

Research Article

A Study on a Salt Solution Concentration Prediction Method Based on CNN-LSTM-Attention

Ziyang Pei¹ , Jianfeng Zhao¹, Ningfeng Wang^{2,*}

¹College of Mechanical Engineering, Qinghai University, Xining, China

²College of Chemical Engineering, Qinghai University, Xining, China

Abstract

The rapid and accurate analysis of ion concentrations in mixed salt solutions is a critical aspect of utilizing salt lake chemical resources. To explore an efficient and non-destructive detection method, this study proposes a deep learning model that fuses a Convolutional Neural Network (CNN), a Long Short-Term Memory (LSTM) network, and an Attention mechanism for the prediction of salt solution concentrations using Near-Infrared Spectroscopy (NIRS). First, single-component and two-component mixed salt solution samples of NaCl, KCl, and MgCl₂ were prepared, and their near-infrared spectral data were collected. After applying Savitzky-Golay smoothing and derivative preprocessing to the spectra, a CNN-LSTM-Attention prediction model was constructed. A comparative analysis was conducted against common models such as Partial Least Squares Regression (PLSR), Support Vector Regression (SVR), and Random Forest (RF), and an ablation study was performed to analyze the contribution of each deep learning module. The results show that for single-component salt solutions, the proposed model's performance is comparable to that of the high-performing SVR and RF models. In complex mixed solutions with severe spectral overlap, the CNN-LSTM-Attention model demonstrated significant superiority, with its prediction accuracy surpassing all traditional baseline models across all mixed datasets, achieving a coefficient of determination (R^2) as high as 0.973. The study concludes that the proposed CNN-LSTM-Attention model can effectively address the challenge of spectral overlap, demonstrating the potential of using deep learning for the quantitative analysis of complex mixture systems via near-infrared spectroscopy.

Keywords

Near-Infrared Spectroscopy, Ion Concentration Prediction, Convolutional Neural Network, Long Short-Term Memory Network, Attention Mechanism, Spectral Analysis Introduction

1. Introduction

The rapid and accurate analysis of ion concentrations in mixed salt solutions is a critical aspect of utilizing salt lake chemical resources. Traditional chemical analysis methods (e.g., titration, ion chromatography), despite their high accuracy, have drawbacks such as being destructive to the sample, having cumbersome procedures, and being time-consuming,

making them unsuitable for real-time, on-site detection needs. Near-Infrared Spectroscopy (NIRS) technology, as a green, non-destructive, and efficient analytical tool, has developed rapidly in recent years. This technology, based on the absorption of near-infrared light by molecular vibrations, can capture information about a substance's composition and

*Corresponding author: 1999990009@qhu.edu.cn (Ningfeng Wang)

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structure and has been widely applied in fields such as food quality monitoring, drug component identification, agricultural testing, and chemical analysis [1-4]. Therefore, indirect detection can be achieved by establishing a quantitative calibration model between spectra and concentration.

However, NIR spectral data are characterized by high dimensionality, high redundancy, and non-linearity, and the absorption peaks of various ions overlap severely, causing serious collinearity issues [5]. Traditional multivariate calibration methods, such as Principal Component Regression (PCR) and Partial Least Squares Regression (PLSR), are widely used but are essentially linear models with limited ability to resolve non-linear relationships in complex systems. Although machine learning methods like Support Vector Regression (SVR) and Random Forest (RF) can capture some non-linear relationships, they still have deficiencies in feature extraction and modeling sequential dependencies [6].

Deep learning technology offers a new approach to solving this problem with its powerful capabilities for automatic feature extraction and modeling complex non-linear relationships. Convolutional Neural Networks (CNNs) are suitable for extracting local features from high-dimensional spectral data. Long Short-Term Memory (LSTM) networks, with their internal "memory" mechanism and gate structures, can capture sequential dependencies in spectral data, thereby learning holistic, order-related features from the entire spectral sequence [7]. The Attention mechanism can adaptively assign higher weights to key wavelength regions most relevant to the target ions, improving the model's interpretability and accuracy. Scholars both domestically and internationally have begun to explore the application of deep learning in spectral analysis. For instance, Acquarelli et al [8], developed a shallow CNN model that achieved an average accuracy of 86% on public spectral datasets, significantly outperforming the PLS method and demonstrating the potential of CNNs in NIRS classification tasks. He T et al [9], proposed a CNN-LSTM model for the quantitative detection of seven components in traditional Chinese medicine, and the results showed that the evaluation coefficients for different components based on the CNN-LSTM model were optimal. Zhang J et al [10], used a CNN-LSTM model to invert soil salinity in an oasis in an arid region, achieving accurate monitoring of soil salinity at multiple depths.

Despite these advances, most existing work focuses on solid or powder samples, or single ions. For complex mixed solution systems, especially for the detection of multiple ion

concentrations, there is still room for improvement in the accuracy and robustness of current methods. Based on this, this paper proposes a CNN-LSTM-Attention hybrid model, aiming to achieve high-precision prediction of ion concentrations in both single and mixed salt solutions by synergistically leveraging the advantages of the three components. By constructing a CNN-LSTM hybrid model, a deep analysis of NIR spectral features from local to global is achieved. Introducing an attention mechanism into the model enhances its ability to assess the importance of key spectral features, making the model more interpretable. This paper aims to study the effectiveness of this model on single and mixed salt solution datasets and to verify the feasibility of deep learning for the NIRS quantitative analysis of salt solutions.

2. Materials and Methods

2.1. Materials

2.1.1. Sample Preparation

Based on the main ion components found in salt lake brines, three salt solutions—NaCl, KCl, and MgCl_2 —were selected for the study. First, stock solutions of 5 mol/L NaCl, 4 mol/L KCl, and 4 mol/L MgCl_2 were prepared. Subsequently, solution samples of different concentrations were obtained by dilution. Then, by simulating salt lake brine, two-component mixed solution samples were prepared by mixing the solutions pairwise.

2.1.2. Spectral Data Acquisition

An Antaris II Fourier Transform Near-Infrared Spectrometer (Thermo Fisher Scientific) was used to scan the prepared samples. The spectral scanning wavelength range was 4000–11000 cm^{-1} , with 32 scans per sample, a resolution of 8.0 cm^{-1} , and an optimized gain of 4x. Each sample was scanned three times, and the average spectrum was used as the original spectrum for analysis. The wavelength range of 5000–7500 cm^{-1} from each original spectrum was used for subsequent operations. The variable ranges for the chloride salt solutions and the final number of spectral data obtained are shown in Table 1. The total concentration of the two-component mixed chloride salt solutions was 5%; the concentration listed in Table 1 for the mixed solutions is the concentration of the first chloride salt added.

Table 1. Variable Ranges and Number of Spectral Data for Each Chloride Salt Solution.

Types of salt solution	Concentration (mol/L)	Number of samples
NaCl	0.2~5	200
KCl	0.1~4	242

Types of salt solution	Concentration (mol/L)	Number of samples
MgCl ₂	0.1~4	259
NaCl + KCl	0.1~4	284
KCl + MgCl ₂	1~4	218
MgCl ₂ + NaCl	0.1~3.6	227

In near-infrared spectral data analysis, the spectrum of water is typically subtracted to eliminate or reduce the negative impact of water as a major interference source on the analysis of the target substance [11]. This is because water has very strong absorption peaks in the near-infrared region, which can affect

other spectral features [12]. Therefore, subtracting the reference spectrum of pure water can help in building more accurate and robust quantitative or qualitative analysis models later on. The original spectra of each chloride salt solution after water subtraction are shown in Figure 1.

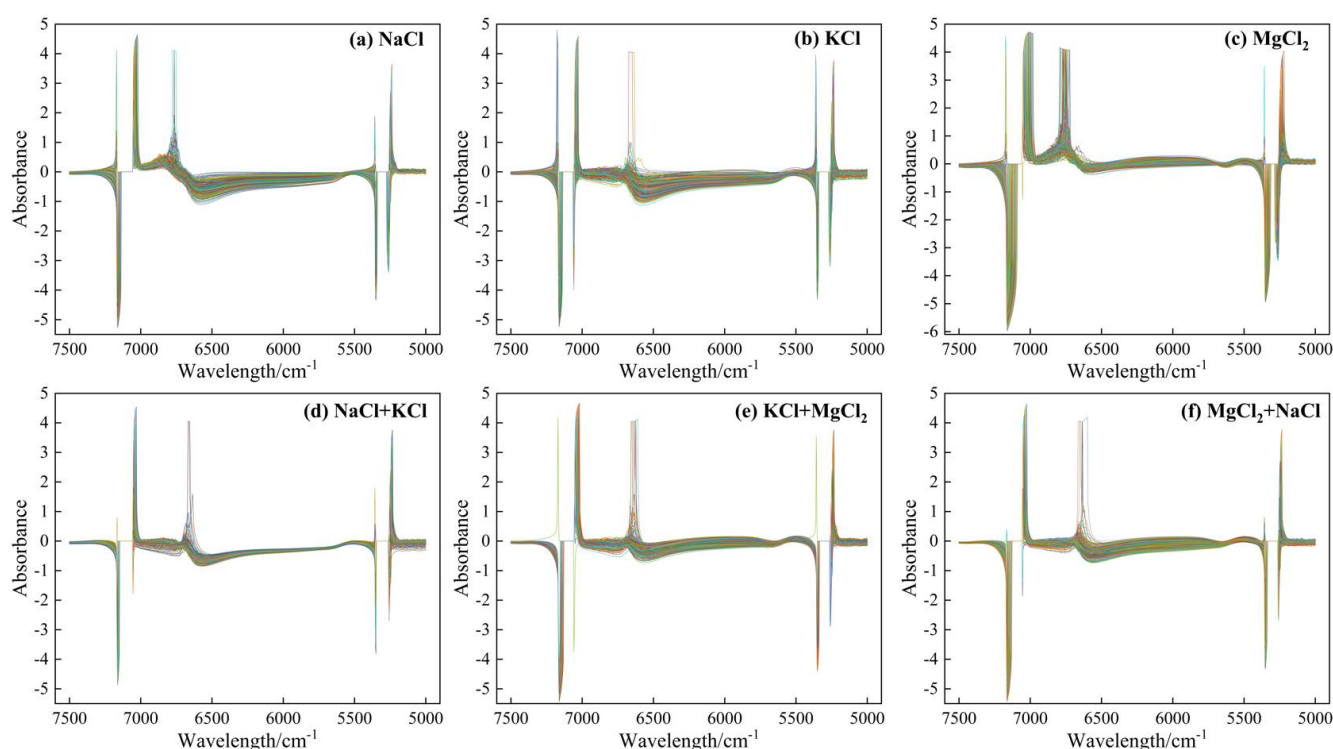


Figure 1. Original Spectra of Each Chloride Salt Solution (Water Subtracted) is omitted here but referenced in the original document.

2.2. Fundamental Algorithms

2.2.1. Spectral Data Preprocessing

During the actual detection process, the original spectral data of samples are often interfered with by environmental noise, baseline drift, and scattering effects, which directly affect the prediction accuracy of subsequent models and the final analysis results. Therefore, preprocessing the spectra is crucial for establishing an accurate analysis model [13, 14]. Spectral data processing methods mainly include smoothing, standard normal variate transformation, multiplicative scatter

correction, derivative processing, normalization, and standardization [15]. However, using only one preprocessing method is often insufficient to obtain good results; a combination of multiple methods is usually required to achieve the desired outcome. Rinnan et al [16] proposed a combination of two preprocessing methods: first using the Savitzky-Golay method to smooth the data and remove noise, and then applying derivatives to highlight feature information, known as the SG-O-P-Q method. Here, O is the window width, P is the polynomial fitting order, and Q is the order of the derivative. This study uses this method to preprocess the near-infrared spectra of each salt solution, setting the window width to 11,

the fitting order to 2, and the derivative order to 1 or 2, presenting the one with the best effect.

2.2.2. Convolutional Neural Network (CNN)

In recent years, deep learning has become a research hotspot in spectral analysis. In particular, the Convolutional Neural Network (CNN) has been widely applied. CNNs are used to directly extract local features from one-dimensional spectral signals; their convolutional kernels can effectively extract features like local absorption peaks and valleys, and their hierarchical structure can fuse local features to form more abstract global representations [17]. A 1D-CNN is a multi-layer neural network stacked with one-dimensional convolutional layers (Conv1D) and pooling layers [18]. The convolutional layer uses multiple kernels of different widths to perform convolutions to capture spectral features at different scales; this process is called the convolution operation, which can be represented by Equation (1). After the convolution operation, a pooling layer, typically max pooling, is connected to reduce the data dimensionality, retain the most significant features, and provide a certain degree of translation invariance [19].

$$F \otimes w = \sum_{k=1}^c \sum_{j=1}^{W_f} \sum_{i=1}^{H_f} (F^k(i, j) w^k(i, j)) \quad (1)$$

Among them, F represents the input data of the convolutional layer, w represents the weight parameters of the convolutional kernel, c , H_f , and W_f are the number of channels, height, and width of the convolutional kernel, respectively.

2.2.3. Long Short-Term Memory (LSTM) Network

Long Short-Term Memory (LSTM) is a special type of Recurrent Neural Network (RNN) specifically designed to solve the problems of vanishing and exploding gradients encountered by RNNs when processing long sequences. Through its sophisticated gate design, LSTM can learn and remember long-term dependencies in spectral sequences [7]. An LSTM unit mainly includes a forget gate, an input gate, and an output gate. The main algorithmic flow is as follows: first, the forget gate examines the current input and the previous time step's output to decide which old information to discard from the cell state (outputting a value between 0 and 1). Then, the input gate decides which new information to store in the cell state. This step creates a new candidate value, which is filtered by the input gate. After that, the cell state is updated by multiplying the old state with the result of the forget gate (discarding information) and then adding the new information filtered by the input gate (adding information). Finally, the output gate, based on the updated cell state, decides the content of the next output. The cell state passes through a tanh activation function and is then multiplied by the result of the output gate to obtain the final output for the current time step [9]. The relevant formulas are not listed here.

2.2.4. Attention Mechanism

In complex full-band spectra, not all bands are equally important for predicting concentration. To enable the model to focus on the most critical feature bands, this study introduces a self-attention mechanism after the LSTM layer. This mechanism can assign an attention weight to each time step (i.e., a feature vector) in the feature sequence output by the LSTM, thereby giving higher weight to important features when generating the final context vector [20]. First, the entire hidden state sequence ($H = [h_1, h_2, \dots, h_T]$) output by the LSTM layer is input into a fully connected layer to calculate an alignment score e_t for each hidden state h_t . This score measures the importance of each feature. Next, the softmax function is used to normalize the alignment scores e_t to obtain attention weights α_t . The sum of all weights is 1, forming a probability distribution. Finally, the obtained attention weights α_t are used for a weighted sum with the corresponding LSTM hidden states h_t to generate a context vector c that contains globally important information. This vector is then fed into subsequent fully connected layers for the final concentration prediction. The relevant formulas are as follows [21]:

$$e_t = v^T \tanh(W_a h_t + b_a) \quad (2)$$

$$\alpha_t = \frac{\exp(e_t)}{\sum_{j=1}^T \exp(e_j)} \quad (3)$$

$$c = \sum_{t=1}^T \alpha_t h_t \quad (4)$$

2.2.5. CNN-LSTM-Attention Model Construction

The structure of the proposed model is shown in Figure 2. First, the original spectral data are divided into a training set and a test set at a 4:1 ratio. The spectral data are input into multiple one-dimensional convolution modules, where each module contains a Convolution1D layer (the last module has 128 kernels of size 1, while the others have 64 kernels of size 3) and a MaxPooling1D layer, with the ReLU function used as the activation function. The feature sequence, after being down-sampled by convolution and pooling, is fed into an LSTM layer with 128 hidden units. The output sequence from the LSTM is weighted by a self-attention module, which is implemented with a fully connected layer, a softmax layer, and a multiplication layer; the fully connected layer has 100 neurons. The weighted feature vector passes through a global average pooling layer, a custom scaling layer, and two fully connected layers, and finally outputs the predicted concentration value through a regression layer. A dropout structure with a value of 0.2 is also added. The model is trained using the Adam optimizer with a maximum of 300 epochs and an initial learning rate of 0.01.

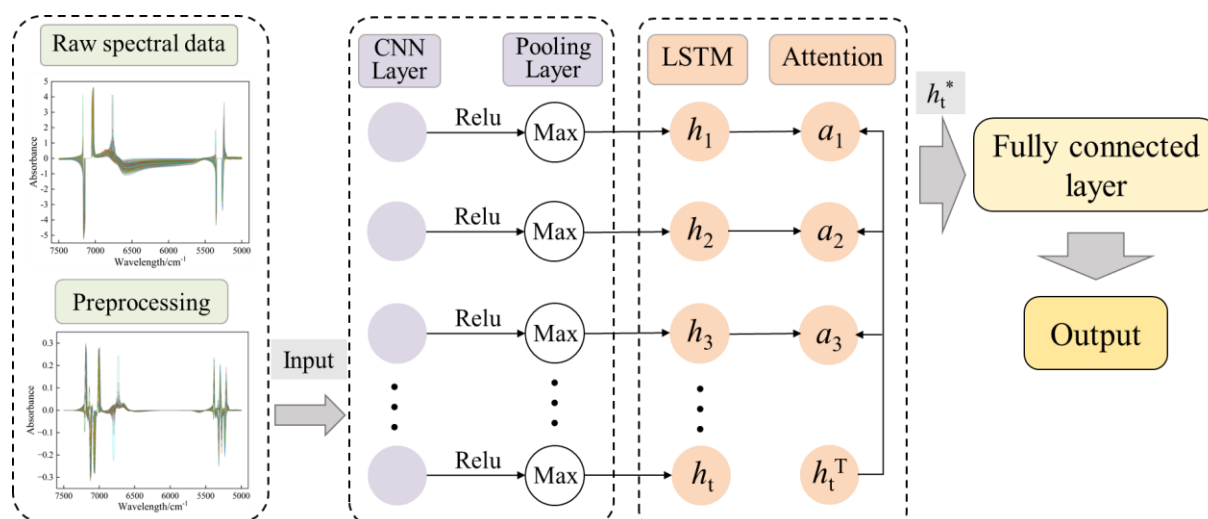


Figure 2. Model Structure Diagram is omitted here but referenced in the original document.

2.2.6. Model Performance Evaluation

The performance of the model is evaluated using the coefficient of determination (R^2) and the root mean square error (RMSE) of the prediction set. An R^2 value closer to 1 indicates a better goodness of fit for the model, while a smaller RMSE indicates higher prediction accuracy. The calculation formulas are as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{\sum_{i=1}^n (\bar{y} - y_i)^2} \quad (5)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2} \quad (6)$$

3. Results and Discussion

The results section should provide an accurate and concise description of the experimental findings, and the resulting conclusions that can be inferred from the experiments. Meanwhile, the results should be presented in a transparent and truthful manner, avoiding any fabrication or improper manipulation of data. Where applicable, results of statistical

analysis should be included in the text or as tables and figures.

3.1. Model Comparison Analysis

To systematically evaluate the effectiveness of the proposed CNN-LSTM-Attention hybrid model and to clarify the actual contribution of its constituent modules, this study compared it with models such as Partial Least Squares Regression (PLSR), Support Vector Regression (SVR), and Random Forest (RF). The evaluation metrics were the R^2 and RMSE of the prediction set. PLSR is a multivariate linear regression method widely used in near-infrared spectral quantitative analysis, particularly adept at handling problems where the number of variables exceeds the number of samples and where multicollinearity exists among variables. SVR is a regression method derived from Support Vector Machines (SVM), which achieves effective data fitting by finding an optimal regression hyperplane in a high-dimensional feature space. RF is a classic machine learning algorithm that performs internal cross-validation, has good prediction performance for complex and non-linear data, and has advantages such as fast training speed, resistance to overfitting, and robust prediction results for data containing outliers and noise [22, 23]. The performance comparison results of each model are shown in Table 2.

Table 2. Model Performance Comparison Results is omitted here but referenced in the original document.

	NaCl		KCl		MgCl ₂		NaCl+ KCl		KCl+ MgCl ₂		MgCl ₂ +NaCl	
	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE
PLSR	0.967	0.280	0.958	0.238	0.978	0.164	0.738	0.607	0.939	0.221	0.965	0.185
SVR	0.971	0.230	0.967	0.177	0.986	0.121	0.777	0.669	0.968	0.143	0.959	0.194

	NaCl		KCl		MgCl ₂		NaCl+ KCl		KCl+ MgCl ₂		MgCl ₂ +NaCl	
	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
RF	0.964	0.253	0.967	0.181	0.984	0.131	0.825	0.444	0.953	0.174	0.975	0.153
CNN+LSTM+Attention	0.968	0.213	0.972	0.168	0.984	0.147	0.925	0.340	0.973	0.146	0.969	0.180

The comparison results show that for single-component salt solutions (NaCl, KCl, MgCl₂), traditional machine learning models demonstrate excellent predictive capabilities. Among them, the performance of SVR and RF is particularly outstanding, with their coefficients of determination (R²) generally above 0.96 and root mean square errors (RMSE) maintained at a low level; the R² for SVR and RF on the MgCl₂ solution is as high as 0.98. This indicates that after effective spectral preprocessing, models like SVR and RF can fully capture the non-linear relationship between single ion concentration and spectra. The PLSR model, being a linear model, performed slightly worse but still achieved high prediction accuracy. The CNN-LSTM-Attention model proposed in this study also performed excellently on such datasets, with its performance being comparable to that of the SVR and RF models, and even slightly superior on the KCl solution with an R² of 0.972, which preliminarily verifies the effectiveness of this deep learning model in processing spectral data.

When dealing with more complex two-component mixed solutions, the performance of all models decreased to varying degrees, highlighting the challenge that severe spectral overlap among ions in mixed solutions poses to quantitative analysis. However, it is precisely in such complex scenarios that the advantages of the CNN-LSTM-Attention model are fully demonstrated. Analysis of the data in Table 2 shows that the prediction accuracy of this model surpassed all comparison models on all three mixed solution datasets. Especially on the most difficult-to-distinguish NaCl+KCl mixed solution, its R² reached 0.925, significantly higher than the best-performing traditional model RF (R²=0.825). This result strongly proves that through the deep feature extraction of CNN, the sequential relationship modeling of LSTM, and the

focusing on key bands by the Attention mechanism, the proposed model can more effectively decouple the effective information related to the concentration of each component from highly overlapping spectra, showing excellent robustness and prediction accuracy.

At the same time, it can be seen from the table that almost all models performed slightly worse on the NaCl and KCl mixed solution dataset. The main reason may be that the chemical properties of NaCl and KCl are the most similar, both being +1 valence alkali metal chlorides, and their effects on water molecules are also very similar, which leads to high overlap in their spectral features, making it difficult for the models to establish an accurate quantitative relationship. For complex data like mixed solutions where patterns are harder to capture, deep learning can, by virtue of its deep network structure, automatically learn and extract potential features from high-dimensional spectral data and model the complex non-linear relationship between spectra and concentration, providing a feasible method to solve such problems.

3.2. Ablation Study Analysis

To investigate the performance improvement brought by the added modules on top of the CNN base, this study conducted an ablation study, with the evaluation metrics still being the R² and RMSE of the prediction set. An ablation study is an experimental method that systematically removes one or more components, functions, or modules from a model or system to study the contribution of that component to the overall performance. This experiment uses CNN as the baseline model and gradually introduces key improvement modules to analyze their effects. The results are shown in Table 3.

Table 3. Ablation Study Results is omitted here but referenced in the original document.

	NaCl		KCl		MgCl ₂		NaCl+ KCl		KCl+ MgCl ₂		MgCl ₂ +NaCl	
	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
CNN	0.901	0.423	0.916	0.288	0.893	0.337	0.494	0.818	0.513	0.588	0.803	0.427
CNN+LSTM	0.943	0.321	0.947	0.230	0.937	0.259	0.835	0.451	0.921	0.225	0.883	0.329
CNN+LSTM+Attention	0.968	0.208	0.972	0.168	0.984	0.147	0.925	0.340	0.973	0.146	0.969	0.180

The results clearly show a stepwise improvement in model performance. First, the standalone CNN model performed the worst on all datasets, indicating that relying solely on local feature extraction from spectra is insufficient to build a high-precision quantitative model. Subsequently, after integrating the LSTM module on top of the CNN, the performance of the CNN+LSTM model was consistently and significantly improved across all six datasets. For example, on the most challenging NaCl+KCl dataset, the R^2 value increased sharply from 0.494 to 0.835. This strongly demonstrates that learning and modeling the sequential dependencies among the features extracted by the CNN is crucial for improving prediction accuracy. Finally, after introducing the attention mechanism, the complete CNN-LSTM-Attention model achieved the best performance on all datasets. Compared to the CNN+LSTM model, its R^2 and RMSE metrics were further optimized, once again verifying that the attention mechanism can effectively en-

hance the model's final prediction ability by focusing on key spectral information.

3.3. Model Performance Analysis

To more intuitively display the prediction performance of the CNN-LSTM-Attention model, a scatter plot is drawn, as shown in Figure 3. In the figure, the data points are basically concentrated around the diagonal line, indicating that the model's predicted values are largely consistent with the true values, and the model has high accuracy. Furthermore, the distribution of data points for the training set and the test set is similar, indicating that the prediction performance of the CNN-LSTM-Attention model is consistent between them, with no obvious overfitting, and it possesses good generalization ability. This further confirms the stability and effectiveness of the CNN-LSTM-Attention model in all test tasks from a quantitative perspective.

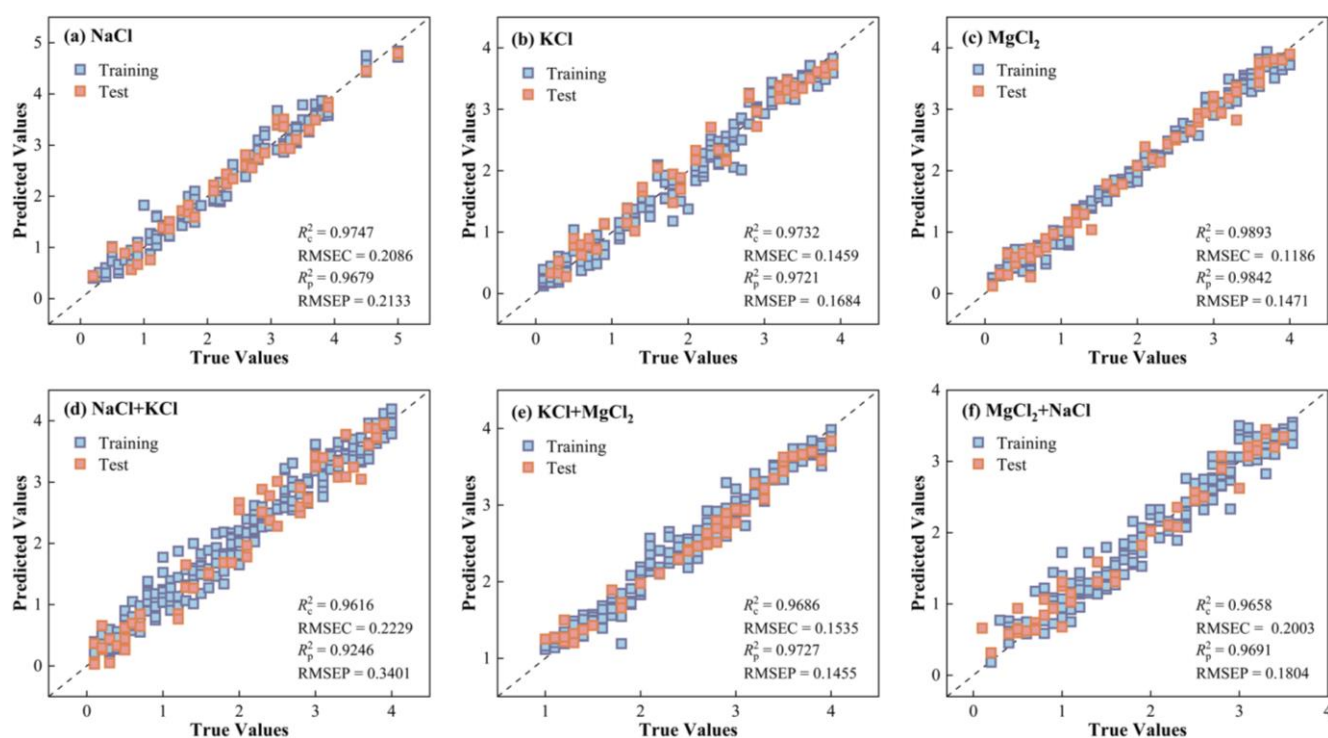


Figure 3. Concentration Model Prediction Results for Each Chloride Salt Solution is omitted here but referenced in the original document.

4. Conclusions

This study aimed to explore a near-infrared spectral salt solution concentration prediction method based on a CNN-LSTM-Attention hybrid model, and systematically evaluated its effectiveness in the quantitative analysis of single and mixed salt solutions through comparison with baseline models such as PLSR, SVR, RF, and an ablation study. The research results show that for single-component

salt solutions with relatively simple compositions, the proposed CNN-LSTM-Attention model is comparable in performance to high-performing traditional machine learning methods (especially SVR and RF), both achieving high-precision concentration prediction. More critically, for two-component mixed solutions with severe spectral collinearity, the CNN-LSTM-Attention model demonstrated significant performance advantages, with its prediction accuracy surpassing that of traditional models on all mixed-substance datasets, proving its excellent capability in

handling complex systems. The ablation study further confirmed that the model's performance shows a stepwise improvement from CNN to CNN+LSTM and then to the introduction of the attention mechanism, verifying the positive contributions of each module in the hybrid model architecture.

In conclusion, this study successfully demonstrates that the proposed CNN-LSTM-Attention hybrid model is an efficient and robust tool for quantitative analysis using near-infrared spectroscopy, especially when dealing with the severe spectral overlap problem in mixture systems, where its performance is superior to that of mature traditional machine learning algorithms, proving the potential of deep learning to solve this problem. Future research directions could focus on further optimizing the model structure to improve computational efficiency, and extending this method to more complex multi-component systems.

Abbreviations

NIRS	Near-Infrared Spectroscopy
CNN	Convolutional Neural Network
LSTM	Long Short-Term Memory
Attention	Attention Mechanism
PLSR	Partial Least Squares Regression
SVR	Support Vector Regression
RF	Random Forest
PCR	Principal Component Regression
SG	Savitzky-Golay (A spectral preprocessing method)
RNN	Recurrent Neural Network
SVM	Support Vector Machine
Conv1D	1D Convolutional Layer
R ²	Coefficient of Determination
RMSE	Root Mean Square Error

Author Contributions

Ziyang Pei: Writing – original draft, Methodology, Formal Analysis

Jianfeng Zhao: Investigation, Validation

Ningfeng Wang: Writing – review & editing, Resources, Supervision

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Conflicts of Interest

The authors declare no conflicts of interest.

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