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Octane Number Prediction of Blend Gasoline Based on Improved Particle Swarm Optimization

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Abstract: *The octane number of hydrogenated gasoline is difficult to be obtained in real time in the modeling of finished gasoline blending formula. Considering the problems of XGBOOST algorithm, gradient lifting tree algorithm and random forest regression algorithm network, a dynamic harmonious search hybrid particle swarm optimization (DSHPHO) algorithm was proposed to predict the octane number of finished gasoline. In this algorithm, the improved HS algorithm is embedded into the PSO algorithm, and all the particles are considered as harmonious memory (HM). Search by harmony search (HS) algorithm of randomness and evolution mechanism to improve the diversity of particle swarm, makes more ergodic particle swarm at the beginning of the search, reduce sensitivity to the initial value of the algorithm and keep randomly generated in the whole evolution process of the possibility of new particles, fundamentally solves the particle swarm optimization algorithm in dimension increase diversity is less defects. The algorithm has faster convergence speed and better global search ability. Finally, based on this method and industrial historical data, the octane number prediction model of hydrogenated gasoline components is established. The simulation results show that the dynamic harmonious search hybrid particle swarm optimization algorithm has better prediction performance than the traditional particle swarm optimization algorithm, and can be used to predict the octane number.*

Keywords: *Octane number, Particle Swarm Optimization, Dynamic Harmonious Search*

1. Introduction

As a major power energy consumption, China's crude oil imports more than 70%, and this part of the import crude oil are sulfur or high sulfur crude oil, in order to effectively use the heavy oil resources, reduce emissions and the impact on the atmospheric environment, need of this part of the heavy oil catalytic cracking process, in order to achieve an heavy oil, thus reduce sulfur and olefin content. At the same time, the qualified finished gasoline is a mixture of various components in different proportions according to the actual quality of each added component and the label index of different finished oil, and the key to ensure the quality of oil is to strictly control its added amount. However, in the actual industry, the addition of component oil is still based on the linear collocation of refined oil label and raw material components. This rough linear blending mode may lead to excess product quality, increase the production cost of enterprises and cause serious waste of resources. Octane number, as the key index to measure the quality of oil, is also the basis of establishing the model of harmonic formula. It is of great significance to establish an appropriate model to predict the octane number and reduce the loss of octane number while reducing the sulfur content.

In recent years, many scholars have also carried out related research in this field [1-3]. The traditional octane number research mainly has two aspects. One is the quantitative structure-property correlation study of gasoline octane number at the molecular level, such as topological index method, group contribution method, etc [4]. Second, based on instrumental analysis, analysis of each gasoline component, component absorbance, component content, using these parameters for linear modeling analysis of gasoline mixture octane number, such as principal component analysis, multiple linear regression combination, etc [5]. Particle Swarm Optimization (PSO) algorithm is an optimization method based on swarm intelligence. It simulates the migration and aggregation behavior of birds in the process of foraging, and searches the optimal solution through the collective cooperation among birds. The POS algorithm searches for the optimal value through a series of iterations after initializing a set of random solutions. Compared with other optimization algorithms based on swarm intelligence,

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such as genetic algorithm (GA) and evolutionary algorithm (EA), PSO algorithm has the characteristics of simple operation, easy implementation and fewer control parameters. It has been studied by many scholars at home and abroad, and has been successfully applied to function optimization, structural optimization and other scientific and engineering fields. However, like most other stochastic optimization algorithms, particle swarm optimization algorithm also has the disadvantages of low accuracy and easy to generate scattered wind. Especially, with the increase of dimension, the diversity of population decreases. The particle swarm may miss the optimal solution and the algorithm does not converge. Potter separates the search Spaces by decomposing the solution vectors into vectors of lower dimension, and then searches each of these smaller search Spaces using a separate GA algorithm. Frans applied Potter's method to the PSO, which ensures that the particle swarm can search every possible region, but at the same time increases the complexity of the algorithm.

Although these methods have improved the optimization performance to varying degrees, most of them are still based on one algorithm and indirectly introduce part of the operation of other algorithms, so they lack of more effective deep fusion. To sum up, the finished product to reconcile formula modeling of octane number of gasoline hydrogenation accurately forecast the demand of drive, based on the principal component analysis (pca) filter mainly from the historical data of some petrochemical enterprise operating variables, and selected the XGBoost, GBDT and random forest three methods comparative research, draw the prediction error density diagram, select prediction effect is the best algorithm as the basis of octane number prediction model is established, at the same time to ensure that the sulfur content is not more than 5ug/g, using the improved particle swarm algorithm, dynamic harmony search (DHSPSO) hybrid particle swarm algorithm, this algorithm, The improved HS algorithm is embedded into the PSO algorithm, and all the particles are considered as harmonious memory (HM). By harmony search (HS) algorithm randomness and evolution mechanism to improve the diversity of particle swarm, makes more ergodic particle swarm at the beginning of the search, reduce sensitivity to the initial value of the algorithm and keep randomly generated in the whole evolution process of the possibility of a new particle, fundamentally solves the dimension increases when the algorithm diversity is less defects. The algorithm has faster convergence speed and better global search ability. The octane number can be predicted in real time, and the loss of octane number can be reduced as far as possible while the oil is desulfurized.

2. Modeling idea of finished gasoline blending formula

2.1 Modeling ideas

Finished gasoline blending refers to the technology of blending non-standard gasoline with various components and additives to meet customers' requirements of national standard gasoline. The blending process is mainly based on the blending formula model. According to the parameters of the component oil input by the operator, it is calculated according to the existing model to obtain a set of blending proportion in line with the product indicators, which is converted into the component oil flow value, which is distributed to the field operator as the initial set value for blending. Octane number measurement is relatively complex. In practice, octane number measurement is based on the processing of original operating variables. Various theoretical models and mathematical methods are used for data analysis, and then cluster analysis is used to eliminate interfering factors and increase the independence between variables, so as to predict the change of octane number. In this paper, the historical data of FCC gasoline refining desulfurization unit of a petrochemical enterprise were selected to conduct principal component analysis on these operating variables, and 26 major operating variables were extracted for modeling, including R102 converter line differential pressure, R102 converter line differential pressure, cold nitrogen filter ME-114 differential pressure, etc.

2.2 Model validation

In order to predict octane number loss as accurately as possible, three methods, Xgboost[5-7], GBDT and random forest, were selected for comparative study, because parameter setting has a crucial influence on model verification, which directly affects the prediction performance of the model. In order to compare the prediction performance of different algorithms, the parameter Settings in this paper are completely consistent. The prediction error density plot is shown below:

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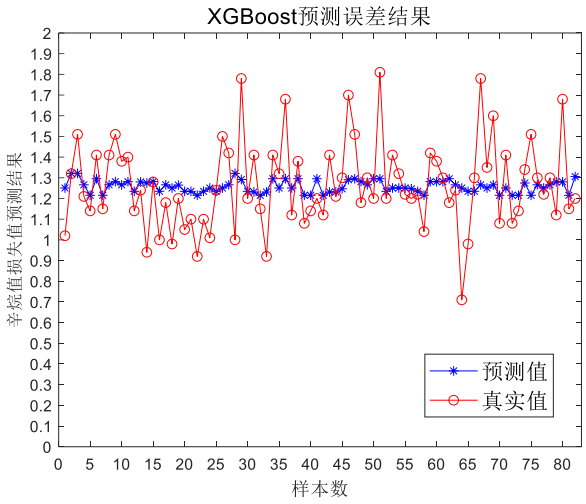

Figure 1: XGBoost predicts error results

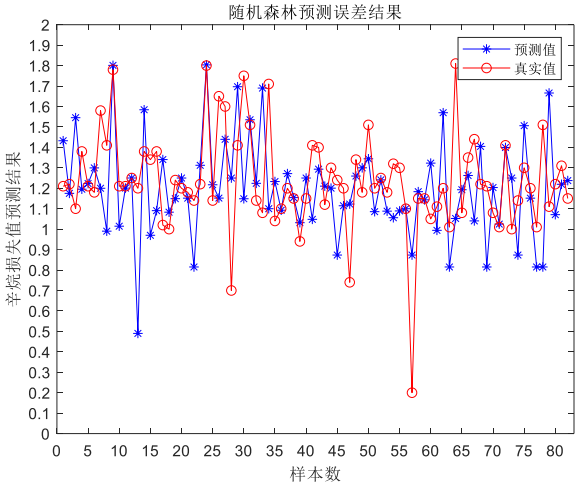

Figure 2: Random forest prediction error results

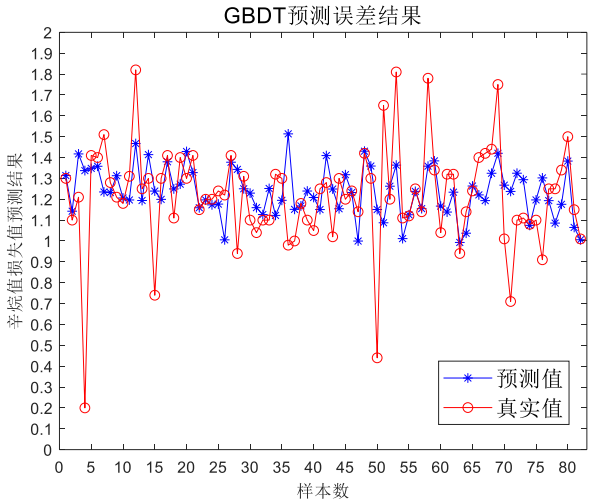

Figure 3: GBDT prediction error results

It can be seen from Table 1 that when the GBDT regression algorithm is used to construct the octane number prediction model[8], the performance of the predicted value, such as mean square error, absolute pair error sum and accuracy within the corresponding error, is greatly improved compared with the other two methods. In the network training time, compared with the other two algorithms, its value also decreased significantly. By comparing the accuracy within the range of 0.05 and 0.15, it can

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also be seen that GBDT regression algorithm has the best accuracy. To sum up, GBDT regression algorithm is used to establish a model for predicting octane number loss.

Table 1: Model performance evaluation

Methods	MSE	RMSE	MAE	R^2	MAPE
XGBoost	4.8034	2.1917	14.5437	0.65	19.7785
GBDT	9.2563	3.0424	20.6466	0.75	8.3320
Random forests	6.2252	2.4950	16.3626	0.58	13.3330

3. Dynamic Harmonious Search Hybrid Particle Swarm Optimization Algorithm

3.1 PSO Algorithm

Particle Swarm Optimization (PSO) algorithm[9] is an optimization method based on swarm intelligence. It seeks the optimal solution through the collective cooperation among birds by simulating the migration and aggregation behavior in the process of bird chamber. A particle is used to simulate the above individual birds, and each particle can be regarded as a searching individual in the n-dimensional search space. The current position of the particle is a candidate solution of the corresponding optimization problem, and the flight process of the particle is the searching process of the individual. The flight velocity of particles can be adjusted dynamically according to the historical optimal position of particles and the historical optimal position of population. A particle has only two properties: speed, which is how fast it is moving, and position, which is the direction it is moving. The optimal solution searched by each particle individually is called individual extremum, and the optimal individual extremum in the particle swarm is regarded as the current global optimal solution. Iterate constantly, updating speed and position. Finally, the optimal solution satisfying the termination condition is obtained.

3.2 DHSPSO lgorithm

The HS[10] algorithm provides a new way to generate a new particle. The difference between HS algorithm and PSO algorithm is that it generates a new vector on the basis of considering all the existing vectors. USES the evolution mechanism in the process of evolution, and in the whole process of evolution to keep randomly generated the possibility of new particles, optimization of operating parameters HM - the introduction of CR and PAR can make the solution vector escape from local optimal solution, thus fundamentally solved the initial random sample's influence on the result, and when the dimensionality increases when the defects of PSO algorithm diversity is less[11-12]. In this algorithm, the improved HS algorithm is embedded into the PSO algorithm, and all the particles are considered as harmonious memory (HM). The algorithm steps can be described as follows:

3.3 Measurement accuracy experiment of ultrasonic sensor

The experimental results are shown in Table 1. It can be seen from the table, from 60cm to 180cm, with the increase of measuring distance, average measurement error of ultrasonic sensor also began to change.

$step1$: Initialize PSO parameters w, c_1, c_2, x_i;

$step2$: According to the following formula:

$$v_{id}(t+1) = w \cdot v_{id}(t) + c_1 \cdot rand_1() \cdot \left(p_{id}(t) - x_{id}(t)\right) + c_2 \cdot rand_2() \cdot \left(p_{gd}(t) - x_{id}(t)\right)$$

$$x_{id}(t+1) = x_{id}(t) + v_{id}(t+1); \quad (1)$$

Particle swarm optimization, calculate the p_{best} and the g_{best};

$step3$: Initialize HS algorithm parameters HM, HMS, $HMCR_{max}$, $HMCR_{min}$, PAR, $iter$, $max\ s\ tep$;

$step4$: The optimization result of $step2$ is taken as the harmonious memory HM;

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$step5$: According to the following formula:

$$x_{id}^{'} = \begin{cases} x_{id}^{'} \in \{x_{id}^{1}, \ldots, x_{id}^{HMS}\} & with\ probality\ 1 - HMCR \\ x_{id}^{'} \in X_{id} & with\ probality\ HMCR \end{cases} ; \quad (2)$$

$$HMCR = HMCR\left(HMCRmin_{max} \times \frac{1+cos\left(\frac{(iter-1)\pi}{(max\ step-1)}\right)}{2}\right)_{min};$$

$$x_{id}^{'} = \begin{cases} Yes & with\ probality\ PAR \\ No & with\ probality 1 - PAR \end{cases};$$

$$x_{id}^{'} = x_{id}^{'} + r \cdot w_b; \quad (3)$$

Produce and improve new particles;

$step6$: Determine whether the fitness of the new particle is better than that of the worst particle in HM, If so, replace the original worst particle with the new particle and update HM, otherwise, it remains unchanged;

$step7$: Determine whether the termination condition of HS is satisfied,if so,enter $step8$, otherwise it renturns $step5$;

$step8$: Renewal particle swarm;

$step9$: According to the set maximum number of cycles, judge whether the termination condition is satisfied. If it is, it ends, otherwise, it returns $step2$.

4. The Simulation Results

In this paper, the historical data of a petrochemical enterprise are selected, 26 main variables obtained according to the GBDT model are taken as input parameters, and the octane number of gasoline is taken as output parameters. There are 325 particles in the network built by the dynamic harmonious search hybrid particle swarm optimization algorithm, and each particle has 26 dimensions. Under the premise that the sulfur content is no more than 5μg/g, all possible solutions are trawled, and the solution with more than 30% reduction in octane number is searched, which is the optimal solution we are looking for. In order to improve the performance of the model, when searching for the optimal solution, the number of iterations is set as 100, 150 and 200 respectively, and the convergence results are as follows.

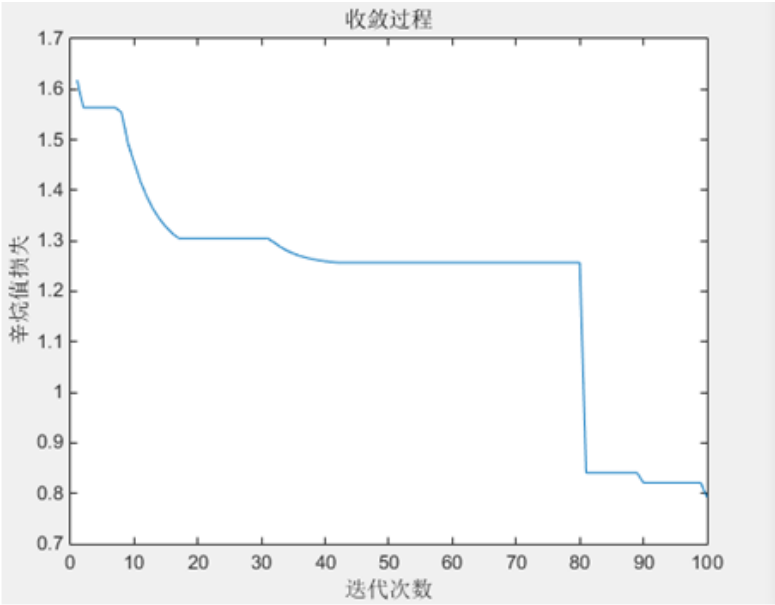

Figure 4: Loss convergence process with iteration number of 100

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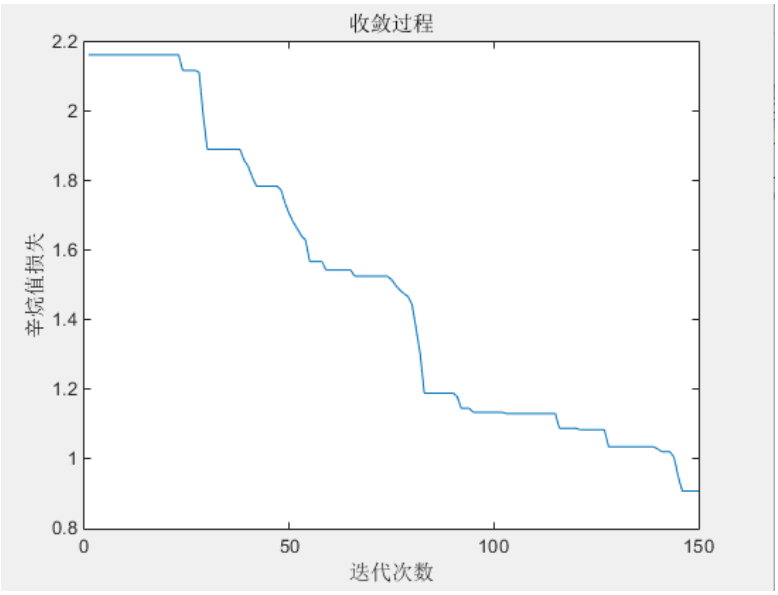

Figure 5: Loss convergence process with iteration number of 150

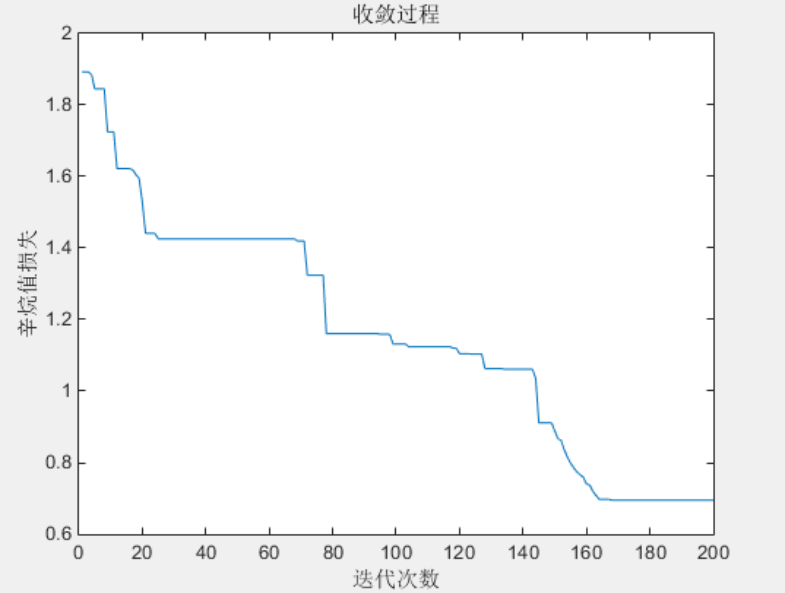

Figure 6: Loss convergence process with iteration number of 200

By analyzing and comparing the convergence process of octane loss with different iterations, it is found that when the number of iterations is 100, the convergence curve is not smooth, the convergence effect is poor, the octane loss decline is small, the operating variables are difficult to aggregate, and the optimization results of main variables cannot be obtained. When the number of iterations increases to 150 times, the convergence curve becomes obviously smooth, the convergence speed is fast, and the convergence effect is good. The objective of optimizing the main variables and reducing the octane number loss has been achieved well. When the number of iterations reaches the set maximum of 200, it can be seen that the smoothness and convergence speed of the convergence curve are significantly better than the result of 150 iterations. That is to say, when the number of iterations is 200, the experiment has the best effect. At this time, the octane loss is reduced by more than 30%, and the optimized main variable is also obtained.

5. Simulation and Analysis

Drived by the demand of mass index octane number prediction and oil sulfur reduction in modeling of finished gasoline blending formulation, a predictive modeling method combining PSO algorithm and HS algorithm for optimizing the parameters of particle swarm network was proposed in this paper, and

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it was applied to the octane number prediction of hydrogenated gasoline components. The results show that:

(1) The DHSPSO algorithm proposed in this paper improves the diversity of the population through the randomness of HS search and the survival of the fittest mechanism, which makes the particle swarm more ergodic in the early stage of search, realizes the deep fusion of the two by the alternating effect of the algorithm, and finds the global optimal solution more easily and quickly.

(2) The loss of octane number is effectively reduced while the sulfur content of the oil is reduced, and the purpose of real-time octane number prediction is realized, which also provides the possibility for the subsequent complete data generation of the demand of finished gasoline blending formula.

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