Simulation and Prediction of Ion Transport in the Reclamation of Sodic Soils with Gypsum Based on the Support Vector Machine

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The effect of gypsum on the physical and chemical characteristics of sodic soils is nonlinear and controlled by multiple factors. The support vector machine (SVM) is able to solve practical problems such as small samples, nonlinearity, high dimensions, and local minima points. This paper reports the use of the SVM regression method to predict changes in the chemical properties of sodic soils under different gypsum application rates in a soil column experiment and to evaluate the effect of gypsum reclamation on sodic soils. The research results show that (1) the SVM soil solute transport model using the Matlab toolbox represents the change in Ca2+ and Na+ in the soil solution and leachate well, with a high prediction accuracy. (2) Using the SVM model to predict the spatial and temporal variations in the soil solute content is feasible and does not require a specific mathematical model. The SVM model can take full advantage of the distribution characteristics of the training sample. (3) The workload of the soil solute transport prediction model based on the SVM is greatly reduced by not having to determine the hydrodynamic dispersion coefficient and retardation coefficient, and the model is thus highly practical.

1. Introduction

The support vector machine (SVM) method was developed based on the Vapnik statistical learning theory and in particular the statistical Vapnik-Chervonenkis Dimension theory and the Structural Risk Minimization Inductive Principle [1]. The basic principle of SVM is to solve the classification problem. Its guiding ideology is to map nonlinear separable sample data to a higher dimensional linear separable space through a kernel function and then to solve the partition hyperplane using an optimization method to determine the parameters of the decision-making function and minimize its structural risk [2]. Theory and practice have proved that the SVM can solve the practical problems of a small sample, nonlinearity, high dimensionality, and local minima points and has good generalizability [3]. The SVM has become a hot topic in machine learning research and has been successfully applied in pattern recognition, data mining, regression, and approximation [4–6]. In the field of agriculture, the problem of reclaiming sodic soils has attracted much attention. Many studies have proved that the effect of the desulfurization byproducts used in the reclamation process on the physical and chemical properties of soil is nonlinear and multifactorial [6–11]. Šimůnek et al. constructed a multicomponent solute transport model of sodic soil reclamation and predicted the solute transport by using the UNSATCHEM and HYDRUS models [12–14]. However, the models use the major ion chemistry module, which have a relatively complex code and require a large number of input parameters that are not always readily available [15–17]. The SVM regression method
is applied here to overcome these issues and determine the variation in the chemical properties of sodic soils with reclaimed time and different application levels of a flue gas desulfurization byproduct (or gypsum) and to evaluate the effect on sodic soils of reclamation with gypsum.

2. Materials and Methods

2.1. Physical and Chemical Properties of Soils and CaSO₄

The soil was sampled from the Changsheng Experimental Station of the Bayannur League Institute of Water Resources in the northwest of China. The soil had typical sodic soil characteristics, that is, a high pH and exchangeable sodium percentage and low hydraulic conductivity. The soil texture was clay and its physical and chemical properties are listed in Table 1. The soil was air-dried, crushed, and passed through a 2 mm sieve before the experiments. The pure CaSO₄ (molecular weight 136) was purchased from the Tianjin Wendaxigui Chemical Reagent Factory.

2.2. Ca²⁺ Penetration Experiment. The experimental device (Figure 1) was a 25-cm-high Plexiglass column with a 5 cm inside diameter (the soil height was 10 cm), and a Mariotte bottle was used to supply the water. The experiment consisted of four treatments (Table 2) with different CaSO₄ rates (0.5, 1, 1.5, and 2 g L⁻¹). The pure CaSO₄ was selected as the reagent and distilled water was used as the solvent to configure the solution.

The experimental procedure was as follows. The tested soil samples were poured homogeneously into the Plexiglass column at a dry soil bulk density of 1.45 g cm⁻³ to a depth of 10 cm. The soil columns were saturated with distilled water from the bottom up at a saturation rate of 2 cm per hour. Once the soils were saturated, the surface water was quickly drained with a vacuum pump and the Ca²⁺ solution that exists among the optimal solutions in (1):}

\[ \min_{\mathbf{w}, b, \varepsilon} \frac{1}{2} \| \mathbf{w} \|^2, \]

s.t. \( y_i ((\mathbf{w} \cdot \mathbf{x}_i) + b) \geq 1, \quad i = 1, \ldots, l \).

This is the decision-making function \( f(x) = \text{sgn}((\mathbf{w}^* \cdot \mathbf{x}) + b^*) \).

Equation (1) can be transformed into the dual problem on duality theory [6]:

\[ \min_{\alpha} \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} y_i y_j \alpha_i \alpha_j (\mathbf{x}_i \cdot \mathbf{x}_j) - \sum_{i=1}^{l} \alpha_i, \]

s.t. \( \sum_{i=1}^{l} y_i \alpha_i = 0, \quad \alpha_i \geq 0, \quad i = 1, \ldots, l \),

where \( \alpha_i \) is a Lagrange multiplier. The following relationship exists among the optimal solutions \( \alpha^* \) in (2) and \( \mathbf{w}^* \) and \( b^* \) in (1):

\[ \mathbf{w}^* = \sum_{i=1}^{l} \alpha_i^* y_i \mathbf{x}_i, \]

\[ b^* = y_j - \sum_{i=1}^{l} \alpha_i^* (\mathbf{x}_i \cdot \mathbf{x}_j). \]

Consider the following linear regression problem.

The regression hyperplane \( y = (\mathbf{w} \cdot \mathbf{x}) + b \) is obtained for the sample set \( T = \{ (x_i, y_i), \ldots, (x_j, y_j) \}, x_i \in \mathbb{R}^n, y_i \in \mathbb{R}, \quad i = 1, \ldots, l \). Intuitively, the difference between the hyperplane value at \( x_i \) and the actual input \( y_i \) value should be as small as possible. A parameter \( \varepsilon > 0 \) is introduced which requires

\[ \min_{\mathbf{w}, \mathbf{b}, \varepsilon} \varepsilon \]

s.t. \( -\varepsilon \leq y_i - ((\mathbf{w} \cdot \mathbf{x}_i) + b) \leq \varepsilon, \quad i = 1, \ldots, l \).

Equation (4) now needs to be converted into a classification problem. It can be envisaged that all of the sample points in the sample set \( T \) are, respectively, moved up and moved down \( \varepsilon \) along the \( y_i \) direction, so that the sample set \( T^+ = \{ (x_i, y_i + \varepsilon) \mid i = 1, \ldots, l \} \) obtained after
Figure 1: Experimental device of Ca\(^{2+}\) penetration.

Table 1: Physical and chemical properties of the soil.

|                | Exchangeable cations/cmol\cdot kg\(^{-1}\) | Soil bulk Density/g cm\(^{-3}\) | pH\(_{1.5}\) |
|----------------|------------------------------------------|---------------------------------|-------------|
| Na\(^+\)       | 8.65                                     | 11.02                           | 9.15        |
| K\(^+\)        | 0.60                                     | 1.45                            |             |
| Ca\(^{2+}\)    | 0.50                                     |                                 |             |
| Mg\(^{2+}\)    | 1.27                                     |                                 |             |
| CEC            | 11.02                                    |                                 |             |
| pH\(_{1.5}\)   | 9.15                                     |                                 |             |

Table 2: Experimental treatments of Ca\(^{2+}\) penetration.

| Experimental treatments | T1 | T2 | T3 | T4 |
|-------------------------|----|----|----|----|
| Concentration of CaSO\(_4\)/g L\(^{-1}\) | 0.5 | 1.0 | 1.5 | 2.0 |
| Concentration of Ca\(^{2+}\)/mmol L\(^{-1}\) | 7.35 | 14.71 | 22.06 | 29.41 |

The upward movement is above the regression hyperplane (positive class) and the sample set \(T^- = \{ (x_i, y_i - \varepsilon) | i = 1, \ldots, l \} \) obtained after the downward movement is below the regression hyperplane (negative class point). The regression hyperplane is thus transformed into a partition hyperplane, and the regression problem is converted into a classification problem.

This problem can be solved by modifying (1):

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + \frac{1}{2} \eta^2,
\]

s.t. \(z_i ((w \cdot x_i) + (y_i + z_i \varepsilon) + b) \geq 1, \quad i = 1, \ldots, 2l,\)

where \(\eta\) is the weight vector corresponding to the \(y\) component of the sample points:

\[
z_i = \begin{cases} 
1, & i = 1, \ldots, l; \\
-1, & i = l + 1, \ldots, 2l.
\end{cases}
\]

The partition hyperplane \((w^* \cdot x) + \eta^* y + b^* = 0\) can be obtained according to the optimal solution \((w^*, \eta^*, b^*)\) to (5), which corresponds to the regression function \(y = (w \cdot x) + b\), where \(w = -w^*/\eta^*\) and \(b = -b^*/\eta^*\).

Letting \(\varepsilon^* = \varepsilon - 1/\eta^*\), (5) is then equivalent to the following:

\[
\min_{w, b} \frac{1}{2} \|w\|^2,
\]

s.t. \((w \cdot x_i) + b - y_i \leq \varepsilon^*, \quad i = 1, \ldots, l,\)

\(y_i - (w \cdot x_i) - b \leq \varepsilon^*, \quad i = 1, \ldots, l.\)
The algorithm is further improved by allowing fitting error through the introduction of slack variables \( \xi \) and a penalty parameter \( C \), which modifies (5) as follows:

\[
\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + \frac{1}{2} \eta^2 + \frac{C}{l} \sum_{i=1}^{l} \xi_i,
\]

\[
\text{s.t.} \quad z_i \left( (w \cdot x_i) + \eta (y_i + z_i) x + b \right) + \xi_i \geq 1, \quad i = 1, \ldots, 2l,
\]

\[
\xi_i \geq 0, \quad i = 1, \ldots, 2l.
\]

Provided that the optimal solution to (8) is \((w^*, \eta^*, b^*, \xi^*)\), then \( \varepsilon = \varepsilon - 1/\eta^* \) and (8) is equivalent to

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + \frac{C}{l} \sum_{i=1}^{l} \xi_i + \xi_i^*,
\]

\[
\text{s.t.} \quad (w \cdot x_i) + b - y_i \leq \varepsilon^* + \xi_i^*, \quad i = 1, \ldots, l,
\]

\[
y_i - (w \cdot x_i) - b \leq \varepsilon^* + \xi_i^*, \quad i = 1, \ldots, l,
\]

\[
\xi_i, \xi_i^* \geq 0, \quad i = 1, \ldots, l.
\]

In the objective function of (9), minimizing \((1/2)\|w\|^2\) renders the regression function flat and increases the generalizability. \((C/l) \sum_{i=1}^{l} (\xi + \xi^*)\) is the total error of the regression function and should be minimized.

Setting the solution to (9) as \((\overline{w}, \overline{b})\), the regression function is then

\[
y = (\overline{w} \cdot x) + \overline{b}, \quad \overline{w} = -\frac{w^*}{\eta^*}, \quad \overline{b} = -\frac{b^*}{\eta^*}.
\]

The dual problem is then written as follows:

\[
\min_{\alpha} \frac{1}{2} \sum_{i,j=1}^{l} \left( \alpha_i^* - \alpha_j^* \right) \left( x_i \cdot x_j \right)
\]

\[
+ \varepsilon^* \sum_{i=1}^{l} \left( \alpha_i^* + \alpha_i \right) - \sum_{i=1}^{l} y_i \left( \alpha_i^* - \alpha_i \right),
\]

\[
\text{s.t.} \quad \sum_{i=1}^{l} \left( \alpha_i^* - \alpha_i \right) = 0,
\]

\[
0 \leq \alpha_i, \alpha_i^* \leq \frac{C}{l}, \quad i = 1, \ldots, l.
\]

The solution to (11) is derived as \( \overline{\alpha} = (\overline{\alpha}_1, \overline{\alpha}_1^*, \ldots, \overline{\alpha}_l, \overline{\alpha}_l^*)^T \).

In general, the solutions to (9) and (11) have the following relationship:

\[
\overline{w} = \sum_{i=1}^{l} \left( \overline{\alpha}^*_i - \overline{\alpha}_i \right) x_i,
\]

\[
\overline{b} = y_j - \sum_{i=1}^{l} \left( \overline{\alpha}^*_i - \overline{\alpha}_i \right) (x_i \cdot x_j) \pm \varepsilon^*,
\]

where \( j \) is the sample index of the corresponding multiplier \( \overline{\alpha} \neq 0 \) (when it is positive) or the sample index of corresponding multiplier \( \overline{\alpha}^* = 0 \) (when it is negative).

As \( \varepsilon^* \) is a constant that is known in advance in the actual process, simplifying \( \varepsilon^* \) will not have any effect in (9), (11), and (12), and after this replacement the linear SVM machine of the insensitive loss function can be obtained.

For a wide range of nonlinear problems, the SVM maps samples to the high-dimensional Hilbert space by skillfully using nuclear transform methods and processing using linear methods. If the mapping is \( \Phi : x \rightarrow \varphi(x) \), then it can be seen that (11) and (12) are only relevant to the inner product (dot product) of the sample points. Given this characteristic, the actual mapping function \( \Phi \) need not be known: only the functional relationship of the sample points in the original space in the dot product of the high-dimensional space after mapping needs to be determined, which is represented by the fact that \( K(x_i, x_j) = (\varphi(x_i) \cdot \varphi(x_j)) \).\( K(x_i, x_j) \) is a kernel function. The Gauss radial basis kernel, polynomial kernel, B-spline kernel, Fourier kernel, and Sigmoid kernel are commonly used kernel functions.

The complete algorithm of the SVM for dealing with nonlinear regression problems is as follows.

1. Select parameters \( \varepsilon \) and \( C \) and the appropriate kernel \( K(x_i, x_j) \).

2. Construct the following optimization problem:

\[
\min_{\alpha} \frac{1}{2} \sum_{i,j=1}^{l} \left( \alpha_i^* - \alpha_j \right) \left( x_i \cdot x_j \right)
\]

\[
+ \varepsilon \sum_{i=1}^{l} \left( \alpha_i^* + \alpha_i \right) - \sum_{i=1}^{l} y_i \left( \alpha_i^* - \alpha_i \right),
\]

\[
\text{s.t.} \quad \sum_{i=1}^{l} \left( \alpha_i^* - \alpha_i \right) = 0,
\]

\[
0 \leq \alpha_i, \alpha_i^* \leq \frac{C}{l}, \quad i = 1, \ldots, l.
\]

Find the optimal solution \( \overline{\alpha} = \left( \overline{\alpha}_1, \overline{\alpha}_1^*, \ldots, \overline{\alpha}_l, \overline{\alpha}_l^* \right)^T \).

3. Construct the decision function

\[
f(x) = \sum_{i=1}^{l} \left( \overline{\alpha}_i^* - \overline{\alpha}_i \right) K(x_i \cdot x) + \overline{b},
\]

where \( \overline{b} = y_j - \sum_{i=1}^{l} \left( \overline{\alpha}_i^* - \overline{\alpha}_i \right) (x_i \cdot x_j) \pm \varepsilon^* \); the positive sign is selected when \( \overline{\alpha}_j \neq 0 \), and the negative sign is selected when \( \overline{\alpha}_j^* \neq 0 \).

2.5. Construction of the SVM Regulation Model. The SVM method is applied to predict the reclamation effect of a desulfurization byproduct (gypsum) on sodic soils. The main factors influencing the reclamation process must first be determined, and then the sample datasets of observations are
selected for training the SVM. Predictions can then be made according to the parameters obtained from the training.

**Conclusion of the Factors of Influence.** The reclamation of sodic soils with desulfurization byproducts is a multi-ion transportation and transformation process that is accompanied by ion exchange-adsorption and precipitation-dissolution reactions. Under one-dimensional vertical infiltration conditions, the factors that affect the soil solute transport include transport time, transport distance, soil texture, soil bulk density, soil moisture, ion concentration in the soil solution, ion concentration in the supply solution, and ion concentration in the solid exchange phase. When the ion concentration in the soil solution, ion concentration in the solid exchange phase, soil texture, soil bulk density, and soil texture are definite, the ion concentration in the supply solution, transport time, and transport distance can be used as the basis for predicting the soil solute transport. After determining the soil solution concentration in multiple profiles in a one-dimensional vertical transport experiment and training the model in terms of the transport time, transport distance, and corresponding soil solute content, the soil solute transport SVM control model can be established to simulate the spatial and temporal variations of the soil solute transport.

**Construction of the Sample Dataset.** To eliminate the effect of each factor caused by differences in dimension and units, the input and output parameters of the sample are normalized using the following equation:

\[
y_i = 2 \left( \frac{z_i - z_{\min}}{z_{\max} - z_{\min}} \right) - 1,
\]

where \(z_i\) and \(y_i\) are the variables before and after normalization, respectively, and \(z_{\min}\) and \(z_{\max}\) are the maximum and minimum values, respectively, of the sample data \(z\).

**Learning and Training the SVM.** The Matlab SVM toolbox is used to build and train the model. The main steps in this process include inputting the input and output parameter files, selecting the kernel function and kernel parameter, and data training and testing.

### 3. Results

#### 3.1. \(Ca^{2+}\) and \(Na^+\) Concentration in the Leachate.

The measured values for the \(Ca^{2+}\) concentrations in the leachate are shown in Figure 2. When the \(Ca^{2+}\) concentrations in the supply water were 14.71, 22.06, and 29.41 mmol·L\(^{-1}\), \(Ca^{2+}\) penetration was realized. When the \(Ca^{2+}\) concentration in
the supply water was higher, Ca$^{2+}$ penetration was faster. Ca$^{2+}$ did not penetrate when the Ca$^{2+}$ concentration was 7.35 mmol·L$^{-1}$. In the initial stage, because the soil solution itself contained a certain amount of soluble Ca$^{2+}$, the Ca$^{2+}$ in the supply water first reacted with the sodic salts and exchangeable Na$^{+}$ in the soil colloid in the top soil. Before the Ca$^{2+}$ reached the bottom of the soil column, the Ca$^{2+}$ in the soil solution was constantly leached from the soil column and the Ca$^{2+}$ concentration in the leachate gradually decreased. However, as the Ca$^{2+}$ gradually reached the bottom of the soil column, the Ca$^{2+}$ concentration in the leachate gradually increased until it reached the Ca$^{2+}$ concentration in the supply water, at which point it stabilized and realized penetration.

The measured values for the Na$^{+}$ concentrations in the leachate are shown in Figure 3. Because there was no Na$^{+}$ in the supply water, the Na$^{+}$ concentration in the leachate gradually decreased. Under higher leachate concentrations, the decrease in Na$^{+}$ was faster due to the increase in the soil’s hydraulic conductivity capacity.

3.2. Prediction of the Ca$^{2+}$ Concentration in a Penetration Experiment. An SVM model of the variations in Ca$^{2+}$ concentration in sodic soils in a penetration test was constructed and used for data prediction. The training process and analytical results are as follows.

The measured Ca$^{2+}$ concentrations of the soil leachate from 0 h to 480 h in 0.5 g·L$^{-1}$, 1.0 g·L$^{-1}$, and 2.0 g·L$^{-1}$ treatments of gypsum and from 240 h to 480 h in a 1.5 g·L$^{-1}$ treatment of gypsum were used as the input data. The measured
3.3. Prediction of the \( \text{Na}^+ \) Concentration in a Penetration Experiment. The measured \( \text{Na}^+ \) concentrations of the soil leachate from 0 h to 480 h in 0.5 g L\(^{-1}\), 1.0 g L\(^{-1}\), and 2.0 g L\(^{-1}\) treatments of gypsum and from 240 h to 480 h in a 1.5 g L\(^{-1}\) treatment of gypsum were used as the input data. The measured \( \text{Na}^+ \) concentrations of the leachate from 0 h to 240 h in a 1.5 g L\(^{-1}\) gypsum treatment were used as the inspection data. The data were normalized, and the prediction model based on the SVM was constructed in Matlab with the following parameters: kernel function rbf (shaped as in (16)), \( \delta = 1.0 \), \( C = 100 \), and \( \varepsilon = 0.001 \).

The SVM model was applied to predict the data. The prediction results and measured data are shown in Figure 6. The results of a regression analysis of the measured data and prediction data are shown in Figure 7. The results show the measured data and prediction data to be strongly correlated. Clearly, the SVM model is able to correctly represent the changes in the \( \text{Na}^+ \) concentration of the soil leachate in the reclamation process.

4. Discussion

4.1. Validation of the SVM Model. The SVM method is a type of lumped parameter prediction method and has broad applicability in determining small changes in a parameter system [11, 18]. In situations where there is a lack of experimental data and system structure, such models are often able to make acceptable simulations and predictions of ion concentrations [6]. This study introduces the SVM to the complex ion change process that occurs during the application of desulfurization byproducts such as gypsum to improve sodic soils and achieves good prediction and simulation results. In addition to the visual check, measured values of \( \text{Ca}^{2+} \) and \( \text{Na}^+ \) were compared with the results of SVM model prediction using the mean absolute error and the root mean square error. The mean absolute error (MAE) given by [19]

\[
MAE = \frac{1}{n} \sum_{i=1}^{n} |X_{mi} - X_{si}|
\]

The SVM model was applied to predict the data. The prediction results and measured data are shown in Figure 4. The results of a regression analysis of the measured data and prediction data are shown in Figure 5. The results show the measured data and prediction data to be strongly correlated. Clearly, the SVM model is able to correctly represent the changes in the \( \text{Ca}^{2+} \) concentration of the soil leachate in the reclamation process.
The Support vector machine (SVM) finds the discriminant function according to the training sample, distribution characteristics of the training sample, constructs a discriminant function unlike SVMs which use a first order insensitivity loss function as a fitness measure [6]. ANN method is more like an art and needs significant skill to obtain a relatively satisfactory result [21, 22]. ANN predictions are not stable and depend on the averages from various network initializations, which may yield a different result each time a model is trained. Converting the SVM algorithm into a quadratic optimization problem should in theory result in a globally optimal solution being obtained [18]. This effectively prevents the local minima problem that neural networks easily fall into, cleverly solves high-dimensional problems by nonlinear transforms and nuclear functions, makes the complexity of the algorithm independent of the sample dimension, and speeds up the training and learning. By contrast, the SVM results are stable and unique. Table 3 shows the results of the comparison between the SVM and ANN methods based on simulated and predicted data. The RMSE using the SVM method was 0.27 mmol L⁻¹ and 15.91 mmol L⁻¹ for Ca²⁺ and Na⁺, respectively, but those of ANN were 0.52 mmol L⁻¹ and 26.15 mmol L⁻¹, indicating that SVM predicted better results than ANN. The maximum error, minimum error, and average error of the SVM results are smaller than those of the ANN [19]. Therefore, the SVM method has better capability to predict ion transport in sodic soils reclaimed by CaSO₄.

### 5. Conclusion

The simulation and prediction model of solute transport was constructed using Matlab toolbox based on nonlinear SVM theory, and the transport and transformation law of Ca²⁺ and Na⁺ in Ca²⁺ penetration process was carried out to simulate and predict. The following conclusions can be drawn from our findings.

1. The change of Ca²⁺ and Na⁺ in leachate can be reflected by SVM soil solute transport model by using Matlab toolbox, and the prediction accuracy is high.

2. Using SVM model to predict the spatial and temporal variations of soil solute content is feasible, and it does not require a specific mathematical model. SVM model can take full advantage of the distribution characteristics of training samples and does not require too much of a priori information and use skills.

3. The workload of soil solute transport prediction model based on SVM was greatly reduced without determination of the hydrodynamic dispersion coefficient and retardation coefficient, and the SVM model has a strong practicality.

### Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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