ground water systems, or assume an open system at fixed CO$_2$. The first assumption is clearly not desirable for a root zone model as large amounts of CO$_2$ are produced by plant decomposition as well as plant root respiration. Specification of a fixed CO$_2$ is a marked improvement over the closed system assumption but still does not consider the spatial and temporal fluctuations. These changes are due to both changes in production of CO$_2$, as well as changes in the transport of CO$_2$, which is mostly related to changes in the air-filled porosity of the soil, but can also be related to the flow of water. In the root zone the quantity of CO$_2$ added or removed by mineral dissolution/ precipitation reactions is usually relatively small compared to the production and flux values and is neglected. Below the CO$_2$ production zone this process may constitute the major control on CO$_2$ gas concentration.

Carbon dioxide production

Simunek and Suarez (1993b) described a general model for CO$_2$ production and transport. They considered CO$_2$ production as the sum of the production rate by soil microorganisms, γ_s [cm^3 cm^{-3}T^{-1}], and the production rate by plant roots, γ_p [cm^{3}cm^{-3}T^{-1}]

$$P = \gamma_s + \gamma_p = \gamma_{s0} \prod_i f_{si} + \gamma_{p0} \prod_i f_{pi} \tag{42}$$

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 γ_{s0} and γ_{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 [cm^{3}cm^{-2}T^{-1}]. The individual reduction functions are given in Simunek and Suarez (1993a) and the discussion of selection of the values for optimal production as well as coefficients for the reduction functions is given in Suarez and Simunek (1993).

Carbon dioxide transport

Gas transport in the unsaturated zone includes three general transport mechanisms (Massmann and Farrier, 1992): Knudsen diffusion, multicomponent molecular diffusion and viscous flow. Thorstenson and Pollock (1989) presented equations to describe these transport mechanisms in a multicomponent gas mixture. They also presented the Stefan-Maxwell approximation of these equations, where Knudsen diffusion and viscous flow are neglected. The original equations, as well as the Stefan-Maxwell approximation, are fully coupled and generally highly nonlinear, thus requiring complex numerical schemes for solution. However, Massmann and Farrier (1992) showed that gas fluxes in the unsaturated zone can satisfactorily be simulated using the single-component transport equation, neglecting Knudsen diffusion, as long as the gas permeability of the media is greater than about 10^{-10} cm^2. They also showed

that overestimation of the gas fluxes using the single component advection diffusion equation becomes large only when permeabilities are as low as 10^{-12} to 10^{-13} cm^2. Use of Fick's law to represent diffusive flux seems to be reasonable since permeabilities smaller than 10^{-12} cm^2 occur only for very fine grained materials or for soils close to saturation. Also, Freijer and Leffelaar (1996) showed that CO_2 concentrations and fluxes can generally be described by Fick's law to within 5% accuracy.

The one-dimensional carbon dioxide transport model presented by Simunek and Suarez (1993a), assumed that CO_2 transport in the unsaturated zone occurs in both the liquid and gas phases. Furthermore, the CO_2 concentration in the soil is governed by two transport mechanisms (Patwardhan et al., 1988), convective transport in the aqueous phase and diffusive transport in both gas and aqueous phases, and by CO_2 production and/or removal. Thus the one-dimensional CO_2 transport is described by the following equation:

$$\frac{\partial c_T}{\partial t} = -\frac{\partial}{\partial z}(J_{da} + J_{dw} + J_{ca} + J_{cw}) - S c_w + P \tag{43}$$

where J_{da} is the CO_2 flux caused by diffusion in the gas phase [cmT^{-1}], J_{dw} the CO_2 flux caused by dispersion in the dissolved phase [cmT^{-1}], J_{ca} the CO_2 flux caused by convection in the gas phase [cmT^{-1}], and J_{cw} the CO_2 flux caused by convection in the dissolved phase [cmT^{-1}]. The term c_T is the total volumetric concentration of CO_2 [cm^{3}cm^{-3}] and P is the CO_2 production/sink term [cm^{3}cm^{-3}T^{-1}]. The term Sc_w represents the dissolved CO_2 removed from the soil by root water uptake. This assumes that when plants take up water the dissolved CO_2 is also removed from the soil-water system.

The individual terms in equation (43) are defined (Patwardhan et al., 1988) as

$$J_{da} = -\theta_a D_a \frac{\partial c_a}{\partial z}$$
$$J_{dw} = -\theta_w D_w \frac{\partial c_w}{\partial z} \tag{44}$$
$$J_{ca} = -q_a c_a$$
$$J_{cw} = -q_w c_w$$

where c_w and c_a are the volumetric concentrations of CO_2 in the dissolved phase and gas phase [cm^{3}cm^{-3}], respectively, D_a is the effective soil matrix diffusion coefficient of CO_2 in the gas phase [cm^{2}T^{-1}], D_w is the effective soil matrix dispersion coefficient of CO_2 in the dissolved phase [cm^{2}T^{-1}], q_a is the soil air flux [cmT^{-1}], q_w is the soil water flux [cmT^{-1}] and θ_a is the volumetric air content [L^{3}L^{-3}].

The total CO_2 concentration, c_T [cm^{3}cm^{-3}], is defined as the sum of CO_2 in the gas and dissolved phases

$$c_T = c_a \theta_a + c_w \theta_w \tag{45}$$

After substituting equations (44) and (45) into (43) we obtain

$$\frac{\partial (c_a \theta_a + c_w \theta_w)}{\partial t} = \frac{\partial}{\partial z} \theta_a D_a \frac{\partial c_a}{\partial z} + \frac{\partial}{\partial z} \theta_w D_w \frac{\partial c_w}{\partial z} - \frac{\partial}{\partial z} q_a c_a - \frac{\partial}{\partial z} q_w c_w - S c_w + P \qquad \textbf{(46)}$$

The total aqueous phase CO_2, c_w, is defined as the sum of $CO_2(aq)$ and H_2CO_3, and is related to the CO_2 concentration in the gas phase by (Stumm and Morgan, 1981)

$$c_w = K_H RT c_a \qquad \textbf{(47)}$$

where K_H is the Henry's Law constant $[MT^2M^{-1}L^{-2}]$, R is the universal gas constant (8.314 $kgm^2s^{-2}K^{-1}mol^{-1}$) and T is the absolute temperature [K]. The value of K_H as a function of temperature is taken from Harned and Davis (1943). Aqueous carbon also exists in the form of HCO_3^-, CO_3^{2-} and other complexed species, such as $CaCO_3^o$, and these species should be included in the definition of c_w. Determination of these species cannot be made without use of a complete chemical speciation program. Substituting equation (47) into (46) gives

$$\frac{\partial R_f c_a}{\partial t} = \frac{\partial}{\partial z} D_E \frac{\partial c_a}{\partial z} - \frac{\partial}{\partial z} q_E c_a - S^* c_a + P \qquad \textbf{(48)}$$

where R_f is the CO_2 retardation factor, D_E is the effective dispersion coefficient for the CO_2 in the soil matrix $[cm^2T^{-1}]$, q_E is the effective velocity of CO_2 $[cmT^{-1}]$, S^* is the CO_2 uptake rate $[T^{-1}]$ associated with root water uptake and θ_a is the volumetric air content $[cm^3cm^{-3}]$. These parameters are defined as

$$R_f = \theta_a + K_H R T \theta_w$$

$$D_E = \theta_a D_a + K_H R T \theta_w D_w$$

$$q_E = q_a + K_H R T q_w \qquad \textbf{(49)}$$

$$\theta_a = p - \theta_w$$

$$S^* = S K_H R T$$

Equation (48) is a nonlinear partial differential equation where, except for c_a and q_a, all parameters are either known or are obtained from solution of the water flow equation. Equation (48) is non-linear due to the term P which is dependent on CO_2 concentration, c_a. The model does not consider coupled water and air movement and the flux of air, q_a, is unknown thus additional assumptions are required. Since significant gas flow can be caused by a relatively small pressure gradient, the gas phase is at or near atmospheric pressure throughout the unsaturated zone. Therefore, under most conditions, the compressibility of the air can be neglected. Then, with the assumption that the air flux is zero at the lower soil boundary and that the water volume changes in the soil profile caused by the water flow must be immediately matched by the corresponding changes in the gas volume, Simunek and Suarez (1993) obtained

$$q_a(z) = q_w(0) - q_w(z) + \int_{L-L_r}^{z} S(z)dz \qquad (50)$$

This latter assumption is not unreasonable, since when water leaves the soil system due to evaporation and root water uptake, air enters the soil at the surface and, vice versa, when water enters the soil during precipitation and irrigation events, soil air is escaping. Only at saturation (typically at the soil surface) does the air become entrapped and compressed under the wetting front.

SOIL AND WATER CHEMISTRY

Transport

The governing equation for one-dimensional advective-dispersive chemical transport under transient flow conditions in partially saturated porous media is taken as (Suarez and Simunek, 1996)

$$\frac{\partial \theta c_{T_i}}{\partial t} + \rho \frac{\partial \bar{c}_{T_i}}{\partial t} + \rho \frac{\partial \hat{c}_{T_i}}{\partial t} = \frac{\partial}{\partial z}[\theta D \frac{\partial c_{T_i}}{\partial z} - q c_{T_i}] \qquad i = 1, n_s \qquad (51)$$

where c_{Ti} is the total dissolved concentration of the aqueous component i [ML^{-3}], $\bar{c}_{Ti}$ is the total adsorbed or exchangeable concentration of the aqueous component i [Mkg^{-1}], $\hat{c}_{Ti}$ is the non-adsorbed solid phase concentration of aqueous component i [Mkg^{-1}], ρ is the bulk density of the soil[ML^{-3}], D is the dispersion coefficient [cm^{2}T^{-1}], q is the volumetric flux [cmT^{-1}], and n_s is the number of aqueous components. The second and third terms on the left side of equation (51) are zero for components that do not undergo ion exchange, adsorption or precipitation/dissolution. The coefficient D is the sum of the diffusion and dispersion components

$$D = \tau D_m + \lambda \frac{|q|}{\theta} \qquad (52)$$

where τ is the tortuosity factor, D_m is the coefficient of molecular diffusion [cm^2T^{-1}], and λ is the dispersivity [cm]. This representation is a simplified treatment of the diffusion process. A more detailed description of the diffusion process requires calculation of the diffusion rates of individual species, with consideration of the coulombic interactions which maintain electroneutrality, requiring coupling of individual ion fluxes to the concentration gradients of all individual species (Lasaga, 1979). However, it appears that in soils, errors generated by uncertainty in determination of the tortuosity factor and velocity vectors are more significant for determination of solute transport than errors associated with a simplified treatment of diffusion.

Realistic modeling of the chemistry in the unsaturated zone requires consideration of various factors which are usually not considered. Among these are the changes in hydraulic properties of the soil as related to the solution chemistry (discussed above), water uptake by plant roots and the spatial distribution of the water uptake, temperature effects on water uptake, gas phase composition and equilibrium and reaction constants, and prediction of the dynamic changes in CO_2 concentration with time and space, all of which affect the water and solute movement and the chemical processes for the solutes of interest.

Chemical model

The chemical model includes consideration of 9 major aqueous components, consisting of Ca, Mg, Na, K, SO_4, Cl, alkalinity NO_3 and B. Alkalinity is defined as

$$\text{Alkalinity} = [HCO_3^-] + 2[CO_3^{2-}] + 2[CaCO_3^0] + [Ca\,HCO_3^+] + $$
$$2[MgCO_3^0] + [MgHCO_3^+] + 2[NaCO_3^-] + [NaHCO_3^0] + [H_2BO_3] - [H^+] + [OH^-]$$

(53)

where brackets represent concentrations (mol kg^{-1}). From these components we obtain 11 species Ca^{2+}, Mg^{2+}, Na^+, K^+, SO_4^{2+}, Cl, HCO_3^-, CO_3^{2-}, NO_3^-, $B(OH)_4^-$ and H_3BO_3. In addition we include the ion pair/complexes $CaHCO_3^+$, $CaCO_3^0$, $CaSO_4^0$, $MgHCO_3^+$, $MgCO_3^0$, $MgSO_4^0$, $NaHCO_3^0$, $NaCO_3^-$, $NaSO_4^-$, and KSO_4^-. We assume that all aqueous species are in equilibrium as defined by the ion association expressions and constants. Alkalinity as defined in equation (53) is a conservative species, in this instance affected only by dissolution or precipitation of a carbonate phase (such as calcite).

After obtaining the air phase CO_2 partial pressure we calculate the $H_2CO_3^*$ (sum of aqueous CO_2 and H_2CO_3) using a Henry's Law expression.

$$K_{co_2} = \frac{(H_2CO_3^*)}{P_{CO_2}(H_2O)}$$

(54)

where P_{CO2} is the partial pressure of CO_2 (atm.). From this value and utilizing the equations for the first and second dissociation constants, conservation of mass and the equations for dissociation of the complexes, we solve the equations using an iterative approach. The soil solution pH is determined as a dependent variable from solution of equation (53) for [H] and

multiplication by the activity coefficient. All equilibrium constants are calculated from available temperature dependent expressions. Soil temperature is calculated from a heat flow submodel, with input of air temperature, as discussed above.

The temperature dependence of the thermodynamic constants are expressed as a power function of the absolute temperature

$$\log K = a_1 + \frac{a_2}{T} + a_3 T + a_4 \log T + \frac{a_5}{T^2} \tag{55}$$

Osmotic pressure

The osmotic pressure is used to calculate the impact of salinity on water uptake and plant yeild. We calculate the osmotic pressure using the following equation

$$P_\varphi = RT \frac{M_s v m \varphi}{V_s m^0} \tag{56}$$

where P_φ (Pa) is the osmotic pressure of the solution, V is the partial molar volume of the solvent, m^0 is unit molality, m is molality of the solution, φ is the osmotic coefficient of the solution and M is the molar weight (Stokes, 1979) . The osmotic pressure in Pa is converted to osmotic pressure in m by the expression

$$h_\varphi = \frac{P_\varphi}{\rho g} \tag{57}$$

The osmotic coefficient is calculated from (Pitzer, 1973) as

$$\sum_i m_i (\varphi - 1) = 2(-\frac{A^\varphi I^{3/2}}{1+1.2I^{1/2}} + \sum_{c=1}^{N_c}\sum_{a=1}^{N_a} m_c m (B_{ca}^\varphi + ZC_{ca}) +$$

$$\sum_{c=1}^{N_c-1}\sum_{c'=c+1}^{N_c} m_c m_{c'} (\varphi_{cc'}^\varphi + \sum_{a=1}^{N_a} m_a \psi_{cc'a}) + \sum_{a=1}^{N_a-1}\sum_{a'=a+1}^{N_a} m_a m_{a'} (\varphi_{aa'}^\varphi + \sum_{c=1}^{N_c} m_c \psi_{aa'c}) + \tag{58}$$

$$\sum_{n=1}^{N_n}\sum_{a=1}^{N_a} m_n m_a \lambda_{na} + \sum_{n=1}^{N_n}\sum_{c=1}^{N_c} m_n m_c \lambda_{nc})$$

Activity coefficients

Activity coefficients are determined either using an extended version of the Debye-Huckel equation (Truesdell and Jones, 1974)

$$\ln\gamma = -\frac{Az^2\sqrt{I}}{1 + Ba\sqrt{I}} + bI \tag{59}$$

where A and B are constants depending on the dielectric constant of water, density and temperature, z is the ionic charge, a and b are adjustable parameters, and I is the ionic strength. The ionic strength is defined as

$$I = 0.5\sum_{i=1}^{M} z_i^2 c_i \tag{60}$$

where M is the number of the species and c is the concentration (mol kg^{-1}). At higher ionic strength (> 0.3 M) the solution is sufficiently concentrated that all ion interactions must be considered for calculation of activity coefficients. In this instance the Pitzer expressions are utilized. The activity coefficients are expressed in a virial-type expansion having the form (Pitzer, 1979)

$$\ln\gamma_i = \ln\gamma_i^{DH} + \sum_j B_{ij}(I)m_j + \sum_j\sum_k C_{ijk}m_jm_k + ... \tag{61}$$

where γ_i^{DH} is a modified Debye-Huckel activity coefficient and B_{ij} and C_{ij} are coefficients specific to each ion interaction. The Pitzer approach considers ion- ion interactions for every species in solution thus it does not consider the individual ion pairs and complexes such as $NaSO_4$ described above as species. The model is considered suitable for prediction of species activity in solutions up to 20 mol kg^{-1}, a concentration well above the intended use of the model. In the FAO-Salinity Lab SWS model the default is set to calculate the activities based on the Pitzer equations in order to obtain accurate calculation of osmotic pressure. The user can select the Debye-Huckel expression via direct editing of the input files.

Solid phases

The model considers a restricted set of solid phases, thus it cannot be used to predict the composition of a evaporating brine. The minerals considered include calcite, gypsum, hydromagnesite, nesquehonite and sepiolite. Since the model attempts to predict the composition of a water it cannot be based only on thermodynamic considerations. Dolomite precipitation is not considered by the present model since it has not been observed at near earth surface conditions. The kinetics of dissolution are also sufficiently slow (Busenberg and Plummer, 1982) that it is not reasonable to assume that a solution is dolomite saturated merely because dolomite is present in the soil profile. It is beyond the scope of this model to consider the detail necessary for a kinetic description of dolomite dissolution. This omission is significant only if calcite is not present.

Calcite Precipitation

The equilibrium condition of a solution with calcite in the presence of CO_2 can be described by the expression

$$(Ca^{2+})(HCO_3^-)^2 = \frac{K_{SP}^C\ K_{CO2}\ K_{a1}}{K_{a2}}\ P_{CO2}(H_2O) = K_{SP}^C\ K_T \tag{62}$$

where parenthesis denote activities, and K_{CO2} is the Henry's law constant for the solubility of CO_2 in water, K_{a1} and K_{a2} are the first and second dissociation constants of carbonic acid in water, and K_{SP}^C is the solubility product for calcite. To obtain equilibrium, i.e., when the ion activity product (IAP) is equal to the solubility product K_{sp}, a quantity x of Ca^{2+} and HCO_3^- must be added or removed from the solution to satisfy the equilibrium condition. The quantity x is obtained by solving the following third order equation

$$[Ca^{2+}+x][HCO_3^-+2x]^2 = \frac{K_{SP}^C\ K_T}{\gamma_{Ca^{2+}}\ \gamma_{HCO_3^-}^2} \tag{63}$$

It has been shown that waters below irrigated regions are supersaturated with respect to calcite (Suarez, 1977, Suarez et al., 1992) thus the equilibrium condition underestimates the Ca solubility in soil water. The cause of supersaturation has been shown to be due to poisoning of crystal surfaces by dissolved organic matter (Inskeep and Bloom, 1986; Lebron and Suarez, 1996).

Calite crystal growth models are not applicable to soil systems as the concentrations of dissolved organic carbon (DOC) in near surface natural environments are usually comparable to levels found by Inskeep and Bloom (1986) to completely inhibit calcite crystal growth. Recently Lebron and Suarez (1996) developed a precipitation rate model which considers the effects of dissolved organic carbon both on crystal growth and heterogeneous nucleation. The combined rate expression is given by

$$R_T = R_{CG} + R_{HN} \tag{64}$$

where R_T is the total precipitation rate, expressed in mmol $L^{-1}s^{-1}$, R_{CG} is the precipitation rate related to crystal growth, and R_{HN} is the precipitation rate due to heterogeneous nucleation. Since for soil systems the crystal growth rate can be neglected only nucleation is an important process. The R_{HN} term is given by

$$R_{HN} = k_{HN}\ f(SA)[\log(\Omega - 2.5)](3.37 \times 10^4\ DOC^{-1.14}) \tag{65}$$

where k_{HN} is the precipitation rate constant due to heterogeneous nucleation, $f(SA)$ is a function of the surface area of the particles (e.g. clay) upon which heterogeneous nucleation occurs (= 1.0 if no solid phase is present), Ω is the calcite saturation value, and 2.5 is the Ω value above

which heterogeneous nucleation can occur. This equation leads to calcite precipitation rates which are independent of the calcite surface area, consistent with the experimental data of Lebron and Suarez (1996).

For the purposes of this model the nucleation rate is sufficiently fast that the calcite solubility can be taken at the point of supersaturation at which there is no further nucleation. This level of supersaturation is very close to the supersaturation (3 fold) based on field measurements (Suarez, 1977a). The model thus uses the apparent solubility of 1.0 x 10^{-8}, with the temperature dependence determined for calcite. This is not an equilibrium value but it is the suitable value to simulate calcium carbonate solubility in the soil zone.

Gypsum

The model allows specification of the initial presence of gypsum, requiring input of the quantity present. If gypsum is present in any soil layer at the given time step, the model forces the solution to gypsum equilibrium. The program tracks changes in the amount of gypsum present, if all gypsum is dissolved in a soil layer, such as during reclamation of a sodic soil, then thus gypsum equilibrium is no longer forced. In all cases gypsum precipitates wherever supersaturation is indicated by solution calculations. The gypsum precipitation/dissolution expression is given by

$$[Ca^{2+}][SO_4^{2-}] = \frac{K_{sp}}{\gamma_{Ca^{2+}} \gamma_{SO_4^{2-}} (H_2O)^2} \tag{66}$$

where γ represents the activity coefficient of the ion and the K_{sp} is the solubility product in solution. To obtain equilibrium, i.e., when the IAP is equal to the solubility product $K_{SP}{}^{G}$, a quantity of gypsum, x, must be added or removed from the Ca^{2+} and SO_4^{2-} concentrations in solution, obtained by solving the quadratic equation.

$$[Ca^{2+} - X][SO_4^{2-} - X] = \frac{K_{sp}}{\gamma_{Ca^{2+}} \gamma_{SO_4^{2-}} (H_2O)^2} \tag{67}$$

For the objectives of this model it is reasonable to assume that kinetics of gypsum dissolution/precipitation are sufficiently fast that the equilibrium condition can be used.

Magnesium precipitation

The model considers that Mg precipitation can occur as a carbonate (either nesquehonite or hydromagnesite), or as a silicate (sepiolite). Since this is a predictive model, it considers only phases that either precipitate under earth surface conditions or occur frequently and are reactive under earth surface conditions, these need not necessarily be the thermodynamically most stable. With this consideration magnesite can be neglected, as it apparently does not form under earth surface temperatures, is relatively rare, and its dissolution rate is exceedingly small, such that its solubility has not yet been satisfactorily determined

from dissolution studies at or near 25° C. Similarly, dolomite precipitation is not considered, as true dolomite appears to very rarely form in soil environments. If dolomite is present in the soil, the model uses the kinetic model of Busenberg and Plummer (1982) to represent the dissolution process. The dissolution rate of dolomite is very slow, especially as the solution IAP values approach within 2-3 orders of magnitude of the solubility product.

If nesquehonite or hydromagnesite saturation is reached, the model will precipitate the predicted Mg carbonate. The Mg carbonate precipitated, combined with calcite precipitation, will likely represent the mixed Ca- Mg precipitate that is observed in hypersaline environments, called protodolomite. However, the resulting solution composition is much different than that produced by simply forcing equilibrium with respect to dolomite, as the model forms this mixed precipitate (calcite+ magnesium carbonate) under conditions of approximately three orders of supersaturation with respect to dolomite. This result is consistent with the high levels of dolomite supersaturation maintained in high Mg waters (Suarez, unpublished data). Precipitation (or dissolution, if present in the soil) of sepiolite is also considered by the model. Sepiolite will readily precipitate into a solid with a $K_{SP}{}^{S}$ greater than that of well crystallized sepiolite. Formation of this mineral requires high pH, high Mg concentrations and low CO_2 partial pressure.

Precipitation of Nesquehonite and Hydromagnesite

At 25^oC and at CO_2 partial pressures above $10^{-3.27}$ kPa, nesquehonite $MgCO_3 \cdot 3H_2O$ is stable relative to hydromagnesite. The precipitation (if saturation is achieved) or dissolution of nesquehonite (if specified as a solid phase) in the presence of CO_2 can be described by

$$MgCO_3 \cdot 3H_2O + CO_2(g) \Leftrightarrow Mg^{2+} + 2HCO_3^- + 2H_2O \tag{68}$$
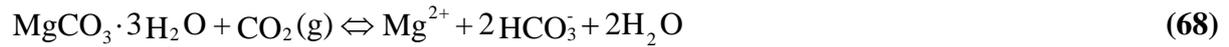
with the solubility product $K_{SP}{}^{N}$ defined by

$$K_{SP}^{N} = (Mg^{2+})\,(CO_3^{2-})\,(H_2O)^3 \tag{69}$$

Substituting the equation for Henry's law for solubility of CO_2 in water, and the equations for the dissociation of carbonic acid in water into the solubility product we obtain:

$$(Mg^{2+})(HCO_3^-)^2 = \frac{K_{SP}^{N}\ K_{CO_2}\ K_{a1}}{K_{a2}}\frac{P_{CO2}}{(H_2O)^2} = \frac{K_{SP}^{N}\ K_T}{(H_2O)^3} \tag{70}$$

This relation is solved for equilibrium in a manner similar to that used for calcite, with a 3rd order equation.

The precipitation or dissolution of hydromagnesite in the presence of CO_2 can be described by

$$Mg_5(CO_3)_4(OH)_2 \cdot 4\,H_2O + 6\,CO_2(g) \Leftrightarrow 5\,Mg^{2+} + 10\,HCO_3^- \qquad \textbf{(71)}$$
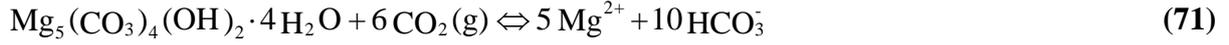
Similarly the equilibrium condition is defined by

$$(Mg^{2+})^5(HCO_3^-)^{10} = \frac{K_{SP}^H K_{CO_2}^6 K_{a1}^{\,6} P_{CO_2}^6}{K_{a2}^{\,4} K_w^2} = K_{SP}^H K_T \qquad \textbf{(72)}$$

Again the equilibrium condition is solved as described for calcite and nesquehonite.

Precipitation of Sepiolite

The precipitation or dissolution of sepiolite in the presence of CO_2 can be described by

$$Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O + 4.5H_2O + 4CO_2(g) \Leftrightarrow 2Mg^{2+} + 3H_4SiO_4^0 + 4HCO_3^- \qquad \textbf{(73)}$$

with the solubility product K_{SP}^S defined by

$$K_{SP}^S = \frac{(Mg^{2+})^2 (H_4SiO_4^0)^3 (OH^-)^4}{(H_2O)^{4.5}} \qquad \textbf{(74)}$$

In this instance we utilize the precipitated sepiolite solubility value given by Wollast et al. (1968) rather than the well crystallized equilibrium value. Freshly precipitated sepiolite has been prepared in the laboratory at IAP values of 10^{-35} comparable to the K_{SP}^S listed by Wollast et al. (1968), thus we consider that a kinetic expression for precipitation is not essential for prediction of unsaturated zone solution composition. The equilibrium condition is expressed as

$$(Mg^{2+})^2 (HCO_3^-)^4 = \frac{K_{SP}^S K_{CO_2}^4 K_{a1}^{\,4} P_{CO_2}^4 (H_2O)^{4.5}}{K_w^4 (H_4SiO_4^0)^3} = K_{SP}^S K_T^+ \qquad \textbf{(75)}$$

Relatively little information exists on the controls on Si concentrations in soil waters, especially in arid zones. In soil systems Si concentrations are not fixed by quartz solubility but rather by dissolution and precipitation of aluminosilicates and Si adsorption onto oxides and

$$\Sigma\,SiO_2 = 0.001\,(\,6.34 - 1.43\,pH + 0.0819\,pH^2\,) \qquad \textbf{(76)}$$

aluminosilicates. As a result of these reactions Si concentrations in soil solution follow a U shaped curve with pH, similar to Al oxide solubility with a Si minimum around pH 8.5 (Suarez 1977b). Data from 8 arid land soils reacted at various pHs for two weeks by Suarez (1977b), were fitted to a second order relationship as follows

where SiO_2 is the sum of all silica species expressed in mol L^{-1}. This relationship likely provides only a rough estimate of Si concentrations, but we consider it acceptable because it is

used only to restrain Mg concentrations at high levels of evapotranspiration, when Mg concentrations become very high at low CO_2 and elevated pH.

Cation exchange

Cation exchange is generally the dominant *chemical* process for the major cations in solution in the unsaturated zone. Generally cation exchange is treated with a Gapon-type expression of the form (White and Zelazny, 1986)

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

(77)

where y, and x, are the respective valences of species i, and j and the overscored concentrations are those of the exchanger phase (concentration expressed in mol_c $mass^{-1}$). It is assumed that the cation exchange capacity c_T is constant, and for non-acid soils

$$\bar{c}_T = \overline{Ca}^{2+} + \overline{Mg}^{2+} + \overline{Na}^+ + \overline{K}^+$$

(78)

Experimentally determined selectivity values are not constant, nor is the cation exchange capacity which varies as a function of pH, due to variable charge materials such as organic matter. It has been observed that soils have an increased preference for Ca^{2+} over Na^+, and Ca^{2+} over Mg^+, at low levels of exchanger phase Ca^{2+}. Suarez and Wood (1993) developed a mixing model which is able to approximate the non constant values of the soil selectivity coefficient by taking into account the organic matter content of the soil and using the published constant selectivity values for clay and organic matter. Calcium preference decreases as the organic matter exchanger sites (which have higher Ca preference than clays) become Ca saturated. This approach is not utilized directly by the model interface but is useful to predict the input exchange constants if the organic matter content is known. This approach is available to the user via direct input to the input file using a standard file editor.

REFERENCES

Allen, R.G., L.S. Peieira, D. Raes, and M. Smith. 1998. Crop Evapotranspiration. FAO Irrigation and Drainage Paper 56. FAO. U.N. Rome.

Busenberg, E. and L.N. Plummer. 1982. The kinetics of dissolution of dolomite in CO_2-H_2O systems at 1.5 to 65 C and 0 to 1 ATM P_{CO2}. Am. J. Sci. 282, 45-78.

Carsel, R.F., and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. Water Resour. Res. 24, 755-769.

Chung, S.-K., and R. Horton. 1987. Soil heat and water flow with a partial surface mulch. Water. Resour. Res. 23(12), 2175-2186.

Felmy, A.R. 1990. GMIN:A computerized chemical equilibrium model using a constrained minimization of the Gibbs free energy. Pacific Northwest Lab. Richland, Wash.

Freijer, J.I., and P.A. Leffelaar. 1996. Adapted Fick's law applied to soil respiration. Water Resour. Res. 32, 791-800.

Gilmore, E., and J.S. Rogers. 1958. Heat units as a method of measuring maturity in corn. Agron. J. 50, 611-615.

Harned, H. S. and Davis Jr., R. 1943. The ionization constant of carbonic acid and the solubility of carbon dioxide in water and aqueous salt solutions from 0 to 50 C. J. Am. Chem. Soc. 653, 2030-2037.

Inskeep, W.P., and P.R. Bloom. 1986. Kinetics of calcite precipitation in the presence of water soluble organic ligands. Soil Sci. Soc. Am. J. 50, 1167-1172.

Lasaga, A. C. 1979. The treatment of multi-component diffusion and ion pairs in diagenetic fluxes. Am. J. Sci. 279, 324-346.

Lebron, I., and D.L. Suarez. 1996. Calcite nucleation and precipitation kinetics as affected by dissolved organic matter at $25^{o}C$ and pH >7.5. Geochem. Cosmochim Acta 60:2767-2776.

Logan, S. H., and P.B. Boyland. 1983. Calculating heat units via a sine function. J. Am. Soc. Hort. Sci. 108, 977-980.

Maas, G. and G. Hoffman. 1977. Crop salt tolerance-current assessmnet. J. Irr. Drainage Div. ASCE. 103:115-134.

Massmann, J., and D.F. Farrier. 1992. Effects of atmospheric pressure on gas transport in the vadose zone. Water Resour. Res. 28, 777-791.

McNeal, B. L. 1968. Prediction of the effect of mixed-salt solutions on soil hydraulic conductivity. Soil Sci. Soc. Am. Proc. 32, 190-193.

Patwardhan, A. S., J. L. Nieber, and I. D. Moore. 1988. Oxygen, carbon dioxide, and water transfer in soils: Mechanism and crop response. Trasactions of ASAE 31, 1383-1395.

Pitzer, K.S. 1973. Thermodynamics of electrolytes I: Theoretical basis and general equations. J. Phys. Chem. 77, 268-277.

Pitzer, K.S. 1979. Activity Coefficients in Electrolyte Solutions, Chapt.7 CRC Press, Boca Raton, Florida.

Richards, L.A. 1952. Water conducting and retaining properties of soils in relation to irrigation, Proc., Inter. Symp. on Desert Res., Jerusalem.

Robbins, C.W., J.J. Jurinak, and R.J. Wagenet. 1980. Calculating cation exchange in a salt transport model. Soil Sci. Soc. Am. J. 44:1195-1200.

Robinson, R.A., and R.H. Stokes. 1965. Electrolyte Solutions. Butterworths, London, 571p.

Shainberg, I., and G.J. Levy. 1992. Physico-chemical effects of salts upon infiltration and water movement in soils, In: R.J. Wagenet, P. Baveye, B.A. Stewart (ed), *Interacting Processes in Soil Science*, Lewis Publishers, CRC Press, Boca Raton, Florida.

Simunek, J., and D.L. Suarez. 1993a. Modeling of carbon dioxide transport and production in soil:1. Model development. Water Resour. Res. 29, 487-497.

Simunek, J., and D.L. Suarez. 1993b. UNSATCHEM-2D Code for Simulating two-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion equilibrium and kinetic chemistry, U. S. Salinity Laboratory Research Report No. 128. U.S. Salinity Laboratory, USDA-ARS, Riverside, CA.

Simunek, J., and D.L. Suarez. 1994. Two-dimensional transport model for variably saturated porous media with major ion chemistry, Water Resour. Res. 30(4), 1115-1133.

Simunek J. and D.L. Suarez. 1996. The UNSCHEM code for simulating one-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion equilibrium and kinetic chemistry. In: Simunek. J., D.L. Suarez, and M. Sejna. 1996. The UNSATCHEM software package for simulating the one-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion equilibrium and kinetic chemistry. Ver 2.0 Research Report No. 141. U.S. Salinity Laboratory, USDA-ARS, Riverside, CA.

Smith, M. 1992. CROPWAT, a computer program for irrigation planning and management. FAO Irrigation and Drainage Paper 46, FAO, Rome.

Sophocleous, M. 1979. Analysis of water and heat flow in unsaturated-saturated porous media. Water Resour. Res., 15(5), 1195-1206.

Stokes, R.H. 1979. Thermodynamics of solutions, In: R.M. Pitkowicz (ed), *Activity Coefficients in Electrolyte Solutions*. CRC Press, Inc., Boca Raton, Florida.

Suarez, D. L. 1977a. Ion activity products of calcium carbonate in waters below the root zone. Soil Sci. Soc. Am. J. 41, 310-315.

Suarez, D. L. 1977b. Magnesium, carbonate, and silica interactions in soils. U. S. Salinity Laboratory Annual Report, USDA, 120 pp.

Suarez, D. L., J.R. Rhoades, R. Lavado, and C.M. Grieve. 1984. Effect of pH on saturated hydraulic conductivity and soil dispersion. Soil Sci. Soc. Am. J. 48, 50-55.

Suarez, D.L., and J. Simunek. 1992. The UNSATCHEM code for simulating one-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion equilibrium and kinetic chemistry. Ver 1.1 Research Report No. 129. U.S. Salinity Laboratory, USDA-ARS, Riverside CA.

Suarez, D. L., and J. Simunek. 1993. Modeling of carbon dioxide transport and production in soil:2. Parameter selection, sensitivity analysis and comparison of model predictions to field data. Water Resour. Res. 29, 499-513.

Suarez, D.L., J.W. Wood, and I. Ibrabim. 1992. Reevaluation of calcite supersaturation in soils. Soil Sci. Soc. Am. J. 56, 1776-1784.

Suarez, D.L., and J. Simunek. 1997. UNSATCHEM: Unsaturated water and solute transport model with equilibrium and kinetic chemistry, Soil Sci. Soc. Am. J., 61, 1633-1646.

Thorstenson, D. C. and D.W. Pollack. 1989. Gas transport in unsaturated zones: Multicomponent systems and the adequacy of Fick's laws. Water Resour. Res. 25, 477-507.

Truesdell, A. H., and B.F. Jones. 1974. WATEQ, a computer program for calculating chemical equilibria of natural waters. J. Res. U. S. Geol. Surv. 2, 233-248.

U.S. Salinity Laboratory Staff. 1954. Diagnosis and Improvement of Saline and Sodic Soils. USDA. Handbook 60. U.S. Gov. Printing Office. Washington D.C.

van Genuchten, M. Th. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44, 892-898.

van Genuchten, M. Th. 1987. A numerical model for waer and solute movement in and below the root zone, Unpub. Research Report, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.

van Genuchten, M.Th., F.Leiji, and S.Yates. 1991. The RETC code for quantifying the hydraulic functions of unsaturated soils. EPA/600/2-91/065. 85pp.

White, N., and L.W. Zelazny. 1986. Charge properties in soil colloids. p.39-81. In: D.L. Sparks (ed.), *Soil Physical Chemistry*. CRC Press, Boca Raton, Florida.

Wollast, R., F.T. Mackenzie, and O. P. Bricker. 1968. Experimental precipitation and genesis of sepiolite at earth-surface conditions. Am. Mineralogist. 53, 1645-1662.

PART 3: USE OF THE MODEL

MAIN PROCESSES

The first screen, labeled main processes, allows the user to select the options, root water uptake, root growth and carbon dioxide production and transport. If plants are growing during the time interval to be simulated then the root water uptake option must be selected. This option allows for evapotranspiration to occur. If this option is not selected there will be no water extraction within the soil and only evaporation from the soil surface may be considered. The no roots option would be used in the case of leaching a field for reclamation, or to simulate evaporation from a bare soil in the presence of a shallow water table.

If root water uptake is selected then it is possible to also select root growth. This option allows for crop development and is used for annual crops, in combination with crop coefficients, as discussed later. If as is the case for many simulations, the reader wants only to know how a series of waters or treatments would affect a soil, or if a perennial crop is considered then this root growth option is not selected.

The carbon dioxide option is to be used whenever a dynamic simulation of CO_2 concentration is desired. This option is especially useful for simulation of reclamation when considering the impact of enhanced calcite dissolution in the presence of organic matter, such as during use of green manure for reclamation. If the user knows the CO_2 concentration in this soil during wetting and drying and for different times of the year (not likely) then they may wish not to select this option, or they can adjust the production function if needed to match their dynamic system. Ordinarily it is recommended that this option be used and that the default parameters be maintained.

GEOMETRY INFORMATION (LAYER, TIME AND DEPTH)

Several layers can be simulated. Layers are defined here as regions in which there are similar physical properties (especially hydraulic properties). Differences in chemical properties will be specified later and need not be associated this the physical property layers. The model allows for a depth of up to 5 m to be simulated. It is suggested that the user avoid unnecessary complexity as selection of a number of soil layers with differing physical properties increases the likelihood of numerical problems and program failure. If possible use one or two physical layers.

Initial time corresponds to the date that the simulation is to be started, it should correspond to the calendar date of the year if crop coefficients are to be considered. For example if the simulation is to start on February 15 then the starting date would be day 46. The final day is the day in which the simulation is ended- it can be after the harvest day and can it extend beyond the end of the year. If the simulation extends into a new calendar year the simulation days must be consecutive i.e., the following year the day for Feb 15 would correspond to day 411. For perennial crops the model can simulate long time periods,

however only one perennial crop can be considered within a single simulation.

In order to avoid boundary layer effects it is generally suggested that the user simulate a depth at least 50% greater than the depth of interest- or simulate the soil down to the water table depth with a specified pressure head as a lower boundary condition. In the case where h=0, this indicates a water table at that boundary. By specifying the depth of the profile to be simulated or specifying the pressure head at the boundary, a water table can be simulated at any desired depth, with the assumption that the water is either of constant composition or a result of the water applications and root zone processes

Output display times correspond to the dates on which there is output to the graphical files. Five times are to be selected. These can be adjusted by the user but should include the final time. The graphs will also present the initial time step thus there will be 6 lines on the graphs. The graphs display the variable against the profile depth, thereby providing information for each depth node.

WATER FLOW PARAMETERS

This menu allows for selection of the hydraulic properties for each of the layers. As many layers can be specified as indicated in the previous menu. The default parameters are obtained based on description of the soil texture from the pull down menu. If the user does not like the indicated hydraulic conductivity value for the soil texture classification, it can be changed. In this instance the texture based soil water retention curve is maintained and the saturated hydraulic conductivity and the scaled unsaturated values are changed accordingly.

The option for reduction of hydraulic conductivity due to solution chemistry is available to simulate the interactions of salinity sodicity and pH on hydraulic parameters. It is assumed that the processes are reversible-while not completely valid it is preferable to the assumption that deterioration of hydraulic properties is irreversible. Selection of this option will result in dynamic changes in the hydraulic properties of the soil. As indicated earlier this response is based primarily on data from the Salinity Laboratory and may be different for other soils. The custom option opens another window allowing for input of the hydraulic parameters, as discussed in Section 1.

SOLUTE TRANSPORT

In this screen the users input the specification of the different number of waters and soil chemical layers to be utilized in the simulation. The layers do not have to coincide with the physical layers specified earlier. In general it is not necessary to enter a lot of chemical information in small layers. The longer the simulation the less important are the initial solution compositions.

Number of different water compositions
This field requires specification of the total number of different water compositions to be considered. This include the irrigation water compositions (there may be more than one water

utilized), rainfall, or any boundary condition, such as the ground water composition, in addition to the initial composition in the soil. If more than one initial composition is used for the soil then these will also have to be specified. As with the physical layers it is best not to provide unnecessary detail in the initial number of soil chemical layers. Usually one or two compositions should be sufficient to describe the solute chemistry at the start. Clearly the longer the simulation the less important will be the initial conditions.

Number of different exchange phase compositions
This entry relates to the number different exchange compositions to be utilized. This can correspond to a layer with different cation exchange capacity and/or layers with different exchange compositions. Ordinarily this would correspond to the layers selected for hydraulic properties and layers selected for chemical composition. If different chemical compositions are indicated above, then it is expected that the exchange composition will also different. The number of layers should be kept to a minimum.

Number of layers with/without calcium carbonate and gypsum
This entry is to specify the number of regions with different solid phase compositions. Specification of different regions can also be made based on the quantity of the solid phase. For example if the entire profile is calcareous. In some instances large inconsistencies between the initial exchange composition and the initial solution composition may cause numerical problems. Typically one or two layers are selected.

SOLUTE TRANSPORT AND REACTION PARAMETERS

Bulk density is required for calculation of the equilibria between the solution and solid phase at a calculated volumetric water content. Solute dispersion is an adjustable parameter relating to the sharpness of the non reactive solute front. A default parameter is provided. In addition, cation exchange selectivities are provided for Ca, Mg, Na and K exchange. The user should input their own values if known, using the selectivity convention described earlier in Section 1.

Solute composition
Ion compositions need to be entered for each of the number of waters specified. Concentrations are in $mmol_c \, L^{-1}$. The solution should be charge balanced although imbalances are adjusted by altering the nitrate values. Designating a tracer (a hypothetical non reactive chemical) is useful to evaluate the extent of infiltration or upward movement of ground water.

Note: The entered compositions are the actual compositions in the soil. If initial chemical data is from a soil water extract the solution must be corrected back to field water content. As a first approximation the composition at field water content can be obtained by multiplying the extract concentrations by the ratio of $\theta_{soil}/\theta_{extract}$.

This correction does not consider cation exchange and dissolution processes that occur as a result of dilution. For any give soil empirical relationship may be established.

The composition of rain should not be input as zero concentration. In the absence of actual data it is suggested that values such as 0.02 be input for Ca, Mg, Na, alkalinity, Cl and SO_4.

Exchange composition

Entry of an exchange composition is required for each exchange number specified. The sum of the exchangeable cations *must* be equal to the specified CEC, with units of $mmol_c$ kg^{-1} of soil. In the absence of specific information the CEC for soil with smectitic clays can be estimated by using the value CEC = %clay x 60. If a water extract of the soil has been made the exchange composition can be estimated by calculating the exchangeable Na percentage from the SAR using the Handbook 60 (U.S. Salinity Laboratory Staff, 1954) relationship

$$ESP = \frac{100(-0.0126 + 0.01475SAR)}{1 + (-0.0126 + 0.01475SAR)}$$

where SAR, the sodium adsorption ratio is equal to $Na/((Ca+Mg)/2)^{0.5}$

Solid concentrations

It is necessary to specify the concentration of the solid phases present in each of the solid layers. These layers will usually correspond to the exchange layers. For each layer the solids and concentration in meq kg^{-1} need to be specified. Specification of the mass allows the model to consider the mass changes, especially important when a solid phase such as gypsum is completely dissolved (over time). To convert the % calcium carbonate or gypsum into units of meq Ca per kg ($mmol_c$ kg^{-1}) of soil, multiply by 200 and 116 respectively.

CARBON DIOXIDE PRODUCTION

This screen will appear only if the carbon dioxide production option was selected earlier. The microbial and plant production terms were taken from Suarez and Simunek, (1993). These terms are modified by the program according to temperature, water and salt stress. The user can modify the optimal term but the stress functions will use this value to calculate a predicted production. The plant root production is only activated by the program if plant water uptake was specified. Also the degree days to maximum production is only activated if plant water uptake was specified.

Root water uptake

This screen appears if root growth was selected as one of the options in the first screen. The initial root growth time corresponds to the date on which the model starts to grow roots. It can correspond to the planting date or more realistically a few days after planting. The harvest time corresponds to the date the plants are removed. The maximum rooting depth is to be specified, in cm. There will be no water extraction below this point (but water can move upward if the hydraulic gradients so indicate). The units for water stress are in -m. A default value of p is normally used. The default parameters are p=3 and h= -50 m for a 50% reduction in water uptake.

The reduction of water uptake due to salinity stress is input next. As these values cannot be generalized it is necessary for the user to select the parameters from the crop list in Table3 3a-c, or provide their own values. In the absence of detailed information p can be set to 3 and the h_{50} value input, in units of -m (as osmotic stress is expressed as a negative pressure).

Root growth parameter

Root growth data
This screen appears if root growth was selected in the main screen. The user must enter the initial root growth time, harvest day, initial rooting depth (cm) and maximum rooting depth. The model will use an exponential distribution for root development. It is suggested that the initial root depth be sufficiently large to span at least 4 nodal spacings (where the node length is equal to the depth of the simulation /100nodes). The maximum rooting depth needs to be specified.

Degree days parameters
Degree days to maturity, Minimum temperature for root growth, optimal temperature and maximum temperature for optimal growth should be entered. Ordinarily the default parameters will be sufficient. The degree day is value should be input if known- if you want to insure that water uptake and biomass production does not shut down then use a sufficiently large number. (at least 1200) The degree days correspond to the summation of the daily average temperature above a minimum (but not counting degrees above a maximum) necessary for the plant to reach maturity under optimal growth conditions.

The minimum temperature corresponds to the temperature at or below which there is no growth. The maximum temperature refers to the temperature above which the growth is reduced.

ET Data Input Source

This screen requires specification of the number of records to be entered. The user must enter as many records as required to represent the soil input. If there is an initial dry period followed by an irrigation followed by a dry period, three records would be input. Any change in ET or water type used for irrigation requires a record. For evapotranspiration (when plants are transpiring) enter the ET_c and leave the E column blank. The model will partition between evaporation and transpiration. In the absence of plant transpiration the ET_c field should be left blank and potential evaporation should be entered in the E column.

Specification of ET to be calculated from crop coefficients opens another section of the window. If this selection is made the user must select to enter crop coefficients manually or to select based on the crop menu. If manual is selected then this information must be provided for each record. If ET is to be calculated from atmospheric records then the user must provide elevation and latitude information for the site.

K$_c$ crop input information
If the user requested this option they can select from the available pull down menu. The selection will automatically fill in the end of various stages of growth, and the corresponding crop coefficient. These can be edited by the user. The user will receive a warning if the crop maturity date exceeds the date of the simulation.

Time variable boundary conditions

This table provides the time dependent boundary conditions. The user interface allows for interpolating. The date corresponds to the *last* date that this boundary condition is used. For example if the user wishes to start the simulation on day 25 the user should have specified this as the starting date in the layer, time depth screen. To start with a one day irrigation then the first day to be entered in the time variable boundary records is day 26.

        More typically the user will start on day 0. If the model specified earlier that the simulation was to start on day 0 then the boundary conditions on record day 25 would be utilized from day 0 to the start of day 26. If records are to be for part of a day then it is necessary to use a decimal notation i.e., specify 25.5 for day 25 at noon. It is possible to specify short time intervals for rain or irrigations.

Precipitation
In this field is to be entered the *rate* of precipitation over the specified time interval. This is used for both irrigation and rain. For example if 6 cm of water are applied over a 2 day interval between day 25 and day 27 there would be a time record ending on day 25 with the previous boundary condition followed by a record on day 27 with a rate of 3 cm/day precipitation.

Evaporation
This field is to be used only when there are no plants. The value corresponds to the potential surface evaporation.

ET$_c$
This corresponds to the rate (cm/day) of the optimal ET of the specified crop at that time in its stage of development. If the value is not known then the model will calculate this value for this time interval based on the climatic data. If the field is left blank the program will calculate the ET$_c$ value before executing the main program. The actual ET of the crop may be lower than the input value depending on water, salt and oxygen stress, as calculated by the model.

Pressure bottom
This input corresponds to the matric pressure at the bottom of the soil profile and must be specified for each time interval. If the boundary condition is a water table at 1 m then the pressure at the bottom corresponds to 0.0 cm. Negative values correspond to suction (-1 bar of pressure is approximately equivalent to -1000 cm). A fluctuating water table can be simulated by changing the bottom boundary for different time records.

Temperature top

Mean temperature for the time interval. This information is used for heat transport and for simulation of crop growth, including calculation of Et_c when this information is not provided.

Input water
This value corresponds to the number of the water to be applied as the top boundary. For example if the irrigation water was selected earlier as water number 1 and an irrigation event is specified for the present time interval then the value of -1 should be entered in this field. The negative sign is added to signify that the infiltration is downward in direction. If a value is entered in this field but no precipitation is specified then the value is ignored.

Ground water
This corresponds to the number assigned earlier to the ground water composition. If a water table condition is specified then this value can be entered for all time records. If more than one ground water composition was specified then the values can be used as desired.

RH max
This column is used if ET is to be calculated rather than input. Maximum relative humidity (%) for the daily period. This can be an average value if daily records are not used.

Wind speed
This column is used if ET is to be calculated rather than input. The speed is that at 2m above the surface, units are in m/s.

delta Temp
This column is used if ET is to be calculated rather than input. This is the difference between the max and min temperature for each day.

n/N
This column is used if ET is to be calculated rather than input. This is the relative sunshine duration. (Relative to the maximum possible for that date)

Crop coefficient
This column is used if ET_c is to be calculated rather than input. Select values from Table 2, or FAO 56 or input if known.

ET_o
Input this number if known and for calculation of ET_c

Max top H (HcritA)
This value corresponds to the most negative pressure head that will be allowed at the upper boundary. It is necessary to place a limit on how dry the surface can get to avoid numerical problems during the simulation. Typically, the value of -10 000 cm is utilized. It is suggested that the same value be used for all time records.

If the ET_c value was specified as unknown then it is necessary to provide additional information. Among the options is input of ET_0 and selection or input of the crop coefficients. If ET_0 is not known then it can be calculated from latitude, altitude, mean temperature

(already specified) (temperature variation from the mean), wind speed, and fraction of sunlight hours in which there is clear sky.

Profile summary
This table is used to input the initial soil conditions. Clearly, the longer the model is run, the less important it is to provide detailed initial conditions.

The first field is the fixed node number 1. The second field z is the depth of each node. The value h corresponds to the initial matric potential for each depth expressed in -cm. It is suggested that a uniform gradient not be used as this is unrealistic and may cause the model to fail. A reasonable approximation in the absence of specific information is to set h=0 at the water table depth (generally the bottom of the profile) and to set the surface pressure at a known value and use the interpolation soft ware to fill in the rest of the node information.

The initial root distribution information is maintained throughout the simulation if the root growth option is not specified. In this case the root distribution would be that of the mature plant, such as the for alfalfa. Input is scaled thus the actual values entered are not important, as they represent only the relative weighing of the individual layers. For example values of 1 can be entered for the depth with the maximum rooting density and values of 0 for layers with no roots. By using the interpolation features it is possible to generate detailed rooting profiles. It is necessary to have some roots specified whenever ET_c is specified as the model will extract the ET specified water from the layers that have roots. For example if ET_c is set to 1 cm per day and roots are specified for only 1 cm the model will attempt to extract 1 cm of water from that depth and a program failure may result.

CO_2
The user should specify an initial condition. In the absence of data the user can select the atmospheric value of 0.00035 for the top node and a value of 0.01 for the bottom node. The value of the bottom node is a constant boundary condition, and no CO_2 is transported below this depth.

Temperature
In a similar manner the initial temperature is set for each node. This can be defaulted to a constant value for the initial condition is unknown. At the bottom node there is a condition of zero flux. Thus no heat is lost or grained from below this depth.

Layer
If one layer was selected earlier than this value (1) is used for all nodes).

Solution concentration
This specifies the number of the solution to be utilized at each depth. The model will apply the concentrations of ions that correspond to that solution number (defined earlier).

Adsorbed concentration
This specifies the number of the exchange phase composition to be utilized at each depth. The model will apply the exchange concentrations of ions that correspond to that number (defined earlier). A number must be selected.

Solid concentration
This specifies the number of the solid to be utilized at each depth. There must be at least one solid. The model will apply the concentrations of the solids that correspond to that number (defined earlier).

Output

The output is in the form of graphs labeled as results in the main menu bar. The options include basic information on water content, CO_2 partial pressure, temperature, and water flux for the selected output times as a function of depth.

The solution concentration section provides for display of the concentrations of the major ions with depth, expressed in $mmol_c\,L^{-1}$, again for the time intervals selected.

Soil information provides for the equivalent Ca (or in the case of Mg minerals, Mg), expressed as $mmol_c\,kg^{-1}$ pool in the soil at various depths as a function of time. This is especially useful for determining the gypsum requirement, as the user can experiment with different amounts of gypsum applications and depths and evaluate the results.

The chemical information graphs display pH, SAR, calculated EC, and osmotic pressure as a function of depth for the selected times

Crop and water flow information
These graphs provide information on the water flow, such as the amount of water that is drained out of the soil. The potential surface flux will no match the predicted flux if the infiltration rate is less than the water application rate. This may occur for a sodic soil when the *K* reduction is enabled. The relative yield is the ratio of the cumulative predicted root water uptake divided by the potential root water uptake without stress (ET_c). Salinity stress will reduce this value.

Table 1   Length of Crop Stages[1]

Crop	Region	Planting Date	Ending date of Stage			
			Initial	Development	Mid	Late
Broccoli	Calif. Desert	240	35	80	120	135
Corn (sweet)	Calif. Desert	0	20	60	130	140
Corn (sweet)	Arid	270	20	50	100	110
Corn (sweet)	Mediterranean	120	20	45	70	80
Corn (grain)	Arid	330	25	65	110	140
Corn (grain)	Mediterranean, California	90	30	70	120	150
Corn (grain)	India	270	20	55	95	125
Cotton	Calif. desert	60	45	135	180	225
Cotton	Pakistan Egypt, California	90	30	80	140	195
Cotton	Texas	90	30	80	135	180
Eggplant	Arid	270	30	70	110	130
Eggplant	Mediterranean	120	30	75	105	140
Barley/Oats	Central India	300	15	40	90	120
Winter wheat	California	330	20	80	150	180
Winter wheat	Mediterranean	300	30	170	210	240
wheat	Calif. desert	330	20	70	130	160
wheat	35°-45°Latitude	60	20	45	105	135
wheat	Central India	300	15	40	90	120
Tomato	Arid	0	30	70	110	135
Tomato	California	90	35	75	125	155
Tomato	Calif. desert	0	25	65	125	155
Tomato	Mediterranean	90	30	70	115	145

[1]FAO Irrigation and Drainage paper 56

Table 2   Crop Co-efficient, K_c[1]

Crop	Region	K_i	K_{mid}	K_{end}
Broccoli	Calif. desert	0.70	1.05	0.95
Corn (sweet)	Calif. desert	0.70	1.15	1.05
Corn (sweet)	Arid	0.70	1.15	1.05
Corn (sweet)	Mediterranean	0.70	1.15	1.05
Corn (grain)	Arid	0.70	1.20	0.60
Corn (grain)	Mediterranean, California	0.70	1.20	0.60
Corn (grain)	India	0.70	1.20	0.60
Cotton	Calif. desert	0.35	1.18	0.60
Cotton	Pakistan Egypt, California	0.35	1.18	0.60
Cotton	Texas	0.35	1.18	0.60
Eggplant	Arid	0.60	1.05	0.90
Eggplant	Mediterranean	0.60	1.05	0.90
Barley/Oats	Central India	0.30	1.15	0.25
Winter wheat	California	0.70	1.15	0.33
Winter wheat	Mediterranean	0.70	1.15	0.33
wheat	Calif. desert	0.70	1.15	0.33
wheat	35°- 45°Latitude	0.70	1.15	0.33
wheat	Central India	0.70	1.15	0.33
Tomato	Arid	0.60	1.15	0.80
Tomato	California	0.60	1.15	0.80
Tomato	Calif. desert	0.60	1.15	0.80
Tomato	Mediterranean	0.60	1.15	0.80

[1]FAO Irrigation and Drainage paper 56

Table 3a   Model parameters[1] for salt tolerance (expressed as osmotic pressure) of grasses and forage crops

Crop	h_{50}(m)	p
alfalfa	-63.00	2.43
barley (forage)	-94.00	3.91
bermudagrass	-106.00	4.00
clover	-72.00	2.09
corn (forage)	-60.00	2.36
cowpea	-50.00	3.12
fescue, tall	-94.00	2.75
rye (forage)	-126.00	3.63
sudangrass	-100.00	2.29
wheatgrass, standard	-112.00	2.39
wheatgrass, tall	-138.00	3.32

[1] Where relative yield $= \dfrac{1}{1+\left(\dfrac{h}{h_{50}}\right)}p$

Table 3b   Model parameters[1] for salt tolerance (expressed as osmotic pressure) of fiber and grain crops

Crop	h_{50}(m)	p
barley	-128.00	3.77
canola	-96.00	8.76
corn	-42.00	2.73
cotton	-124.00	3.77
flax	-42.00	2.73
peanut	-36.00	6.55
rice, paddy	-52.00	3.57
rye	-116.00	8.10
sorghum	-72.00	7.36
soybean	-54.00	6.91
sugarcane	-110.00	3.84
sunflower	-106.00	2.93
triticale	-182.00	2.43
wheat	-94.00	3.92
wheat (semidrawf)	-178.00	3.01
wheat (durum)	-134.00	2.84

$$^{1}\,\text{Where relative yield} = \frac{1}{1+\left(\dfrac{h}{h_{50}}\right)^{p}}$$

Table 3c   Model parameters[1] for salt tolerance (expressed as osmotic pressure) of vegetable and fruit crops

Crop	$h_{50}(m)$	p
bean, common	-26.00	2.64
broccoli	-58.00	3.03
cabbage	-50.00	2.58
corn, sweet	-42.00	2.73
cowpea	-64.00	4.76
cucumber	-46.00	3.38
eggplant	-58.00	2.03
lettuce	-36.00	2.54
potato	-42.00	2.73
spinach	-60.00	2.46
squash	-46.00	4.36
squash, zucchini	-70.00	4.38
sweet potato	-42.00	2.51
tomato	-54.00	2.97

[1] Where relative yield $= \dfrac{1}{1+\left(\dfrac{h}{h_{50}}\right)^p}$

Appendix for ET Calculations

U_2 windspeed [m s^{-1}] at 2 m height

R_a extraterrestrial radiation [MJ $^{-2}$ d^{-1}]

ω_s sunset hour angle [rad]

ψ latitude [rad]

δ solar declination [rad]

J   calender date

d_r relative distance, Earth-Sun

$\dfrac{n}{N}$ relative sunshine fraction

R_{ns} net shortwave radiation [MJ $^{-2}$ d^{-1}]

R_{nl} net outgoing longwave radiation [MJ $^{-2}$ d^{-1}]

G soil heat flux [MJ m^{-2} d^{-1}]

Δ slope if vapor pressure curve [kPa ^{o}C^{-1}]

γ psychometric constant [kPa ^{o}C^{-1}]

λ latent heat [MJ Kg^{-1}]

RH_{max} maximum relative humidity [%]

T   Kelvin

z elevation above sea level [m]

P atmospheric pressure [kPa]

e^o_{tmax} saturation vapor pressure at daily maximum temperature [kPa]

e^o_{tmin} saturation vapor pressure at daily minimum temperature [kPa]

e_a actual vapor pressure [kPa]

PART 4: EXAMPLES, CASE INPUT AND OUTPUT

EXAMPLE 1 - Irrigation with saline water

In this case we have a non saline soil and part way through the irrigation season we switch to a saline water source for irrigation, The model simulates a case where the water table is at 3m, and the CO_2 production routine is enabled but root growth is not considered. Cation exchange is neglected in this case. The soil is a loam with a saturated K_s of 25 cm/d (default value). Two different waters are considered. The initial condition is that of a non saline soil that has been leached with a dilute water. At the start of the simulation a salt sensitive crop is simulated (50 % reduction in yield at -50 m or -5 bars of osmotic pressure). There are a series of irrigation events. Every 10 days the soil is irrigated for 2 days at a rate of 6 cm/d. The ET_c is constant throughout at a rate of 1 cm/d. At steady state this corresponds to a *potential* leaching fraction of 0.167. On day 70 (about half way through the season) the irrigation water is switched to that of the saline ground water.

The graphical output file shows the predicted yield (biomass) relative to a non-stressed crop. Initiation of the irrigation with saline water caused a salinization of the root zone as shown by the output files for EC. This resulted in a small decrease in yield. As a management tool the user can evaluate if it would be beneficial to increase the amount of saline water applied, or to delay its application until all the fresh water was consumed.

Screen 1: Select project or create a new project. Files can be copied and modified.
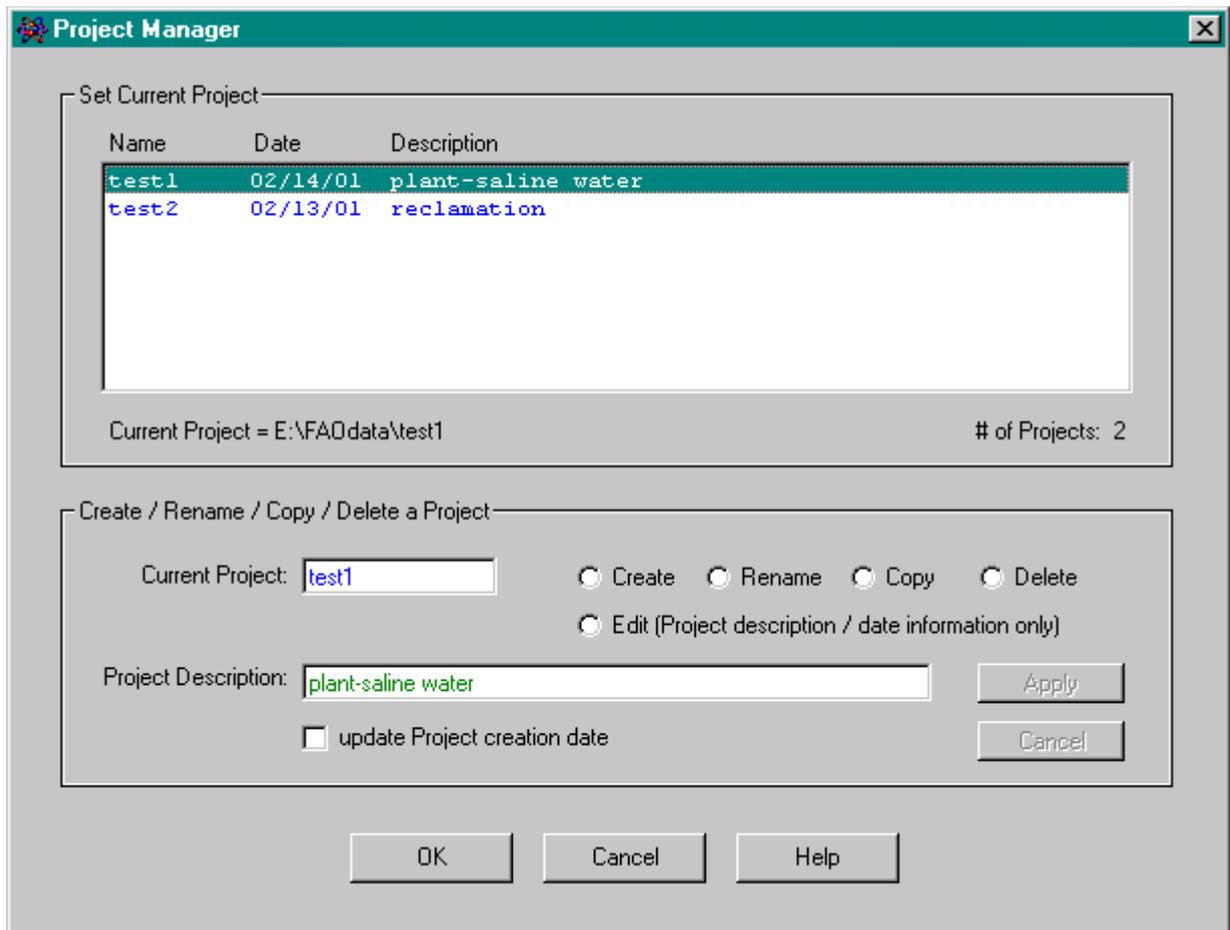
Step 2: Main process

Water flow and chemistry are always activated. Select if CO_2 production/ transport is desired. Otherwise CO_2 concentration is fixed by the user.
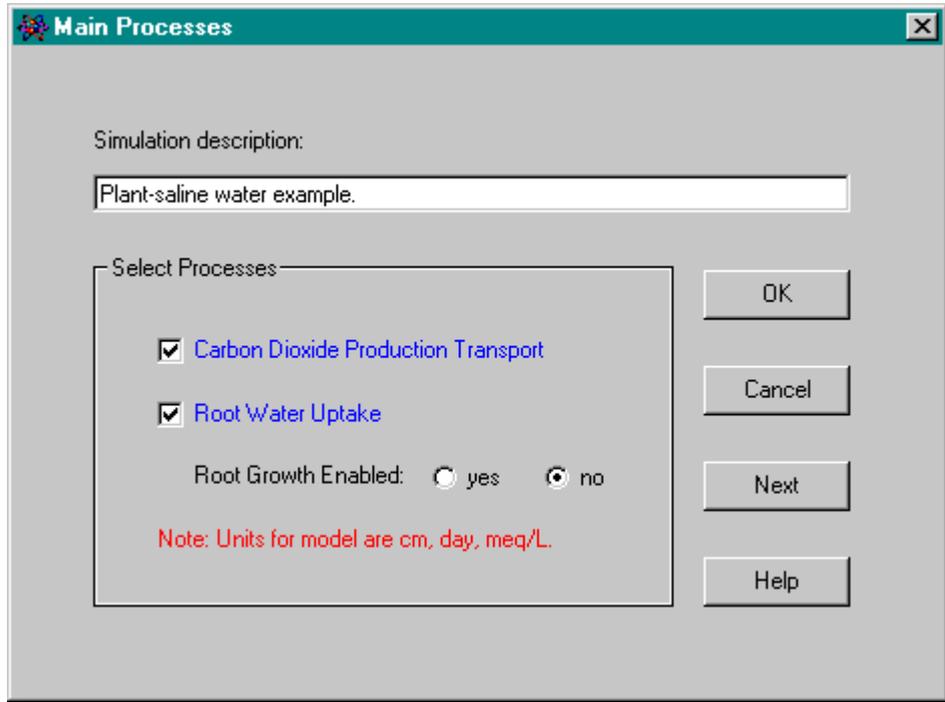
Step 3:

In this instance the last output requested was at time 100 d. The output will also plot the data for the last day of the simulation, day 130, as well as the initial condition.

Step 4:

The default parameters for loam were selected from the pull down menu. Only one layer was selected. If a second layer was specified earlier the pull down selection for layer would allow selection of properties for the second layer.
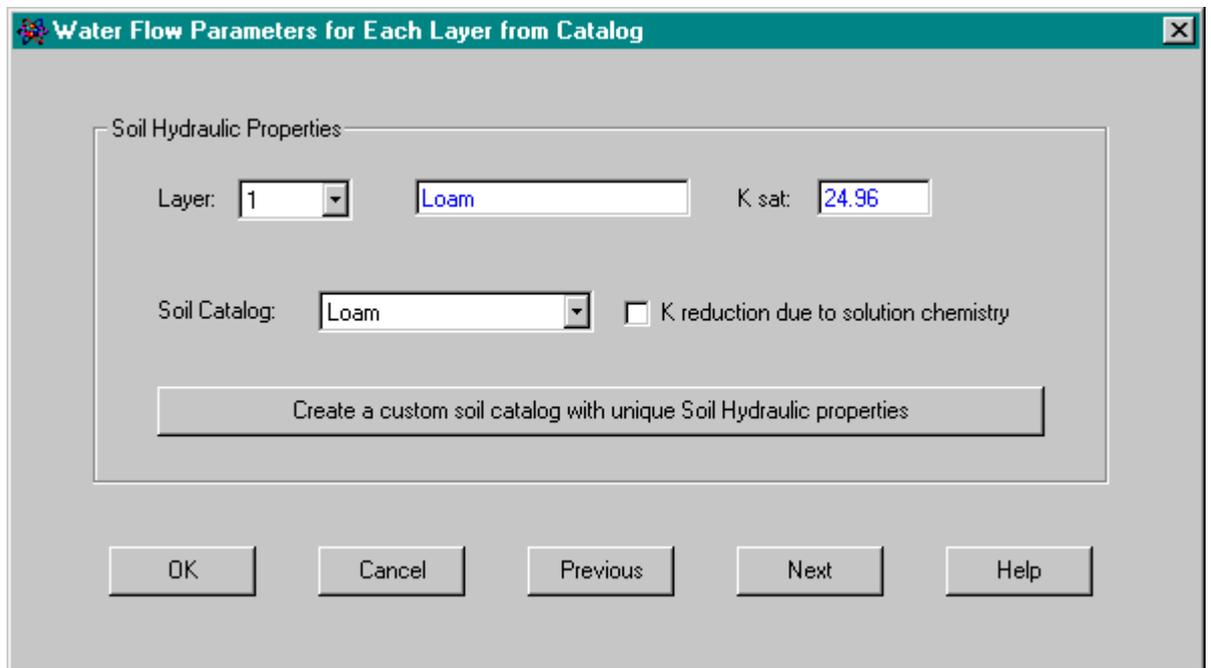
Step 5:

Two waters are selected; one for the initial non saline conditions and one for the saline irrigation water.

Step 6:

Default parameters for exchange. The bulk density is used to calculate the masses of salt in the solid and solution phase and allow for mass transfer as required.

Step 7:

Solution composition of the two waters are entered. A tracer is added to the saline water so that the infiltration front can be monitored. Use of a tracer on the ground water allows for assessment of upward water movement. No exchanger phase composition was specified, in this case we neglect cation exchange by assigning a zero value to CEC.

Solute Composition

Solution Composition

	Ca	Mg	Na	K	Alk	SO4	Cl	NO3	Tracer
1	1	1	1	0	1	1	1	0	0
2	5	5	50	0	1	7	52	0	1

Exchange Concentrations, meq/Kg (must sum to CEC)

	Ca	Mg	Na	K	CEC
1	0	0	0	0	0

Concentrations in Solid, meq/Kg soil

	Calcite	Gypsum
1	400	0

OK Cancel Previous Next Help

Step 8:

Step 9:

These are the standard default production values for CO_2. The salt tolerance values can be obtained from Tables 3a-3c.

Step 10:

Selection of the number of records. If an insufficient number is selected the user can come back to this screen later. In this case we specify the ET_c values.

Step 11:

Only 11 o f the 26 records are seen. Additional records can be entered by scrolling down the button on the left side. The bottom pressure is 0.0 and the applied water is -1. The bottom boundary water is also specified as 1. The hCritA is set to -10000 cm.

Step 12:

The initial conditions are entered. If a column has a constant value it can be entered by selecting the header which will highlight the entire column. Delete existing values and input the new constant value. In this case a trapezoidal root distribution was created using the assign editor, and selecting the root distribution option.

	z	h	Root	CO2	Temp
1	0	-5.0000000	0.0000000	0.0003500	25.0000000
2	3	-4.9500000	0.1111111	0.0004465	25.0000000
3	6	-4.9000000	0.2222222	0.0005430	25.0000000
4	9	-4.8500000	0.3333333	0.0006395	25.0000000
5	12	-4.8000000	0.4444444	0.0007360	25.0000000
6	15	-4.7500000	0.5555556	0.0008325	25.0000000
7	18	-4.7000000	0.6666667	0.0009290	25.0000000
8	21	-4.6500000	0.7777778	0.0010255	25.0000000
9	24	-4.6000000	0.8888889	0.0011220	25.0000000
10	27	-4.5500000	1.0000000	0.0012185	25.0000000
11	30	-4.5000000	1.0000000	0.0013150	25.0000000
12	33	-4.4500000	1.0000000	0.0014115	25.0000000
13	36	-4.4000000	1.0000000	0.0015080	25.0000000
14	39	-4.3500000	1.0000000	0.0016045	25.0000000
15	42	-4.3000000	1.0000000	0.0017010	25.0000000
16	45	-4.2500000	1.0000000	0.0017975	25.0000000
17	48	-4.2000000	1.0000000	0.0018940	25.0000000
18	51	-4.1500000	1.0000000	0.0019905	25.0000000

Soil Profile Summary

OK Cancel Previous Next Assign Help

Step 13: Run the SWS program.

If okay is selected the files are updated before running the program.
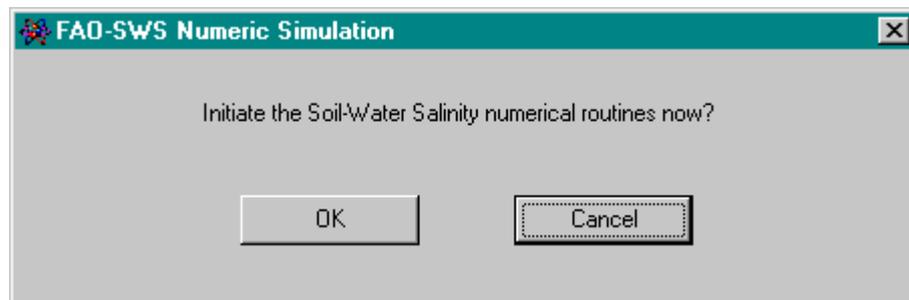
Step 14: View the output plots. Example of the relative yield output. At the end of the simulation the relative yield is predicted to be 91%. Note that the predicted yield was at 100% until introduction of saline water.
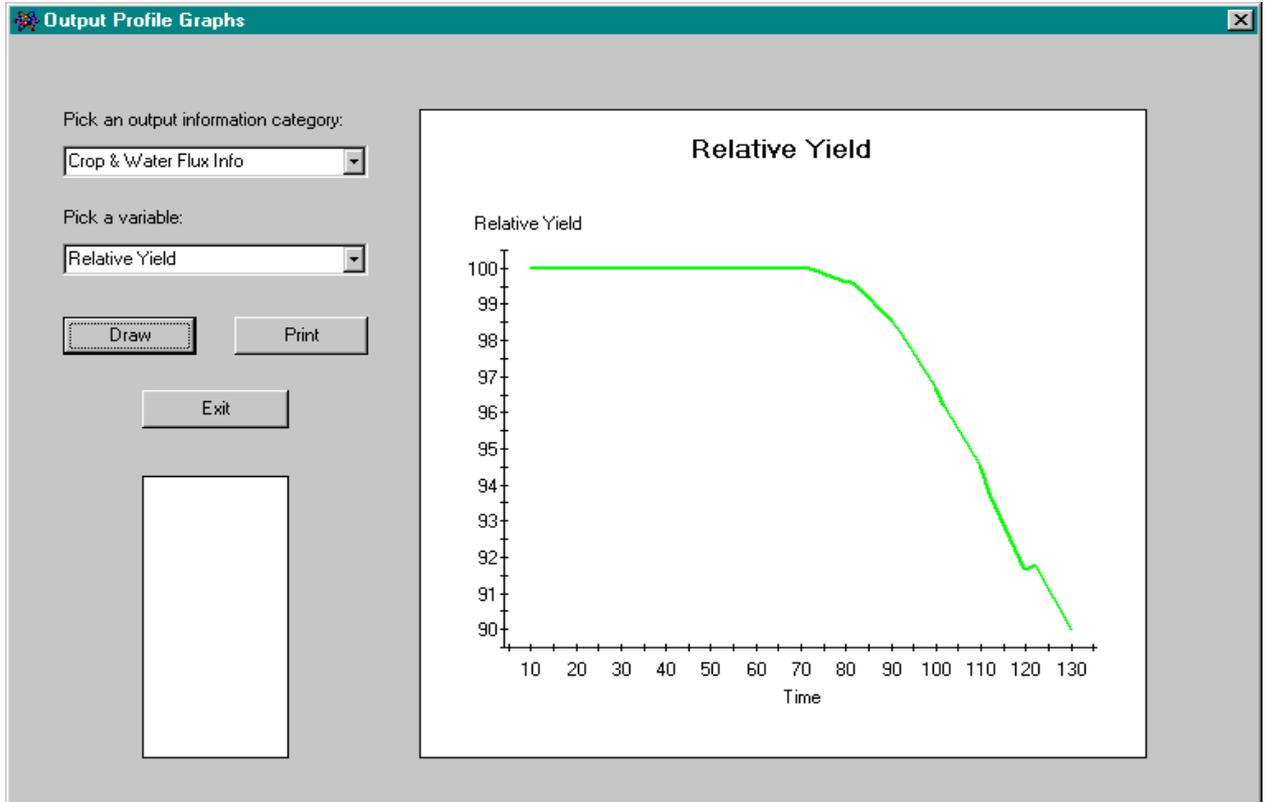
EXAMPLE 2 - Reclamation

In this simulation we are evaluating the reclamation of a sodic soil with the use of gypsum and consideration of the reclamation contribution of high CO_2 and calcite. This is a 100 day simulation with a sandy clay soil and a water table at 3 m.

Step 1:

Creation of new file and description
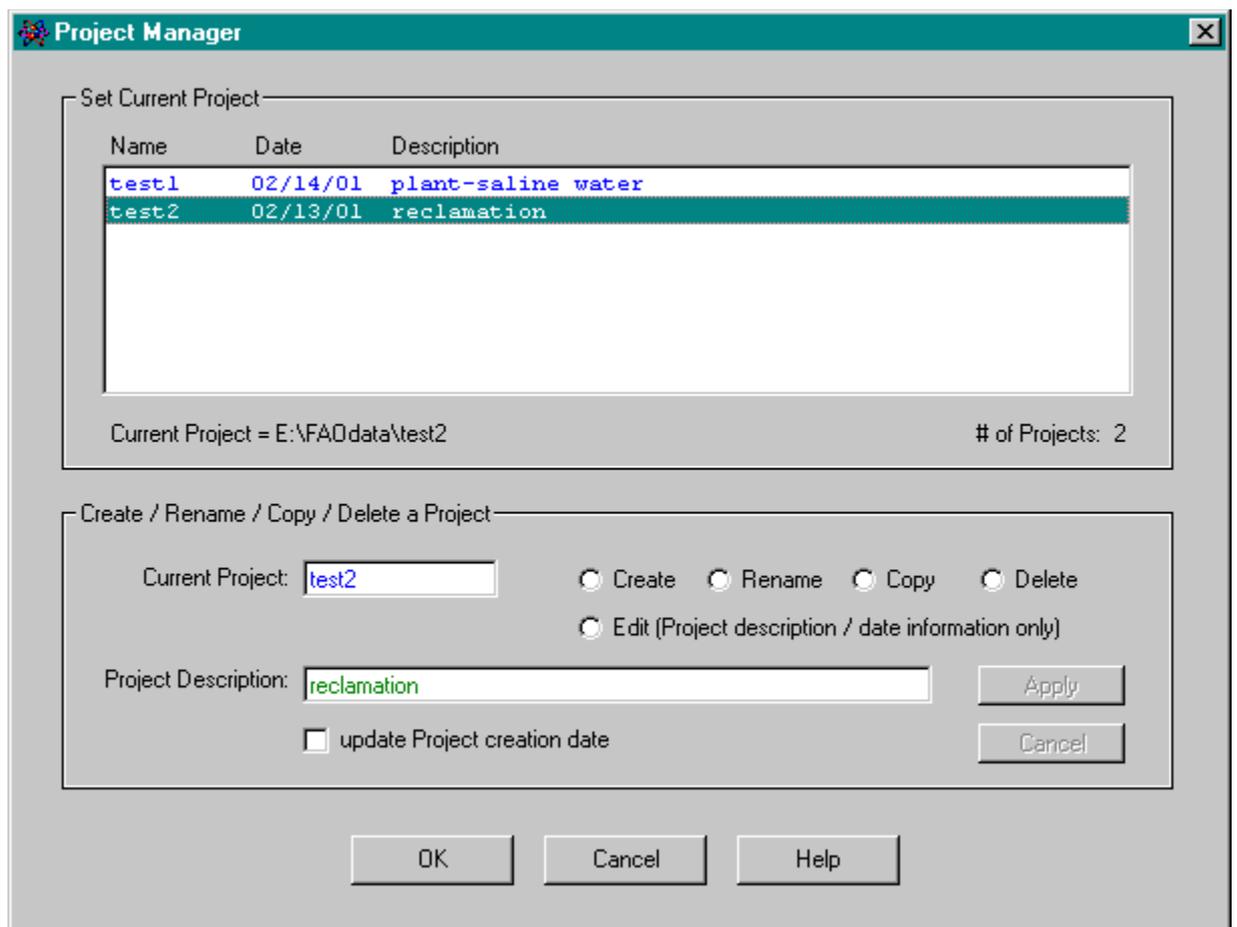
Step 2:

Specification of CO_2 production. There will be no plants grown during initial leaching/reclamation as the soil will be very wet.
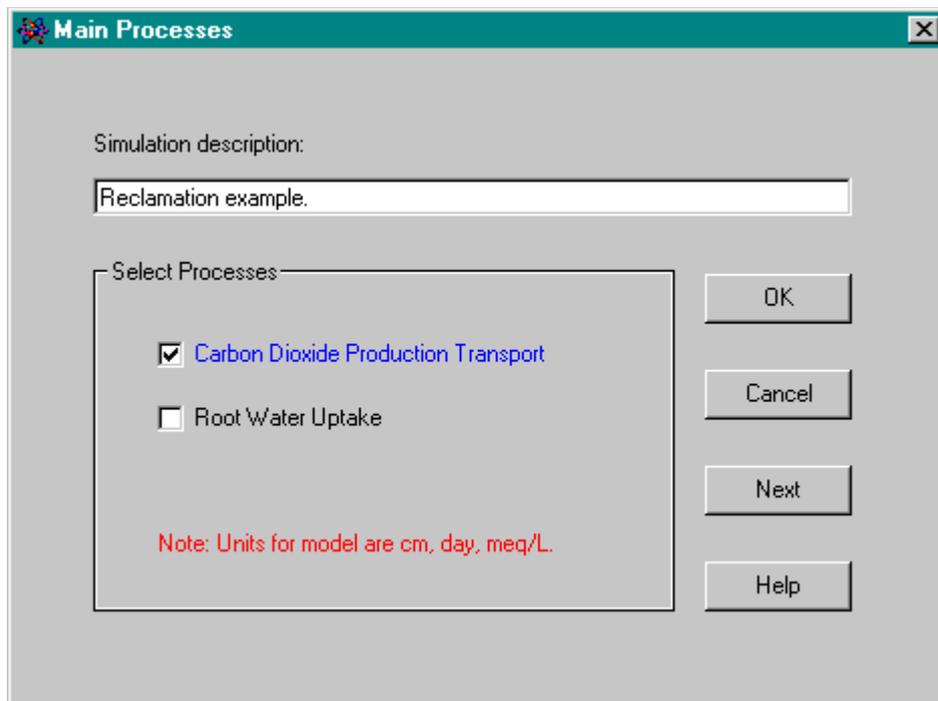
Step 3:

Input of depth of simulation, time and specification of 1 layer.

Step 4:

Selection of soil material. Saturated hydraulic conductivity is relatively low. The option for consideration of chemical effects on K was not selected.

Step 5:

Two waters are selected the initial water and the leaching water. Two mineral layers are selected, the top layer will contain added gypsum and the second layer will be the native calcareous soil.
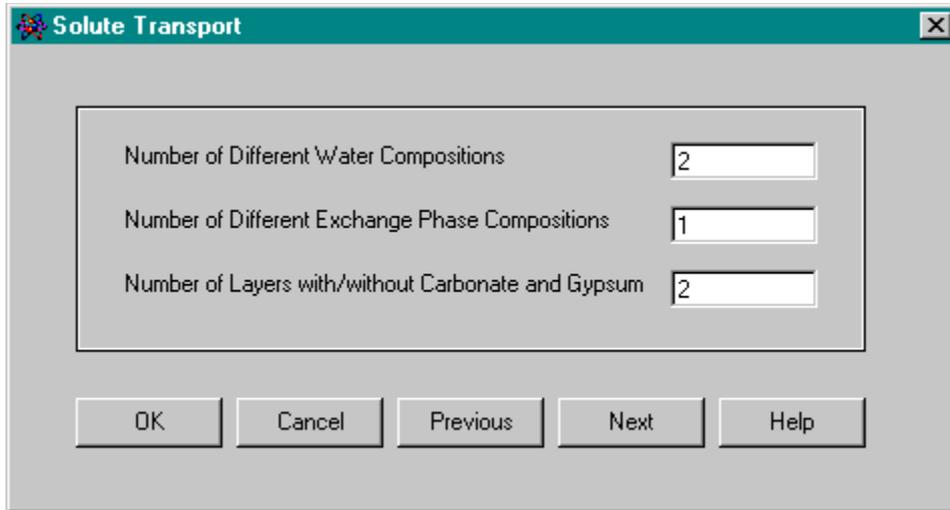
Step 6:

Default parameters

Solute Transport and Reaction Parameters

	b.d.	Disp.	K[Ca/Mg]	K[Ca/Na]	K[Ca/K]
1	1.4	10	0.81	4	0.36

OK   Cancel   Previous   Next   Help

Step 7:

Input of the water to be used for leaching (1) and the initial sodic water (2) in the soil. The user should attempt to match the water and the exchange composition for a realistic set of initial conditions. In this instance the CEC is 200 mmol$_c$/kg an the ESP is 30%. Gypsum was added at the rate of 50 mmol$_c$/kg. The tracer is placed in the irrigation water.

Solute Composition

Solution Composition

	Ca	Mg	Na	K	Alk	SO4	Cl	NO3	Tracer
1	2	1	1	0	1	1	2	0	1
2	2	2	20	0	2	18	4	0	0

Exchange Concentrations, meq/Kg (must sum to CEC)

	Ca	Mg	Na	K	CEC
1	80	60	60	0	200

Concentrations in Solid, meq/Kg soil

	Calcite	Gypsum
1	1000	50
2	1000	0

| OK | Cancel | Previous | Next | Help |

Step 8:

Default parameters. As there are no plants, the plant production term is ignored.

Step 9:

Two records are specified. The initial record will show the chemical conditions after addition and mixing of gypsum. Water will be applied starting after day 1

Step 10:

The application rate is specified as 2 cm/d, slightly below the saturated *K* value. The water table is at 3 m. The applied water is -1. The bottom boundary is given as water 2 (the sodic water initially in the profile).

Time Variable Boundary Conditions

Obs	Time	Precip	Evap	ETc	Press. Bot	Temp. Top	applied
1	1	0	0	0	0	20	
2	100	2	0	0	0	20	

Maximum negative pressure head:

hCritA: -10000
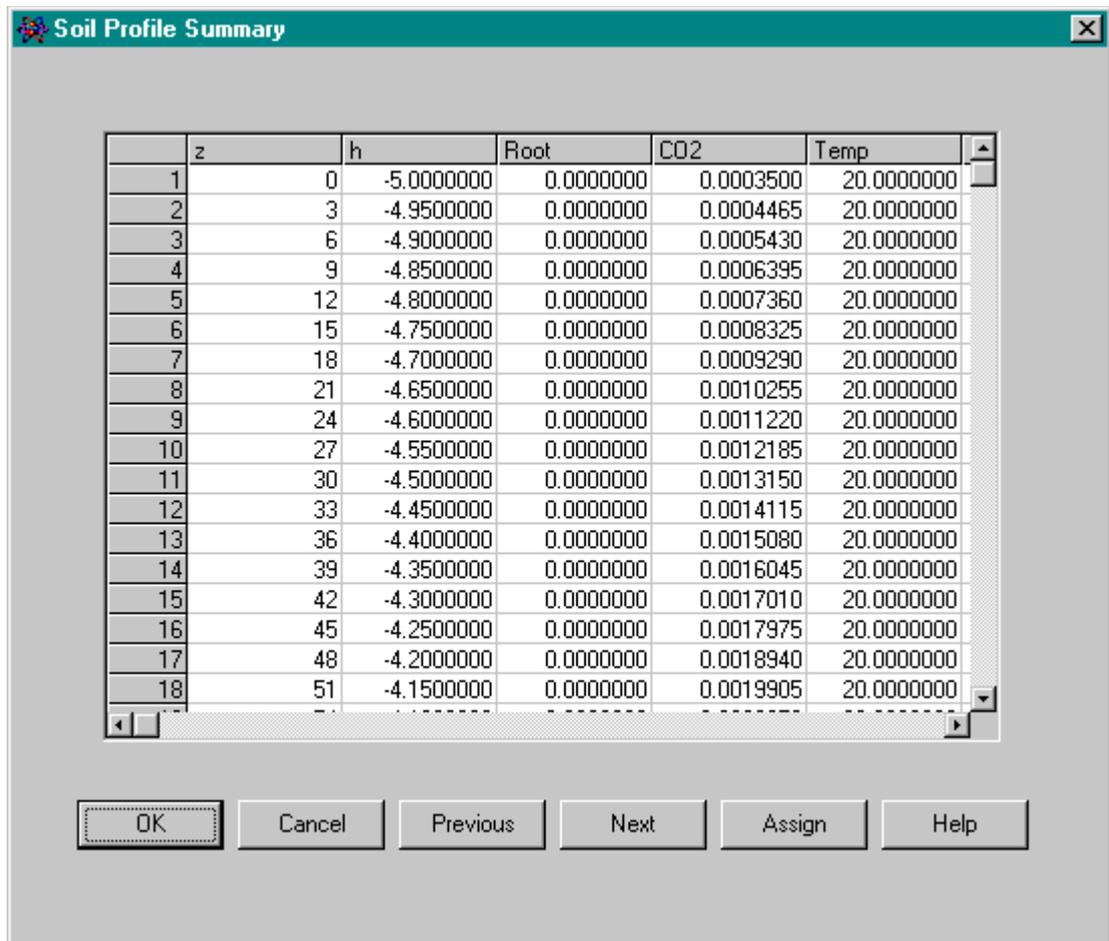
Calculate crop coefficients

Calculate ETo values

Calculate ETc values

OK   Cancel   Previous   Next   Help

Step 11:

Initial conditions. Water type 2 is specified throughout the profile, and exchanger 1is utilized. These columns must be assigned a number. The solid is specified as 1 for the top 50 cm and 2 for the rest of the profile.

	z	h	Root	CO2	Temp
1	0	-5.0000000	0.0000000	0.0003500	20.0000000
2	3	-4.9500000	0.0000000	0.0004465	20.0000000
3	6	-4.9000000	0.0000000	0.0005430	20.0000000
4	9	-4.8500000	0.0000000	0.0006395	20.0000000
5	12	-4.8000000	0.0000000	0.0007360	20.0000000
6	15	-4.7500000	0.0000000	0.0008325	20.0000000
7	18	-4.7000000	0.0000000	0.0009290	20.0000000
8	21	-4.6500000	0.0000000	0.0010255	20.0000000
9	24	-4.6000000	0.0000000	0.0011220	20.0000000
10	27	-4.5500000	0.0000000	0.0012185	20.0000000
11	30	-4.5000000	0.0000000	0.0013150	20.0000000
12	33	-4.4500000	0.0000000	0.0014115	20.0000000
13	36	-4.4000000	0.0000000	0.0015080	20.0000000
14	39	-4.3500000	0.0000000	0.0016045	20.0000000
15	42	-4.3000000	0.0000000	0.0017010	20.0000000
16	45	-4.2500000	0.0000000	0.0017975	20.0000000
17	48	-4.2000000	0.0000000	0.0018940	20.0000000
18	51	-4.1500000	0.0000000	0.0019905	20.0000000

Soil Profile Summary

OK   Cancel   Previous   Next   Assign   Help

Step 12: Run the SWS program.

Files are saved and program executed. The simulation run time information will scroll on the screen. Press return when run is completed.
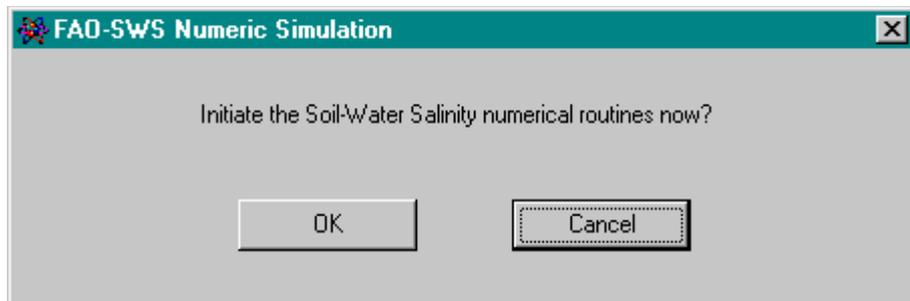
Step 13: View the output plots (SAR plot shown below).

In this instance reclamation was effective. All of the gypsum was dissolved and some of the reclamation was achieved via calcite dissolution. This can be evaluated by examining the alkalinity values in the concentration output.
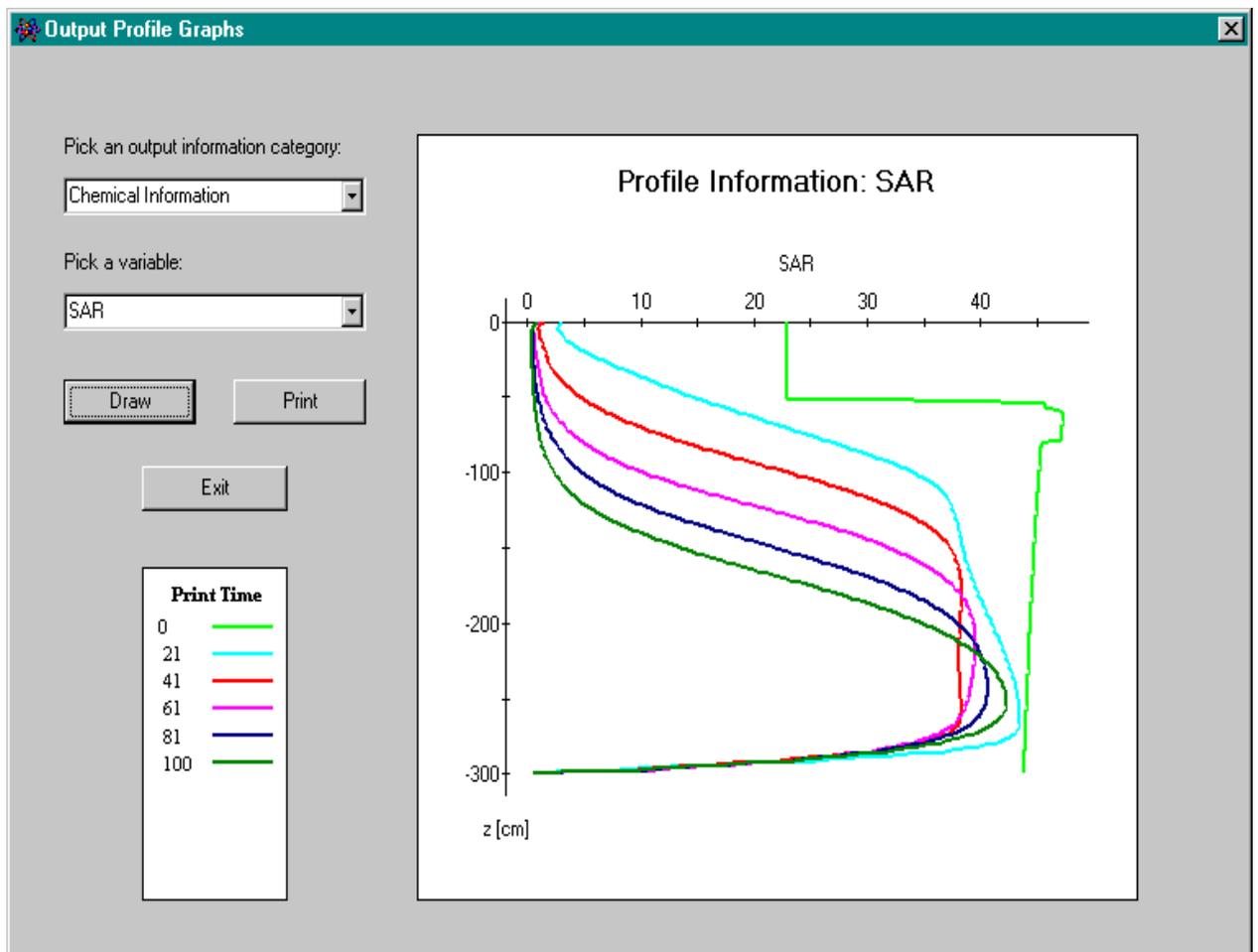
Step 13 continued:

View the output plots (EC plot shown below).

The initial high EC was the result of gypsum dissolution, enhanced by Ca exchange. This graph and the previous indicates that much less water and less gypsum was sufficient to reclaim the upper part of the profile. The user can evaluate different gypsum applications, and turn off or reduce the CO_2 production if organic matter was not present.