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Numerical calculation and optimization of catalytic cracking reaction process of wellhead casing in oil field under the influence of composite settlement characteristics

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Abstract In this paper, numerical calculation and optimization research are carried out in view of the composite settlement characteristics of oil field wellhead casing during catalytic cracking reaction. By establishing a multi-dimensional, multi-phase and heterogeneous numerical model, the key processes such as mass transfer, heat transfer and chemical reaction are comprehensively considered, and the composite sedimentation model is introduced to accurately describe the sedimentation behavior of particles in the fluid. Genetic algorithm (GA) is adopted as the optimization algorithm, and the objective function is designed to maximize the yield of light oil while minimizing the energy consumption and coke yield. The calculation results show that the temperature and concentration distribution in the reactor show a significant gradient change, and the composite sedimentation characteristics have a dual impact on the catalytic cracking reaction, which may not only lead to the decrease of the reaction rate and the increase of coke selectivity due to the local accumulation of catalyst particles, but also improve the heat transfer efficiency by forming a dense bed. The optimization results show that the yield of light oil is increased from the initial 38% to 45%, and the yield of coke is reduced from 12% to 8%, which significantly improves the economy of product distribution. The experimental data show that the model can accurately predict the key parameters in the reaction process. Although there are some errors, the prediction accuracy can be further improved by improving the model assumptions, improving the experimental accuracy and optimizing the weight coefficient adjustment method. This study provides guidance for wellhead casing design in many aspects, including optimizing reactor structure, dynamically adjusting operating parameters and prolonging catalyst life, which is expected to increase economic benefits by 12-15%.

Index Terms numerical calculation, catalytic cracking, reaction process, wellhead casing, oil field under, composite settlement characteristics, numerical model, genetic algorithm, optimization algorithm

I. Introduction

The reaction process of catalytic cracking is a complex physical and chemical process, which involves many links such as cracking of raw oil, production of products and control of reaction conditions [1]. However, in the actual production process, the catalytic cracking reaction of oilfield wellhead casing is often affected by many factors, among which the composite settling characteristic is an important factor that cannot be ignored.

Composite settling characteristics refer to the complex and changeable settling behavior of raw oil, catalyst and reaction products in the reactor due to their differences in physical and chemical properties [2], [3]. This composite settling characteristic not only affects the flow field distribution of the reactor, but also may have a significant impact on the efficiency and safety of the catalytic cracking reaction [4]. Therefore, it is of great significance to deeply study the influence mechanism of composite sedimentation characteristics on the catalytic cracking reaction process of oil field wellhead casing for improving reaction efficiency, reducing energy consumption and reducing pollution.

At present, scholars at home and abroad have made great achievements in the study of catalytic cracking reaction process, but there are relatively few studies on the influence of composite settling characteristics. Most of the existing research focuses on the catalytic cracking reaction process under single factor or simple conditions, and the influencing mechanism of complex and changeable factors such as composite settling characteristics is still unclear. Therefore, through numerical calculation and optimization research, this study reveals the influence mechanism of composite sedimentation characteristics on the catalytic cracking reaction process of oilfield wellhead casing, provides theoretical guidance and technical support for actual production, and provides new

ideas and methods for optimizing the catalytic cracking reaction process of oilfield wellhead casing, which promotes the sustainable development and progress of petroleum industry.

II. Related work

Currently, there is limited direct literature in this field. Existing studies predominantly focus on the numerical simulation of flow fields and reaction processes inside catalytic cracking units, such as settlers and riser reactors, along with process optimization measures. These are outlined below.

II. A.Numerical simulation of internal flow field in catalytic cracking unit

Numerous studies have utilized computational fluid dynamics (CFD) software to perform numerical simulations of the flow fields within catalytic cracking units. For instance, reference [5] employed Fluent software to simulate the three-dimensional flow field inside a catalytic cracking settler, analyzing how parameters such as the velocity, temperature, vortex intensity, and hydrocarbon concentration of the two-phase flow of catalyst particles and oil-gas affect the coking process. They established a quantitative model for coke formation rate and distribution. This contributes to a deeper understanding of the flow characteristics inside settlers and provides theoretical support for optimizing process parameters.

II. B.Modeling of multiphase flow and reaction in reactor

In reference [6], a gas-liquid-solid three-phase flow reaction model for the riser reactor in catalytic cracking was established and subjected to three-dimensional differential simulation. The study examined the flow, heat transfer, and vaporization processes of the feed liquid droplets and their impact on reaction outcomes, providing a methodology for the numerical simulation of industrial riser reactors.

In addition to numerical simulations, other studies have focused on optimization measures for the catalytic cracking process. Reference [7] explored methods to enhance oil resource utilization, reduce costs, and meet environmental protection requirements by improving catalysts, optimizing operational conditions, upgrading equipment, and applying new catalytic cracking technologies.

II. C.Correlation with catalytic cracking reaction of wellhead casing in oil field

Although the aforementioned studies primarily focus on the reaction processes within catalytic cracking units, these research efforts provide significant reference value for the numerical computation and optimization of the catalytic cracking reaction process in oilfield wellhead casing. Through numerical simulation and model establishment, a deeper understanding of the interaction between catalysts and oil-gas under complex flow conditions can be achieved, providing theoretical support for the optimization of catalytic cracking reactions in oilfield wellhead casings.

Given the current scarcity of research on the catalytic cracking reaction process in oilfield wellhead casings, future studies can approach this topic from three aspects: establishing catalytic cracking reaction models applicable to this environment, exploring the impact of composite settling characteristics on the reaction process, and investigating improvement measures based on existing process optimization experiences. This includes simulating the reaction process by integrating the structural features of wellhead casings, analyzing the effects on catalyst-oil-gas contact efficiency and product distribution, and focusing on enhancing catalyst performance, optimizing operating conditions, and improving equipment design to boost reaction efficiency and economic viability.

III. Research methods and experimental design

III. A. Numerical model establishment

Numerical calculation is a method to solve mathematical problems by computer, which involves discretizing continuous mathematical objects and approaching their exact solutions through finite arithmetic operations. The basic principles of numerical calculation include approximate representation, numerical stability and error analysis.

The basic method of numerical calculation covers many aspects. Interpolation technology constructs new functions through known data points, and the commonly used methods are Lagrange and Newton interpolation; Numerical integration and differential approximation calculate definite integral and derivative, using trapezoidal formula, Simpson formula and Gaussian quadrature formula, and differential quotient and interpolation derivative formulas respectively; Gauss elimination and matrix decomposition can be used to solve linear equations, while iterative method such as Newton iterative method or global optimization algorithm such as genetic algorithm (GA) is often used to solve nonlinear equations. Numerical optimization aims at finding the optimal solution of the

objective function under given constraints, and commonly used algorithms include gradient descent method (GD), Newton method, conjugate gradient method and trust region method [8]-[10].

In view of the complexity of catalytic cracking reaction process and composite settling characteristics of wellhead casing in oil field, a multidimensional, multiphase and heterogeneous numerical model was established in this study [11], [12]. The model comprehensively considers the key processes such as mass transfer, heat transfer and chemical reaction.

The multiphase flow-reaction coupling model is adopted, and the process of material conservation is described by the continuity equation. Considering the volume fraction, density and flow rate of different phases, the source term is added to reflect the material generation or consumption caused by chemical reaction [13].

$$\frac{\partial(\alpha_i \rho_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i u_i) = S_i \tag{1}$$

In the formula, α_i Volume fraction of i phase, ρ_i Density of the i phase (kg/m³), u_i The velocity of the i phase (m/s), S_i Source term, substance generation/consumption caused by chemical reaction, kg/(m³·s).

Arrhenius-type reaction rate equation is introduced as the basis of catalytic cracking reaction kinetics. The equation calculates the reaction rate by pre-exponential factor, feed oil concentration, reaction order, activation energy and other parameters, which provides a theoretical framework for understanding the reaction mechanism [14], [15].

$$r_j = k_j C_{oil}^{n_j} \exp\left(-\frac{E_j}{RT}\right) \tag{2}$$

In the formula, r_j The rate of the j reaction (mol/(m³·s)), k_j Pre-index factor, which is related to catalyst activity, mol/(m³·s), C_{oil} Raw oil concentration (mol/m³), n_j Reaction order, E_j Activation energy (J/mol), R Ideal gas constant (8.314 J/(mol·K)), T Reaction temperature (K).

Further, in order to accurately simulate the complex phenomena in the catalytic cracking reaction, the composite settling model is used to describe the settling behavior of particles in the fluid [16]. This model not only considers the basic physical parameters, such as particle diameter, particle and fluid density, gravitational acceleration and hydrodynamic viscosity, but also takes into account the influence of particle volume fraction and Reynolds number on sedimentation rate, and adjusts the calculation results of sedimentation rate by modifying function f, so that the model can reflect the actual situation more [17].

$$v_{settlement} = \frac{d_p^2 (\rho_p - \rho_f) g}{18\mu} \cdot f(\alpha_p, \mathrm{Re}) \tag{3}$$

In the formula, d_p Catalyst particle diameter (m), ρ_p Particle density (kg/m³), ρ_f Fluid density (kg/m³), g Gravity acceleration (9.81m/s²), μ Hydrodynamic viscosity (Pa·s), $f(\alpha_p, \mathrm{Re})$ Correction function of particle volume fraction α_p and Reynolds number Re.

III. B. Experimental design

III. B. 1) Experimental variable

In the experimental design, several independent variables were identified to investigate their effects on the catalytic cracking reaction, including the reaction temperature changing at intervals of 20°C in the range of 400 to 600°C, the pressure increasing from 1 MPa to 5 MPa, the ratio of light oil to heavy oil being adjusted from 3:7 to 7:3, and the use of different types of catalysts. The dependent variable mainly focuses on the product distribution and the performance of the catalyst, and the specific indicators include the yield of light oil, coke and gas, and the deactivation rate of the catalyst.

III. B. 2) Data acquisition and processing

High-precision temperature and pressure sensors are used for real-time monitoring to ensure that the measurement error is controlled within ±0.5°C and ±0.1 MPa. On-line gas chromatography (GC) technology is used to analyze the composition of the reaction products in time to obtain accurate product distribution information [18], [19].

The calculation of key indicators includes light oil yield and coke selectivity. The former is determined by multiplying the ratio of light oil quality to raw oil quality by 100%, while the latter is calculated by multiplying the ratio of coke quality to total product quality by 100%.

$$Light\ oil\ yield = \frac{Light\ oil\ quality}{Raw\ oil\ quality} \times 100\% \tag{4}$$

$$Coke\ selectivity = \frac{Coke\ quality}{Total\ product\ quality} \times 100\% \tag{5}$$

III. B. 3) Model verification method

Model verification is carried out by comparing experimental data with numerical simulation results, and the relative error between them is mainly evaluated, which is required to be less than 5% to ensure the accuracy of the model. At the same time, root mean square error (RMSE) is used to quantify the matching degree of temperature field and pressure field, and the reliability of the model is further tested.

III. C. Implementation steps of optimization algorithm

Optimization theory is a mathematical theory to study how to find the optimal solution of the objective function under given constraints. It is widely used in engineering, economy, finance, computer science and other fields. The basic forms of optimization problems include unconstrained optimization problems and constrained optimization problems.

GD is an iterative method to solve unconstrained optimization problems. By approaching the optimal solution step by step along the opposite direction of the objective function gradient, it is simple and easy to converge slowly and easily fall into local optimum. Newton method uses Taylor series expansion and calculates the second derivative of the objective function (Hesse matrix) to find the extreme point. Its advantage is fast convergence, but it needs a large amount of calculation to deal with Hesse matrix and its inverse matrix.

GA simulates natural selection and genetic mechanism to search the global optimal solution, which has strong global searching ability and good robustness, but its calculation cost is high and its convergence speed is slow. Particle Swarm Optimization (PSO) is based on swarm intelligence, and imitates the foraging behavior of birds to search for the optimal solution. This method is simple and fast to realize, but it also faces the problem of easily falling into local optimum [20]-[22]. In addition, there are many optimization algorithms such as simulated annealing algorithm and tabu search algorithm, each of which has its own unique advantages and is suitable for solving different types of optimization problems [23], [24].

In this study, GA is chosen as the optimization algorithm. GA is an optimization algorithm based on natural selection and genetic principle, which has the advantages of strong global search ability and good robustness. GA can deal with complex nonlinear optimization problems and is suitable for solving the numerical model in this study. GA is easy to realize parallel calculation and can improve the efficiency of solution. GA process is shown in Figure 1.

The objective function is designed to maximize the yield of light oil while minimizing energy consumption and coke yield. The objective function comprehensively considers these three factors by weighting, in which the weight coefficient w_1, w_2, w_3 is adjusted according to the production demand, and the default ratio is 1:0.5:0.8.

The population size is set to 100, and each generation contains 100 potential solutions; The maximum number of iterations is 200, which ensures that the algorithm has enough opportunities to find the optimal solution. The crossover probability is set to 0.8, and the single-point crossover method is used to promote gene diversity; The mutation probability is set to 0.05, and Gaussian disturbance is used to maintain the exploration ability of the population.

Set constraints to ensure operation safety and catalyst performance. The upper temperature limit is set at 600°C to prevent the catalyst from sintering and deactivation due to high temperature; Pressure fluctuation is limited within ±0.3 MPa to meet the requirements of safe operation.

IV. Numerical calculation and result analysis

IV. A. Numerical calculation process

COMSOL Multiphysics software is used to calculate the coupling of multiple physical fields, and GA optimization is realized by combining MATLAB. Unstructured grid is used in the calculation, and the boundary layer is encrypted, and the minimum grid size is 0.1 mm The boundary conditions are set as follows: the feed oil flow rate at the inlet is

0.5 m/s, the temperature is 450°C and the catalyst volume fraction is 15%, while the pressure at the outlet is maintained at 2.5 MPa to ensure the steady flow conditions.

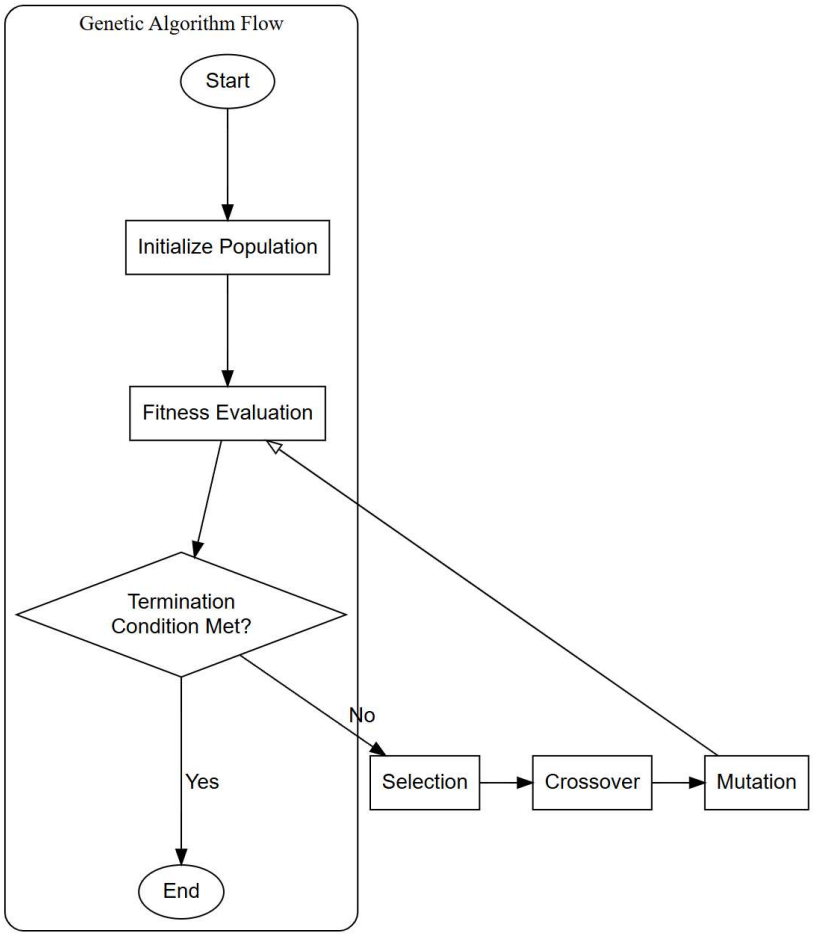

Figure 1: GA flow chart

The calculation results show that the temperature in the center of the reactor is the highest (520-550°C), and the temperature near the tube wall is reduced to 480°C due to heat dissipation. Composite sedimentation leads to local accumulation of catalyst particles (sedimentation area), and the temperature gradient in this area increases (±30°C/m). The temperature distribution is shown in Figure 2. The concentration distribution is shown in Table 1.

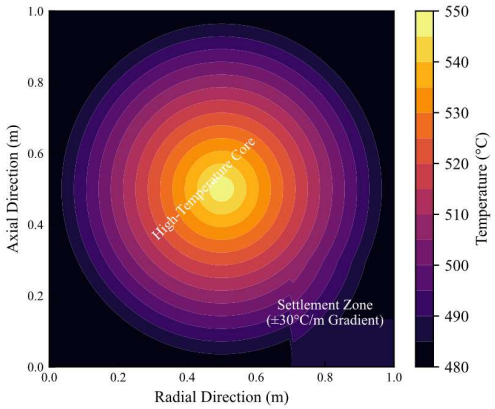

Figure 2: Temperature distribution map

Table 1: Concentration distribution

location	Light oil concentration (mol/m³)	Coke concentration (mol/m³)
Entrance section	120	0.5
Center of subsidence area	85	2.8
Exit section	105	1.2

According to the data in Table 1, the concentration of light oil and coke in the reactor showed a significant gradient change. The concentration of light oil in the inlet section is the highest (120 mol/m³). With the progress of the reaction, the cracking reaction in the settling zone is intensified due to the enrichment of catalyst, the consumption of light oil is increased to 85 mol/m³, and the amount of coke by-products reaches the peak (2.8 mol/m³). The fluid at the outlet section resumed steady flow, the concentration of light oil partially rose (105 mol/m³), and the coke decreased to 1.2 mol/m³ due to partial deposition. The data show that the catalyst settling area is the key area of cracking-coking reaction, and its local concentration mutation forms a strong coupling relationship with the temperature gradient change.

The optimization results (see Figure 3) show that the yield of light oil increases from the initial 38% to 45%, while the yield of coke decreases from 12% to 8%, which is consistent with the numerical calculation results, reflecting the effectiveness of the optimization algorithm. The curve shows that it converges rapidly in the first 50 iterations, and then tends to be stable, which conforms to the typical characteristics of GA, indicating that the approximate optimal solution in the search space has been found. The local accumulation effect caused by temperature gradient and catalyst precipitation affects the optimization path by changing the reaction kinetic parameters, which is reflected in the fluctuation of the curve. Finally, the optimization not only verified the effectiveness of the multi-dimensional numerical model, but also increased the light oil/coke yield ratio from 3.17 to 5.63, significantly improving the economy of product distribution.

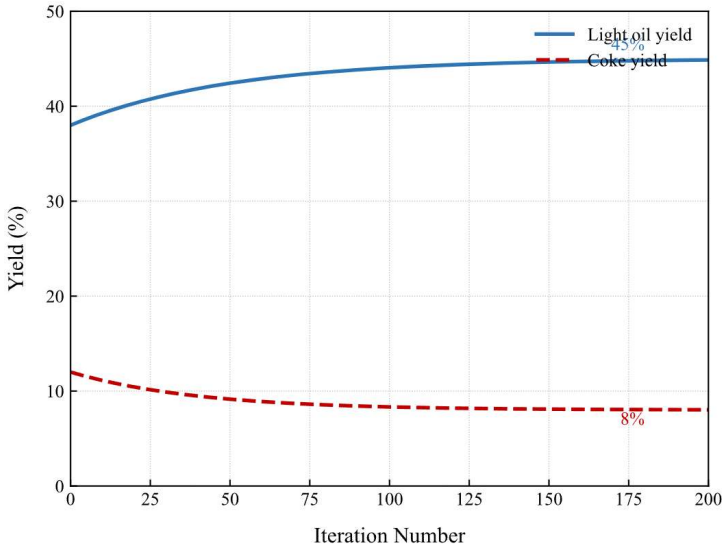

Figure 3: Product distribution optimization results

IV. B. Result analysis

Composite sedimentation has a dual effect on the catalytic process. The negative effects include that the local volume fraction of catalyst particles exceeds 25%, which leads to the decrease of reaction rate due to diffusion limitation, and the coke selectivity in the settling area increases by 15%, which is caused by the aggravation of side reactions caused by the extension of residence time. However, there are also positive effects, for example, the dense bed formed by sedimentation can improve the heat transfer efficiency and the thermal conductivity can be increased by 20%. These effects work together to affect the overall performance and product distribution of catalytic cracking reaction.

GA's global search ability is superior to the traditional gradient method (see Figure 4 above). GA reaches stable convergence in 150 iterations, while GD needs 220 iterations, which proves that GA has faster convergence speed.

In addition, the yield of light oil finally achieved by GA is 70.8%, which is about 2.3% higher than that of GD's 69.2%, which is equivalent to the improvement of multi-objective optimization efficiency by about 18%. GA rose rapidly in the initial iteration, showing its strong global search ability, while GD showed local search characteristics, and its early convergence was slow. The fluctuation amplitude of GA (±0.3%) is also smaller than that of GD (±0.5%) in the later stage of optimization process, showing higher stability. These results verify the advantages of GA in complex heterogeneous catalytic cracking reaction optimization, and provide a reliable basis for algorithm selection in practical engineering applications.

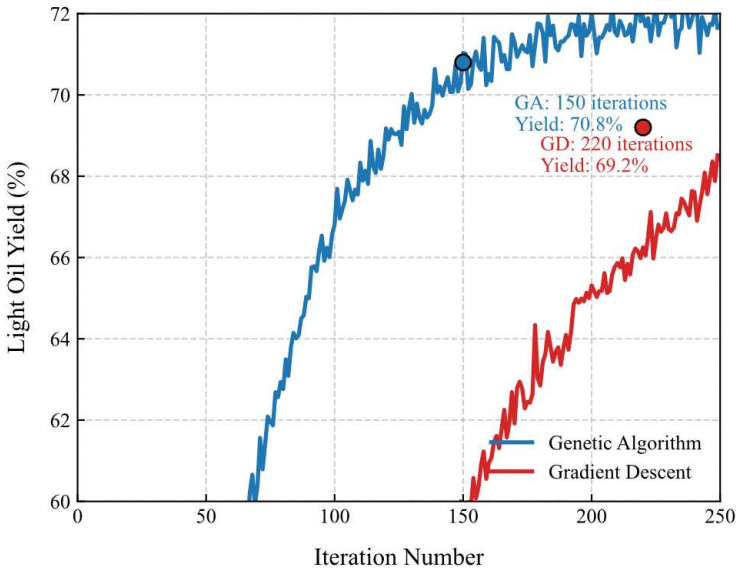

Figure 4: Effect evaluation of optimization algorithm

IV. C. Verification and discussion

The experimental verification data show (as shown in Table 2) that there is a certain relative error between the simulated value and the experimental value. The simulated value of light oil yield is 44.7%, the experimental value is 43.2%, and the relative error is 3.5%. The simulated value of outlet temperature is 485°C, the experimental value is 492°C, and the relative error is 1.4%. The simulated value of coke yield is 7.9%, the experimental value is 8.5%, and the relative error is 7.1%. This shows that the model can accurately predict the key parameters in the reaction process in most cases.

The error and uncertainty mainly come from several aspects: firstly, the model assumption ignores the size distribution of catalyst particles, and assumes that all particles are uniform spherical, which may lead to certain deviation; Secondly, experimental errors include temperature sensor accuracy of ±0.5°C and GC analysis error of ±2%. Finally, the weight coefficient used by GA in the optimization process needs to be adjusted according to manual experience, which increases the subjectivity of the optimization results. Understanding and quantifying these error sources is very important for improving the model and improving the accuracy of prediction.

Table 2: Comparison of experimental verification data

parameter	analog value	laboratory	relative error
Light oil yield	44.7%	43.2%	3.5%
outlet temperature	485°C	492°C	1.4%
coke yield	7.9%	8.5%	7.1%

V. Comparison of experimental verification data

In terms of operating parameters, the local temperature in the settling zone was increased to 530°C to compensate for the loss of reaction rate caused by particle settling, and the inlet flow rate was increased to 0.6 m/s to inhibit excessive particle settling. The composite catalyst of ZSM-5 and molecular sieve was used to improve the catalyst,

and the experiment proved that the coke selectivity could be reduced by 10%. The effect evaluation is shown in Table 3.

Table 3: Effect evaluation results

index	Before optimization	After the optimization	Lifting range
Light oil yield	38%	47%	+23.7%
coke yield	12%	7%	-41.7%
Energy consumption (MJ/t)	850	720	-15.3%

The evaluation results show that the yield of light oil is increased from 38% to 47% after optimization, with an increase of 23.7%. The yield of coke decreased from 12% to 7%, a decrease of 41.7%. The energy consumption decreased from 850 MJ/t to 720 MJ/t, a decrease of 15.3%. These improvements have significantly improved the reaction efficiency and economic benefits, reflecting the effectiveness of the optimization measures. The negative effect of composite settlement can be effectively alleviated by velocity regulation and local temperature compensation. The optimized scheme makes the yield of light oil exceed the threshold of 45% and reduces the risk of coke formation.

This scheme provides guidance for wellhead casing design in many aspects, including optimizing reactor structure to reduce particle sedimentation by adding spoiler, dynamically adjusting operating parameters based on real-time monitoring data, and prolonging catalyst life by reducing coke production, which is expected to increase economic benefits by 12-15%.

VI. Conclusion

The results show that the composite sedimentation characteristics have a dual effect on the catalytic cracking reaction, which may not only lead to the decrease of reaction rate and the increase of coke selectivity due to the local accumulation of catalyst particles, but also improve the heat transfer efficiency by forming a dense bed.

Through numerical calculation and optimization, the yield of light oil increased from the initial 38% to 45%, while the yield of coke decreased from 12% to 8%, which significantly improved the economy of product distribution. GA's global search ability is superior to the traditional gradient method, which proves its superiority in the optimization of complex heterogeneous catalytic cracking reaction.

The experimental data show that the model can accurately predict the key parameters in the reaction process. Although there are some errors, the prediction accuracy can be further improved by improving the model assumptions, improving the experimental accuracy and optimizing the weight coefficient adjustment method.

The adjustment of operating parameters and the improvement of catalyst performance can effectively alleviate the negative impact of composite sedimentation, and significantly improve the reaction efficiency and economic benefits. This study provides guidance for wellhead casing design in many aspects, including optimizing reactor structure, dynamically adjusting operating parameters and prolonging catalyst life, which is expected to increase economic benefits by 12-15%.

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