

Chapter 2

Soil Salinity Modeling, Approaches, and Key Issues

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Abstract Salinization is a progressive soil and water degradation process. Soil salinity can be natural or induced by human affecting aquifers and the most productive irrigated agroecosystems in arid and semiarid regions, representing an increasing environmental concern. Root zone soil salinity can be managed using advanced tools and adjusting irrigation application and using the concept of leaching requirement. Modeling the reactive transport in soil uses simplified representations of the reality, but can reveal complex interrelations of properties of the system under study, and is best suited for drawing scenarios for investigating “what-if...” questions. Each modeling effort tries to give answer to a particular question; hence, the input information required for running the models ranges in complexity as does the data acquisition efforts. The scale of application, geometry of the system, and biological, chemical, and physical processes represented, as well as the capability of representing an evolving system, are main differences among models. Some aspects important under normal agricultural practices are not well reproduced by some codes nowadays. Management practices, geometry of irrigation and evaporation, sinks of solutes (plant uptake), and interaction of fertilizers with soil components are incorporated in an uneven way in the available codes and should be further developed. Currently models become more and more mechanistic and require very intensive research efforts. There are uncertainties associated to the values of the input parameters, to the computation procedure, or to the inaccurate description of the system. The parameter estimation, analysis of sensitivity, and validation procedures are refinements applicable to most models. This chapter presents an overview of different modeling approaches, discusses the limits of application of models, and develops a study case.

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Keywords Irrigation • Leaching requirements • Modeling • Reactive transport • Salinity

2.1 Introduction

Soil salinity is high concentration of ions in the soil solution, more specifically in soil saturation extract. This condition is very restrictive for plant's growth due to high osmotic potential of the solution that restricts the plant water uptake and induces specific ion effects causing nutritional imbalances. Soil salinity affects crop productivity and feasibility, especially in arid and semiarid zones, where mostly irrigated agriculture is practiced. The chemical equilibrium established between the exchange complex of clays, organic soil components, and soil solution can cause dispersion of fine-sized clays that ultimately degrade soil structure.

In areas where potential evapotranspiration (PET) exceeds water application plus rainfall, the soil solution can be concentrated until that solids can precipitate from liquid phase, forming solid salt accumulations at the soil surface or inside the soil. Also in areas where water table is high and soils are fine textured, the soil water reaches surface through capillary ascent capability and precipitates at surface through evaporation.

Salinity is a transient condition in most salt-affected soils. A concentration of the soil solution follows to the water uptake from the soil by the plant roots, as well as to water loss by evaporation at soil surface. Subsequent irrigation or rainfall can dilute the soil solution, or the solutes can be removed from the system by leaching of the soil to drains or by deep drainage. In a scenario of water scarcity, an irrigated agriculture should minimize the volume of water required for optimum yield and ensure the leaching of salts from the root zone.

Leaching requirement is the extra water applied (above the plant water requirements – PET) to an irrigated field (under risk of salinization), to keep dissolved the solutes that concentrate during the root uptake and allow their drainage from the root zone (U.S. Salinity Laboratory Staff 1954; Rhoades 1974).

The electrical conductivity (EC) of the irrigation water and the EC of the resultant drainage water (specific crop-threshold EC) determines the leaching requirements for the irrigated soil (Rhoades et al. 1992). It is essential to know the threshold EC value of the crop under cultivation to assure the saline water available for irrigation can be used successfully. Highly saline irrigation waters are unfeasible for economical crop production under any leaching fraction (salt-sensitive crops). The use of very solute-concentrated waters for irrigation can induce groundwater degradation by high salt loadings of drainage water.

Inadequate irrigation practices can lead to soil and aquifers salinization (Milnes and Renard 2004; Misra and Mishra 2007; Petheram et al. 2008; Fakir et al. 2001) and impact the hydrological resources of a region. The human-induced secondary soil salinization is a progressive soil and water degradation process, affecting the most productive irrigated agroecosystems in the arid and semiarid regions,

representing an increasing environmental concern. A dramatic example is soil salinization in the Aral Sea area (Kitamura et al. 2006); also many salinized areas in the world exist at any latitude, requiring high economical cost for their reclamation (Janmaat 2004). An environmentally sound and economically feasible land management should take advantage from the most advanced tools for adjusting irrigation application (de Clercq et al. 2009; Jorenush and Sepaskhah 2003; Metternicht and Zinck 2003; Wang et al. 2007) to tackle soil salinity in irrigated agricultural fields taking into account the leaching requirements.

2.2 Modeling Water Flow and Reactive Transport

There exist many models addressing soil-water-plant-atmosphere-aquifers system, as a whole or as subsystems, taking into account several biological, physical, and chemical processes. All models are simplifications of the reality, but considering several coupled processes together, they can derive in models of great complexity. In most soil-centered models, the atmospheric processes, the plant growth, and the aquifers loading, rather than modeled, are considered as input variables that should be given for the model run. Modeling the reactive transport in soil can reveal complex interrelations of properties of the system under study. This can also serve as a tool to answer questions of the type “what-if...” in particular scenarios. Each modeling effort tries to give answer to relevant questions, and the type, amount, and precision of data required for running the models ranges in complexity.

The first task for a soil transport model is to solve the water flow. A recent review of water transport models by Ranatunga et al. (2008) reports the application that can be used for each model and highlights that the elaboration of models of increasing complexity and wide-range application is often hampered by a lack of the required input data.

In the simplest soil water transport models, the soil water content is computed considering the soil as tipping bucket of a certain capacity. The bucket loses water due to the plant water uptake, and the irrigation and rainfall fill in the bucket. The size of the bucket determines the reserve of water during the periods of no infiltration. If the capacity of the bucket is surpassed by the water inflow, drainage occurs. Those models can be monolayer or multilayer (cascade) and cannot simulate water capillary raise. More complex models incorporate a continuous soil profile where water flows (in any direction) are based on the Richards equation (Richards 1931) for computing the movement of water and solute through porous media.

Some of those models approach the system considering it under steady-state conditions, what is an oversimplification of the real conditions, allowing easy calculations with limited input data, although they are of limited value for a satisfactory irrigation design. An example of this is the WATSUIT model (Rhoades and Merrill 1976) that considers the composition of the irrigation water and includes the processes of salt precipitation and the dissolution of calcite and gypsum present in soil. Other models approach the system considering transient conditions and much

more adjusted to the reality but also need more intensive data acquisition efforts. The capability of steady-state models versus transient models is compared by Corwin et al. (2007) for optimizing the calculus of the leaching fraction under risk of salinization. Another review of the relative merits of the transient versus steady-state models is given by Letey and Feng (2007) with respect to the evaluation of the irrigation management using saline waters. Bastiaanssen et al. (2007) make a literature review of the models suitable to describe irrigation and drainage processes for the unsaturated zone.

Some soil models can simulate very complex processes as reactive transport of water, solutes, and heat in the vadose zone in interaction with vegetation development. Those models employ the Richards equation including root water extraction to simulate soil moisture movement in variably saturated soils, considering the processes of convection, dispersion, adsorption, and decomposition. The existing models differ in their capability of the hydrological part, for simulating bypass flow, hysteresis, dual porosity, dual density, variable conditions of the upper and lower limit of the soil, pedotransfer functions for estimating the unsaturated hydraulic conductivity at any soil moisture content, resolution of texture discontinuities, and changes in permeability due to clays dispersion, among others.

Only a reduced number of complex models can solve the reactive transport of solutes, including the cation exchange of the soil solution with the solid phase of the soil, the precipitation or dissolution of numerous mineral phases, the simulation of nonequilibrium conditions, or the kinetic aspect of some reactions, that take place during the reactive transport. The capability to simulate the transport of CO_2 affects the carbonate chemistry in a decisive way, and only a few models are capable of simulating this chemical aspect.

In most salt-affected soils, the concentration of ions is so high that the equilibrium constants for the possible reactions, applicable to the dilute systems, are no longer valid. This is a very serious constraint of models that try to make chemical predictions for the equilibria that are established in media of high ionic strength. The most advanced models (Simunek and Suarez 1993, 1997; Simunek et al. 1996) used Pitzer approach (Pitzer 1973) for calculating ion activity that could be used to reliably model the solubilities of solutes present in complex, highly concentrated, natural brines and to model the diagenetic precipitation sequences resulting from evaporation of diverse types of natural waters. Very recently, the Brönsted-Guggenheim-Scatchard Specific Ion Interaction Theory (SIT) approach (Sipos 2008) has been introduced in the PHREEQC (Parkhurst and Appelo 1999), which is one of the more robust geochemical models. This is one of the few models that can deal with reducing conditions that appear in soils under stagnant-anoxic circumstances.

The transport processes, which are predominantly vertical, can be considered one-dimensional, that is, the simplest case of water and solute movement, as in furrow or flood irrigation. In cases of drip irrigation, 2D or 3D models are needed to take into account the lateral movements as well as the vertical fluxes. This increases the complexity for obtaining the input information for the model.

In the domain of hydrogeology exist many computer programs that can be used for simulating groundwater flow, solute transport, and multicomponent geochemical reactions, but most of the existing models consider only saturated water flow,

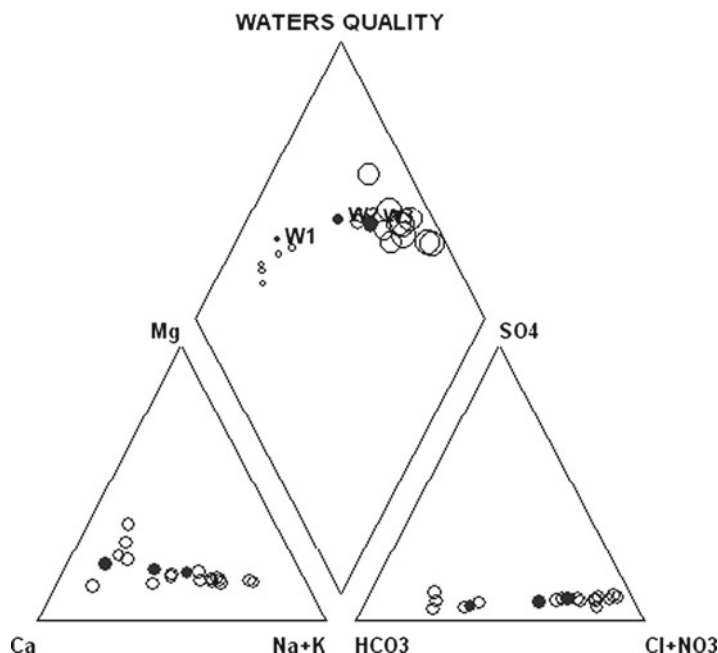


Fig. 2.1 Piper diagram of the quality of water wells

whereas soil salinity models are focused in modeling an unsaturated depth with time-changing boundary conditions. In this sense a coupling of a model for the vadose zone and a model for the aquifers is necessary because the downward output of water and solutes from the vadose zone is the input for the hydrogeological model.

2.3 Case Study: Optimization of Irrigation with Low-Quality Water

An agricultural area of the Western Mediterranean region (Castellon Province, Spain) was selected for studying the long-term effect of irrigation with low-quality waters on the soils and on the underlying aquifers of the area. Two different detritic aquifers exist, one free aquifer and the other a confined aquifer; both are affected by marine intrusion due to the disruption of the fringe freshwater/seawater by over pumping the wells used for irrigation. The occurrence of marine intrusion in the aquifers of the study area (Torreblanca) has been studied by Gimenez (Gimenez et al. 1996).

The chemical composition of the waters is presented in Fig. 2.1, as a Piper plot, each point in the rhomboidal area with radius proportional to the water electrical

conductivity. The shape of the distribution of points close to aligned suggests a process of mixing of freshwater and seawater, modified by processes of cation exchange and sulfates reduction (Batlle-Sales et al. 2002).

The scarcity of volumes of low-conductivity water and the use of solute-concentrated water for irrigation increase the risk of soil salinization processes as well as promote a higher solute loading of the aquifers that receive the deep drainage of agricultural parcels.

Although the tendency in the agricultural area is changing to drip irrigation for saving water and allowing fertigation, there still exist many fields irrigated by furrow, with periodical availability of water (not on demand). One of such plots was selected for modeling purposes, using two different one-dimensional models, LEACHC (Hutson and Wagenet 1992) and UNSATCHEM (Simunek and Suarez 1997). The objective is to optimize the irrigation rotation to avoid the exposure of the crop both to hydric and to osmotic stress.

2.3.1 *Description of the Experiment*

A soil under cultivation of *Citrus sinensis*, classified as a Typic Calcixerept in the soil taxonomy (Soil Survey Staff 1999), was selected to perform the study. Its effective depth is 100 cm, with free depth drainage. Four distinct horizons were recognized in the profile and were sampled for subsequent analysis of physical, chemical, and mineralogical properties.

The texture of the first horizon is loamy, and the other horizons have clay-loamy texture. The upper two horizons have around 20% of their mass in coarse fraction (>2 mm). The calcium carbonate equivalent content (w/w) ranges from 10% in the upper horizon to 29% at the bottom horizon, part of this is in the form of calcium carbonate nodules. The pH of the extract of the saturated paste ranges from 8.21 to 8.45 (moderately alkaline) and the $EC_e < 1$ dS m^{-1} in all horizons.

Soil mineralogy is dominated by calcite ($CaCO_3$) and clay minerals kaolinite and weathered illite with minor proportion of montmorillonite, and gypsum ($CaSO_4 \cdot 2H_2O$) was undetectable. Cation-exchange capacity (CEC) ranges from 209 to 235 mmol(+) kg^{-1} and the exchangeable sodium percentage (ESP) less than 1. This suggests the soil to be moderately alkaline, nonsaline, and non-sodic (US Salinity Lab Staff 1954).

A computerized station capable of measuring solar radiation, temperature, humidity, wind direction and velocity, as well as precipitation measured the meteorological data during the course of the experiment, with records at every 5-min interval. Evapotranspiration was computed using Penman-Monteith method.

Several devices were installed in the profile: a groundwater-level observation well, a fiberglass guide for measuring soil volumetric moisture (theta) with a time-domain reflectometry (TDR) meter at any depth, several sensors of matric potential, and captors for measuring soil solution and soil atmosphere, located at different depths.

The placement of all these devices allowed obtaining real-time data from soil, at fixed dates, the same dates that were requested to the models giving predictions for soil conditions, allowing comparison of observed data versus properties predicted, for purposes of calibration and validation of the models. Such measurements were performed six times during the 376 days duration of the experiment. During this period the soil was irrigated with water of $EC = 2.09 \text{ dS m}^{-1}$ and composition indicated as “W2” (Table 2.1). PHREEQC (Parkhurst and Appelo 1999) was used for computing the saturation indices of the water for calcite and gypsum, revealing that water “W2” at 25°C and atmospheric P_{CO_2} is in equilibrium with calcite and undersaturated to gypsum.

The models UNSATCHEM and LEACHC were calibrated with the soil information measured initially; the soil hydraulic properties were estimated using the pedotransfer functions included in both models that use different equations for calculus. Gapon coefficients for cation exchange were provided from experimental measurement.

2.4 Results and Discussion

Figure 2.2 presents, with bars, the water balance for the soil during the experimental period. The upper part presents details of water inputs (rainfall+irrigation), whereas the bottom part details the outputs (evaporation, crop transpiration, drainage, and runoff), computed on a daily basis, but for clarity they are expressed on a weekly basis. Lines represent the soil matric potential at each of four depths, grouped weekly.

Neither measurements nor predictions were advised from development of osmotic stress at any time for the crop, under the conditions of irrigation, but an unwanted high hydric potential was measured and predicted by the two simulation models at the middle of the experiment (the driest and hotter part of the year in the area). This was a clear evidence that the irrigation scheme was incorrect and should be corrected.

The validation of the goodness of fit of the predictions made by the models was evaluated using a set of statistical indices (Hagi-Bishow and Bonnell 2000) that give different information about the performance of the models. The index RMSE (root-mean-square error) highlights how the simulations over the measures are overestimated or underestimated. The CD (coefficient of determination) statistic shows the relationship between the dispersion of the values of the simulation from the mean of the observations. The EF (efficiency of the model) index compares the simulated values with the average of the measured values so that a negative value of EF indicates that the average of the measures provides a better estimate than the simulations. Finally, the CRM (coefficient of residual mass) index is an indicator of the tendency of the model to overestimate or underestimate the measurements. The CRM positive values indicate an underestimation by the model, while positive

Table 2.1 Chemical composition of waters used for irrigation

Reference water	pH	EC (dS m ⁻¹ 25°C)	Ca ²⁺ (mmolc L ⁻¹)	Mg ²⁺ (mmolc L ⁻¹)	Na ⁺ (mmolc L ⁻¹)	K ⁺ (mmolc L ⁻¹)	Alkalinity (mmolc L ⁻¹)	Cl ⁻ (mmolc L ⁻¹)	SO ₄ ²⁻ (mmolc L ⁻¹)	SI calcite	SI gypsum
W2	7.00	2.09	7.49	3.40	8.13	0.09	4.50	12.91	1.70	-0.04	-1.58
W3	6.98	3.15	14.44	3.74	11.13	0.06	3.90	23.94	1.53	0.10	-1.17

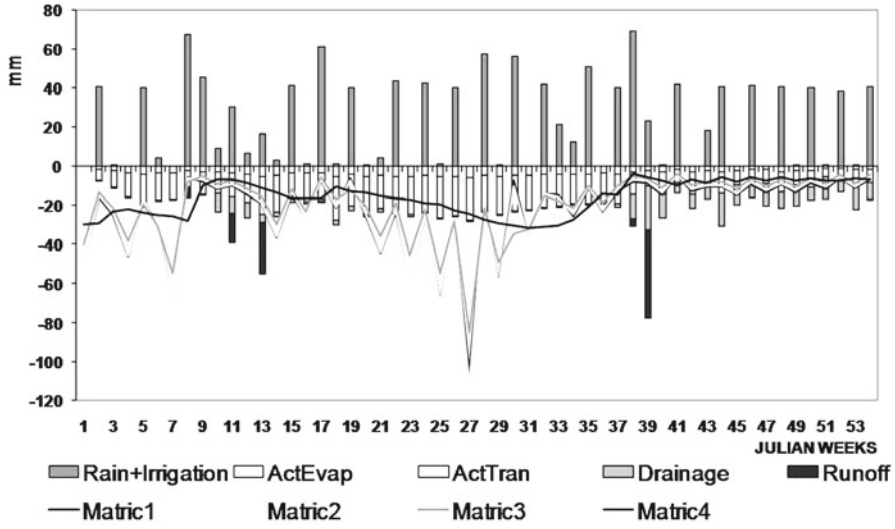


Fig. 2.2 Soil water balance after simulation

values indicate a tendency to overestimate the measurements. A perfect fit between observations and simulations gives the following values: RMSE=0.0, CRM=0.0, CD=1.0, and EF=1.0.

$$\text{RMSE} = \left[\frac{\sum_{i=1}^n (P_i - O_i)^2}{n} \right]^{0.5} * \frac{100}{\bar{O}} \quad (2.1)$$

$$\text{CD} = \frac{\sum_{i=1}^n (O_i - \bar{O})^2}{\sum_{i=1}^n (P_i - \bar{O})^2} \quad (2.2)$$

$$\text{EF} = 1 - \frac{\sum_{i=1}^n (P_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2} \quad (2.3)$$

$$\text{RMSE} = \left[\frac{\sum_{i=1}^n (P_i - O_i)^2}{n} \right]^{0.5} * \frac{100}{\bar{O}} \quad (2.4)$$

Table 2.2 Statistical indices for theta

Index	RMSE %	CD	EF	CRM
Optimal value	0	1	1	0
Statistical indices UNSATCHEM (theta)				
0–20 cm	7.42	0.67	0.80	–0.05
20–40 cm	8.62	0.51	0.79	0.02
40–60 cm	3.63	0.88	0.97	0.02
60–80 cm	5.31	0.94	0.92	–0.03
Average	6.15	0.63	0.87	0.00
Statistical indices LEACHC (theta)				
0–20 cm	15.61	0.99	0.13	0.02
20–40 cm	7.15	1.51	0.86	0.04
40–60 cm	11.46	3.06	0.67	–0.02
60–80 cm	5.21	1.39	0.92	–0.04
Average	10.64	1.62	0.60	0.01

Table 2.3 Statistical indices for chloride

Index	RMSE %	CD	EF	CRM
Optimal value	0	1	1	0
Statistical indices UNSATCHEM (Cl [–])				
0–20 cm	17.63	0.74	0.77	0.07
20–40 cm	12.13	0.89	0.93	–0.01
40–60 cm	21.98	0.65	0.44	0.17
60–80 cm	23.33	0.33	0.32	0.03
Average	16.52	0.83	0.81	0.06
Statistical indices LEACHC (Cl [–])				
0–20 cm	45.13	1.00	–0.52	–0.12
20–40 cm	79.81	0.49	–1.91	–0.39
40–60 cm	28.32	1.48	0.08	0.07
60–80 cm	11.85	0.89	0.82	–0.02
Average	53.12	0.57	–1.10	0.12

where O_i are observed values, P_i are predicted values, \bar{O} is the mean of observed values, and n is number of observations.

The Table 2.2 presents the indices elaborated for the comparison between the values of soil volumetric water content, measured in the field, and the values predicted by the models UNSATCHEM and LEACHC, at different soil depths. This gives information about how well the water flow in the soil is modeled. The values suggest a better performance of the UNSATCHEM model for the case under study.

Chloride ion experiment-anion exclusion in soils is very soluble and can serve as autotracer of the efficiency of the modelization of the chemical part (reactive transport). The comparison of observed and predicted values for the chloride ion can be found in the Table 2.3. The chloride indices reveal again a superior performance of the

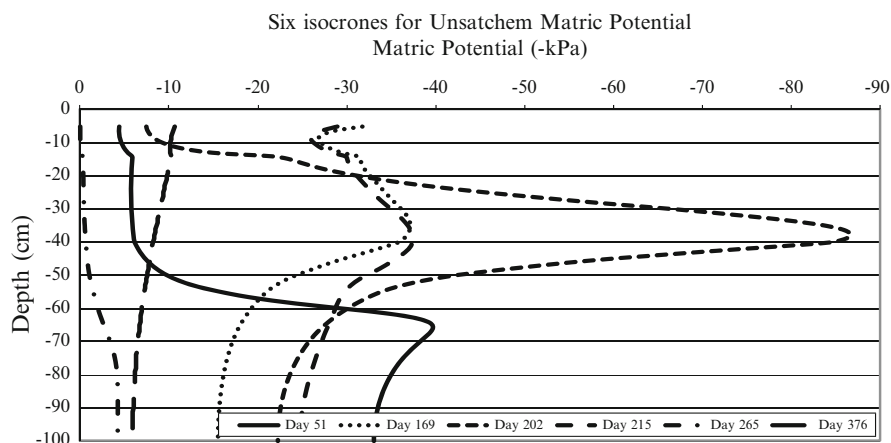


Fig. 2.3 Isochrones for UNSATCHEM. Matric potential

UNSATCHEM model over the LEACHC model in part because the errors of the hydraulical part (solute flow) are added to the errors in the chemical part, for the whole modeled reactive transport process.

On the basis of the information of the soil water balance (Fig. 2.2), the irrigation was adjusted (increased in the critical period) to reduce the water matric potential. Once adjusted, the same irrigation doses were considered for a simulation of the risk of soil salinization using the water quality labeled “W3” in Table 2.1, of $EC=3.15 \text{ dS m}^{-1}$. This water at 25°C and atmospheric P_{CO_2} is slightly oversaturated with calcite and undersaturated to gypsum.

Both models UNSATCHEM and LEACHC were reset with the same initial soil conditions, climatic data, as well as schedule and irrigation doses (adjusted), but using water of quality “W3.” Predictions for the matric potential are shown in Figs. 2.3 and 2.4, and predictions for electrical conductivity are shown in Figs. 2.5 and 2.6. Both models give similar results for the values of matric potential at different dates, but differ a few in the predictions for electrical conductivity: UNSATCHEM gives a maximum of close to $EC=2 \text{ dS m}^{-1}$, whereas the predictions for the LEACHC are higher, with a maximum of $EC=3 \text{ dS m}^{-1}$ and higher EC in the middle of the soil depth at any time.

Due to the high calcite content of the soil and the composition of the irrigation water, oversaturated to calcite, the soil Na exchangeable remains low, the soil solution sodium adsorption ratio – $SAR < 6$; hence, no risk of clays dispersion is anticipated. The conditions of water matric potential, electrical conductivity, and SAR predicted by the two models do not affect the normal growth of the citrus, even with water labeled as “B.” Whatsoever the use of water “B” instead of water “A” will increase the salt loading of the underlying aquifers, with respect to the loadings produced by using water “A.”

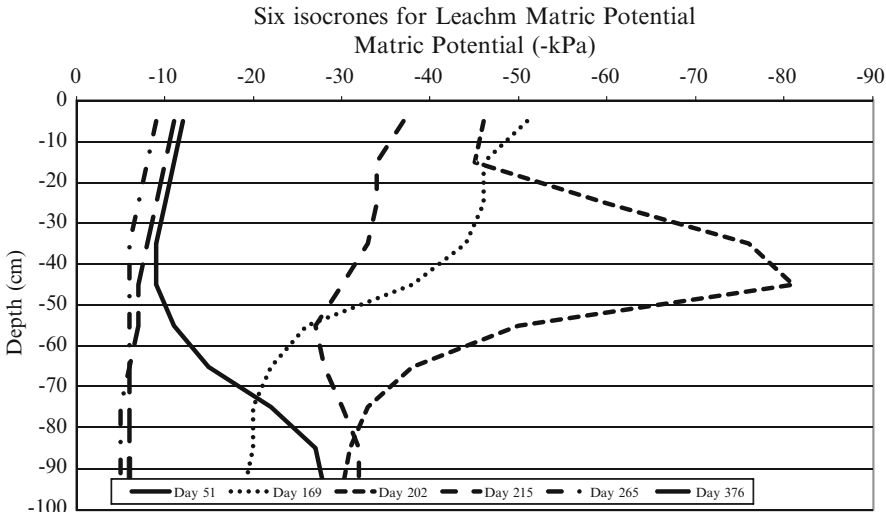


Fig. 2.4 Isochrones for LEACHC. Matric potential

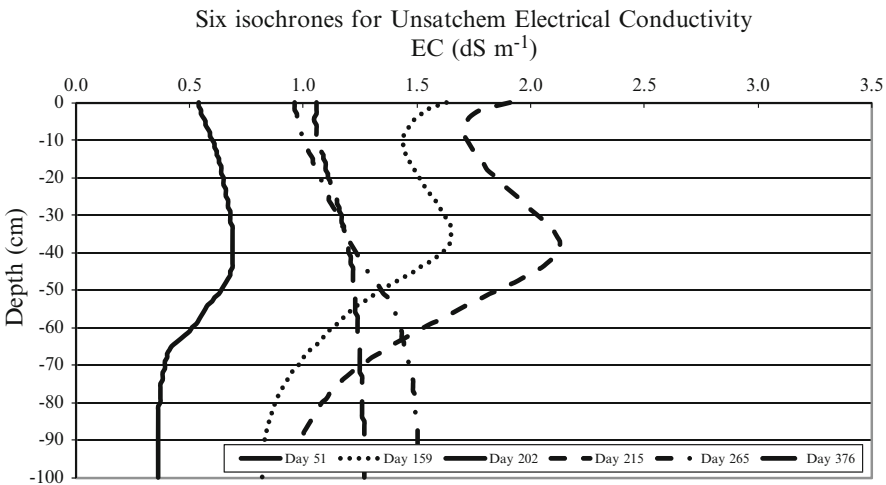


Fig. 2.5 Isochrones for UNSATCHEM. Electrical conductivity

2.5 Conclusions and Recommendations

The versions of both models LEACHC and UNSATCHEM used in this work are unidimensional; hence, heterogeneous fields can affect the results and validation of the models. Bypass flow cannot be represented by the codes used, so even small cracks can lead to divergence in the salts distribution in the upper part of the soil.

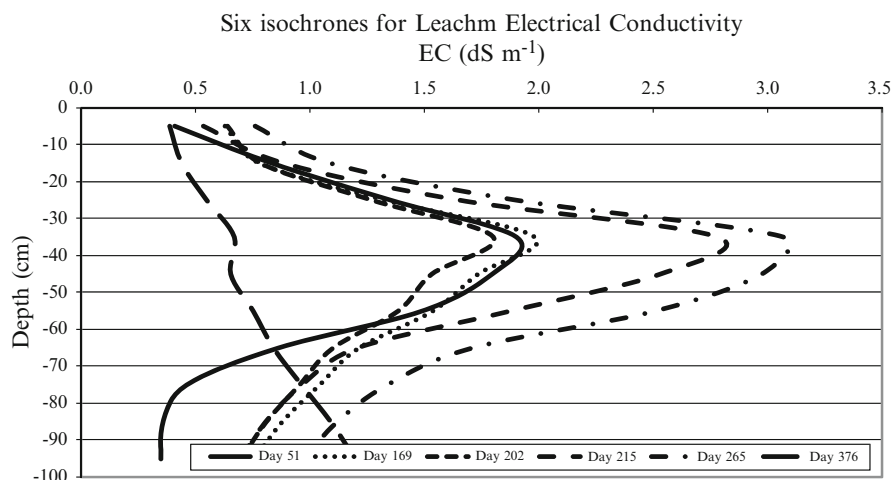


Fig. 2.6 Isochrones for LEACHC. Electrical conductivity

Most models do not consider the case of soils with high portion of soil particles in the coarse fraction (>2 mm), affecting soil hydraulic conductivity computed only on the basis of the textural class. Plant uptake of fertilizers and solutes is not simulated by any of the two models used. Small differences in outputs from both models can be attributed to their different codes, pedotransfer functions used, and capability of dealing with high ionic strength of solutions, although tendencies for both models were congruent with observed data. Results can be used for recommendations about irrigation strategies and management practices, as well as for estimating salt loading of underlying aquifers due to percolation of drainage waters, giving an input for hydrogeological modeling. Models can be used for simulating hypothetical future conditions derived from use of several water types within the composition existing in the area.

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Reclamation

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Resources in Irrigated Agriculture

Shahid, S.A.; Abdelfattah, M.A.; Taha, F.K. (Eds.)

2013, LI, 808 p. 212 illus., 116 illus. in color.,

ISBN: 978-94-007-5684-7