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Research on the Optimization Model of Octane Loss Based on Genetic Algorithm

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Abstract: This paper develops an optimisation model for octane loss under the constraints of genetic algorithm based desulphurisation. A model on product sulphur content is established, five main variables for modelling product sulphur content are selected based on the process related to product sulphur content in the gasoline refining process, containing three operational variables and two non-operational variables, and LSSVM is used to build the model for product sulphur content. Based on the optimization model, the optimized operating conditions for the main variables were obtained, with a view to providing some reference for other enterprises in the industry and providing some social research significance and value for gasoline clean-up.

1. Introduction

Nowadays, China's crude oil resources rely heavily on sulfur-containing and high-sulfur crude oils from abroad, especially from the Middle East. Heavy oil accounts for 40-60% of such crude oil. As heavy oil is difficult to be applied directly, in order to use this resource more effectively, heavy oil lightening process technology with catalytic cracking as the core has been vigorously developed, and with the increasing awareness of environmental protection, gasoline clean-up technology has been developed rapidly [1]. How to effectively reduce the olefin and sulphur content of gasoline while maintaining the octane value of the oil has become the focus of gasoline cleaning research.

In this paper, a model was established for the sulphur content of the product, combine the process principles related to sulphur content in gasoline catalytic cracking refineries with the main variables of the octane loss model, jointly select the variables required to establish the product sulphur content model and then establish the octane loss optimisation model [2].

The data in the paper comes from a real sample of companies in the industry provided by the 17th China Postgraduate Innovation and Practice Competition "Huawei Cup", and the historical data provided by this company are used in this paper to solve the modelling and optimisation problem of octane loss.

2. Product sulfur content model

2.1 Determination of main variables in modeling

In the production process of catalytic cracking refined gasoline, the main desulfurization methods to control the sulfur content of products include raw material desulfurization, process desulfurization, hydrodesulfurization and oxidative desulfurization. The quality of raw materials is inconvenient to improve, and industrial verification shows that hydrodesulfurization and adsorption desulfurization have good production effects [3]. Therefore, in the input variables of the product sulfur content model, the hydrogen-oil ratio of MV_1 was selected, the hydrogen sulfide gas flow rate of MV_4 reducer and the bottom temperature of MV_6 reactor related to hydrodesulfurization. In addition, the property S of PV_{13} regenerated adsorbent related to adsorption desulfurization process and the sulfur content of PV_1 raw material related to raw materials are selected, with five variables, which are shown in Tab.1.

Table 1. Main variables of product sulfur content model.

Type	Variable sequence number	Name
Operate variable	MV_3	Reducer pressure
	MV_4	Flow rate of fluidized hydrogen in reducer
	MV_6	Reactor bottom temperature
Nonoperational variable	PV_1	Sulfur content of raw materials
	PV_{13}	Regenerated adsorbent S

2.2 Establishment of least squares support vector machine model

2.2.1 Modeling process of support vector machine model

The modeling process of LSSVM is to first determine the kernel function, its parameters and regularization parameters of the function model, and then train the model through input and output. The support vector and threshold are solved by the least square method [4]. Given the data training set T, construct a prediction function with the following form, so that the output of the prediction function is close to the actual output function value of the sample:

$$f(x)=\omega^T\varphi(x)+b \tag{1}$$

$$T=\left\{(x_1,y_1),\leftrightharpoons(x_N,y_N)\right\} \tag{2}$$

The algorithm is as follows:

Step1:build the objective function of LSSVM optimization problem.

$$\min\frac{1}{2}\omega^T\omega+\frac{1}{2}r\sum_{i=1}^{N}\xi_i^2 \tag{3}$$

Step2:construct constraints.

$$y_i=\omega^T\varphi(x_i)+b+\xi_i \tag{4}$$

Step3:build Lagrange function:

$$L=\frac{1}{2}\omega^T\omega+\frac{1}{2}r\sum_{i=1}^{N}\xi_i^2-\sum_{r=1}^{N}\alpha_i\left\{\omega^T\varphi(x_i)+b+\xi_i-y_i\right\} \tag{5}$$

Step4:from KKT condition, get the condition that the partial derivative of each variable is 0 at the optimal value:

$$\begin{cases} \omega = \sum_{i=1}^{N} \alpha_i \varphi(x_i) \\ -\sum_{i=1}^{N} \alpha_i = 0 \\ \alpha_i = r\xi_i \\ \omega^T \varphi(x_i) + b + \xi_i - y_i = 0 \end{cases} \tag{6}$$

Step5: solve.

$$\begin{cases} Z = [\varphi(x_1), \ldots \varphi(x_N)]^T \\ y = [y_1, \ldots y_N]^T \\ I = [1, 1 \ldots 1]^T \\ a = [a_1, \ldots a_N]^T \end{cases} \tag{7}$$

$$f(x) = \sum_{r=1}^{N} \alpha_i k(x, x_i) + b \tag{8}$$

2.2.2 Establishment of Product Sulfur Content Model Based on LSSVM

In this paper, a product sulfur content model with five input variables and one output variable based on LSSVM is established. Here, the sample data are also randomly divided into training sample set and test sample set according to the ratio of 8: 2, that is, 325*80%=260 training data and 325*20%=65 test data. RBF_kernel function is selected for LSSVM kernel function. The network is trained by training data to extract the deep mapping relationship between input variables and output variables, and then the accuracy of the model is verified on the test set, and the product sulfur content model based on LSSVM is continuously adjusted and finally constructed.

In this paper, the LSSVM model is built in Matlab software, and the parameters are constantly adjusted. C is the regularization parameter as 500 and σ is the kernel function parameter as 2.5. Is the maximum number of neurons in MN RBF network, DF is the display interval, and epoch is the iteration number of model training.

The input of RBF kernel function only activates the nearby sample points, and the kernel function has fewer parameters, so the complexity of the model is smaller, as shown in the following formula:

$$k(x_i, x) = e^{-\frac{\|x - x_i\|_2^2}{2\sigma^2}} \tag{9}$$

2.2.3 Modeling results of product sulfur content

Fig.1 is the final product sulfur content model result based on LSSVM. The blue dots in the figure are the real values of the test data, and the red dots are the predicted values output by the model. It can be seen that the trends among the data points are basically consistent, and the difference between the real values and the predicted values is about 3.5 on average, indicating that

the model has achieved a good result, which meets the requirements and lays a good foundation for the subsequent optimization model construction.

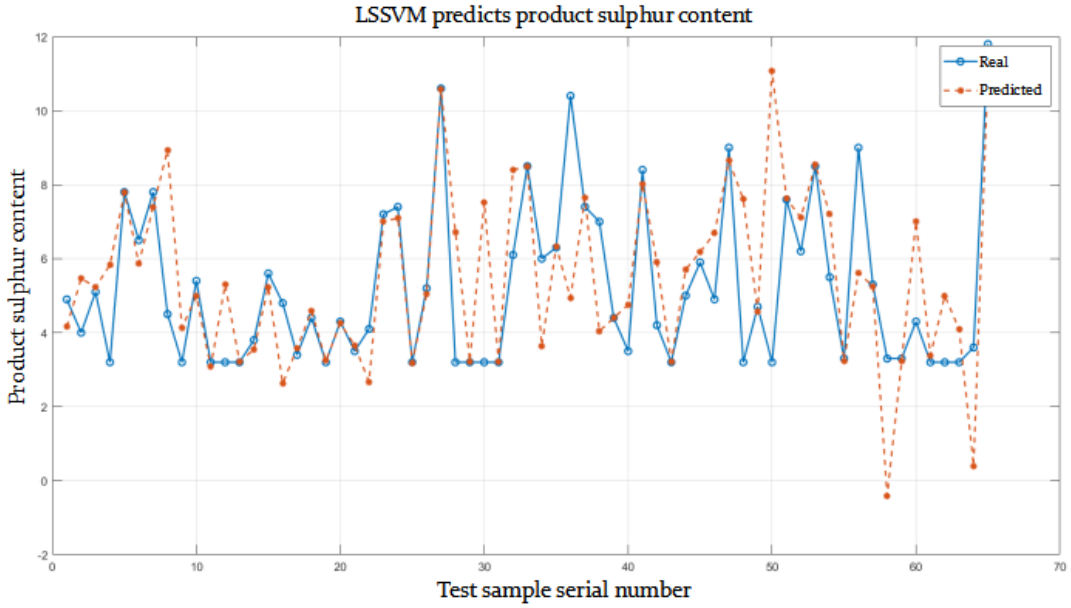

Figure 1. Results of product sulfur content model based on LSSVM.

3. Model building

3.1 Determination of the optimisation objective function

As the optimization of gasoline catalytic cracking must meet the premise of ensuring that the sulfur content of the product is not higher than $5\,\mu g/g$, so that the octane loss of the product is as low as possible [5]. Therefore, the optimization condition is set to be the minimum octane loss, and the optimal solution of octane loss is solved for each sample, and then the sample with the optimal solution greater than 30% is selected, which is the sample that the model is looking for, so the optimization condition is:

$$\min J(t) = \min(\Delta R)^2 \tag{10}$$

f_{ls_svm} is a minimum support vector machine model for the sulphur content of the product, with the constraint:

$$f_{ls\_svm}(PV_{1,}PV_{13,}MV_{1,}MV_{4,}MV_{6}) \le 5 \tag{11}$$

$$Min \le MV_i \le Max \tag{12}$$

The operational variables for product sulphur content and product octane loss are selected and concentrated, and the elements in the set MV_i.

$$MV_i \in \left\{MV_{1,}MV_{4,}MV_{6}\right\} \tag{13}$$

The adjustment of operating variables in the production of refined gasoline cannot be done in one go, otherwise it may easily lead to production safety accidents. The adjustment of the operating variables needs to be adjusted slowly according to the values of the operating variables solved by the optimisation to push the process reaction to a state with low product octane loss and low product

sulphur content, so the upper and lower limits of the operating variable adjustment value ΔMV_j were defined as 30% of the upper and lower limits of the range of values of the operating variables.

$$\Delta MV_j \in S = \left\{\Delta MV_{1,}\Delta MV_{4,}\Delta MV_6\right\} \tag{14}$$

$$-0.051 \le \Delta MV_1 \le 0.051 \tag{15}$$

$$-120 \le \Delta MV_4 \le 120 \tag{16}$$

$$-9.3 \le \Delta MV_6 \le 9.3 \tag{17}$$

The smaller the adjustment value of the corresponding operating variables, the better, while reducing the loss of octane and ensuring that the sulphur content of the product meets the requirements. Therefore the final optimisation objective and constraints for the octane loss optimisation model under the desulphurisation constraints developed in this paper are given by the following equation, where λ is a weighting factor.

$$\begin{aligned}
&\min J(t) = \min\{(\Delta R)^2 + \lambda \sum_{\Delta \mathrm{MV}_j \in S} \Delta \mathrm{MV}_\mathrm{j}^2\} \\
&s.t.\begin{cases} f_{ls_svm}(PV_{1,}PV_{13,}MV_{1,}MV_{4,}MV_6) \le 5 \\ Min \le MV_i \le \mathrm{Max} \\ -0.051 \le \Delta MV_1 \le 0.051 \\ -120 \le \Delta MV_4 \le 120 \\ -9.3 \le \Delta MV_6 \le 9.3 \end{cases} \\
&MV_i \in \left\{MV_{1,}MV_{4,}MV_6\right\} \\
&\Delta MV_j \in S = \left\{\Delta MV_{1,}\Delta MV_{4,}\Delta MV_6\right\}
\end{aligned} \tag{18}$$

3.2 Determination of the overall structure of the optimisation model

The operating conditions are optimised subject to an upper limit of the product sulphur content constraint. The radial basis neural network model for product octane loss is therefore passed to the optimisation solver as the objective function and the product sulphur content model is passed to the optimisation solver as the constraint. The optimisation solver regulates the smallest possible objective jointly with the variable operating variables and converts the multi-objective optimisation into a single objective optimisation to solve for the optimised solution, i.e. the *MV* operating conditions. The operating conditions are passed to the product octane radial basis neural network model to obtain the optimised octane loss, compared with the initial octane loss to obtain the octane loss reduction, and finally to obtain the sample with an optimised octane loss reduction greater than 30%, i.e. the sample for which the model requires a solution, and the *MV* operating solution for this part of the sample is the optimised operating condition for the main variable corresponding to the sample.

4. Model solving

4.1 Genetic algorithm based solution method

After building a RBF neural network model for octane loss of gasoline catalytic cracking

products, an optimised MV value is solved by giving an optimised feasible solution within a set acceptable range.

$$\min J(t) = \min\{(\Delta R)^2 + \lambda \sum_{\Delta \mathrm{MV}_j \in S} \Delta \mathrm{MV}_j^2\}$$

$$s.t. \begin{cases} f_{ls\_svm}(PV_{1,}PV_{13,}MV_{1,}MV_{4,}MV_6) \le 5 \\ Min \le MV_i \le \mathrm{Max} \\ -0.051 \le \Delta MV_1 \le 0.051 \\ -120 \le \Delta MV_4 \le 120 \\ -9.3 \le \Delta MV_6 \le 9.3 \end{cases} \tag{19}$$

$$MV_i \in \{MV_{1,}MV_{4,}MV_6\}$$

$$\Delta MV_j \in S = \{\Delta MV_{1,}\Delta MV_{4,}\Delta MV_6\}$$

Where ΔR is calculated from the RBF prediction model, Matlab simulations were performed on the developed octane loss optimisation model under desulphurisation constraints until the algorithm finally converged to a steady state. The basic experimental parameters were set to 50 for the population size, 0.8 for the crossover probability, 0.2 for the variation probability and 200 for the maximum number of evolutions. The simulation of the model showed a linear increase in the initial individual values as the number of iterations increased, proving that this solution method is effective.

After solving the optimisation model using the genetic algorithm, the optimisation solution will be obtained for 325 samples. Based on the overall structure of the optimisation model, it can be seen that the next step is to select the samples with an optimised octane loss value reduction greater than 30%, i.e. the target samples, and to determine the operating conditions for the optimisation of the main variables corresponding to these samples.

4.2 Model solution results

4.2.1 Results of changes in target variables before and after optimisation

Based on the above work, the final optimization results for 325 samples were obtained in this paper, i.e. the changes in the sulphur content variables and the changes in the octane loss variables of the sample products before and after optimization. Some of the results are shown in Tab.2.

Table 2. Partial sample optimization results.

Sample number	Before adjustment	After adjustment	Before adjustment	After adjustment
	PV_8Sulfur content of product($\mu g/g$)		ΔR	Loss of RON
1	3.2	4.0	1.4	0.6687
2	3.2	4.8	1.2	0.6474
3	3.2	4.6	1.4	0.6366
4	3.2	4.7	1.4	0.6880
5	3.2	4.6	1.3	0.6847
6	3.2	5.0	1.4	0.6251
7	4.6	3.0	1.2	0.6302
8	6.6	3.5	1.3	0.6212

Fig.2 shows the before and after optimization of sulfur content in the product. In the figure, the blue line is the sulfur content of the original product of the sample. Because the title requires that the sulfur content of the product should not exceed 5 $\mu g / g$, the yellow line is the sulfur content value of the optimized sample product, which can be obtained after optimization. The sulfur content of all sample data does not exceed 5 $\mu g / g$, which meets the optimization constraints and the model solution is effective [6].

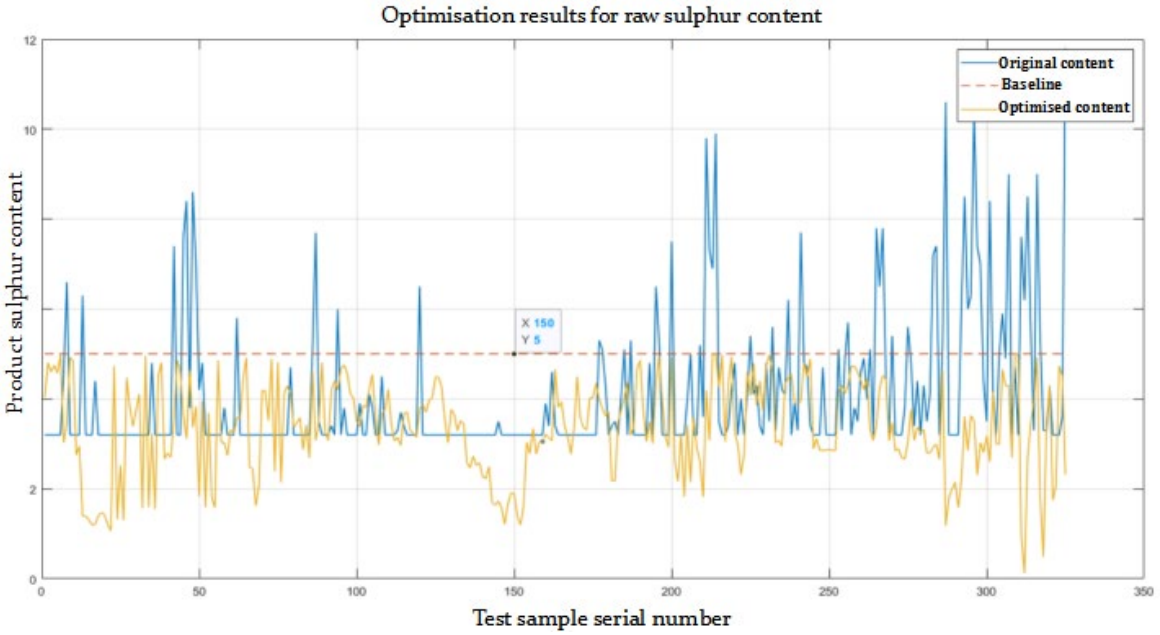

Figure 2. Before and after optimisation of product sulphur content.

Fig.3 shows the before and after graphs of octane loss optimisation. In the graph, the blue line is the original octane loss value of the sample and the yellow line is the octane loss value of the sample after optimisation. As can be seen from the graph, most of the samples were optimised to have an octane loss greater than 30%, with only some samples failing to meet this target. 23 samples in total were calculated to have failed to meet the requirement.

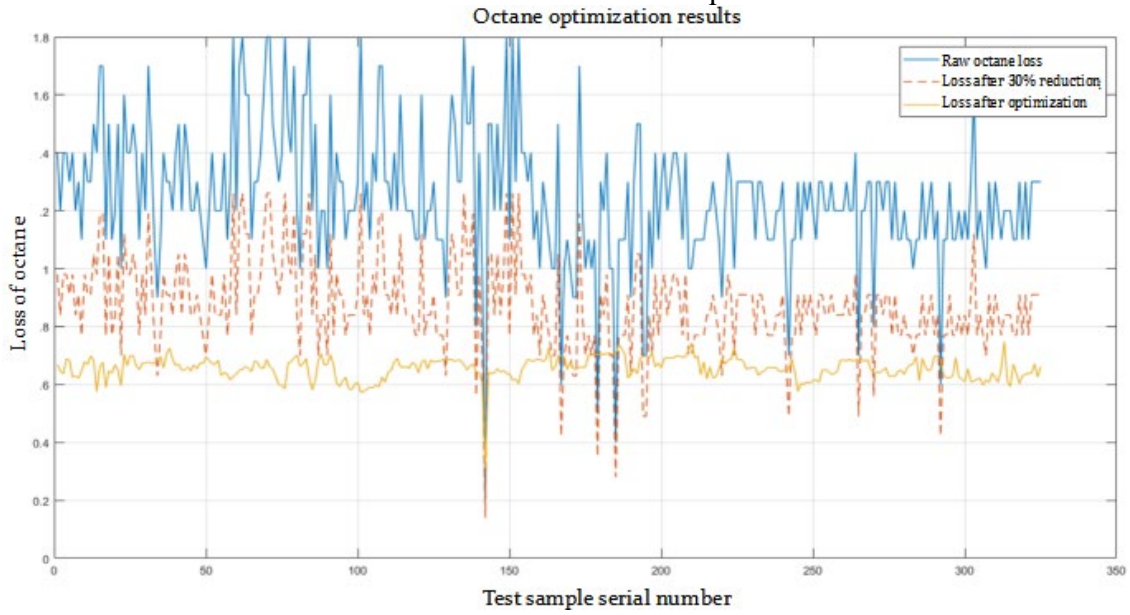

Figure 3. Before and after octane loss optimisation.

4.2.2 Optimize the operating condition results of the corresponding operating variables.

According to the above results, a total of 23 samples failed to meet the requirements, and the results are shown in Tab.3. In addition, it also shows that a total of 302 samples are optimized, and the octane number loss is more than 30%.

Table 3. Some samples with RON loss decreasing by less than 30%.

Sample number	Original RON loss	RON loss after optimization	RON loss reduction
34	0.9	0.6811266	24.32%
129	0.9	0.686326205	23.74%
139	0.8	0.643719084	19.54%
142	0.2	0.311788411	-55.89%
…	…	…	…
270	0.8	0.641110236	19.86%
292	0.6	0.68685614	-14.48%

It is known that 302 samples have lost more than 30% of octane number after optimization. For these samples, the changes of the main variables that make them achieve this goal are the solutions obtained by these sample optimization models, that is, the optimized operating conditions of the main variables corresponding to these samples [7]. Some changes of optimization operations are shown in Tab.4.

Table 4. Changes of partial optimization operation.

Sample number	Before adjustment	After adjustment	Before adjustment	After adjustment	Before adjustment	After adjustment
	Hydrogen-oil ratio MV_1		Flow rate of fluidized hydrogen in reducer MV_4		Reactor bottom temperature MV_6	
1	0.27632	0.3100	647.7524	820.0000	421.6081	411.0000
2	0.27713	0.3100	651.8219	820.0000	417.9278	411.0000
3	0.27701	0.3100	650.7472	820.0000	420.0035	411.0000
4	0.27722	0.2300	652.6691	820.0000	419.9648	411.0000
5	0.27731	0.3100	649.3409	820.0000	422.1289	411.0000
6	0.27661	0.3000	650.1234	820.0000	422.1307	411.0000
7	0.27741	0.3100	649.1494	820.0000	421.3018	411.0000
8	0.27692	0.3100	649.7636	820.0000	418.6726	411.0000
…	…	…	…	…	…	…
11	0.28884	0.2300	648.6645	600.0000	418.0324	411.0000

5. Conclusion

This paper focuses on the optimization model of octane loss under desulphurization constraints based on real sample data from an industrial unit of an enterprise. Firstly, a model on product sulphur content was developed, and five main variables for modelling product sulphur content were selected based on the processes related to product sulphur content in the gasoline refining process, containing three operational variables and two non-operational variables. The LSSVM was then used to model the product sulphur content, determine the objective function and constraints of the octane loss optimisation process, and build the overall structure of the octane loss optimisation

model; next, a genetic algorithm belonging to a heuristic algorithm was used to solve the octane loss optimisation model under the established desulphurisation constraints. The results show that a total of 302 samples were optimised with an octane loss greater than 30%. Based on the optimisation model, the optimised operating conditions for the main variables corresponding to these samples were also obtained.

References

[1] Bao Liu, Weiqi Ni. Analysis of factors influencing octane loss of gasoline in S Zorb unit[J]. Qilu Petrochemical, 2019, 47(02):102-104+124.

[2] Hongtao Li, Wenping Wei, Guoquan Jiang, Rongbin Zhao,Liankun Feng. Balance between gasoline hydrodesulfurization and octane loss[J]. Petrochemical Technology and Applications, 2017, 35(04):326-328.

[3] Zongxuan Li. An analysis of methods to control octane loss in gasoline hydrodesulfurization[J]. Chemical Management, 2020(06):148-149.

[4] Afshin Tatar, Ali Barati, Adel Najafi, Amir H. Mohammadi. Radial basis function (RBF) network for modeling gasoline properties[J]. Petroleum Science and Technology, 2019, 37(11).

[5] Yueqing Li, Siyi Jin, Shaohui Tao, Ning Li. Least squares support vector machine for soft measurement of gasoline dry points in atmospheric pressure towers[J]. Computers and Applied Chemistry, 2008(08):928-930.

[6] Chao Li, Jie Wang, Yuntao Shi, Jinlong Li. Genetic algorithm-based gasoline blending optimization system[J]. Industrial Control Computer, 2018, 31(10):79-81.

[7] Feleke Bayu, Debashish Panda, Munawar A. Shaik, Manojkumar Ramteke. Scheduling of gasoline blending and distribution using graphical genetic algorithm[J]. Computers and Chemical Engineering, 2020, 133.