Operation optimization of SCR system based on denitration efficiency prediction model

Guilin Wang*, Yigang Zhoua, Yue Zhao and Sen Wangb

Tianjin Electric Power Science & Research Institute, Tianjin, 300384, China

*Corresponding author e-mail: guilin602@163.com, a13920246723@163.com, bzhaoyue_1214@126.com, cwangsen429@163.com

Abstract. In this paper, models for NO\textsubscript{x} emission prediction and denitration costs are built with support vector machine. The effects of the factors such as SCR inlet NO\textsubscript{x} content, unit load, oxygen content of exhaust gas, ammonia injection rate, air distribution condition, and coal type on NO\textsubscript{x} reduction are discussed. The denitration costs under different working conditions are calculated. The ammonia injection rate is optimized with genetic algorithm. It can be shown that the actual ammonia injection rate is 1%-3.5% lower than the optimal value.

1. Introduction

With the increasing requirement of the environment protection, the fee standard of NO\textsubscript{x} emissions is becoming increasingly high. Now China government charges the thermal power plants steadily higher fees based on the NO\textsubscript{x} emission values. According the pollutant discriminative charge policy in Tianjin, the charge standard is 8.50 yuan per kilogram in the key cities since July 1, 2014 and it is increased by 10 times than before.

Now selective catalytic reduction (SCR) has become the major denitration technology in thermal power plants with high NO\textsubscript{x} removal efficiency, low secondary pollution and mature technology. The basic principle of SCR is converting NO\textsubscript{x} into nitrogen (N\textsubscript{2}) and water (H\textsubscript{2}O) by dosing ammonia under the condition of catalyst. The main factors that influence the system inlet NO\textsubscript{x} content and denitration efficiency are active power, oxygen content of exhaust gas, air distribution condition, ammonia injection rate, coal type, denitration reaction temperature and catalyst activity. It is showed from the actual stable operation situation that the reaction temperature could be controlled by gas bypass, the catalyst can only be replaced after failure and the ammonia injection rae is one of the key controllable operating factors [1].

The ammonia injection control had been studied by many scholars [2-8]. Most of researches aim to decrease the NO\textsubscript{x} emission content, reduce the ammonia escape rate and improve the ammonia injection device, but few of them focus on minimizing the total costs of combustion and denitration while considering both the combustion and denitration efficiency.

In this paper, the ammonia injection rate is optimized to obtain the minimum total costs of combustion and denitration. The SCR inlet NO\textsubscript{x} content and denitration efficiency are predicted using support vector machine, then the total denitration cost is calculated based on the prediction, and genetic algorithm is designed to optimize the ammonia injection rate. A 300MW boiler is tested on the basis of the method.
2. Research Object

The denitration reactor and catalyst of SCR system are arranged with “2+1” mode. The reducing agent storage and preparation system are designed to meet the requirement that the NO\textsubscript{x} emission concentration is no more than 100mg/Nm\textsuperscript{3}. 2-layer catalyst is initial assembled to meet the emission requirement. High ash type SCR technique is employed and it is designed based on that the inlet NO\textsubscript{x} concentration is 600mg/Nm\textsuperscript{3}, 100 percent of the flue gas is treated and the final NO\textsubscript{x} emission concentration is below 100mg/Nm\textsuperscript{3}. The reducing agent is prepared with liquid ammonia by reducing agent public system. The Ammonia area system include ammonia unloading system, ammonia storage system, ammonia preparation system, valves, pipes and accessories. The denitration system is as shown in Fig.1.

![Denitration system](image)

*Figure 1. Denitration system.*

3. Research Method and Model Establishment

The denitration efficiency is predicted based on Support Vector Machine and then the NO\textsubscript{x} emission is calculated according to the predicted denitration efficiency. Denitration costs consist of ammonia consumption cost, electricity power consumption cost, pollution charge, electricity price compensation if meeting the standard and the fixed costs such as labor cost, depreciation cost and maintenance cost. The ammonia consumption cost is calculated with the ammonia consumption and the unit price. The numerical relations of denitration equipment current and ammonia dosing amount are obtained using data fitting method based on the power plant operation data to estimate denitration electricity power cost. The pollution charge is calculated according to the NO\textsubscript{x} emission concentration based on the related standard. It is concluded that whether to benefit the electricity price compensation is based on the calculated NO\textsubscript{x} emission concentration and the related policy. Other costs are basically fixed and considered as constant.

3.1. Denitration Efficiency Prediction Model

Multiple sets of data are chosen to train the model. Input parameters and output parameters are expressed as \( \{x_i, y_i\}^N \). \( x_i \) is used to express the input parameter from group \( i \), \( y_i \) is used to express the output parameter from group \( i \) and \( N \) is the sample size.

Radial basis function is used as the key function of Support Vector Machine.
The decision function is set as \( f(x_i) = w \cdot \Phi(x_i) + b \), \( f(x_i) \) is the model prediction, \( w \) is the weight coefficient vector and \( b \) is the intercept. The relaxation factors \( \xi_i \) and the allowed fitting error \( \epsilon \) are also introduced with \( \xi_i \geq 0 \) and \( \xi_i^* \geq 0 \). Constraints are as below:

\[
\begin{align*}
\xi_i^* & \geq 0 \\
\xi_i & \geq 0 \quad i = 1, \ldots, N
\end{align*}
\]

The model is set as:

\[
\min R(w, \xi, \xi^*) = \frac{1}{2} w \cdot w + C \sum_{i=1}^{k} \xi_i + \xi_i^*
\]

The constant \( C \) represents penalty coefficient and \( C \geq 0 \). The Lagrange function is introduced as below:

\[
L(w, b, \xi_i, \xi_i^*, \alpha_i, \alpha_i^*, \gamma_i, \gamma_i^*) = \frac{1}{2} w \cdot w + C \sum_{i=1}^{N} \left( \xi_i + \xi_i^* \right) - \sum_{i=1}^{N} \alpha_i \left( y_i - (\xi_i + \epsilon + f(x_i)) \right) - \sum_{i=1}^{N} \gamma_i^* \left( \xi_i + \xi_i^* \right)
\]

\( \alpha_i, \alpha_i^*, \gamma_i \) and \( \gamma_i^* \) represent Lagrange multiplier and they are all above zero. Minimum value points with respect to \( w, b, \xi_i \) and \( \xi_i^* \) of the function are calculated as below:

\[
\frac{\partial}{\partial w} L = 0 \Rightarrow w = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) \phi(x_i)
\]

\[
\frac{\partial}{\partial b} L = 0 \Rightarrow \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) = 0
\]

\[
\frac{\partial}{\partial \xi_i} L = 0 \Rightarrow C - \alpha_i - \gamma_i = 0
\]
\[
\frac{\partial}{\partial \xi_i} L = 0 \Rightarrow C - \alpha_i^* - \gamma_i^* = 0
\]  

(11)

The Lagrange dual function is obtained as below:

\[
\overline{\omega}(\alpha, \alpha^*) = -\frac{1}{2} \sum_{i, j=1}^{N} (\alpha_i - \alpha_j^*) (\alpha_j - \alpha_j^*) K(x_i, x_j) - \sum_{i=1}^{N} (\alpha_i + \alpha_i^*) + \sum_{i=1}^{N} (\alpha_i + \alpha_i^*) y_i
\]  

(12)

Then

\[
w = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) \varphi(x_i)
\]  

(13)

\[
f(x) = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) K(x, x_i) + b
\]  

(14)

According to the KKT theorem, the relations at the extreme value point are as below:

\[
\alpha_i [\xi_i + y_i - f(x_i)] = 0
\]  

(15)

\[
\alpha_i [\xi_i + y_i + f(x_i)] = 0
\]  

(16)

\[
i = 1, \ldots, N
\]  

(17)

It follows that \( \xi_i \gamma_i = 0, \xi_i^* \gamma_i^* = 0, i = 1, \ldots, N \).

Finally the decision function can be determined as:

\[
f(x) = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) K(x, x_i) + b
\]  

(18)

Active power, oxygen content of exhaust gas, ammonia injection rate, gas flow rate and coal type are chosen to be input parameters. SCR inlet NO\(_x\) concentration \(RNOx\) (mg/m\(^3\)) and denitration efficiency \(\eta\) are chosen to be output parameters. The relations of input parameters and output parameters are obtained based on the boiler operating data using the model established.

3.2. Verification of the prediction model

13 groups of data at different loads are chosen to be predicted and compared with the measured values [11]. The results are as follows:
Table 1. Predicted value vs. measured value of denitration efficiency.

| Group number | Unit Load | Measured Denitratio Efficiency | Predicted Denitratio Efficiency | Percentage Difference |
|--------------|-----------|--------------------------------|----------------------------------|-----------------------|
| 1            | 159.56    | 86.4                           | 87.92                           | 1.76%                 |
| 2            | 198.79    | 83.2                           | 88.02                           | 5.79%                 |
| 3            | 199.45    | 82.85                          | 84.75                           | 2.29%                 |
| 4            | 228.57    | 86.49                          | 87.98                           | 1.72%                 |
| 5            | 239.34    | 88.8                           | 87.74                           | -1.19%                |
| 6            | 270.11    | 90.93                          | 88.34                           | -2.85%                |
| 7            | 272.31    | 93.19                          | 90.81                           | -2.55%                |
| 8            | 273.08    | 93.95                          | 89.73                           | -4.49%                |
| 9            | 274.17    | 93.13                          | 89.53                           | -3.87%                |
| 10           | 278.35    | 95.38                          | 92.87                           | -2.63%                |
| 11           | 278.9     | 94.23                          | 89.98                           | -4.51%                |
| 12           | 287.69    | 93.83                          | 90.87                           | -3.15%                |
| 13           | 288.46    | 92.44                          | 89.95                           | -2.69%                |

As shown in Table 1, the selected validation sample covers all the load parts of the power plant. The percentage difference between prediction results and actual measured results is below 5% and can be accepted in engineering application. The prediction results could be considered accurate enough to calculate the costs in the next step.

4. Calculation of Denitration Costs

Denitration costs includes ammonia consumption cost, electricity power consumption cost, pollution charge, electricity charge compensation if meeting the standard and fixed costs such as labor cost, depreciation cost and maintenance cost [12].

The ammonia consumption cost [13-14] \( F_1 (\text{yuan/kg}) \) is calculated with the ammonia consumption \( W_a (\text{kg/h}) \) and the unit price \( D_1 (\text{yuan/kg}) \) as follows:

\[
F_1 = W_a \cdot D_1
\]  \hspace{1cm} (19)

The numerical relations of denitration equipment current and ammonia injection rate are obtained using data fitting method based on the power plant operation data. Usually electricity power cost would increase as the ammonia dosing increased, so the easiest linear relationship could be used as fitting equation:

\[
I = k \times W_a + b
\]  \hspace{1cm} (20)

Where \( k \) and \( b \) are constants and obtained by data fitting.

The electricity power consumption of denitration system could be estimated according to the load and the electricity power consumption cost \( D_2 (\text{yuan/kwh}) \) could be calculated with the electricity price \( F_2 (\text{yuan/h}) \).

\[
F_2 = 1.732 \times 6000 \times I \times 0.83 \times D_2 / 1000
\]  \hspace{1cm} (21)

\[
F_2 = \frac{1.732 \times 6000 \times (k \times W_a + b) \times 0.83 \times D_2}{1000}
\]  \hspace{1cm} (22)
The NOX concentration without denitration \(PNO_x (mg/m^3)\) could be calculated according to the predicted denitration efficiency, the measured SCR inlet NO\(_x\) concentration \(RNO_x (mg/m^3)\) and the gas flow rate \(Vq (m^3/h)\). Emission cost per unit \(D (yuan/kg)\) could be obtained with the state pollution charge standards. Then the pollution charge could be calculated.

NO\(_x\) emission concentration without denitration is calculated as below:

\[
PNO_x = RNO_x \times (1 - \eta)
\]

Pollution charge is calculated as below:

\[
F_3 = PNO_x \cdot Vq \cdot D_3 / 10^6
\]

\[
D_3 = f_p (PNO_x) = f_p (RNO_x, \eta)
\]

The specific equation \(f_p\) is based on the requirements of environment protection department.

It is concluded that whether to benefit the electricity price compensation \(F_4' (fen/kwh)\) according to the calculated NO\(_x\) emission concentration and the related policy.

\[
F_4 (yuan/h) = 10 \cdot F_4' \cdot P
\]

\[
F_4' = f_b (PNO_x) = f_b (RNO_x, \eta)
\]

The specific equation \(f_b\) is based on the requirements of environment protection department.

Other costs such as depreciation cost, maintenance cost, catalyst cost and labor cost are basically fixed and expressed as \(G [15]\).

The cost per unit power unit generation of the denitration system \(F(yuan/kwh)\) is calculated as below:

\[
F = \frac{F_1 + F_2 + F_3 - F_4 + G}{P}
\]

5. Optimization and Effects of Ammonia injection rate

Genetic algorithm is used to optimize the Ammonia injection rate. The load, oxygen content in exhaust gas, SCR inlet NO\(_x\) concentration and gas flow rate are considered as fixed. The ammonia injection rate is the only variable to reach the lowest cost. The denitration efficiency is considered as a function of ammonia injection rate and the total cost is also considered as a function of ammonia injection rate.

The ammonia injection rate ranged from 50t/h and 350t/h and it basically covered all states of 300MW unit. Then the original problem is transformed into a search for the best ammonia injection rate from the interval [50-350] that could make the cost minimum. A fitness function \(F (Wa)\) is defined on the interval to express the relation between ammonia injection rate and total costs. The population size \(N\) is set to 8, the crossover probability \(P_c\) is set to 0.8, the mutation probability \(P_m\) is set to 0.01 and the maximum Iterations \(T\) is set to 200. The interval is encoded using a binary system based on the required accuracy. Nine-figure binary coding is used in this paper and the precision reached 1t/h.

\(N\) individuals are randomly generated from the binary interval as \(N, S, s, S, s, S, s, S, s\). The algebraic counter is set to 1.
The fitness of each individual \( F(s_i) \) is calculated based on the decimal numbers to which the binary numbers corresponded.

The individual with the minimum fitness is chosen to be exported.

\[
P(W_{a_i}) = F(W_{a_i}) / \sum_{j=1}^{N} F(W_{a_j})
\]  

(29)

One individual from \( S \) is selected randomly to copy the chromosome each time with the selection probability \( P(W_{a_i}) \) and it would be repeated \( N \) times. Then \( n \) copied chromosomes would form the population \( S_1 \).

According to the crossover probability \( P_c \), \( c \) chromosomes are determined from \( S_1 \) and they are paired to perform crossover operations. The new generated chromosomes would form the population \( S_2 \).

According to the mutation probability \( P_m \), \( m \) chromosomes are determined from \( S_2 \) and they performed mutation operation separately. The new generated chromosomes would form the population \( S_3 \).

Population \( S_3 \) is considered as the new generation and \( S \) is replaced by \( S_1 \), \( t = t+1 \). The fitness is calculated again and copying, crossover and mutant process would be cycling.

The final result is the minimum ammonia injection rate of all.

For example, when active power is 229.12MW, oxygen content is 4.94%, gas flow rate is 1081km\(^3\)/h, ammonia injection rate is 195kg/h, the predicted NO\(_x\) production rate is 551.16mg/m\(^3\), denitration efficiency is 88%. Taking the ammonia injection rate as independent variable and the minimum cost as searching target, the calculated ammonia injection rate is 198.37kg/h. Costs of before optimization vs. Costs of after optimization are shown in Table 2.

| Cost subentry            | Before optimization (yuan/kWh) | After optimization (yuan/kWh) | Percentage difference |
|--------------------------|--------------------------------|------------------------------|-----------------------|
| ammonia consumption      | 0.00384                        | 0.0039                       | 1.56%                 |
| Electricity consumption  | 0.00072                        | 0.00079                      | 9.72%                 |
| pollution charge         | 0.00105                        | 0.00067                      | -36.19%               |
| compensation             | 0.01                           | 0.01                         | 0.00%                 |
| Others                   | 0.01813                        | 0.01813                      | 0.00%                 |
| Sum                      | 0.03374                        | 0.03352                      | -0.65%                |

It is shown from Fig.2 and that ammonia consumption cost, Electricity consumption cost and pollution charge cost change while electricity price compensation and other costs remain the same basically. After optimization, the ammonia consumption cost increase by 1.56%, the Electricity consumption cost increase by 9.72% while pollution charge cost decrease by 36.19%. Finally the total costs decrease by 0.65%. After optimization, however ammonia consumption cost and electricity consumption cost increase a little, the total costs decrease slightly because of the pollution charge cost reduction. It can be concluded that the proportion of each subentry of denitration costs changes because of the change of pollution charge cost. Even increasing the ammonia injection rate will increase the ammonia consumption, it can also reduce the NO\(_x\) emission and the pollution charge to make total costs decrease.

Repeat the same procedure and calculate the best ammonia injection rate under different working conditions.
Table 3. The amount of ammonia spray before and after optimization in different work conditions.

| Condition | Load (MW) | Measured injection rate (t/h) | Injection rate after optimization (t/h) | Percentage difference (%) |
|-----------|-----------|-------------------------------|----------------------------------------|---------------------------|
| 1         | 162.42    | 175                           | 180.42                                 | 3.10                      |
| 2         | 198.79    | 189.53                        | 196.32                                 | 3.58                      |
| 3         | 229.67    | 195                           | 198.07                                 | 1.57                      |
| 4         | 239.34    | 193.68                        | 193.42                                 | -0.13                     |
| 5         | 273.08    | 205.16                        | 207.77                                 | 1.27                      |
| 6         | 278.9     | 238.1                         | 241.34                                 | 1.36                      |

As shown in Table 3, the ammonia injection rate under 5 conditions increases and the ammonia injection rate under 1 condition decreases. It probably because that the NO\textsubscript{x} removal rate increasing caused by ammonia injection rate increasing will reduce the pollution charge cost even it can also increase the ammonia consumption cost.

6. Conclusion
In this paper, models for Relationship between active power, oxygen content of exhaust gas, ammonia injection rate, gas flow rate, SCR inlet NO\textsubscript{x} content and denitrification efficiency are established and then the model for relationship between the ammonia injection rate and denitration costs is established. The ammonia injection rate is optimized using the genetic algorithm to achieve the minimum total denitrification costs. It is shown from the results that the total denitration costs decrease even the ammonia injection rate increases by about 4.5%. The research method in this paper can be used to guide the ammonia injection rate control of denitrification system in power plants to make power plants achieve higher economy and lower costs at the premise of meeting environment requirements.

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