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Prediction of Adsorption Efficiency of Lithium Hydroxide Based on an Enhanced NSGAII-LSTM Model

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Abstract: With the continuous advancement of aerospace and deep-sea technologies, the safety of enclosed spaces has increasingly garnered attention, particularly concerning the control of carbon dioxide (CO_2) concentrations. However, there are challenges with existing CO_2 control methods. For instance, the adsorption efficiency cannot be measured when utilizing Lithium Hydroxide for absorption. To address this challenge, this paper presents a new model to quantify LiOH AC. This study integrates Long Short-Term Memory (LSTM) networks with a self-attention mechanism, refined utilizing Non-Dominated Sorting Genetic Algorithm II (NSGA-II) for optimization. The results indicate that the supposed model surpasses traditional LSTM model leading to improved predictive precision and enhanced overall performance in the prediction of LiOH AC.

1. Introduction

With the continuous advancement of aerospace and deep-sea technologies, the safety of enclosed spaces has been increasingly emphasized. Among them, the Environmental Control and Life Support System (ECLSS) is an essential component for ensuring the safety of personnel within enclosed spaces, with one of its primary tasks being the removal of carbon dioxide (CO_2) [1]. Among the various methods developed for the control of carbon dioxide (CO_2) concentrations, lithium hydroxide (LiOH) as a chemical adsorption material has been widely used due to the advantages of low energy consumption and high adsorption capacity [2]. In the aerospace and marine industries, LiOH is used as a CO_2 absorbent in the filtration units to reduce the side effects of high CO_2 concentrations on human operators. A simplified diagram of the use of LiOH to adsorb CO_2 in a filtration apparatus is shown in Fig. 1. When CO_2 is generated in a confined space, according to the operator's environment, mainly including temperature and humidity, and carbon dioxide concentration, the amount of CO_2 removal can be estimated, and further to find the fan air volume. LiOH filling volume can be calculated accordingly. In the apparatus device under the action of the fan, CO_2 will enter into the LiOH filter layers through the air inlet on both sides of the apparatus device to chemically react with LiOH to form, resulting in lithium carbonate (Li_2CO_3) and water (H_2O). The generated Li_2CO_3 will be retained in the filtration device, and the water can be removed by other water separation devices.

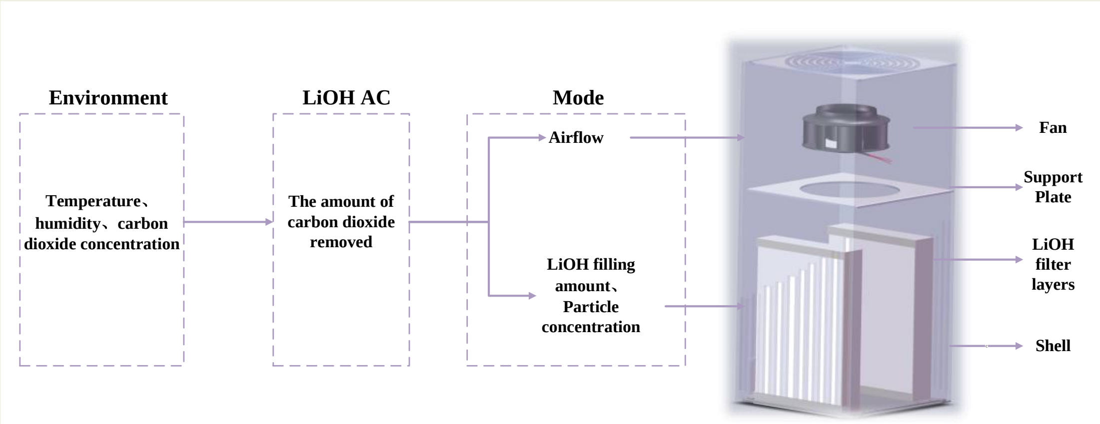

Figure 1: The flowchart of CO_2 adsorption by LiOH.

$$2\mathrm{LiOH(solid)} + \mathrm{CO_2(gas)} \rightarrow \mathrm{Li_2CO_3(solid)} + \mathrm{H_2O(gas)} \tag{1}$$

An issue arises in conjunction with using LiOH. According to formula 1, the adsorption efficiency of LiOH (LiOH AC) is estimated based on the coefficient ratio of 2:1 for LiOH to CO_2. However, formula 1 is under ideal conditions but not accurate in various practical conditions. As in Fig. 1, the chemical reaction can be affected by several factors, including the particle reaction time (PRT), carbon dioxide concentration (CC), airflow (A), humidity (H), particle filling amount (FV), temperature (T), and particle concentration (PFM). Different ranges of values for these factors can be combined to form a complex set of chemical reactions. The diversity of chemical reaction conditions is seen as critical in influencing LiOH AC. The problem is how to quantify LiOH AC.

To address the above problems, in this study, this paper presents a new model to quantify LiOH AC with the following innovations: The model combines Long Short-Term Memory (LSTM) networks with the self-attention mechanism to predict LiOH AC with multiple input factors, including PRT, CC, A, H, FV, T, and PFM. The hyperparameter optimization is conducted by utilizing the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) within this model. The trained model does not need experiments, and it helps users obtain LiOH AC under different reaction conditions. This provides engineering guidance for future researchers to apply LiOH in various environmental conditions.

2. Experiments and Methods

2.1 Overall flow

Fig. 2 shows the flowchart of how LiOH AC can be predicted using the enhanced NSGAII-LSTM model. After experiments are designed and raw data from the experiments are collected, the data are used to train and test the established models for LiOH AC prediction under different reaction conditions. Because of the temporal nature of the collected data, this study employs the LSTM model to forecast LiOH AC, utilizing R^2 and MSE as evaluation metrics. To enhance the predictive ability of the model, a multi-head self-attention mechanism is integrated into the LSTM to better capture the crucial features within the input data. Furthermore, the NSGA-II algorithm is utilized to optimize the model's hyperparameters, thereby further enhancing the predictive performance.

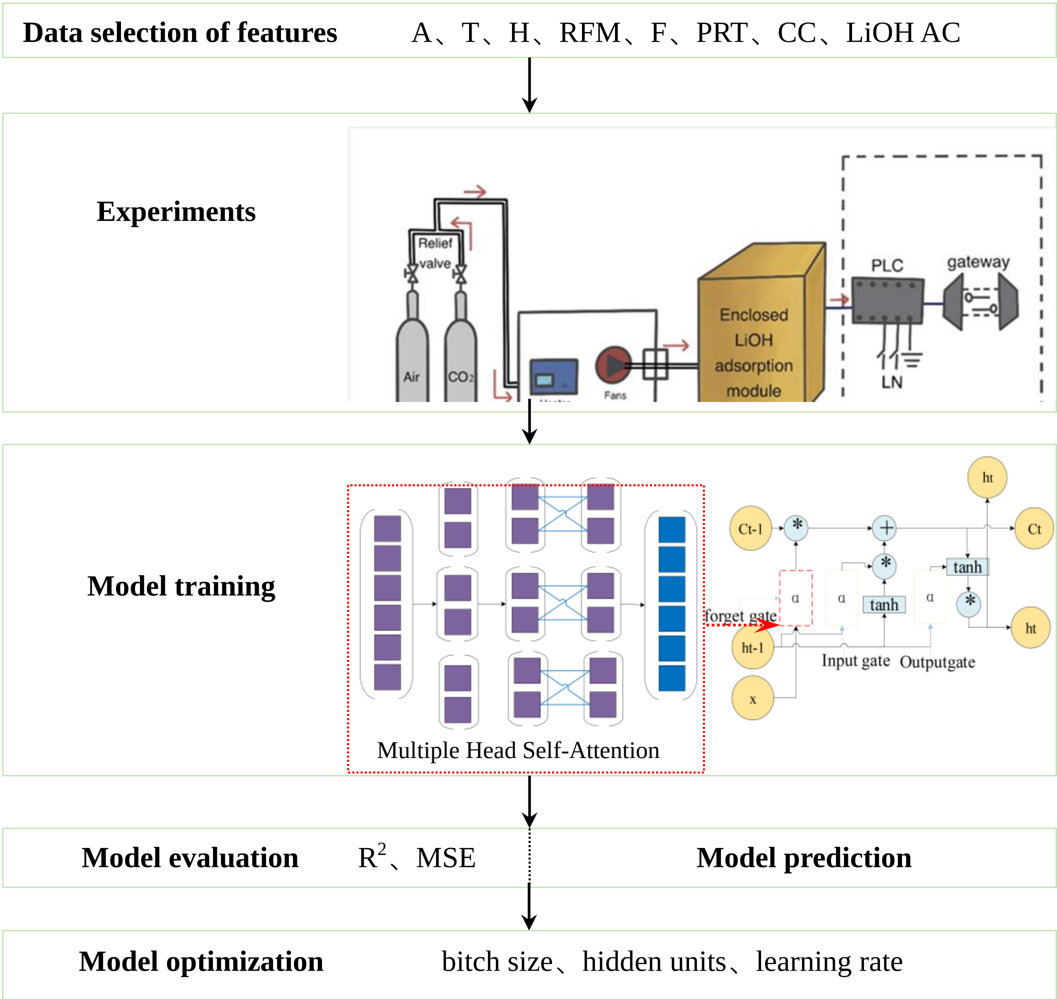

Figure 2: The flowchart of the developed methodology.

2.2 Methodology

In this study, an enhanced NSGAII-LSTM model is designed for LiOH AC prediction. The input includes the particle reaction time (PRT), carbon dioxide concentration (CC), airflow (A), humidity (H), particle filling amount (FV), temperature (T), and particle concentration (PFM). A, T, and RH data are collected in the form of a time series. Therefore, the model should adequately consider the dynamic features within the time series. Long Short-Term Memory (LSTM) is a type of recurrent neural network (RNN) specifically designed for processing and predicting time series data. LSTM employs gate mechanisms are integral components in the architecture of neural networks.

The input gate plays a crucial role in deciding the necessity of updating the data within the memory unit. Herein lies its formal explanation.

$$i_t = sidmoid(W_{ii} * x + W_{hi} * h_{t-1} + b_i) \tag{2}$$

where W_{ii} and $W_{hi}$are the weights establishing the connection between the input gate and the prior hidden state, and $b_i$is the bias value of the input gate.

The operational function of the forget gate, denoted as f_t, is to regulate the decision-making process regarding the retention or removal of information stored within the memory unit.

$$f_t = sigmoid(W_{if} * x + W_{hf} * h_{t-1} + b_f) \tag{3}$$

where x is the input of the LSTM network.h_{t-1} is the previous hidden state. $W_{if}$and $W_{hf}$are the weights that link the forget gate to the prior hidden state, and b_f is the bias value of the forget gate.

The decision regarding the dissemination of the status details from the concealed layer hinges upon the output gate denoted aso_t, as elaborated in the subsequent definition.

$$o_t = sigmoid(W_{io} * x + W_{h0} * h_{t-1} + b_0) \tag{4}$$

Whether the status information of the hidden layer is output is determined by the output gate o_t. The following is its definition.

The candidate state c'_t retains information about candidates and undergoes updates through the utilization of the preceding concealed state in conjunction with the present input in the subsequent manner.

$$c'_t = i_t * tanh(W_{ic} * x + W_{hc} * h_{t-1} + b_c) \tag{5}$$

where $W_{ic}$and W_{hc} are the weights connecting the previous hidden state to the candidate state, and b_c is the bias value of the candidate state.

The following is how output gates and cell states are used to update the hidden state h_t.

$$h_t = o_t * tanh(c'_t) \tag{6}$$

The LSTM network regulates the flow of new information through the input gate. The input gate determines whether to retain or discard information in the memory cells through the forget gate. It generates potential new information to update the memory based on candidate states, which dynamically manages the cell state according to the forget gate and candidate state. Finally, the output gate decides which parts of the cell state are to be output as hidden states, effectively transmitting information to the next time step and subsequent network layers.

However, traditional LSTM models still encounter issues of information loss and insufficient selection of important features when dealing with long sequences. Additionally, for neural network-based models, hyperparameter tuning is a crucial task that demands a significant amount of time and effort to determine the optimal set of hyperparameters [3]. To address the limitations of the LSTM model, we have introduced a self-attention mechanism and NSGA-II algorithm. By employing a self-attention mechanism, the LSTM model is facilitated to autonomously select the features that have the most significant impact on LiOH AC. The self-attention mechanism, when dealing with sequential data, dynamically weights the relationships between elements in a sequence to assist models in focusing on crucial features. The incorporation of attention mechanisms facilitates the capturing of long-term temporal patterns in LSTM models, thereby enhancing their generalization capability. The formula for this mechanism is as follows:

$$H = LSTM(X) \tag{7}$$

where X represents a sequence comprising seven input features in the present study, where H denotes the hidden states of all time steps in the LSTM model.

$$Q = H_T \tag{8}$$

where Q represents queries, and H_T denotes the final hidden state of the LSTM model.

Using all hidden states of LSTM as keys and values.

$$K = V = H \tag{9}$$

Where the attention mechanism consists of values V, K is keys, H is hidden states. The aggregation of the output A from each attention head, denoted as $\mathrm{head_i}$, is calculated.

$$head_i = Attention(Q * W_Q^i, K * W_K^i, V * W_V^i) \tag{10}$$

$$A = MultiHead(Q,K,V) = Contact(head_1, head_2, \ldots, head_h) * V \tag{11}$$

where W_Q^i, W_K^i, W_V^i are learned projection matrices for each head. The outputs of each attention head are concatenated and linearly transformed.

$$\hat{Y} = W_{out} * A \tag{12}$$

Where the matrix W_{out} represents the weights of the output layer in the neural network architecture. The symbol $\hat{Y}$ denotes the predicted values generated by the model.

Furthermore, NSGA-II operates by simulating a natural evolutionary process, wherein multiple potential solutions are evaluated based on defined objectives to determine the optimal hyperparameter configuration. This not only enhances the model's performance but also ensures its robustness by exploring a diverse solution space, thereby avoiding local optima [4]. This optimization problem aims to minimize MSE and maximize R^2, thus the mathematical model for the optimization problem is as follows:

$$min(F(l,h,b)) = min(MSE, \frac{1}{R^2}) \tag{13}$$

$$s.t. = \begin{cases} 0.00001 < l < 0.1 \\ 26 < h < 1500 \\ 16 < b < 526 \end{cases} \tag{14}$$

The symbol l represents the learning rate, h denotes the number of hidden units, and b signifies the batch size. Determination coefficient (R^2) and mean square error (MSE) were used for evaluation. The higher the value of R^2 and the lower the values of MSE, the more accurate the model's prediction result is. The calculation equations are shown in formula 15 and formula 16.

$$R^2 = 1 - \frac{\sum_{n=1}^{N}(y_{pred} - y_{act})^2}{\sum_{n=1}^{N}(y_{pred} - y_{mean})^2} \tag{15}$$

$$MSE = \frac{1}{N}\sum_{n=1}^{N}(y_{act} - y_{pred})^2 \tag{16}$$

where N is the total number of data points, and y_{pred}, y_{act}, and y_{mean} denote the predicted, actual, and mean values of the LiOH AC, respectively.

3. Conclusion

A novel approach is presented in this study, introducing a model that employs Long Short-Term Memory (LSTM) networks with a self-attention mechanism to quantify LiOH AC. The optimization of this model is achieved through the utilization of the Non-Dominated Sorting Genetic Algorithm II (NSGA-II).

The results indicate that the LSTM model, enhanced with the self-attention mechanism and NSGA-II algorithm, exhibits superior accuracy in predicting LiOH AC. The model achieves an R^2 of 0.987 and MSE of 0.04, outperforming the traditional LSTM model which only attains an R^2 of 0.92 and MSE of 0.21. The incorporation of the self-attention mechanism and NSGA-II algorithm effectively addresses the limitations of the LSTM model, enhancing its predictive accuracy and overall performance.

Subsequent research endeavors may focus on evaluating the performance of this model across different datasets and application scenarios, thereby providing more robust predictive capabilities.

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