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Determination of Leaching Water Norm by Mathematical Modelling in Reclamation of Boron Soils

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Abstract

A considerable part of study area has boron-sodic and saline properties. In this study, in reclamation of boron soils were used water and sulphur (S). Empirical models were used in determining of leach water norm in the reclamation of soils. Analytical expressions of these models are hyperbolic, force, exponential and logarithmic. At the same time, by choosing the most appropriate from these models, will use these models in large-scale leaches. Nine (2 x 2 m) parcels were used to obtain the necessary data to construct these models. Soil samples were taken from the parcels at depths of 0-25, 25-50, 50-75, 75-100 cm and leach water norm models were established with the obtained values. The parcels; sulphur in the amounts of control (S_0), 4 kg (S_1) and 8 kg (S_2) were applied into the soil. Model selection criteria were applied to determine suitability of models. The following values were obtained for each application after the comparison of the eligibility criteria of the obtained models: For S_0; Correlation Index (η) 65.3172, Root Mean Square Error (σ) 0.0547, Agreement Index (D) 0.7698 and Akaike Information Criterion (AICc)- 5.6368 with the power model, S_1; the Logarithmic model with η: 77.8010, σ: 0.0958, D: 0.8655 and AICc: -4.5163 and $S_{2;}$ the Exponential model with η: 71.4723, σ: 0.0688, D: 0.8159 and AICc: -5.1790 reflected the most appropriate of the test data.

Keywords: Boron, Boron soils, Leaching Water Norm, Modelling

INTRODUCTION

In problematic soils, even a very small amount of boron has toxic effects on the plant. For this reason, it is important. The boron concentration ratio in the soil solution is very low in the benefit-damage margin range [1]. Boron soils usually occur in arid and semi-arid regions. For this reason, the boron concentration of the soil solution is high [2] and is quite difficult to control the solubility of boron [3,4]. Boron deficiency is seen frequently in plants grown in sandy soils.This shows that the soil structure is effective in the removal of boron from the soil [5]. Reclamation of boron soils is very difficult. The amount of water used in the reclamation of these soils is 2 or 3 times the amount of water used in the leaching of salted soils. The cost of reclamation of boron soils is high and a process that requires a long time and labour. The shortage and increasing need for water make water more important in the soil reclamation. The calculation of the amount of water and the application time is one of the important problems of the theory of the reclamation of salt- affected soils. Until now, researchers have obtained a large number of leaching formulas and suggested their use. These are simple-logical, empirical (experimental) and theoretical models [6,7]. In this area first as Reeve (1957), (S_i / S_f or EC_i/ EC_f) of the mean salt concentrations before (S_i-EC_i) and after (S_f or EC_f), the quantity of leaching water (N_w or D_w) and soil depths to be leached (D_s or L_s) ratio (D_w or N_w/D_s or L_s) of the relation between the analytical expression is given in the following format (D_w or N_w/D_s or L_s) of the relation between the analytical expression is given in the following format [8]:

$$\frac{EC_f}{EC_i} = f\left(\frac{D_w}{D_s}\right),\ \frac{S_f}{S_i} = f\left(\frac{N_w}{L_s}\right) \qquad \text{or}$$

$$\frac{D_w}{D_s} = f^{-1}\left(\frac{EC_f}{EC_i}\right),\quad \frac{N_w}{L_s} = f^{-1}\left(\frac{S_f}{S_i}\right) \qquad (1)$$

Safoora et al., obtained the following 2 and 3 logarithmic models from the saline soils of the Khuzestan region of Iran [9].

$$y = 0.07 - 0.16ln(x) \qquad (2)$$

$$y = 0.11 - 0.16ln(x) \qquad (3)$$

Bahçeci [10], obtained the following logarithmic equation in the leaching result of salty alkaline soil.

$$D_{lw} = D_s exp\left[\left(-\frac{1}{0.25}\right)\left(\frac{C}{C_0} - 0.76\right)\right] \qquad (4)$$

Reeve at al. as a result of field experiments, obtained the following curve (Figure 1) [11].

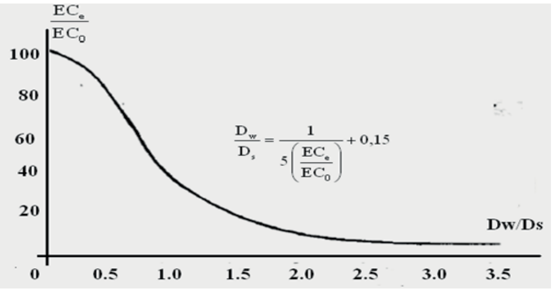

Figure 1. Leaching curve

The purpose of this study is; to find and model the amount of leaching water required to effectively leach the boron in the soil. The result of this modeling is to propose to the most appropriate model selected large-scale reclamation work and to spread it to reclamation efficiency and also to the rational use of water.

MATERIALS AND METHODS

The research was carried out in Aksaray- Center between 38° 32’ northern latitudes 34° 98’ east longitudes in Aksaray University (ASU) campus. The amount of sulphur given to the soil; S_0; Control, S_1 and S_2, respectively applied to the parcels 4 and 8kg sulphur indicates. Some physical and chemical properties of the study soils are given in Table 1.

Table 1. Some physical and chemical properties of study soils

Soil depth (cm)	Volume weight (g. cm^{-3})	Particle density (g. cm^{-3})	Saturation (%)	Field capacity (volume %)	Fading point (volume %)	Soil texture	Saturation extract	
							EC$_e$ (dS. m^{-1})	pH
0-25	1.23	2.60	110.0	62.6	40.0	C	4.10	9.2
25-50	1.25	2.68	140.0	65.0	42.8	C	13.3	8.6
50-75	1.24	2.66	123.3	59.8	40.3	C	5.76	8.4
75-100	1.30	2.54	80.30	42.5	26.9	S- C	4.00	8.0

Table 1 continue

Soil depth (cm)	CEC (me.100g^{-1})	Exchangeable cations(me. 100 g^{-1})				ESP (%)	Organic material (%)	Lime (%)	B$_i$ (mg. l^{-1})
		Na$^+$	K$^+$	Ca^{++}	Mg^{++}				
0-25	23.6	5.0	2.7	12.6	2.7	21.2	2.1	48.0	43.7
25-50	19.9	4.5	1.8	9.9	2.8	22.6	1.5	51.2	24.3
50-75	21.8	2.9	1.1	14.5	2.7	13.5	0.8	52.6	2.2
75-100	20.2	2.5	1.0	13.4	2.7	12.4	0.7	57.3	5.8
Ave.	21.4	3.7	1.7	12.6	2.7	17.4	1.3	52.3	19.0

Some chemical properties of the leach water used in the study are given in Table 2.

Table 2. Some chemical properties of the leaching water used for the leaching of boron soils

pH	EC µmhos. cm^{-1} (25 °C)	Water soluble									
		Anions (me. l^{-1})					Cations (me. l^{-1})				
		CO$^{=}_3$	HCO$^-_3$	Cl$^-$	SO$^{=}_4$	Total	Na$^+$	K$^+$	Ca^{++}	Mg^{++}	Total
6.70	690	-	0.72	4.31	2.39	7.42	1.29	0.40	3.96	1.64	7.29

Table 2 continue

SAR	Na (%)	Irrigation water class	B (mg. l^{-1})
0.77	17.68	C_2S_1	0.87

The study area is shown in Figure 2 and 3.

Figure 2. The study area

Figure 3. The study area surface

The relationship between x and y variables of the amount of leaching water is given below [8,11];

$$x = \frac{D_{lw}}{D_s}, \qquad (5)$$

$$y = \frac{B_f - B_{eq}}{B_i - B_{eq}}, \qquad (6)$$

$$y = f(x) \quad \text{or} \quad \frac{B_f - B_{eq}}{B_i - B_{eq}} = f\left(\frac{D_{lw}}{D_s}\right) \qquad (7)$$

In which; D_{lw} is depth of applied leaching water (cm), D_s is depth of soil (cm), B_i and B_f are the initial and final boron quantity (mg. l^{-1}), B_{eq} is quantity of boron at equilibrium (mg.·l^{-1}).

Models commonly used in all these studies; four mathematical models including power, exponential, hyperbolic and logarithmic functions were applied to the obtained experimental data using the curve estimation method.

These:

Hyperbolic function;

$$y = \frac{a}{x+b}\,, \qquad y = \frac{a}{x} + b \tag{8}$$

Exponential function;

$$y = a.e^{b.(x)} \tag{9}$$

Power function;

$$y = a.(x)^b \tag{10}$$

Logarithmic function;

$$y = a + b.\ln(x) \tag{11}$$

When more than one model is taken into consideration, different statistical criteria can be used depending on the structure of the model in choosing the best model among the models compared [12-16].

The following model selection criteria were used to determine the suitability of these models.

-The sum of squared errors (ESS or SSE) is defined as follows [13]:

$$\boldsymbol{ESS} = \sum_{i=1}^{n} (u_i - \tilde{u}_i)^2 \tag{12}$$

The main goal in modeling is to minimize the value of this parameter.

-The root mean squared error (RMSE) has many names, including the standard error of the estimate, the standard error of regression, the estimated noise standard deviation, and the root mean squared residuals ($\mathrm{RMS}_{\mathrm{residual}}$). This statistical parameter is often used to test the validity of models when several mathematical models are compared [13-16]. The lower limit of the RMSE is 0, which indicates complete agreement between the model estimates and the measurements [17].

$$\boldsymbol{MSE} = \boldsymbol{\sigma} = \begin{cases} \sqrt{\frac{1}{n-np-1}\boldsymbol{ESS}} & if \leq 30 \\ \sqrt{\frac{1}{n-p}\boldsymbol{ESS}} & if \quad n > 30 \end{cases} \tag{13}$$

-The coefficient of determination (R^2) can also be used to quantitatively describe the accuracy of model outputs. It is defined as follows:

$$\boldsymbol{\eta} = \boldsymbol{R^2} = 1 - \frac{\boldsymbol{ESS}}{\boldsymbol{TTS}}$$

$$= 1 - \sum_{i=1}^{n}(u_i - \tilde{u}_i)^2 / \sum_{i=1}^{n}(u_i - \bar{u})^2 \tag{14}$$

The coefficient of determination is a positive value that ranges from 0 to 1, and it is the square of the correlation coefficient.

Clearly, $0 \leq R^2 \leq 1$, and larger R^2 values indicate a better fit of the model to the data. In particular, a model is a perfect fitif $R^2=1$, and this statistic does not account for any variation in y if $R^2=0$ [18].

-To what extent the observed variate is correctly predicted by the simulated variate [19] is reflected by the index of agreement (D), which is given by

$$\boldsymbol{D} = \mathbf{1.0} - \frac{\boldsymbol{ESS}}{\sum_{i=1}^{n}(|u_i - \bar{u}| + |\tilde{u}_i - \bar{u}|)^2} \tag{15}$$

The index D ranges from 0 to 1, where the value 1 indicates perfect agreement with of estimated data, and the value 0 indicates complete disagreement, similar to the interpretation of the coefficient of determination R^2.

-The Akaike information criterion (AIC; Akaike, 1973) is a popular method for comparing the adequacy of simple and multiple linear or nonlinear and nested or non-nested models. The Akaike information criterion is applied to select the best model from among the candidate models considered [20].

This quantity is calculated according to the equations below:

$$\boldsymbol{AIC}_{cor.} = \begin{cases} \boldsymbol{ln}\left(\frac{\boldsymbol{ESS}}{\boldsymbol{n}}\right) + \frac{\boldsymbol{2p}}{\boldsymbol{n}}, & if \ \frac{n}{p} > 40 \\ \boldsymbol{ln}\left(\frac{\boldsymbol{ESS}}{\boldsymbol{n}}\right) + \frac{\boldsymbol{2p}}{\boldsymbol{n-(p+1)}}, & if \ \frac{n}{p} < 40 \end{cases} \tag{16}$$

In equations (12) - (16), the following notation is adopted:

$\boldsymbol{u_i} -$ represents the observed values of the dependent variable,

$\boldsymbol{\tilde{u}_i} -$ represents the estimated values of the dependent variable,

$\boldsymbol{\bar{u}} = \sum_{i=1}^{i=n} \boldsymbol{u_i}/\boldsymbol{n} -$ represents the average of the observed values,

n -represents the number of data points,

p -represents the number of estimable parameters in the approximating model, including the intercept term,

where **p<n**; $\mathbf{R^2}$ represents the coefficient of determination; **RSS**-represents the regression sum of squares and is given by,

$\boldsymbol{RSS} = \sum_{i=1}^{i=n}(\boldsymbol{\tilde{u}_i} - \boldsymbol{\bar{u}})^2 -$ **ESS** represents the sum of squared errors and is given by,

$\boldsymbol{RSS} = \sum_{i=1}^{i=n}(\boldsymbol{u_i} - \boldsymbol{\tilde{u}_i})^2 -$ **MSR** represents the mean square due to regression and is given by,

$\boldsymbol{MSR} = \boldsymbol{RSS}/(P-1) -$ and **MSE** represents the mean squared error and is given by,

$\boldsymbol{MSE} = \boldsymbol{ESS}/(\boldsymbol{n}-\boldsymbol{p})$ $-\mathbf{R^2}$ represents the coefficient of determination.

In our study, the computation of model parameters is carried out using the **Statistica-7** software package.

RESULTS AND DISCUSSION

According to the results of the analysis of the values obtained after leaching, logarithmic, power, exponential and hyperbolic empirical models are obtained by using the variables x and y derived from equations 5 and 6.

The suitability of these mathematical models is determined according to equations (12) - (16) and is shown below according to the amount of sulphur application.

For S_0;

Table 3. Empirical models of x and y parameters and adequacy values

	Functions		**a**	**b**	**η, %**	**σ**	**D**	**AICc**
S_0	**1**	**y=a+blnx**	0.9208	-0.0600	65.2954	0.0547	0.7692	-5.6363
	2	**$y=a.e^{bx}$**	0.9667	0.0394	60.1043	0.0578	0.7197	-5.5288
	3	**$y=a.x^b$**	**0.9198**	**-0.0659**	**65.3172**	**0.0547**	**0.7698**	**-5.6368**
	4	**y=a+b/x**	0.8554	0.0502	61.1010	0.0572	0.7306	-5.5479

In table 3, η; 65.3172, σ; 0.0547, D; 0.7698 and AIC$_c$; -5.6368 force model best reflect the experimental data.

The power model equation is as follows:

$$y = 0.92(x)^{-0,066} \tag{17}$$

In equation 17, If the x and y variables in Equation 5 and 6 are replaced;

$$\left[\frac{B_f - B_{eq}}{B_i - B_{eq}}\right] = 0.92\left(\frac{D_{lw}}{D_s}\right)^{-0.066} \tag{18}$$

$$D_{lw} = D_s\left[0.92\left(\frac{B_i - B_{eq}}{B_f - B_{eq}}\right)\right]^{\frac{1}{0.066}} \tag{19}$$

For S$_1$;

Table 4. Empirical models of x and y parameters and adequacy values

		Functions	**a**	**b**	**η, %**	**σ**	**D**	**AICc**
S$_1$	**1**	**y=a+blnx**	**0.8121**	**-0.1508**	**77.8010**	**0.0958**	**0.8655**	**-4.5163**
	2	**y=a.e^{bx}**	0.9486	0.1286	74.2174	0.1022	0.8435	-4.3870
	3	**y=a.x^b**	0.8045	-0.1908	77.6910	0.0960	0.8649	-4.5119
	4	**y=a+b/x**	0.6462	0.1276	73.5499	0.1033	0.8348	-4.3652

In table 4, η; 77.8010, σ; 0.0958, D; 0.8655 and AIC$_c$; -4.5163 logarithmic model best reflect the experimental data.

The logarithmic model equation is as follows:

$$y = 0.812 - 0.151\ln(\frac{D_{lw}}{D_s}) \tag{20}$$

In equation 20, If the x and y variables in Equation 5 and 6 are replaced;

$$\left[\frac{B_f - B_{eq}}{B_i - B_{eq}}\right] = 0.812 - 0.151\ln(\frac{D_{lw}}{D_s}) \tag{21}$$

$$D_{lw} = D_s exp\left\{\left(-\frac{1}{0.151}\right)\left[\left(\frac{B_f - B_{eq}}{B_i - B_{eq}}\right) - 0.812\right]\right\} \tag{22}$$

For S$_2$;

Table 5. Empirical models of x and y parameters and adequacy values

		Functions	**a**	**b**	**η, %**	**σ**	**D**	**AICc**
S$_2$	**1**	**y=a+blnx**	0.8840	-0.0859	68.7613	0.0714	0.7944	-5.1041
	2	**y=a.e^{bx}**	**0.9623**	**-0.0677**	**71.4723**	**0.0688**	**0.8159**	**-5.1790**
	3	**y=a.x^b**	0.8816	-0.0967	68.0176	0.0721	0.7871	-5.0850
	4	**y=a+b/x**	0.7964	0.0664	59.3235	0.0792	0.7144	-4.8977

In table 5, η;71.4723, σ; 0.0688, D; 0.8159 and AIC$_c$; -5.1790 exponential model best reflect the experimental data. The exponential model equation is as follows

$$y = 0.962\, e^{-0.068\left(\frac{D_{lw}}{D_s}\right)} \tag{23}$$

In equation 23, If the x and y variables in Equation 5 and 6 are replaced;

$$\left[\frac{B_f - B_{eq}}{B_i - B_{eq}}\right] = 0.962e^{-0.068\left(\frac{D_{lw}}{D_s}\right)} \tag{24}$$

$$D_{lw} = -0.558\, D_s + 14.70\, D_s\, ln\left[\frac{B_i - B_{eq}}{B_f - B_{eq}}\right] \tag{25}$$

It is obtained.

DISCUSSION

In the research, 0-50 cm soil profile of the soil is heavily clayed boron in this layer is caused by stronger adsorption, therefore the effectiveness of leaching has been reduced. In all three sulphur applications, it was seen that force, logarithmic and exponential models define leaching data better than others.

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