Water Suitability Determination Model Watsuit Help

Introduction

Watsuit calculates the chemical composition of soil water based on the composition of irrigation water and various management practices including: leaching fraction and amendment additions to the water.

The model does not use the depth (or volume) of applied water as an input. Rather it uses leaching fraction, the ratio of the depth of subsurface drainage water divided by the depth of applied water. If one wishes to relate the results to the depth of applied water (AW), it equals crop evapotranspiration (ET), expressed in depth of water, divided by one minus the leaching fraction. In other words, AW = ET/(1-LF).

Because the depth or volume of applied water is not used, the concentrations of ions as well as the amount of precipitated or dissolved salt are expressed as concentrations. Further comments about concentration of salts are given below.

This is a steady state model and assumes a particular leaching fraction remains constant over time. Consequently cation exchange reactions can be and are assumed to be at equilibrium: there is no cation exchange in the model.

The model assumes a 40/30/20/10 water-uptake function through the rootzone. The relative water uptake is assumed to be 40, 30, 20 and 10 % of the total for first (upper), second, third and fourth (bottom) quarters of the rootzone, respectively. The depth of the rootzone is assumed to be constant, but it is not defined.

The user can define the total depth of the rootzone and assume the depth of each quarter of the rootzone is ¼ of the total depth. Or the user can define the depth of each quarter of the rootzone based on the depths at which 40% (bottom of the first quarter), 70 % (bottom of the second quarter), 90% (bottom of the third quarter), and 100% (bottom of the rootzone) of the water uptake has occurred.

The model calculates pH assuming a partial pressure of CO2 in that increases with depth through the soil. At the surface, the PCO2 is set at 0.07 kPa and 0.5, 1.5, 2.3, and 3.0 kPa going from the upper quarter of the rootzone to the last quarter.

Inputs

The chemical composition of the applied water (irrigation water) has to be in meq/L, or mmolc/L (1 mmolc/L = 1 meq/L). If ionic composition data is given in units of mg/L (ppm), then the conversion to mmolc/L requires division of the mg/L by the following numbers:

Ca ²⁺	Mg^{2+}	Na^+	K ⁺	Cl⁻	SO4 ²⁻	CO3 ²⁻	HCO ₃ ⁻	NO_3^-
20.0	12.2	23.0	39.1	35.5	48.0	30	61.0	62.0

The concentrations of the following ions are required: calcium, magnesium, sodium, potassium, chloride, sulfate, and bicarbonate. If the analysis includes carbonate, add its concentration to bicarbonate before entering the bicarbonate concentration. If the analysis includes nitrate, add its concentration to chloride before entering the chloride concentration.

Leaching Fractions

Choose the leaching fractions that interest you. One, any, or all may be chosen.

Saturation With CaCO3

The model allows the user to decide if the soil is calcareous and the irrigation water should be brought up to calcite (lime) saturation. This decision is made at the data-input stage. If the box labeled, "Saturate with $CaCO_3$ " is <u>not</u> checked, calcite – also referred to as lime in the model---is allowed to precipitate if saturation is reached within the soil, but the dissolution does not occur. Precipitation is indicated by positive values in the column marked "lime" in the output file. If the box <u>is</u> checked and the irrigation water is undersaturated with calcite, "lime" dissolves from the surface of the soil, increasing the Ca and HCO₃ concentrations. The column marked "lime" in the output file will have negative numbers.

The units for precipitated or dissolved "lime" are meq/L. How would one convert this to the weight of lime precipitated (positive numbers) or dissolved (negative numbers)? First, remember the comment that the volume, or depth, of applied water is not specified and only leaching fraction is specified. Consequently one cannot convert meq/L of lime into weight of lime without first determining the 'liters' of applied water. Dividing your estimate of crop ET, in units of depth, by one minus the leaching fraction, will result in depth of infiltrated water. Appropriate conversion factors would convert this depth to volume in units of liters per hectare or liters per acre. Multiply this number by meq/l of dissolved or precipitate lime and divide the result by 0.050 g/meq to obtain the grams of precipitated or dissolved calcite. This works for only the first quarter of the rootzone.

For the other quarters of the rootzone, one begins in the same way, but an additional step is required at the end. Namely, one subtracts the grams precipitated at shallower quarters. This is a consequence of the way the compositions are calculated for each depth. That is, the first step for each quarter of the rootzone is to divide the ion concentrations of the irrigation water by the leaching fraction corresponding to the bottom of each quarter.

The leaching fractions at the bottom of each quarter of the rootzone are a function of the overall leaching fraction and the assumed 40/30/20/10 water uptake distribution. Should you

want to calculate these numbers Ayers and Westcot provides an example of how to do this on pages 16 and 17 of their FAO Irrigation and Drainage Paper 29, Rev. 1 entitled Water quality for Agriculture, FAO Rome, 1985.

Calcite saturation is assumed to occur when the ion activity product (Ca x CO_3 activities) exceeds $10^{-8.2}$. Ion activities are calculated using chemical speciation equations, taking into account ion pairing and ionic strength effects.

Gypsum precipitation can also occur if the ion activity product (Ca activity time SO_4 activity) exceeds $10^{-4.6}$. This may occur if the irrigation water is amended with gypsum or the original irrigation water has high concentrations of Ca and SO_4 .

The weight of precipitated gypsum would be calculated the same way as for lime, except that one would divide the result of volume times concentration by 0.086 g/meq instead of 0.050 g/meq.

Water Amendments

The program allows the user to test the effect of adding sulfuric acid and gypsum to the irrigation water. The amendments can be chosen on the data input page. Sulfuric acid is added at a rate to convert 90% of the alkalinity (HCO_3) to sulfate. Gypsum can be added at a rate of 1.0 meq/L A 1.0 meq/L amendment rate simulates a gypsum injector or a top dress of gypsum to the soil.

An amendment rate of 20 meq/L simulates soil-incorporated gypsum. The model will run any and all of the amendment treatments on the same computer run.

<u>Outputs</u>

<u>Data Table</u>

Column	Description					
1	Depth , with 0 being the soil surface, 1 is the bottom of the first quadrant of the rootzone, and 4 is the bottom of the rootzone. The chemical composition at depth 4 is assumed to be drainage water.					
2	Leaching fraction (LF) for each layer. The leaching fraction is defined as the volume of drainage water divided by the total applied water. For the surface layer, the LF is always 1. The LF is given for each of the four rootzone depths.					
3	The concentration factor (1/LF) indicates the multiplier by which the ion concentrations in the original irrigation water is converted to the initial concentration used in the model to calculate the final concentrations corrected for calcite and gypsum precipitation.					
4-10	The chemical composition (meq/L) of the <u>soil water</u> at each depth. Conservative ions not involved in precipitation reactions (Na, K, Cl, and Mg) increase in proportion to the concentrating factor. Calcium, carbonate, bicarbonate, and sulfate may be different due to lime dissolution or precipitation, gypsum precipitation, or amendment addition.					
11	The soil solution pH is calculated from the alkalinity and assumed PCO_2 at each depth.					
12	The Ca/Mg ratio is used to identify possible problems with Ca deficiency. If this ratio is less than 1.0, potential problems with Ca deficiency or magnesium toxicity may occur.					
13	The sum of all the cations in meq/L.					
14	The Electrical Conductivity (dS/m) of the soil water is calculated using a sophisticated set of equations (see McNeal, B.L., J.D. Oster and J. Hatcher. 1970. Calculation of electrical conductivity from solution composition data as an aid to in-situ estimation of soil salinity. Soil Sci. 110:405-414.).					
15	The sodium adsorption ratio (SAR) of the soil water at each depth is calculated from the following equation: SAR = $[Na]/v[(Ca+Mg)/2]$. The SAR is used to predict changes to the physical properties of soils due to excess exchangeable sodium. If the "Saturate with CaCO ₃ " box was checked at input, the SAR of the surface layer is equal to the "Adjusted SAR" as would be calculated using the Suarez method (give reference).					
16-17	The amount of calcite or gypsum that had dissolved or precipitated in the soil. The units are meq/L.					

Summary Table

Column	Description				
1	Leaching fraction treatment.				
2	Average electrical conductivity (EC) of the soil water for the whole rootzone: This is the most important information that the model provides because it can be used to estimate yield reductions based on salinity. Use the following rule of thumb to convert the Ave EC as calculated by watsuit to an average EC that is used with the Mass-Hoffman coefficients. Divide the Avg. EC by 2.				
	Avg. EC divided by 2 often will not equal the EC of the saturation paste extract. However it is the right number to use with the Mass-Hoffman salt tolerance coefficients.				
	The salt tolerance tables for crops, which give salinity threshold values for a decrease in yield, were reported in terms of the EC of the saturation extract (EC sat. ext), averaged over the rootzone (Maas, E.V. and S. R. Grattan, 1999. Crop yields as affected by salinity. 111 – 144. In R. W. Skaggs, and J. van Schilfgaarde, eds. Agricultural Drainage. Agronomy Monograph no. 38. ASA, CSSA, SSSA. Madison Wisconsin.). For example, if Watsuit calculates and Avg. EC. of 3.2 dS/m, the corresponding EC(sat. ext.) for the chloride solutions used to determine crop salt tolerance would have been 1.6 dS/m. Maas and Grattan (1999) provide more details on how to relate EC to the salt tolerance characteristics of many crops.				
3	The average EC of the soil water in the upper profile (layers 1 and 2). Units are dS/m.				
4	The average sodium adsorption ratio (SAR) of the soil water in the root zone. Units are (mmol/L) ^{1/2} .				
5	The average SAR of the soil water in the upper profile. Units are (mmol/L) ^{1/2} .				
6	The average chloride concentration in the rootzone soil water in meq/L. Divide this concentration by 2 to convert to saturation extract CI concentration and identify potential CI toxicity problems based on the Maas tables.				
7	The average chloride concentration in the upper profile. Units are in meq/L.				
8	EC of water in the surface layer of the soil . Use this number in conjunction with Surface SAR to estimate infiltration hazards that the water may pose. (Figure 21 in Ayers, R.S. and D.W. Westcot. 1985. Water quality for agriculture. FAO Irrigation and Drainage Paper 29 rev. 1. FAO Rome. Or, Table 3 in Oster. 1994. Irrigation with poor quality water. Agric. Water Management 24:271-197.)				
15	Surface soil SAR ; use this to predicts problems with crusting. Give guidelines. If Surface EC less than 0.5 dS/m, poor infiltration and crusting problems can occur even when Surface SAR equals zero. When Surface SAR equals 10, Surface EC should be higher than 1 dS/m to prevent problems with infiltration and crusting. At higher SAR's, Surface EC needs to be greater than 0.1 times Surface SAR to prevent problems with infiltration and crusting. These quidelines should be used with care, since infiltration characteristics vary considerably among soils. For further information about (Oster, J.D., I. Shainberg, and I.P. Abrol. 1999. Reclamation of salt-affected soils. P. 659-691. In R.W. Skaggs and J. van Schilfgaarde (ed.) Agricultural drainage. Agron. Monogr. 38. ASA, CSSA, SSSA, Madison, WI.)				

References

Oster, J.D. and J.D. Rhoades. 1990. Steady state root zone salt balance. 410 – 431. In K.K. Tanji ed. Agricultural salinity assessment and management. ASCE Manuals and Reports on Engineering Practice No. 71. ASCE. New York.

Rhoades J.D., A. Kandiah and A.M. Mashali. 1992. The use of saline waters for crop production. FAO Irrigation and drainage paper 48. FAO Rome.