

# A machine learning NO<sub>x</sub> emission model for SCR system considering mechanism knowledge and catalyst deactivation

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**Abstract.** In this work, an adaptive NO<sub>x</sub> emission model is proposed for a SCR system of a 660 MW utility boiler. First, 3-years operating data was collected from the plant SIS system as raw data, which was then filtered using the R-statistic method and clustered by the condensed nearest neighbor (CNN) rule to form a classified steady-state database. In addition, a sliding window approach was used to deal with the continuous data stream. As the newest steady state sample was introduced into the database, the most similar old sample in the same data class was replaced. The crowding distance (CD) operator was also used to eliminate the redundant samples. This new method RCNN-CD is proven to be a good tool to improve the representatives of the samples. Based on the selected samples, a fusion monotony support vector regression (FM-SVR) was used to establish the NO<sub>x</sub> emission model. The results show that, this model can reasonably reflect SCR mechanism and follow the degradation of SCR performance.

## 1 Introduction

Thermal process modelling can be divided into mechanism method and data-driven method. The mechanism model is established based on the intrinsic characteristics of the system, which ensures that the relationship among operating parameters strictly abides by the physical and chemical theorems. However, since the thermal process is very complicated, as the running time increases, the mechanism model cannot follow the changes of the system in real time. Taking the Selective Catalytic Reduction (SCR) system of the power station as an example, factors such as the modification of the deflector, the adjustment of the reducing agent distribution strategy, and the deactivation of the catalyst [1] will affect the accuracy of the mechanism model.

Data-driven modelling method directly learns the relationship among the parameters, which accordingly resulting in a high predicting accuracy. Smrekar et al. [2] performed data cleaning, steady-state screening, and variable selection on the operating data of a power station in the last 12 days, and based on the filtered data, established a main steam parameter model that can accurately reflect the current performance status of the unit. Fan et al. [3] combined continuous restricted Boltzmann machine and SVR in NO<sub>x</sub> emissions prediction of a tangential firing boiler. However, while pursuing high modelling accuracy, data-driven models are prone to overfitting.

This paper used data-driven method to establish a prediction model of NO<sub>x</sub> emissions from a 660 MW power plant SCR system, and introduced mechanism knowledge and adaptive strategies into this model. The

results show that the model can maintain the correct relationship among parameters, and can reasonably track the performance changes of the catalyst.

## 2 SCR system and raw data

### 2.1. SCR system

The SCR DeNO<sub>x</sub> system in this work contains an ammonia injection grid (AIG) and three catalyst layers, arranged at the tail of a 660 MW coal-fired boiler, as shown in Fig. 1. Each catalyst layer fills with an amount of plate-type catalysts, whose service life is 24,000 hours.

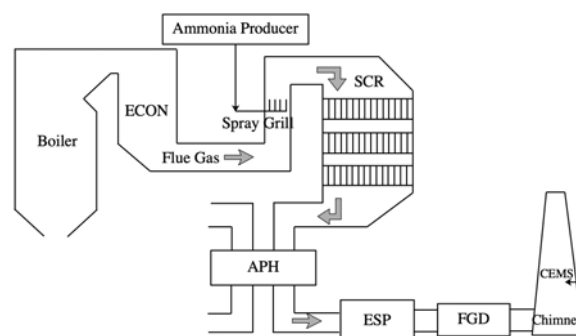


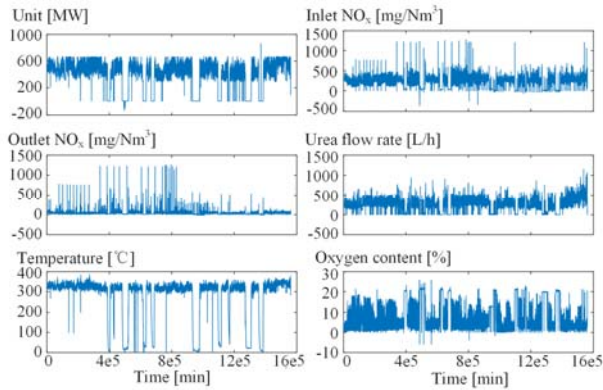
Fig. 1. Schematic of boiler and SCR system.

### 2.2. Raw data

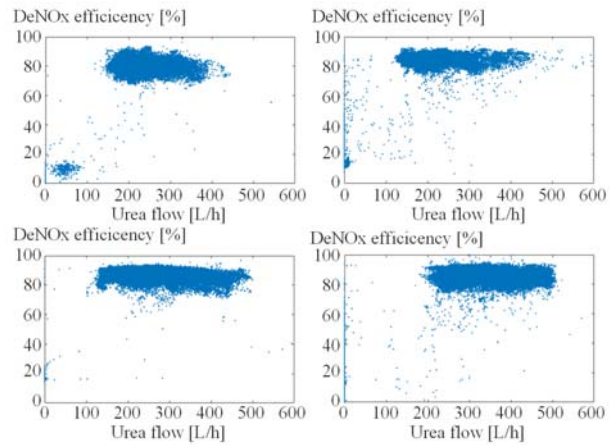
Taking a total of 1,560,990 raw data as the original samples, which is collected from the Supervisory Information System (SIS) of the power plant with a

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period of 1084 days and a sampling interval of 1 minus. Fig. 2 shows several historical curves of these data, including the key parameters like load, oxygen content, temperature, flow rate of urea, and NO<sub>x</sub> concentration at inlet and outlet of the SCR reactor. It is hard to observe any degradation for SCR performance over time due to many useless data mixed in the data collection.



**Fig. 2.** 3-years historical operating data for SCR system  
 Fig. 3 shows the relationships between the DeNO<sub>x</sub> efficiency and the urea flow rate, each sub-figure displays the data of a month. It also cannot see a mechanism trend that the NO<sub>x</sub> reduction efficiency increases with the amount of the reducing agent. This phenomenon can be attributed to the variation of gas condition during the boiler operation.

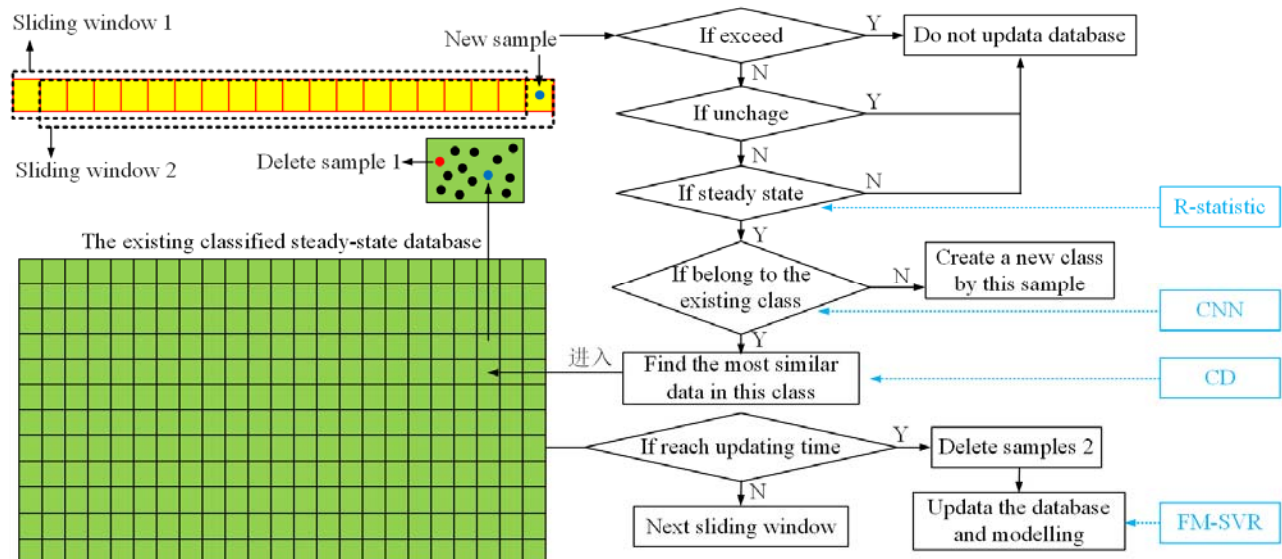


**Fig. 3.** Parameters relationship observed from the raw data.

### 3 Modelling method

#### 3.1. RCNN-CD

A machine learning method named RCNN-CD was proposed to deal with the raw data, which combined the R-statistic method, the condensed nearest neighbor (CNN) rule, and the crowding distance (CD) operator. As shown in Fig. 4, after choosing the high quality samples using RCNN-CD method, a fusion monotony support vector regression (FM-SVR) was further applied to establish the NO<sub>x</sub> emission model.



**Fig. 4.** Schematic diagram of the proposed model.

#### 3.2. FM-SVR

According to the mechanism of SCR reaction, the NO<sub>x</sub> reduction efficiency is increased with the mole ratio of NH<sub>3</sub>/NO<sub>x</sub>. Thus, FM-SVR was proposed to describe this monotony increasing relationship. Based on training method of Least Square-Support Vector Regression (LS-SVR), FM-SVR adds the constraint that the first-order

partial derivative of the function must be equal or greater than zero.

The function of LS-SVR can be written as:

$$f(x) = \sum_{i=1}^n \alpha_i K(x, x_i) + b \quad (1)$$

The first-order partial derivative of LS-SVR can be written as:

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}^j} = \frac{1}{\sigma^2} (\mathbf{X}_i^j - \mathbf{x}^j) \sum_{i=1}^n \alpha_i \exp \left( -\frac{\sum_{k=1}^d (\mathbf{x}^k - \mathbf{X}_i^k)^2}{2\sigma^2} \right) \quad (2)$$

To improve the training efficiency, an additive kernel method was introduced by adding separate kernels for each input dimension, which can be written as:

$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i (K_1(\mathbf{x}^1, \mathbf{X}_i^1) + \dots + K_d(\mathbf{x}^d, \mathbf{X}_i^d)) + b \quad (3)$$

$$= \left( K_1(\mathbf{x}^1, (\mathbf{X}^1)^T) + \dots + K_d(\mathbf{x}^d, (\mathbf{X}^d)^T) \right) \boldsymbol{\alpha} + b$$

The training problem of FM-SVR containing  $n$  equality constraints and  $m$  inequality constraints can be described as:

$$\min_{\boldsymbol{\alpha}, b} \quad \frac{1}{2} \|\boldsymbol{\alpha}\|^2 + C \sum_{i=1}^n \eta_i^2 \quad (4)$$

s.t.  $\sum_{k=1}^n \alpha_k K(\mathbf{x}_i, \mathbf{X}_k) + b - y_i = \eta_i, i = 1, 2, \dots, n$

$$\frac{1}{\sigma^2} (\mathbf{X}^j - \mathbf{e} \mathbf{x}_p^j)^T \text{diag}(K_j(\mathbf{x}_p^j, \mathbf{X}^j)) \boldsymbol{\alpha} \geq 0, p = 1, 2, \dots, m$$

### 4 Results and discussion

The data exceeding the upper and lower limits and the data with an unchanged value were regarded as the error data. These data was first cleaned from the raw data, and the number of the samples was decreased from 1,560,990 to 949,524. After that, R-statistic method [4] was employed to deal with the remaining data. As shown in Fig. 5,  $S$  represents the steady factors. The greater the value of  $S$ , the more unstable the SCR system is. This work treats the data with a steady factor less than 1.2 as the useable data for modelling, and put them into the database. Finally, the number of samples dropped to 203,221.

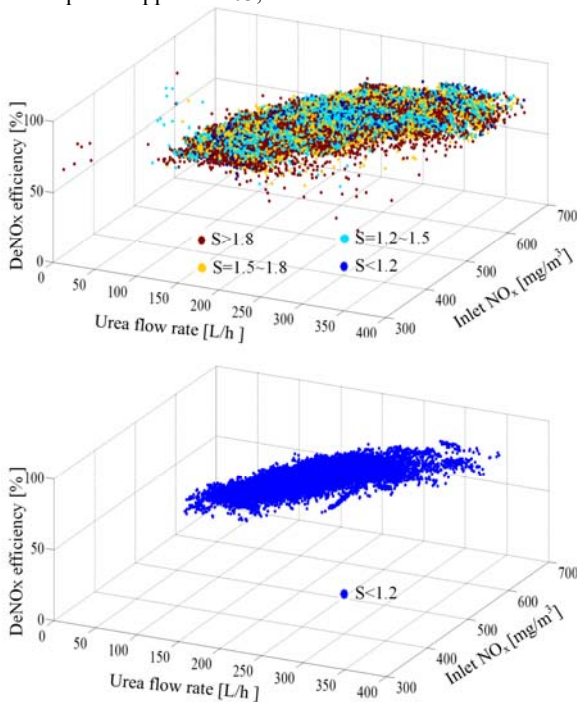


Fig. 5. Data processing results after R-statistic method.

CNN was used to classify the steady-state database. As shown in Fig. 6, the cluster algorithm can eliminate the effects of environmental difference on data relationship. The data in a certain class have similar environmental parameters such as temperature, load, and inlet NO<sub>x</sub> concentration. These samples clearly show the SCR mechanisms [5]; one is that the DeNO<sub>x</sub> efficiency increases with urea flow, and the other is to keep a same DeNO<sub>x</sub> efficiency, the urea flow rate will rise over time due to the catalyst deactivation.

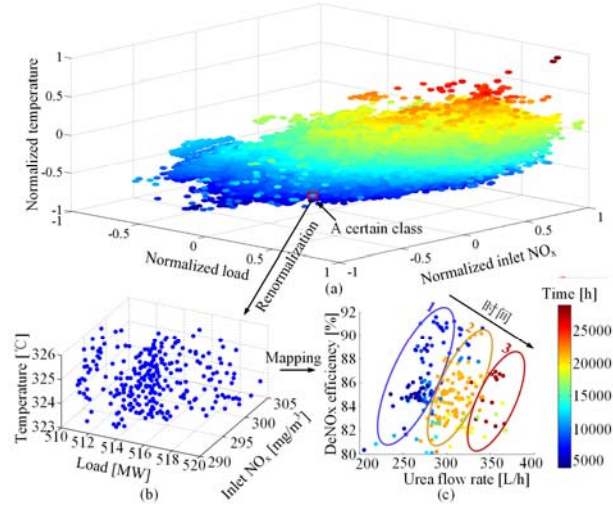


Fig. 6. Data processing results after CNN.

This work used CD method to update database for a continuous data stream. To validate the effect of CD strategy, a simple test was conducted. In this test, the data from the first month were used to form an initial steady-state database, then the data from the next two months were constantly imported to update the database. The First in First out (FIFO) strategy, the RCNN with CD strategy, and the RCNN without CD strategy were compared in the test. As shown in Fig. 7, when the data updating is finished, two data classes were selected to analyse. It can be seen that, in both classes, the data through RCNN-CD filtration have a better distribution, which is well dispersed and covers the whole sample space. This ability to select the great representative samples is essential for the modelling.

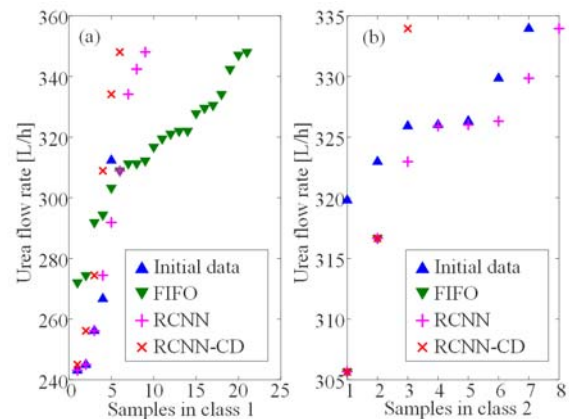
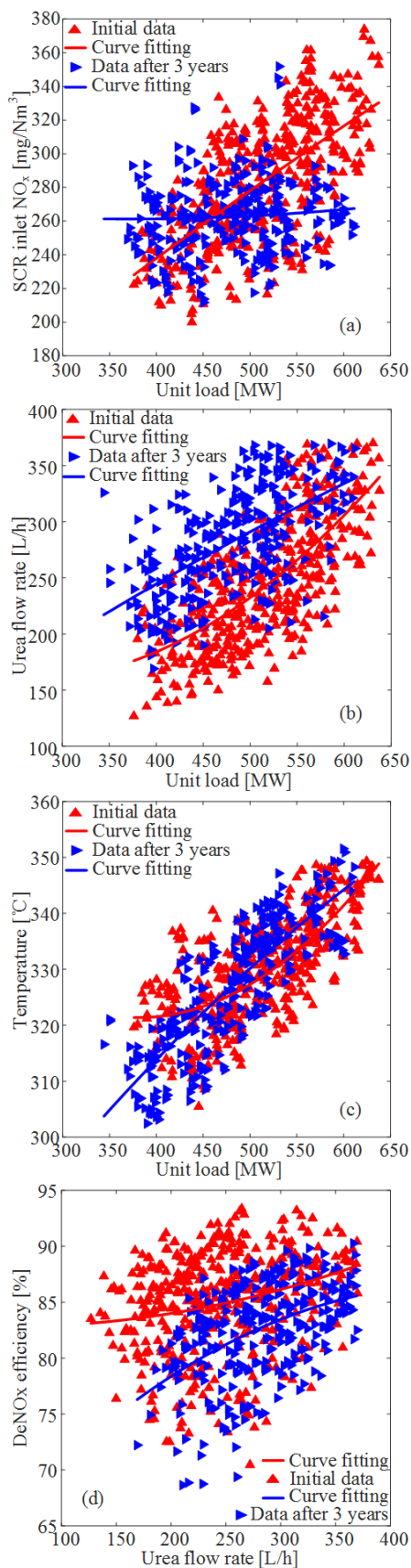


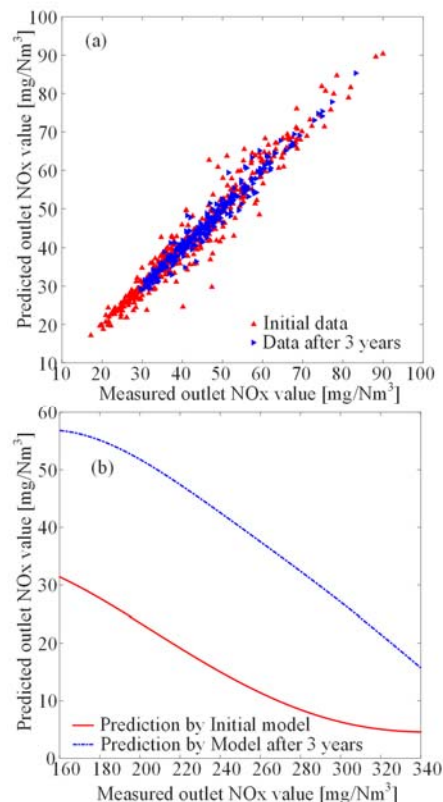
Fig. 7. Comparison of data processing results by FIFO, RCNN, and RCNN-CD.





**Fig. 8.** Initial data and the data chosen by RCNN-CD. Taking 3-years raw data from SCR system for analysis, the period is from the first time that the fresh catalyst was arranged into SCR reactor to the time that

the catalyst operating for 3 years. The mechanical trend for SCR system becomes clear. Fig. 9 shows the modelling results predicted by FM-SVR according to these high quality samples. The Mean Relative Error (MRE) for the initial model and the model after 3 years are 5.26% and 2.68%, respectively.



**Fig. 9.** Modelling results by RCNN-CD and FM-SVR.

## 5 Conclusion

In this work, an integrated machine learning method combined RCNN-CD and FM-SVR was proposed to predict the NO<sub>x</sub> released from a 660 MW utility boiler. 3-years plant historical data were obtained as the samples. The results show that the present method has adaptive ability to follow the degradation of SCR performance, and can reflect a reasonable mechanism relationship between different operating parameters in the SCR system.

## References

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