

## TECHNICAL NOTE:

# A SHORT NOTE ON CALCULATING THE ADJUSTED SAR INDEX

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**ABSTRACT.** A simple algebraic technique is presented for computing the adjusted sodium adsorption ratio (SAR) index. The statistical formula presented in this note facilitates the computation of the adjusted SAR without the use of a look-up table, custom computer software, or the need to compute exact individual ion activity coefficients and complexes. A short data analysis example is also presented that demonstrates the application of this technique.

**Keywords.** Adjusted SAR, Salinity, Sodium hazard, Water quality.

The sodium adsorption ratio (SAR) is commonly used as an index for evaluating the sodium hazard associated with an irrigation water supply. The SAR is defined as the square root of the ratio of the sodium (Na) to calcium + magnesium (Ca + Mg), i.e.:

$$\text{SAR} = \frac{\text{Na}}{\sqrt{\text{Ca} + \text{Mg}}} \quad (1a)$$

where all cation measurements are expressed in millimoles per liter (mmol/L). Alternatively, if the cation measurements are expressed in milliequivalents per liter (meq/L), then the SAR is defined to be:

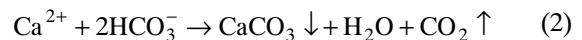
$$\text{SAR} = \frac{\text{Na}}{\sqrt{(\text{Ca} + \text{Mg})/2}} \quad (1b)$$

Irrigation waters having high SAR levels can lead to the build-up of high soil Na levels over time, which in turn can adversely effect soil infiltration and percolation rates (due to soil dispersion). Additionally, excessive SAR levels can lead to soil crusting, poor seedling emergence, and poor aeration.

Measurements of the electrical conductivity ( $\text{EC}_w$ , dS/m) and/or total dissolved solids (TDS, mg/L) also represent commonly used indexes for evaluating the salinity hazard of the irrigation water. Generally, the potential for water infiltration and/or soil dispersion problems can only be adequately addressed when the salinity and SAR indexes are considered together. Increasing  $\text{EC}_w$  levels tend to mitigate negative sodium effects, but can simultaneously induce crop stress (by degrading the quality of the available water for the crop via salinization). Hence, to properly assess the suitability

of a particular irrigation water supply, the apparent salt tolerance of the specific crop must also be taken into consideration.

The standard SAR formulas (eqs. 1a or 1b) represent a suitable sodium hazard index for typical irrigation waters. However, when waters having appreciable concentrations of calcium (Ca) and/or bicarbonates ( $\text{HCO}_3^-$ ) are employed for irrigation, a variable fraction of this constituent will precipitate in the soil as  $\text{CaCO}_3$  according to the equation:



For high calcium and/or bicarbonate waters (primarily groundwater at elevated  $\text{CO}_2$  content), many soil scientists recommend that an adjusted SAR formula be used in place of equations 1a or 1b. Various adjustments have been proposed in the literature (Bower et al., 1968; Rhoades, 1968; Suarez, 1981). The formula derived by Suarez (1981) is generally recognized as the most applicable technique for determining the adjusted SAR hazard index; this formula is currently used by both the United Nations Food and Agricultural Organization (Ayers and Westcot, 1994) and the USDA Natural Resource Conservation Service (NECD, 2005).

An exact calculation of the adjusted SAR can be obtained by making use of the equations given in Suarez (1981) along with the extended Debye-Huckel equation, and/or by use of numerical software such as Extract-Chem or UnSatChem (Suarez and Taber, 2007; Suarez, 2001). Likewise, accurate approximations can be obtained using the formulas and numeric look-up table (table 1) in Suarez (1981). While this latter approach clearly avoids the need for extensive numeric calculations and/or custom software, it is not convenient when more than a few adjusted SAR calculations need to be performed. Ideally, a simple technique that is amenable to spreadsheet calculations would be desirable, particularly when multiple water content samples need to be processed by extension specialists and practitioners.

The objective of this note is to describe and demonstrate a computationally simple technique for calculating the adjusted SAR formula of Suarez (1981) without the use of a look-up table, custom computer software, or the need to compute exact individual ion activity coefficients and complexes. A short data analysis example is also presented that demonstrates the step-by-step application of this computational technique.

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## THE TRADITIONAL (LOOK-UP TABLE) COMPUTATIONAL TECHNIQUE

Suarez (1981) describes how to compute the adjusted SAR ( $SAR_{adj}$ ) via the use of a look-up table. Specifically, on a mmol/L basis, the  $SAR_{adj}$  is defined as:

$$SAR_{adj} = \frac{Na}{\sqrt{Ca_{eq} + Mg}} \quad (3)$$

where  $Ca_{eq}$  represents the expected Ca concentration, after equilibrating with the  $CaCO_3$  solid phase present in the soil. The equilibrated Ca concentration can in turn be calculated as:

$$Ca_{eq} = \left( \frac{\kappa_1 \cdot \kappa_2 \cdot \kappa_3}{\kappa_4 \cdot (HCO_3/Ca)^2 \cdot \gamma_{Ca} \cdot \gamma_{HCO_3}} \right)^{1/3} \times (P_{CO_2})^{1/3} \quad (4)$$

where  $\kappa_1$  through  $\kappa_4$  represent four known chemical equilibrium constants,  $HCO_3$  and Ca represent the bicarbonate and calcium concentrations (in mmol/L) in the irrigation water,  $\gamma_{Ca}$  and  $\gamma_{HCO_3}$  represent the activity coefficients associated with these bicarbonate and calcium concentrations, and  $P_{CO_2}$  represents the partial  $CO_2$  pressure in the near surface soil. Note that this latter value is typically assumed to be 0.0007 atm, but other values can also be employed as appropriate (Suarez, 1981).

The main burden encountered when calculating equation 4 is the computation of the activity coefficients and determining the degree of solution complexation. To minimize this problem, Suarez (1981) rewrote equation 4 as:

$$Ca_{eq} = X \times (P_{CO_2})^{1/3} \quad (5)$$

and then produced a table of  $X$  values for various combinations of  $HCO_3/Ca$  ratios and ionic strength ( $I_S$ ) values. A similar table can be found in Ayers and Westcot (1994), where irrigation water salinity values ( $EC_w$ , dS/m) have been derived from the ionic strength table in Suarez (1981). In practice, the ionic strength term can be adequately estimated from the sum of the Na, Ca, and Mg cations (SC), where the cation concentrations are expressed in meq/L units. Following Bower et al. (1965), one can employ the published U.S. Salinity Laboratory relationship, i.e.:

$$I_S = \frac{(1.3477 \times SC + 0.5355)}{1000} \quad (6)$$

Hence, given the  $HCO_3/Ca$  ratio and the estimated  $I_S$  value, table 1 of Suarez (1981) can be conveniently used to determine the approximate  $X$  value for input into equation 5.

## A NUMERIC FORMULA FOR COMPUTING $X$

The above methodology can be easily employed if/when only a few adjusted SAR calculations are required. However, if a large number of water quality measurements need to be analyzed, then a convenient computational technique for computing  $X$  is desirable. Working directly from equations 4 and 5, note that we can express  $X$  as:

$$X = \left( \frac{\kappa_1 \cdot \kappa_2 \cdot \kappa_3}{\kappa_4 \cdot (HCO_3/Ca)^2 \cdot \gamma_{Ca} \cdot \gamma_{HCO_3}} \right)^{1/3} \quad (7)$$

$$\Rightarrow X^3 = \psi \cdot \left( \frac{Ca}{HCO_3} \right)^2 \cdot \left( \frac{1}{\gamma_{Ca}} \right) \cdot \left( \frac{1}{\gamma_{HCO_3}} \right) \quad (8)$$

for  $\psi = (\kappa_1 \cdot \kappa_2 \cdot \kappa_3) / \kappa_4$

$$\Rightarrow 3 \log(X) = \log(\psi) - \log(\gamma_{Ca}) - \log(\gamma_{HCO_3}) + 2 \log \left( \frac{Ca}{HCO_3} \right) \quad (9)$$

$$\Rightarrow 3 \log(X) \approx \beta_0 + \beta_1 [\log(I_S)] + \beta_2 [\log(I_S)]^2 + 2 \log \left( \frac{Ca}{HCO_3} \right) \quad (10)$$

where ( $\beta_0, \beta_1, \beta_2$ ) represent empirical regression model coefficients. This last step is justified because  $\psi$  represents a fixed constant and we can expect a very precise (abet nonlinear) relationship to exist between the solution ionic strength and the combined values of the two activity coefficients.

Consider the 27  $X$  values reported in table 1 of Suarez (1981) that are associated with  $HCO_3/Ca$  ratios of 0.1, 1.0, and 10.0 and  $I_S$  levels of 0.001, 0.005, 0.01, 0.02, 0.04, 0.07, 0.1, 0.25, and 0.5, respectively. Note that these  $HCO_3/Ca$  ratios and  $I_S$  levels effectively span the entire range of  $X$  values reported by Suarez (1981). Upon defining  $y = 3 \log(X) - 2 \log(Ca/HCO_3)$  and fitting these 27 selected values to a quadratic function of ionic strength values, we obtain an  $R^2$  value of 0.999, a root mean square error estimate of 0.0092, and the following parameter estimates (and standard errors):  $\hat{\beta}_0 = 4.6629$  (0.0063),  $\hat{\beta}_1 = 0.6103$  (0.0087), and  $\hat{\beta}_2 = 0.0844$  (0.0026). In turn, these estimates yield a simple formula for producing extremely precise  $X$  value approximations. Specifically, we find that:

$$\log(X) = \frac{1}{3} \left[ 4.6629 + 0.6103 \log(I_S) + 0.0844 \{ \log(I_S) \}^2 + 2 \log \left( \frac{Ca}{HCO_3} \right) \right] \quad (11)$$

where all log transformations are taken with respect to the base 10 scale and the cation/anion ratio term is expressed in mmol/L units. An example of the approximation accuracy of equation 11 is shown in table 1 for 12 selected  $X$  values. This accuracy is generally as good (or better) than one would obtain when using linear interpolation techniques, and more than sufficient for all practical applications.

**Table 1. Exact versus equation 11 approximated  $X$  values (approximations shown in parentheses).**

Ionic Strength	$HCO_3/Ca$ Ratio (mmol/L basis)		
	0.1	1.0	10.0
0.001	73.4 (73.1)	15.8 (15.8)	3.41 (3.39)
0.010	84.1 (84.5)	18.1 (18.2)	3.90 (3.92)
0.100	112.0 (111.1)	24.1 (23.9)	5.20 (5.16)
0.500	144.0 (145.3)	30.9 (31.3)	6.66 (6.74)

## THE STEP-BY-STEP SPREADSHEET PROCEDURE

Since nearly all commercial laboratories measure and report ion levels in either meq/L or mg/L units, in this section we present the necessary formulas for calculating the adjusted SAR using cation and anion data expressed in meq/L units. These same formulas can also be used for laboratory data expressed in other units, provided that the ion measurements are first converted into meq/L units. Table 2 shows how to change cation and anion measurements reported in mg/L, parts per million (ppm), or mmol/L units into meq/L units using the atomic weight and valence conversion relationships.

The specific computational steps and corresponding formulas that need to be incorporated into the spreadsheet are as follows:

Step 1: If necessary, convert the Na, Ca, Mg, and HCO<sub>3</sub> measurements into meq/L units using the conversion factors shown in table 2.

Step 2: Calculate the sum of cations (SC) and ionic strength (I<sub>S</sub>) as:

$$SC = Na + Ca + Mg$$

$$I_S = \frac{(1.3477 \times SC + 0.5355)}{1000}$$

Step 3: Calculate the log(X) value (using meq/L ion measurements) as:

$$\log(X) = \frac{1}{3} [4.6629 + 0.6103 \log(I_S) + 0.0844 \{ \log(I_S) \}^2 + 2 \log \left( \frac{Ca}{(2HCO_3)} \right)]$$

Step 4: Calculate the equilibrated Ca concentration (on a meq/L unit basis) as:

$$Ca_{eq} = 2 \times 10^{\log(X)} \times (P_{CO_2})^{1/3}$$

**Table 2. Atomic weights, valence numbers, and conversion factors for common ions.**

Ion	Element	Atomic Weight (AW)	Valence (V)
Na <sup>+</sup>	Sodium	22.99	1
Ca <sup>2+</sup>	Calcium	40.08	2
Mg <sup>2+</sup>	Magnesium	24.31	2
Cl <sup>-</sup>	Chloride	35.45	1
SO <sub>4</sub> <sup>2-</sup>	Sulfate	96.06	2
HCO <sub>3</sub> <sup>-</sup>	Bicarbonate	61.02	1

### Conversion Factors

For a Concentration Expressed in:	To Convert to a Concentration Expressed in:	Multiply by:
mg/L (or ppm) <sup>[a]</sup>	meq/L	V / AW
mmol/L	meq/L	V

<sup>[a]</sup> ppm = parts per million; for practical purposes 1 ppm = 1 mg/L in a water sample; thus, these two measurement systems can be taken to be equivalent.

where  $P_{CO_2}$  represents the partial CO<sub>2</sub> pressure in the near surface soil. If this latter value is assumed to be 0.0007 atm, then the equilibrated Ca concentration can be calculated as:

$$Ca_{eq} = 10^{\log(X)} \times 0.17758$$

Step 5: Calculate the adjusted SAR as:

$$SAR_{adj} = \frac{Na}{\sqrt{(Ca_{eq} + Mg)/2}}$$

## A DATA ANALYSIS EXAMPLE

In the following example, we consider an irrigation water quality sample obtained from a municipality treated wastewater plant in Orange County, California (and used to irrigate a private Orange County golf course). Table 3 shows the relevant chemical measurements. Note that the cation and anion measurements were originally reported in mg/L units; these values can be converted to meq/L units using the atomic weight and valence conversion factors shown in table 2. For example, Ca (meq/L) = (2/40.08) × 65.5 = 3.27, etc. The EC<sub>w</sub> level suggests that this water contains insufficient salts to represent a salinity hazard. However, from equation 1b, the ordinary SAR index value is found to be 4.01, suggesting that this water might pose a slight to moderate (unadjusted) sodium hazard.

To determine the adjusted sodium hazard, we can use the step-by-step procedure to calculate the adjusted SAR. In step 2, we find that the sum of cations is SC = 11.90 and thus calculate the ionic strength to be I<sub>S</sub> = 0.01657, (log(I<sub>S</sub>) = -1.78060). In step 3, we first note that the Ca/2HCO<sub>3</sub> ratio is 0.61932 (corresponding log value = -0.208085). Inputting the (log transformed) ionic strength and ratio values into the log(X) equation then yields log(X) = 1.14254 ⇒ 10<sup>log(X)</sup> = 13.885. Using this result along with an assumed  $P_{CO_2}$  value of 0.0007 atm, in step 4 we compute the adjusted (equilibrium) calcium value to be 2.466 meq/L. Finally, in step 5, we calculate the adjusted SAR index to be 4.36. Had we chosen to use the tabular X values in Suarez (1981) and standard linear interpolation techniques, we would have calculated X to be approximately 13.9 and thus derived an identical adjusted SAR index value.

In this example, the adjusted SAR index is found to be about 10% higher than the standard SAR index because the equilibrium calcium concentration is calculated to be about 25% lower than the measured calcium concentration in the treated wastewater sample. Nonetheless, the adjusted sodium hazard would again be classified as slight to moderate. Thus, we would still conclude that this municipality treated wastewater can be used as an irrigation source for the golf course (in terms of its SAR hazard), provided that (1) proper irrigation practices are employed, and (2) the soil(s) receiving this water are not particularly susceptible to developing sodicity-related problems.

**Table 3. Municipality treated wastewater sample, chemical water quality measurements (primary measurements: EC<sub>w</sub> = 1.25 dS/m, pH = 7.0).**

Units	Cations			Anions		
	Na	Ca	Mg	Cl	SO <sub>4</sub>	HCO <sub>3</sub>
mg/L	150.8	65.5	25.2	167.0	235.8	161.1
meq/L	6.56	3.27	2.07	4.71	4.91	2.64

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