

Article

PINN-Assisted Low-Carbon Operation Configuration for Catalytic Cracking Units: An Economic–Environmental–Energy Co-Optimization Framework Based on Life Cycle Assessment

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Abstract

This study addresses challenges in fluid catalytic cracking (FCC) units, including inaccurate quantification of carbon emissions, difficulties in implementing low-carbon operational optimization, and low computational efficiency in solving complex process kinetics. A low-carbon operation optimization method based on physics-informed neural networks (PINNs) is proposed. First, a unit-level carbon footprint assessment model is established using process life cycle assessment (PLCA) to achieve high-resolution quantification of both direct and indirect carbon emissions. Second, a multi-objective low-carbon operation optimization model is developed considering carbon tax scenarios, incorporating carbon emissions and corresponding carbon tax costs into the optimization objectives to achieve economic and low-carbon synergistic optimization. Finally, a PINN-assisted surrogate model is designed by embedding material balance constraints into the neural network training process, enabling efficient approximation of complex product yield kinetics and improving optimization solution efficiency and predictive reliability. The proposed method is applied to optimize the operation of an FCC unit at a refinery site. The results indicate an increase of 12,048.851 CNY/h in profit, a reduction of 1088.921 kgCO₂eq/h in CO₂ emissions, and a decrease of 324.281 m³/h in steam consumption. Meanwhile, the PINN model exhibits excellent performance in product yield prediction, with an average R^2 of 0.9968 and an average RMSE of 0.1482, outperforming conventional data-driven methods. The proposed approach balances carbon emission quantification accuracy, physical consistency in yield prediction, and optimization solution efficiency, providing a systematic and implementable technical framework for low-carbon operation optimization of FCC units.

Keywords: fluid catalytic cracking; multi-objective operation optimization; physics-informed neural networks; life cycle assessment



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1. Introduction

As a core secondary processing unit in refineries, the fluid catalytic cracking (FCC) unit accounts for over 20% of the total refining capacity and plays a dominant role in the economic performance and energy efficiency of the refinery system [1]. The primary function of the FCC process is to convert heavy oil feedstocks into high-value light products, including gasoline, light diesel, and liquefied petroleum gas, while emitting approximately

0.4 kg of carbon dioxide (CO₂) per ton of feedstock processed, thereby representing a substantial contribution to the refinery's overall carbon footprint. With the global pursuit of carbon neutrality and increasingly stringent environmental regulations, reducing carbon emissions during FCC operation has become a significant challenge for the refinery industry. Low-carbon operation not only mitigates greenhouse gas emissions in compliance with national carbon reduction policies in China, but also aligns with international climate initiatives, such as the European Green Deal and the EU "Fit for 55". In addition to reducing CO₂ emissions, low-carbon operation enhances energy utilization efficiency, optimizes feedstock and energy allocation, and improves the economic–environmental performance of the unit. Therefore, research on low-carbon operation optimization of FCC units holds both practical engineering value and theoretical significance, providing technical support for the green transformation of the refining industry in both national and global contexts.

Conventional research on FCC unit operation optimization has primarily focused on single-objective problems aiming to maximize economic benefits, by adjusting key operating parameters such as reactor temperature, pressure, steam flow, and air flow to increase product yields and unit profitability [2]. Liu et al. [3] conducted steady-state simulation of the separation processes of a 2-million-ton-per-year FCC unit using industrial production data combined with Aspen Plus, and implemented multi-objective optimization of the separation system by integrating Aspen Plus with MATLAB via an improved non-dominated sorting genetic algorithm (NSGA-II), achieving enhanced system performance. Tian et al. [4] proposed an optimization framework combining a multi-output artificial neural network with NSGA-II, constructing a sensitivity dataset through steady-state modeling and Latin hypercube sampling to enable simultaneous optimization of system safety, energy consumption, and product quality. The optimization results demonstrated a 3.76% reduction in operational interruptions, an 8.38% decrease in energy consumption, and stable product quality compared with the baseline process. Li et al. [5] developed a two-level data-driven robust optimization framework to optimize feed selection and reaction temperature for an industrial FCC unit under feedstock property uncertainty. Based on two years of historical industrial and simulation data, two sets of uncertainty parameters were derived. This framework, by nesting numerical and mathematical problem-solving, ensured profitability of the FCC unit under uncertainty, verifying its practical applicability in industrial operations. Although these studies have achieved certain improvements in unit economic performance, they are primarily limited by their focus on product yield or economic indicators, while overlooking comprehensive factors such as energy consumption and environmental impact, making it difficult to fully reflect the sustainability of unit operation [6].

In recent years, some studies have attempted to incorporate energy savings or conversion efficiency into multi-objective optimization frameworks to achieve a balance between economic benefits and energy efficiency [7]. Han et al. [8] proposed an FCC simulation optimization framework integrating process simulation, thermodynamic analysis, and industrial constraints. Multi-objective optimization of energy efficiency, product yield, and economic returns was performed using a genetic algorithm (GA) and the non-dominated sorting genetic algorithm II (NSGA-II), with the TOPSIS method employed to select the optimal compromise solution from the Pareto front. The optimization results indicated that an energy-capacity trade-off could reduce energy consumption by 3.28% and increase product yield by 1.95%, while compared with single-objective yield maximization, energy consumption was reduced by 9.63%. Reyes et al. [9] proposed integrating various process intensification strategies within the absorption-stable process (ASP) to enhance the operational and energy efficiency of FCC units. Through combined simulation, validation, and life cycle energy assessment, this approach achieved a 17.72% reduction in total energy

consumption and an increase in stabilized gasoline yield from 54% to 60.15%, benefiting from synergistic optimization of feed allocation, thermal energy recovery, and resource utilization. Despite these advances, such studies, while considering feedstock utilization and energy consumption, still do not fully address the environmental impacts generated during operation, particularly carbon dioxide emissions [10]. Due to the lack of quantification and analysis of the carbon footprint, multi-objective optimization strategies in practical operation struggle to simultaneously achieve both economic performance and environmental sustainability.

To address this limitation, recent studies have attempted to incorporate carbon emissions as either a constraint or an optimization objective, regulating operating conditions by limiting emission caps or introducing carbon emission costs [11]. Wan et al. [12] proposed a multi-objective optimization framework that integrates an FCC-RR centralized kinetics model based on a path evolution reproduction operator with the SPEA-2 algorithm, incorporating CO₂ and SO₂ emissions as optimization constraints. Furthermore, the study introduced an improved SPEA-2 algorithm that integrates the path evolution operator to enhance the convergence speed and quality of the optimization solutions. Case studies applied to practical FCC-RR units demonstrated the significant advantages of this framework in achieving multi-objective optimization during the catalytic cracking process. Cuadros et al. [13] proposed a multi-objective hybrid optimization strategy that sequentially combines a genetic algorithm (GA) with sequential quadratic programming (SQP) for FCC processes. This method aims to maximize process conversion while satisfying CO emission constraints. Considering the high nonlinearity and significant coupling between variables in FCC processes, GA is employed to generate a global initial estimate and avoid local minima, followed by SQP using the GA results as initial values to accelerate convergence, thereby achieving the optimization objectives while reducing computational burden and time. However, despite improving the feasibility of low-carbon operation to some extent, these methods still exhibit significant limitations. First, carbon emissions are typically approximated using empirical formulas or simple constraints, lacking precise tracking and dynamic quantification of emissions across multiple stages, including reaction processes, catalyst regeneration, and flue gas treatment. Second, existing studies remain focused primarily on economic and energy efficiency optimization, providing insufficient consideration of carbon emissions and environmental impacts, which limits the ability of low-carbon operational strategies to accurately reflect their environmental benefits.

Moreover, operation optimization models of FCC units typically involve complex multiphase reaction kinetics, heat transfer, and multi-component distillation equations, exhibiting highly nonlinear behavior and strong multivariable coupling [14]. These equations are often described by partial differential equation (PDE) systems representing reactant conversion, product distribution, and by-product formation. Directly solving such systems is computationally intensive and technically challenging, which limits the practical application of multi-objective optimization [15]. To overcome this computational bottleneck, researchers have proposed surrogate-assisted optimization approaches, wherein data-driven surrogate models approximate the complex kinetic mappings as computationally tractable functions, thereby significantly reducing the computational cost of optimization. Song et al. [16] proposed a surrogate-assisted optimization framework that couples 23 riser kinetics models based on molecular-type homology sequences (MTHS) with four reaction regenerators to predict flue gas composition and heat release, while intrinsically enforcing unit-level mass and energy balances. Optimization results based on this surrogate model indicated that by coordinating air rates, feed preheating, and heat extraction, profit could be increased by 7.76%, demonstrating the efficiency and physical interpretability of the surrogate-assisted framework for industrial FCC unit operation optimization. Yu et al. [17]

employed Fe-K loaded biochar for catalytic steam gasification to produce hydrogen-rich syngas and constructed a surrogate model using the response surface methodology (RSM) to systematically optimize gasification temperature, reaction time, steam content, and gas hourly space velocity (GHSV). The model exhibited high predictive accuracy for carbon conversion and hydrogen yield. Optimization based on the surrogate model showed that under mild operating conditions at 667 °C, carbon conversion could reach 97.52%, while hydrogen yield and effective syngas production reached 140.25 mol/kg and 3.99 Nm³/kg, respectively, validating the efficiency and reliability of surrogate modeling in biochar gasification process optimization.

In the field of surrogate-assisted optimization, mainstream approaches include machine learning models such as XGBoost [18] and random forests [19], Gaussian process regression methods (Kriging [20], GPR [21]), deep neural networks (CNN [22], BiLSTM [23], Transformer [24]), and Bayesian optimization [25] combinations. These methods excel at high-dimensional nonlinear data fitting and pattern recognition, enabling rapid prediction of the mapping relationships between operating variables and product yields, thereby providing efficient tools for multi-objective optimization. Li et al. [26] constructed a feed-stock molecular matrix containing over 1600 full-range feature carriers based on molecular reconstruction techniques, enabling automatic generation of catalytic cracking reaction networks. On the basis of this molecular-level kinetic model, a surrogate-assisted optimization framework was developed, in which XGBoost was combined with the NSGA-III algorithm to optimize process parameters. The results demonstrated that the surrogate model could accurately quantify hydrocarbon distribution characteristics during the reaction, establish quantitative relationships between reaction conditions and product distribution, and identify optimal process parameters and product distribution schemes. Zhou et al. [27] proposed a hybrid framework that integrates molecular mechanism modeling with data-driven surrogate optimization for multi-objective optimization of industrial chemical processes. This framework utilizes molecular-level mechanistic modeling to construct a high-accuracy deep learning database to support optimization of novel processing pathways, aiming to maximize chemical yields while incorporating CO emission constraints. Compared with conventional direct-solving methods, this approach exhibits significant computational efficiency advantages under various operating modes. Life cycle assessment further indicated that the optimized scheme, while maintaining product yields, could reduce non-renewable energy consumption required for high-octane gasoline by 2.91% and CO emissions by 4.85%. However, conventional data-driven surrogate models exhibit several inherent limitations. First, these approaches are typically “black-box” models that neglect physical laws and mass conservation constraints, which may result in predictions that deviate from actual physical behavior under certain operating conditions [28]. In FCC units, disregarding physical consistency can lead to non-conservation of total product mass and inaccurate estimation of energy losses, thereby compromising the reliability of optimization results. Second, traditional surrogate models struggle to capture the complex coupling of multi-phase flow, catalyst activity variation, and non-ideal kinetic processes [29]. Consequently, their generalization capability is limited, and predictive accuracy deteriorates significantly under extreme operating conditions or novel process configurations.

In summary, the field of low-carbon operation optimization for FCC units still faces several critical research gaps that need to be addressed: (1) Lack of a system capable of precise carbon emission quantification at the unit level. Existing studies largely rely on empirical formulas or simple constraints to estimate carbon emissions, making it difficult to comprehensively reflect the dynamic carbon flows across multiple stages, including the reaction process, catalyst regeneration, and flue gas treatment. Such coarse carbon accounting not only limits the analysis of carbon flow responses to operating variables but

also reduces the practical implementability of low-carbon operation strategies. (2) Insufficient integration of carbon emissions and environmental sustainability into multi-objective optimization. Although multi-objective optimization approaches have partially balanced economic performance and energy efficiency, most studies still prioritize economic benefits as the primary optimization goal, providing inadequate consideration of carbon emissions and overall environmental sustainability. As a result, proposed low-carbon operational strategies are often difficult to implement in industrial practice, and their environmental benefits cannot be reliably quantified. (3) Lack of physical consistency constraints in existing data-driven surrogate models. Under highly nonlinear and strongly coupled operating conditions, such models struggle to ensure predictive reliability and robustness of optimization results, potentially introducing deviations that violate mass or energy conservation. Precise carbon quantification, multi-objective synergistic optimization, and physically consistent surrogate models remain the core directions in which breakthroughs are urgently needed for low-carbon operation optimization of FCC units.

This study focuses on addressing the aforementioned challenges by developing a physics-informed neural network (PINN)-assisted low-carbon operation optimization model for FCC units, aimed at systematically exploring the energy-saving, emission-reduction potential, and economic optimization space of the production system. Specifically, first, a unit-level carbon emission accounting model was established based on process life cycle assessment (PLCA) to achieve high-resolution quantification of both direct and indirect carbon emissions of FCC units. This model precisely captures the dynamic distribution of carbon flows across multiple stages, including feedstock conversion, fuel combustion, and flue gas treatment, providing a scientific basis for low-carbon operation optimization. Subsequently, a multi-objective low-carbon operation optimization model incorporating carbon tax scenarios was developed, in which carbon emissions and carbon tax costs are integrated into the objective function. This enhances the model's decision-making capability in balancing economic performance and environmental outcomes, enabling synergistic optimization of profitability and carbon reduction. To address the highly nonlinear, multivariable-coupled characteristics of FCC units and the complex, higher-order kinetic relationships between operating variables and product yields, a PINN-based surrogate-assisted model was further designed. By embedding material balance constraints into the neural network training process, this approach enables efficient approximation of complex process kinetics, improving computational efficiency and predictive reliability of the optimization model. Compared with conventional carbon emission constraints based on empirical formulas and purely data-driven surrogate optimization models, the proposed low-carbon operation optimization method simultaneously ensures the accuracy of carbon emission quantification, the physical consistency of product yield prediction, and the computational efficiency of the optimization process. It thus provides a systematic and implementable technical framework for low-carbon operation optimization of FCC units and offers a reliable decision-making tool for energy saving, emission reduction, and sustainable operation in industrial-scale facilities. The main contributions of this study are summarized as follows:

(1) A unit-level carbon footprint assessment model for FCC units based on process life cycle assessment (PLCA) is proposed. This model enables high-resolution quantification of both direct and indirect emissions at the unit level, accurately capturing the dynamic distribution of carbon flows across multiple stages, including feedstock conversion, fuel combustion, and flue gas treatment. It provides a scientific and reliable basis for carbon emission quantification to support low-carbon operation optimization.

(2) A unit-level low-carbon operation optimization model incorporating carbon tax scenarios is developed. In this model, carbon emissions are converted into corresponding

carbon tax costs and integrated into the objective function, achieving joint optimization of economic profitability and carbon emission reduction. This approach provides quantifiable decision support for low-carbon operational strategies while balancing production economics and environmental performance, thereby promoting sustainable operation of FCC units.

(3) A physics-informed neural network (PINN)-assisted surrogate model is developed. By embedding physical constraints, such as material balance, into the neural network training process, this model enables efficient approximation of complex process kinetics. This approach not only significantly improves the computational efficiency of multi-objective optimization but also ensures the physical consistency of product yield predictions and the reliability of optimization results, providing effective technical support for low-carbon operation optimization of highly nonlinear, multivariable-coupled industrial units.

2. Process Description

As a critical secondary processing unit, the FCC unit processes more than 20% of the total crude oil throughput and plays a dominant role in the overall production system. The core objective of the FCC process is to convert heavy oils into light products, which requires substantial participation of catalysts in chemical reactions and is accompanied by significant CO₂ emissions. Figure 1 [30] illustrates the typical process flow of an FCC unit, which primarily consists of three sections: the reaction–regeneration system, the distillation system, and the absorption–stabilization system.

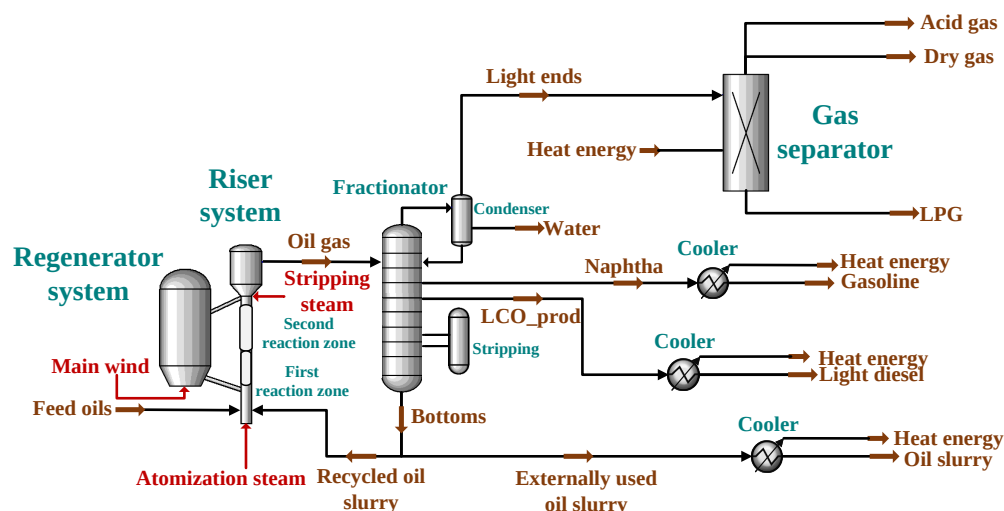


Figure 1. The typical process flow of an FCC unit.

The reaction–regeneration system comprises a furnace, a reactor, and a regenerator. The feedstock, assisted by atomizing steam, is atomized and introduced into the riser. The riser is designed with a two-stage reaction structure to ensure sufficient contact between the fluidized catalyst and the hydrocarbon vapors for cracking reactions. The reaction products, consisting of hydrocarbon vapors and entrained catalyst, exit the riser and enter a cyclone separator for rapid separation. The hydrocarbons are discharged from the top to the distillation and stabilization system, while the spent catalyst, carrying coke deposited during the cracking reactions, returns to the regenerator for reactivation. In the regenerator, carbon deposited on the catalyst surface is combusted under high-temperature air conditions, restoring catalyst activity and generating direct CO₂ emissions. Part of the heat released during regeneration is returned to the reactor with the regenerated catalyst to provide the necessary thermal energy for cracking, while the remainder is absorbed by a heat exchanger to generate steam and maintain thermal balance. The hydrocarbon

products from the reaction system are sent to a distillation column for fractionation. The overhead vapor mixture is condensed and separated into two streams: one containing wastewater with impurities, and the other being rich gas, which subsequently enters the absorption-stabilization system. Two product streams are withdrawn from the middle of the column as light diesel and naphtha, while unreacted oil at the column bottom is recycled and further processed. Cooling and separation allow recovery of light components such as propylene as well as heavier fractions. Fuel consumption and steam usage during distillation contribute to indirect carbon emissions. The absorption–stabilization system is responsible for the separation and purification of gasoline, liquefied petroleum gas, and dry gas, and mainly consists of a gas separator and a cooler. During the purification of light diesel, naphtha, and oil slurry, heat is released through the cooling process. Rich gas enters the gas separation unit, where, under heating conditions, acidic gases and dry gas are separated from the column top, and liquefied petroleum gas is withdrawn from the bottom. Energy consumption and rich gas treatment in this system may result in indirect CO₂ emissions, particularly during gas heating, compression, and absorption processes.

3. Carbon Footprint Assessment Model Based on Process Life Cycle Assessment

3.1. Assessment Boundary

This study focuses on the FCC unit as the research object and employs the PLCA [31] methodology to quantify its carbon footprint. The rationale for selecting PLCA is threefold. First, compared with conventional LCA methods, PLCA provides high-resolution carbon emission quantification at the unit or process level, avoiding the reduced accuracy in LCA results caused by high data uncertainty during upstream feedstock extraction and downstream product utilization. Second, relative to hybrid LCA approaches, PLCA offers greater operational simplicity and specificity, enabling clear differentiation between direct and indirect emissions based on unit-specific process parameters, material flows, and energy consumption data. This facilitates precise tracking of carbon flows and systematic quantification of unit-level carbon footprints. Third, PLCA is particularly suitable for FCC units, in which material, energy, and carbon flows are highly coupled, direct and indirect emissions coexist, and multiple operational modules and multiphase systems are involved, necessitating precise tracking and quantification of carbon flows at the unit level.

As illustrated in Figure 1, the assessment boundaries in this study cover the entire process from feedstock input to product output, including key production stages such as feedstock and by-product input and pretreatment, cracking reactions, catalyst regeneration, product separation, and flue gas treatment. This boundary setting allows comprehensive capture of both direct and indirect carbon emissions during unit operation, including carbon conversion from feedstocks and auxiliary materials, emissions from fuel combustion, coke combustion during catalyst regeneration, and indirect emissions associated with energy consumption.

3.2. Assessment Category

Given that CO₂ is the predominant greenhouse gas emitted during the FCC process, accounting for the vast majority of emissions from fuel combustion, catalyst regeneration, and process flue gas streams, while methane (CH₄), nitrous oxide (N₂O), and other greenhouse gases are comparatively minor and exhibit high measurement uncertainty, this study focuses exclusively on CO₂. This approach ensures the reliability and quantifiability of the assessment results and provides a scientific basis for carbon footprint evaluation and sustainability analysis of industrial production systems.

Figure 2 illustrates the integrated carbon hub of an FCC unit. As a typical secondary processing unit, the FCC carbon hub exhibits a high degree of coupling among material flows, energy flows, and carbon flows, comprising material handling modules, production reaction modules, energy consumption modules, and steam supply modules. In this work, to ensure the completeness and comparability of carbon emission quantification, the carbon hub system classifies carbon flows according to their sources into direct emission carbon flows and indirect emission carbon flows, while explicitly defining the inflow and outflow paths of each type of carbon stream.

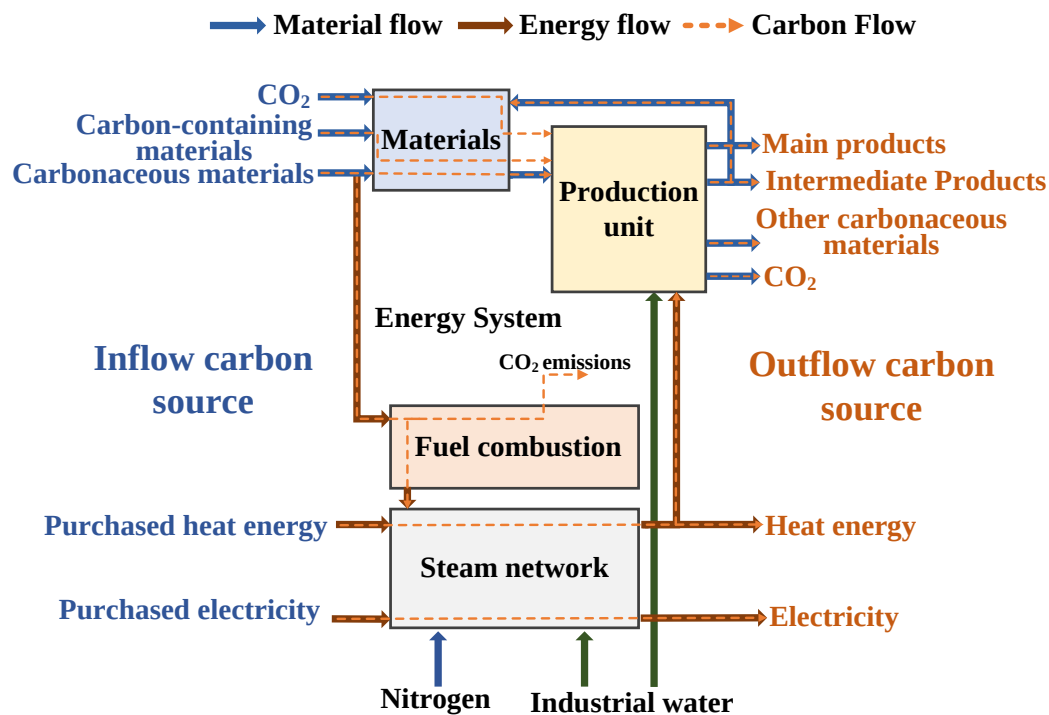


Figure 2. The integrated carbon hub of an FCC unit.

(1) Direct emission carbon flows:

Direct emission carbon flows primarily originate from chemical reactions and fuel combustion occurring within the unit, involving feedstock conversion, catalyst regeneration, and flue gas discharge. The inflows and outflows of these carbon streams include:

1. Carbon inflows: Carbon-containing feedstocks and other carbon-bearing materials entering the FCC unit, such as heavy oils, vacuum residues, and carbon-containing components in by-product streams.
2. Carbon outflows: Carbon in products and intermediate streams, including light diesel, naphtha, liquefied petroleum gas, propylene, and intermediates such as oil slurries and heavy oil. This portion of carbon is not directly oxidized to CO₂ but exits the unit with products or by-products. Process emissions: CO₂ generated from the partial oxidation of feedstocks and intermediates during cracking reactions. Fuel combustion emissions: CO₂ produced from fuel combustion in furnaces, steam boilers, and auxiliary combustion devices. Exhaust emissions: CO₂ released from coke combustion during catalyst regeneration, as well as carbon components present in the cracking reaction flue gas.

(2) Indirect emission carbon flows:

Indirect emission carbon flows are primarily associated with purchased energy consumption during unit operation. The inflows and outflows of these carbon streams include:

1. Carbon inflows: Carbon equivalents associated with purchased electricity, steam, and thermal energy. Although these energy sources do not undergo chemical reactions within the FCC unit, CO₂ emissions are generated during power or heat production.

2. Carbon outflows: Indirect CO₂ emissions resulting from energy consumption. These emissions do not originate directly from chemical reactions within the FCC unit but are transmitted to the unit via utility systems, representing indirect carbon flows.

By distinguishing between direct and indirect emission carbon flows and clearly defining their inflows and outflows, the FCC carbon hub provides a comprehensive representation of carbon cycling and emission characteristics within the unit. This framework offers quantitative support for the development of carbon reduction strategies and energy optimization measures.

3.3. Assessment Method

For carbon emissions from a single production unit, a hybrid approach combining the emission factor method [32], the lower heating value (LHV) method [33], and the carbon balance method [34] is adopted. Specifically, the carbon emissions of an individual unit consist of direct emissions and indirect emissions:

$$C_u = C_u^{DE} + C_u^{IE} \quad (1)$$

where C_u represents the total CO₂ emissions from the unit, and C_u^{DE} and C_u^{IE} denote the direct and indirect emissions, respectively.

Direct emissions consist of process emissions C_u^{PE} , fuel combustion emissions C_u^{CE} , and exhaust emissions C_u^{EE} :

$$C_u^{DE} = C_u^{PE} + C_u^{CE} + C_u^{EE} \quad (2)$$

Indirect emissions are generated by the consumption of purchased electricity, thermal energy, and other external utilities:

$$C_u^{IE} = C_u^{PW} \quad (3)$$

The fuel combustion emissions C_u^{CE} of a single unit are evaluated using the lower heating value (LHV) method:

$$C_u^{CE} = \sum_{j \in J} F_j(u, j) \cdot CC_j \cdot LLC_j \cdot CC_{rmm}, \forall u \in U \quad (4)$$

where $F_j(u, j)$ is the consumption of fuel j in unit u , CC_j is the carbon conversion rate (typically assumed to be 100%), and LLC_j is the lower heating value of the fuel. CC_{rmm} is defined as the relative molecular mass ratio of carbon atoms to carbon dioxide, which is generally set to 44/12. This method accurately reflects the carbon emission contribution from different fuel combustion processes.

The process emissions C_u^{PE} of a single unit are calculated using the carbon balance method, which determines emissions based on the difference in carbon content between the inlet and outlet material streams:

$$C_u^{PE} = \sum_{s' \in S^{in}} F_{s'}^{in}(u, s') \cdot CC_{s'} \cdot CC_{rmm} - \sum_{s \in S^{out}} F_s^{out}(u, s) \cdot CC_s \cdot CC_{rmm}, \forall u \in U \quad (5)$$

where $F_{s'}^{in}(u, s')$ and $F_s^{out}(u, s)$ are the inlet and outlet flow rates of stream s to and from unit u , and CC_s represents the carbon content percentage of stream s .

Exhaust emissions C_u^{EE} mainly originate from coke formation during catalyst regeneration and are estimated using the emission factor method:

$$C_u^{EE} = \sum_{l \in L} F_l(u, l) \cdot CF_u \cdot CC_c \cdot CC_{rmm}, \forall u \in U \quad (6)$$

where $F_l(u, l)$ denotes the consumption of catalyst l in unit u , CF_u is the coking factor for unit u , and CC_c is the emission factor for coke.

Emissions from utility or indirect energy consumption are quantified using the emission factor method:

$$C_u^{PW} = \sum_{r \in R} F_r(u, r) \cdot CDF_r \cdot CEF \cdot CC_{rmm} \quad (7)$$

where $F_r(u, r)$ is the consumption of energy r in unit u , CDF_r is the coal equivalent conversion factor for energy r , and CEF is the carbon emission factor, typically set as a constant. Notably, due to differences in energy units, all energy consumption in this study is converted to standard coal equivalent using the coal-equivalent factor method, allowing uniform calculation. This approach is applicable for quantifying indirect CO₂ emissions associated with electricity, steam, and thermal energy consumption, effectively reflecting energy-related emissions during unit operation.

Notably, in this work, carbon emission calculations and LCA are rigorously based on China's energy mix and associated emission factors, and this selection is justified for several reasons. First, the study focuses on typical FCC units operating within China, whose operational data, energy consumption patterns, and fuel composition accurately reflect domestic industrial practices. Therefore, employing China-specific standard coal equivalents and local emission factors ensures both the precision and applicability of carbon emission assessment. Second, substantial differences exist between China and regions such as Europe in terms of power generation structure, fuel composition, and carbon emission factors. For instance, European power systems feature a higher proportion of renewable energy and a lower share of coal. Direct application of European emission factors could result in assessments that deviate from actual operational conditions, thereby diminishing the engineering relevance of the study. Finally, the objective of this work is to establish a practical low-carbon optimization methodology whose core technical framework and optimization strategies possess cross-regional applicability. By grounding the analysis in China-specific emission factors, the study not only accurately captures the carbon emission characteristics of real industrial operations but also provides a comparative reference and theoretical basis for future extension of the methodology to other regions.

4. Low-Carbon Operation Optimization Framework for FCC Units Considering Carbon Tax Scenarios

4.1. Multi-Objective Operational Optimization Model for Production Units

In this section, a multi-objective operational optimization model is developed for FCC production units, aiming to simultaneously achieve carbon emission reduction and economic benefits. The optimization model primarily consists of three core components: operating variables, constraints, and objective functions. The following subsections systematically describe these components to clarify the model structure and implementation logic.

(1) Operating Variables and Constraints:

The process performance of an FCC unit is influenced by a variety of operating parameters. Based on conventional process design specifications and expert knowledge, eleven key process variables that significantly affect unit performance are selected in this study. These include: Feed Mass Flow (FM), Regenerator Pressure (REP), Reactor Pressure (RP), Reactor Outlet Temperature (ROT), Atomisation Steam (AS), Pre-lift Steam (PLS),

Stripping Steam (SS), Main Air (MA), Loose air (LA), Distribution Air (DA), and Return Conveyor Air (RCA) (see Table 1).

Regarding product classification, this study focuses on the main products and by-products of FCC units, including sour gas, dry gas, liquefied petroleum gas (LPG), gasoline, light diesel oil, oil slurry, propylene, and coke. To ensure the rationality of the operating variables and the safe operation of the unit, corresponding constraints are imposed on the selected process variables, as detailed in Table 1. The chosen variables and their constraint settings adequately represent the operational characteristics of the FCC unit and provide essential information for subsequent process optimization and multi-objective analysis.

Table 1. Operating variables and constraints for the FCC unit.

Process Variables	Constraints	Indicators
Regenerator pressure (kPa)	[300, 305]	Sour gas
Reactor pressure (kPa)	[270, 275]	Dry gas
Reactor outlet temperature (°C)	[510, 515]	Propylene
Atomisation steam (m ³)	[8950, 9050]	LPG
Pre-lift steam (m ³)	[8950, 9050]	Gasoline
Stripping steam (m ³)	[14,150, 14,350]	Light diesel oil
Main air (m ³)	[333,000, 334,500]	Oil slurry
Loose air (m ³)	[1200, 1300]	Coke
Distribution air (m ³)	[2750, 2850]	-
Return conveyor air (m ³)	[4500, 4600]	-
Feed mass flow (kg)	[695, 735]	-

(2) Objective Functions:

The operational optimization model for the FCC unit is formulated as a multi-objective framework, with the objective functions consisting of maximizing economic benefits and minimizing carbon emissions. The total production profit of the unit can be expressed as

$$profit_u = \sum_i^n F_i^{out} \times price_i - \sum_t^m F_t^{in} \times price_t - Cost_{unilty} \quad (8)$$

where n denotes the number of product types, m represents the number of feedstock types, $price_i$ is the sales price of the i -th product, $price_t$ is the cost of the t -th feedstock, and $Cost_{unilty}$ represents the cost of utility consumption. It should be noted that for certain intermediate materials, direct market prices are unavailable. To address this issue, the shadow price method [35] is introduced to quantify the opportunity cost of these intermediates during the production process. By assigning an implicit economic value to intermediate materials lacking market prices, the shadow price method enables a reasonable evaluation of their impact on production costs and resource allocation within the optimization model. Table 2 presents the sales prices and cost prices of feedstocks and products in the FCC unit.

Table 2. Material and product price list for the FCC unit.

Raw Material	Price	Products	Price
Mixed fractions	5.55 CNY/kg	LPG	4.85 CNY/kg
Residual oil	5.2 CNY/kg	Propylene	7 CNY/kg
Steam	0.14 CNY/kg	Light diesel oil	7.66 CNY/kg
Electricity	1.8 CNY/kwh	Oil slurry	2.2 CNY/kg
Water	0.28 CNY/m ³	Gasoline	8 CNY/kg
Air	0.1 CNY/m ³	Dry gas	0.5 CNY/kg
-	-	Coke	2.6 CNY/kg

Additionally, F_i^{out} and F_t^{in} represent the production quantity of product i and the feedstock input of type t , respectively, which are subject to the following constraint:

$$F_i^{out} = \sum_t^m F_t^{in} \times k_i \quad (9)$$

where k_i denotes the yield of product i , generally determined from actual production data. Notably, all operating variables can be mapped to product yields through kinetic equations:

$$K = \{k_1, k_2, \dots, k_i\} = f(x|x = Tp, Pr, St, Wi) \quad (10)$$

where Tp , Pr , St , and Wi correspond to various operating parameters, such as temperature, pressure, steam flow, and air flow, respectively.

The carbon emission objective function is quantified based on the unit-level carbon footprint assessment model established in Section 3, and can be expressed as the sum of direct and indirect emissions:

$$C_u = C_u^{DE} + C_u^{IE} \quad (11)$$

In summary, the multi-objective operational optimization model for the FCC unit, oriented toward carbon emission reduction, can be formulated as

$$\begin{aligned} \text{obj} & \begin{cases} \max \text{profit}_u \\ \min C_u \end{cases} \\ \text{s.t.} & \begin{cases} \text{Equations (1)–(7)} \\ \text{Equations (9) and (10)} \\ 0 \leq \text{Var}^L \leq \text{Var} \leq \text{Var}^U \\ i = 1, 2, \dots, I \\ t = 1, 2, \dots, T \\ s \in S, r \in R, l \in L \\ j \in J, u \in U \end{cases} \end{aligned} \quad (12)$$

Notably, although the constructed multi-objective optimization model systematically integrates operating variables, economic benefits, and carbon emissions, the kinetic relationship between product yields and operating variables is typically described by a set of complex partial differential equations. Directly solving these equations is computationally intensive and time-consuming, significantly increasing the computational cost of the optimization. To overcome this bottleneck and improve optimization efficiency, it is necessary to introduce a surrogate-assisted model that approximates the complex process kinetics as a rapidly computable functional form.

4.2. Surrogate Model Assisted by PINNs

The kinetics of product yields in the FCC process are typically described by a set of partial differential equations (PDEs), whose derivation and solution rely on in-depth theoretical foundations and complex engineering models. However, solving such PDEs is computationally intensive and process-intensive, representing a major technical bottleneck in multi-objective operational optimization. To improve computational efficiency and reduce solution costs, surrogate models can be introduced as an approximate tool. Surrogate models simplify the computation by mapping complex physical processes into rapidly computable functional forms and training these models using experimental or simulation data. Although conventional machine learning or deep learning-based “black-box” surrogate models excel in high-dimensional data fitting and pattern recognition, they often fail to guarantee physical consistency and lack interpretability, limiting their application in

high-reliability engineering scenarios. To address these limitations, this study develops a surrogate model assisted by a PINN [36], embedding mass conservation constraints into the neural network loss function to ensure that the predicted product yields satisfy the law of mass conservation.

Specifically, FCC product yields are influenced not only by operating variables (e.g., feed rate, reaction temperature) but also by underlying physical mechanisms, such as reactant conversion, product distribution, and by-product flows. Accordingly, a multi-layer perceptron (MLP) architecture is employed in combination with the PINN approach, incorporating mass conservation constraints [37] into the training process to ensure that the predictions are physically consistent while maintaining high data fitting accuracy. A detailed description of the MLP architecture can be found in the literature [38]. The total loss function constructed in this study is expressed as follows:

$$\ell_{total} = (1 - \lambda_p) \cdot \ell_{data} + \lambda_p \cdot \ell_{phys} \quad (13)$$

where λ_p represents the weighting coefficient for the physical loss.

The data fitting loss ℓ_{data} measures the discrepancy between the neural network predictions and the actual observations. It is a typical supervised learning mean squared error (MSE) term, defined as

$$\ell_{data} = \frac{1}{N} \sum_{i=1}^N \|\hat{y}_i - y_i^{true}\|_2^2 \quad (14)$$

where N is the number of training samples, $\hat{y}_i$ denotes the predicted value of the i -th sample, and y_i^{true} is the corresponding observed value.

The mass conservation loss ℓ_{phys} is introduced to constrain the neural network predictions of product yields to satisfy the principle of mass conservation. In FCC units, mass conservation is a fundamental physical law. Let F_{in} and F_{out} denote the total feed and total product mass per unit time, respectively. The mass conservation relationship can be expressed as

$$F_{in} = F_{out} \quad (15)$$

In practice, both feed and products are multi-component systems. Assume the feed contains n components, with the mass of the j -th component denoted as F_j . The products consist of m components, with the yield of the k -th component denoted as y_k . The mass of each product per unit time can be expressed as

$$P_k = y_k \cdot \sum_{j=1}^n F_j \quad (16)$$

Thus, the mass conservation equation for a multi-component system is given by

$$\sum_{j=1}^n F_j = \sum_{k=1}^m P_k = \sum_{k=1}^m y_k \cdot \sum_{j=1}^n F_j \quad (17)$$

In the neural network surrogate model, the network outputs the predicted yields $\hat{y}_k$ of each product. To ensure that the predictions satisfy the mass conservation principle, a mass conservation constraint is incorporated into the loss function, defined as the mean squared difference between the total feed mass and the total predicted product mass per unit time:

$$\ell_{phys} = \frac{1}{N} \sum_{i=1}^N \left(\sum_{j=1}^n F_{i,j} - \sum_{k=1}^m \hat{y}_{i,k} \cdot \sum_{j=1}^n F_{i,j} \right)^2 \quad (18)$$

where i is the sample index, N is the total number of training samples, and $\hat{y}_{i,k}$ denotes the predicted mass of the k -th product in the i -th sample. By incorporating this mass conservation loss during training, the network is guided to produce physically feasible outputs even under limited data conditions, ensuring that the predicted yields satisfy the law of mass conservation and improving the model's reliability and generalization capability.

4.3. Optimization Solution Strategy Considering Carbon Tax Scenarios

To effectively reduce carbon emissions in the FCC process, after introducing a carbon accounting framework and incorporating carbon emission minimization as an optimization objective, the scale and complexity of the operational optimization problem increase significantly, making it challenging for conventional solution methods to handle efficiently. To enhance computational efficiency, a carbon tax scenario [39] is introduced into the optimization model, converting the CO₂ emissions into corresponding carbon tax costs and incorporating them into the total production cost. In this way, the original multi-objective optimization problem can be transformed into a single-objective optimization problem, expressed as

$$\begin{aligned} \text{obj} \{ & \max (\text{profit}_{\text{unit}} - CT \cdot C_u) \\ \text{s.t.} \{ & \begin{cases} \text{Equations (1)–(7)} \\ \text{Equations (9) and (10)} \\ \text{Equations (13)–(18)} \\ 0 \leq \text{Var}^L \leq \text{Var} \leq \text{Var}^U \\ i = 1, 2, \dots, I \\ t = 1, 2, \dots, T \\ s \in S, r \in R, l \in L \\ j \in J, u \in U \end{cases} \end{aligned} \quad (19)$$

where CT denotes the carbon tax rate, expressed in CNY per kilogram of CO₂ equivalent (CNY/kgCO₂eq). Finally, based on this single-objective optimization model, the Particle Swarm Optimization (PSO) algorithm [40] is employed to obtain the optimal operating strategy that balances economic performance and low carbon emissions.

5. Case Study

5.1. Case Description

The FCC unit used in this case study is located at an integrated refinery and petrochemical production site in Jiujiang, Jiangxi Province, China. The operational data were collected on-site in March 2021. The operational optimization was conducted in the MATLAB 2023b environment. The computer hardware configuration included an Intel CPU i7-6700K (4.0 GHz), 16 GB of RAM, and an NVIDIA RTX 1060 8 GB GPU. In the surrogate-assisted experiments, the input–output relationships of the PINN model are presented in Table 3, providing a concise overview of the variables and dataset partitioning used for model training. The dataset used for training the surrogate model consists of 4650 samples, which are divided into training, testing, and validation sets in a ratio of 7:2:1. Prior to training, all input variables are normalized to the [0, 1] range, and output variables are scaled to facilitate convergence and ensure numerical stability of the neural network.

In this case study, the FCC unit feedstock input was 501.658 kt/month, and the carbon tax price was set at 1000 CNY/tCO₂eq, based on current market data from the Chinese carbon trading system, to reflect a typical carbon pricing level in the domestic industrial context. This value was selected according to the empirical range of carbon prices observed in domestic carbon markets and related policy practices, ensuring that the economic impact of carbon emissions is appropriately represented. By adopting this carbon tax rate, the case

study maintains practical relevance and analytical consistency, providing a sound basis for evaluating the effects of low-carbon optimization on the unit's economic performance.

Table 3. Training sample features in surrogate model experiments.

Category	Variable Type	Variables/Outputs
Input	Operating parameters	Feedstock flow rate, regenerator pressure, reactor pressure, reaction outlet temperature, atomisation steam flow, pre-lift steam flow, stripping steam flow, main air flow, loose air flow, distribution air, return conveyor air
Output	Product yields	Sour gas, dry gas, propylene, LPG, gasoline, light diesel oil, oil slurry, coke
Number of Samples	Data Partition	Preprocessing
4650	7:02:01	Normalization to [0, 1]

Additionally, the constructed PINN surrogate model adopts a multilayer perceptron (MLP) architecture with two hidden layers. The input layer receives the key operational variables of the FCC unit (as listed in Table 3), while the output layer predicts the yields of various product components. Each hidden layer consists of 64 neurons and employs the ReLU activation function. To mitigate overfitting during training, a dropout rate of 0.1 is applied to the hidden neurons. All input variables are normalized to the [0, 1] range prior to training, and the output variables are scaled correspondingly to enhance numerical stability during network training. The model is trained using the AdamW optimization algorithm with an initial learning rate of 1×10^{-3} for 1000 iterations. After extensive empirical tuning and cross-validation, the physical loss weight λ_p is set to 0.7, achieving an optimal balance between data-driven fitting and adherence to physical laws. This weighting ensures both high prediction accuracy of FCC unit yields and effective enforcement of mass conservation. The physical loss term is incorporated into the MSE loss function by embedding the mass conservation constraint of the FCC unit, thereby enabling the network to maintain predictive accuracy while satisfying fundamental physical principles. Training termination is based on a fixed number of iterations, with continuous monitoring of loss convergence on both training and validation sets to ensure stable model convergence. The PINN model is implemented in MATLAB 2023b, utilizing the Deep Learning Toolbox to construct the MLP network, with the physical loss term manually integrated within the training loop to achieve a unified framework of data-driven learning and physical constraint enforcement. Detailed model training parameters and network architecture are summarized in Table 4.

Table 4. The training parameters for the PINN model.

Category	Parameter	Value
Optimization & Training	Optimization Algorithm	AdamW
	Learning Rate (η)	1×10^{-3}
	Physical Loss Weight (λ_p)	0.7
	Number of Epochs (epoch)	1000
Multilayer Perceptron	Hidden Layer Dimension (H)	64
	Hidden Layer Number	2
	Dropout (p)	0.1
	Activation Function	ReLU
	Input Preprocessing	Normalization of inputs to [0, 1]
	Data Loss	Mean Squared Error
	MATLAB Implementation	Constructed using Deep Learning Toolbox

5.2. Optimization Results Analysis

Figure 3 illustrates the operational performance of the FCC unit following the implementation of the proposed optimization strategy over the production cycle. The results

indicate improvements across key performance indicators, thereby validating the effectiveness of the proposed optimization approach in terms of economic performance, energy utilization, and environmental impact. Based on the trained PINN surrogate model, the optimization process converges to the optimal solution within only 3.2 min, demonstrating the high computational efficiency and practical applicability of the proposed methodology for industrial low-carbon operation optimization.

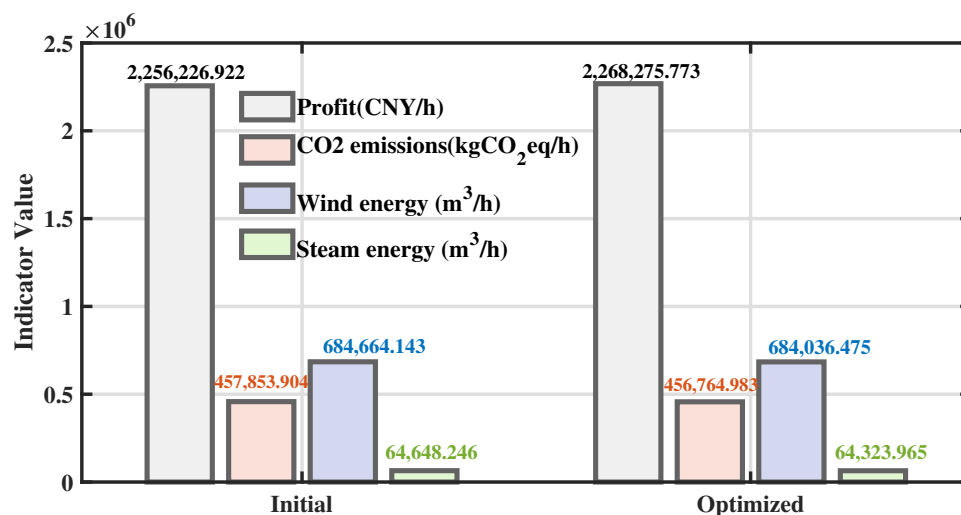


Figure 3. Distribution of operational optimization metrics for the FCC unit.

After optimization, the unit-time profit increased from 2,256,226.922 CNY/h to 2,268,275.773 CNY/h, representing an increase of approximately 0.5%. This indicates that under high-load continuous operation, resource utilization efficiency within the unit was enhanced, leading to improved economic returns. Although the profit increment is relatively modest, it can accumulate to significant benefits over extended operational periods. In terms of environmental performance, CO₂ emissions decreased from 457,853.904 kgCO₂eq/h to 456,764.983 kgCO₂eq/h, representing a reduction of approximately 0.24%, demonstrating that a degree of emission control can be achieved concurrently with economic improvement, thereby realizing the synergistic optimization of economic and environmental objectives. Furthermore, air flow and steam consumption decreased from 684,664.143 m³/h and 64,648.246 m³/h to 684,036.475 m³/h and 64,323.965 m³/h, respectively, indicating enhanced energy utilization efficiency. In particular, the reduction in steam consumption can further lower operational costs and associated carbon emissions. Overall, the proposed low-carbon operational optimization method not only improves the unit-time economic output of the FCC unit but also demonstrates positive effects on energy efficiency and emission control. These results provide a scientific basis for the optimization and sustainable operation of industrial units and offer strong support for achieving energy management and environmental protection objectives.

5.3. Carbon Emission Characteristics Analysis

Figure 4 presents the carbon emission characteristics of the FCC unit before and after optimization. According to the optimization results, CO₂ emissions from fuel combustion decreased from 130,448.304 kgCO₂eq/h to 129,795.383 kgCO₂eq/h, representing a relative reduction of approximately 0.07%, indicating the effectiveness of operational optimization in reducing fuel consumption and improving combustion efficiency. Process emissions decreased from 89,481 kgCO₂eq/h to 89,215.5 kgCO₂eq/h, representing a relative reduction of approximately 0.013%, suggesting that the optimization of operating conditions helped control incomplete conversion and energy losses in the reaction process, thus achieving a

reduction in carbon emissions at the micro-level. Flue gas emissions remained unchanged at 144,992.5 kgCO₂eq/h, indicating that the optimization measures had limited impact on the flue gas generation and treatment system. This is primarily because flue gas emissions are largely constrained by combustion conditions and the characteristics of the gas treatment units and therefore did not exhibit significant changes during operational optimization. Emissions from utility systems decreased from 92,932.1 kgCO₂eq/h to 92,761.6 kgCO₂eq/h, reflecting energy savings in steam, air, and other utility consumption, thereby reducing indirect carbon emissions. In summary, operational optimization of the FCC unit achieved significant reductions in fuel combustion and process emissions, while utility emissions were also slightly decreased, leading to an overall downward trend in carbon emissions. Although flue gas emissions did not change markedly, the optimization measures positively influenced overall carbon control by improving energy efficiency and reducing energy waste in reaction and utility systems. These results demonstrate that through scientific design and adjustment of operating conditions, low-carbon operation can be achieved while maintaining production stability, providing a reliable strategy for the green and sustainable operation of FCC units.

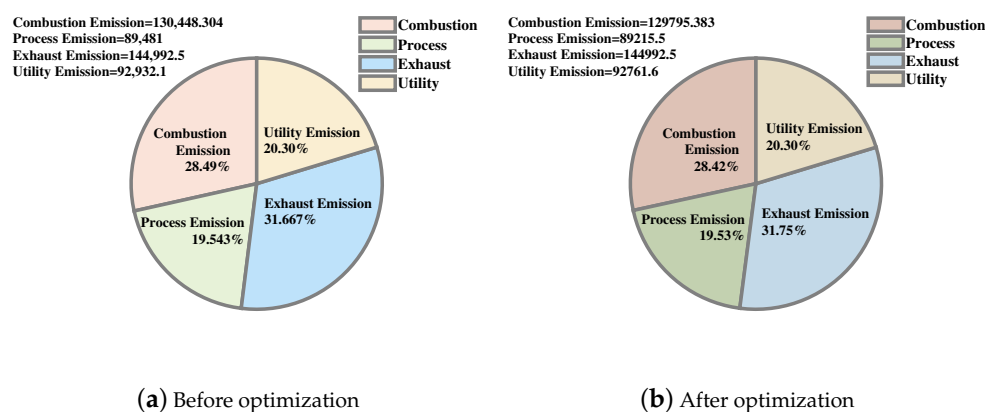


Figure 4. The carbon emission characteristics of the FCC unit before and after optimization.

Figure 5 compares the key operating variables of the FCC unit before and after optimization. It is evident that several critical operating parameters underwent significant adjustments, demonstrating the effectiveness of the optimization strategy in improving production efficiency and reducing energy consumption.

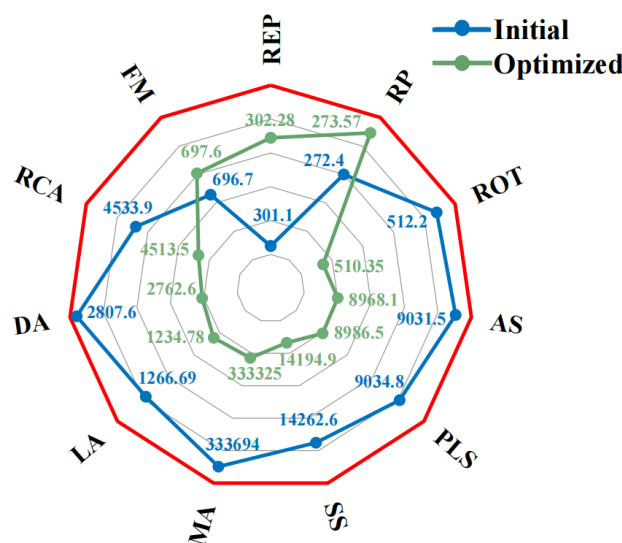


Figure 5. Comparison results of operating conditions.

Specifically, the regenerator pressure increased from 301.1 kPa to 302.28 kPa, an increase of approximately 0.4%. This slight adjustment helps enhance catalyst regeneration capability while maintaining reaction efficiency, suppressing coke formation, and improving overall unit stability. Reactor pressure increased from 272.4 kPa to 273.57 kPa, an increase of approximately 0.43%, which helps improve internal reactor hydrodynamics, enhancing contact efficiency between oil–gas and catalyst, thereby promoting cracking reaction conversion and improving product yield and quality. The reactor outlet temperature slightly decreased from 512.2 °C to 510.35 °C, a reduction of about 0.4%. This adjustment helps suppress excessive cracking and coke formation, alleviates high-temperature stress on equipment and catalyst, extends equipment lifespan, and improves product composition. Atomizing steam and pre-lift steam flows decreased from 9031.5 m³/h to 8968.1 m³/h and from 9034.8 m³/h to 8986.5 m³/h, respectively, corresponding to reductions of 0.7% and 0.5%. Stripping steam flow decreased from 14,262.6 m³/h to 14,194.9 m³/h, approximately a 0.5% reduction. These adjustments indicate that optimization can effectively control steam consumption, improve energy efficiency, and reduce system load. In terms of air distribution, the main air flow decreased slightly from 333,694 m³/h to 333,325 m³/h, a reduction of about 0.1%; the loosened air flow in the external heat exchanger decreased from 1266.69 m³/h to 1234.78 m³/h, a 2.5% reduction. The external circulation bottom distribution flow and external return transport air flow also decreased. These changes reflect the role of the optimization strategy in reducing air consumption and improving system energy efficiency. The material feed rate changed minimally from 696.7 t/h to 697.6 t/h, indicating that optimization primarily targeted operational efficiency and energy management while maintaining feed stability and continuous production. Overall, the optimization of operating conditions in the FCC unit resulted in reasonable adjustments to multiple key process parameters. The measures not only effectively improved operational efficiency but also reduced steam and air consumption, thereby lowering energy input, reducing production costs, and enhancing process sustainability. This optimization strategy supports both economic performance and environmental load control.

Table 5 presents the changes in product yields of the FCC unit under optimized operating conditions. The results indicate a significant increase in the yield of high-carbon liquid products, with light diesel oil increasing from 22.396% to 22.629% and oil slurry increasing from 4.584% to 4.656%. Low-carbon light fractions experienced a slight decrease, including a reduction from 3.637% to 3.603% for dry gas, from 15.139% to 15.01% for LPG, from 40.492% to 40.41% for gasoline, and from 6.976% to 6.915% for the light fraction of oil slurry. Sour gas yield remained unchanged, and coke yield increased marginally from 6.775% to 6.776%, indicating stable by-product formation. From the perspective of carbon flow distribution, the optimization increases carbon incorporation into high-value liquid products while reducing low-carbon light fractions, enhancing carbon utilization efficiency. The decrease in light fraction yields also reflects suppression of side reactions and a shift of carbon flow toward liquid fuels, contributing to reduced carbon emissions per unit product. The stable coke yield indicates that the increase in high-carbon liquid products did not significantly exacerbate negative effects from catalyst regeneration or coke deposition, ensuring stable and sustainable reactor operation. The observed yield changes are attributed to the regulation of reaction temperature, steam flow, and gas–solid distribution through operating condition optimization, which favors the formation of medium- to heavy-carbon chain liquid products while suppressing the generation of light fractions such as LPG and dry gas. This redistribution of carbon flow not only increases high-value product yield but also optimizes carbon emission structure, thereby reducing the carbon footprint per unit of product. Overall, the optimized operation enhances both high-carbon product yields and carbon utilization efficiency, achieving concurrent economic

and environmental benefits, and provides a theoretical basis and quantifiable data for low-carbon operation and energy optimization in industrial FCC units.

Table 5. Variation in product yield distribution of the FCC unit.

Product Category	Yield Before Optimization (%)	Yield After Optimization (%)
Sour gas	0.001	0.001
Dry gas	3.637	3.603
LPG	15.139	15.01
Gasoline	40.492	40.41
Light diesel oli	22.396	22.629
Oil slurry	4.584	4.656
Propylene	6.976	6.915
Coke	6.775	6.776

5.4. Validation of the PINN Model

To evaluate the training performance of the constructed surrogate-assisted model, operational data from the FCC unit were used to train the model. During training, the evolution of the loss function was recorded, including mean squared error (MSE) loss, physics-constrained loss, and total loss. Figure 6 illustrates the variation of each loss function with training iterations, providing a visual assessment of convergence behavior and fitting performance, thereby validating the model's ability to maintain both data fitting accuracy and physical consistency.

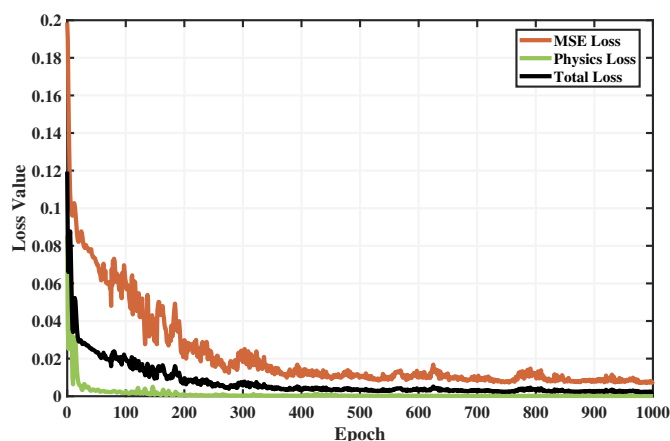


Figure 6. Trends of various loss functions during training.

As shown in Figure 6, all loss functions decreased and gradually stabilized with increasing iterations. During early training stages, the physics-constrained loss decreased significantly, indicating its critical role in guiding the model optimization and influencing total loss convergence. The incorporation of physics loss enhances the model's adherence to actual physical processes, improving prediction accuracy and reliability. These results validate the effectiveness of the material balance loss as a training objective, improving model fitting performance and promoting stable convergence during training. Overall, optimizing the physics-constrained loss significantly enhances model robustness, reduces overfitting risk, and ensures the physical feasibility and reliability of the surrogate model in practical applications.

To further evaluate the performance of the proposed surrogate-assisted model, systematic comparative experiments were conducted against several mainstream surrogate-assisted models, including BO-XGBOOST [41], NOS-Kriging [42], CNN-BiLSTM [43], Transformer [44], and BO-GPR [45]. Model performance was assessed using operational data from a single FCC unit, with predictive accuracy quantified by R^2 and RMSE values on the test set. Each experiment was repeated 50 times to ensure statistical robustness,

and the optimal, mean, and variance values were recorded to evaluate model stability and performance variability. The use of a single FCC unit provides a consistent and controlled dataset, facilitating reliable benchmarking of the surrogate models.

As shown in Table 6, the surrogate-assisted model based on the PINN demonstrates significant advantages in predicting product yields for the FCC unit. Specifically, the PINN model achieved an optimal R^2 of 0.9973, an average R^2 of 0.9968, and a variance of 1.2×10^{-5} , substantially higher than other comparison models (BO-XGBOOST: average $R^2 = 0.9182$, variance = 4.5×10^{-4} ; NOS-Kriging: average $R^2 = 0.9705$, variance = 2.1×10^{-5} ; CNN-BiLSTM: average $R^2 = 0.955$, variance = 3.8×10^{-5} ; Transformer: average $R^2 = 0.985$, variance = 1.6×10^{-5} ; BO-GPR: average $R^2 = 0.9618$, variance = 3.2×10^{-5}). In terms of prediction error, the PINN model achieved a minimum RMSE of 0.1437, an average RMSE of 0.1482, and a variance of 2.5×10^{-4} , which is significantly lower than other methods (BO-XGBOOST average RMSE = 0.6013; NOS-Kriging = 0.3521; CNN-BiLSTM = 0.3842; Transformer = 0.1975; BO-GPR = 0.3689). These results indicate that the PINN model can achieve high-precision predictions when handling complex, multivariable, and nonlinear production data of FCC units, while ensuring stability and reproducibility of outputs. The superior performance of the PINN model primarily stems from embedding physical laws into the neural network during training, ensuring that predictions not only fit the statistical characteristics of observed data but also satisfy physical consistency constraints. This approach enhances generalization in highly nonlinear and strongly coupled FCC processes and significantly reduces prediction errors. In contrast, traditional data-driven models, such as BO-XGBOOST and BO-GPR, may achieve certain fits under specific conditions but lack direct integration of physical laws, resulting in lower prediction accuracy and stability under complex operating conditions. Overall, experimental results fully validate the effectiveness and reliability of the PINN-assisted surrogate model in predicting FCC product yields. The model demonstrates clear advantages in achieving high predictive accuracy, low error, and physical consistency, providing robust technical support for operational optimization and low-carbon decision-making in industrial units.

Table 6. Evaluation results of metrics for different surrogate models fitting.

Indicator Name	Indicator Type	PINN	BO-XGBOOST	NOS-Kriging	CNN-BiLSTM	Transformer	BO-GPR
R^2	Best	0.9973	0.9236	0.9731	0.9596	0.9864	0.9650
	Mean	0.9968	0.9182	0.9705	0.955	0.985	0.9618
	Variance	0.000012	0.000450	0.000021	0.000038	0.000016	0.000032
RMSE	Best	0.1437	0.5841	0.3467	0.3785	0.1919	0.3635
	Mean	0.1482	0.6013	0.3521	0.3842	0.1975	0.3689
	Variance	0.00025	0.00580	0.00060	0.00090	0.00030	0.00110

5.5. Discussion

5.5.1. Advantages of the Proposed Method

This study integrates a PINN-assisted surrogate model with PLCA to achieve low-carbon operational optimization for FCC units. The advantages of this method can be summarized in three aspects: (1) PINN model advantages: By embedding physical constraints during neural network training, the model strictly adheres to mass balance and reaction mechanism requirements, ensuring physically reasonable predictions. In complex, nonlinear, and multivariable production systems, the PINN model achieves high-precision predictions, significantly reduces prediction errors, and enhances generalization. Moreover, the model transforms complex kinetic mappings into efficiently computable functions, substantially reducing the computational cost of multi-objective optimization and providing feasibility support for continuous industrial optimization. (2) Life cycle assessment advantages: PLCA enables high-resolution quantification of direct and indirect carbon

emissions at the single-unit level, allowing precise tracking and dynamic analysis of carbon flows. This method quantifies carbon flow changes before and after optimization, providing reliable data support for low-carbon operational strategies while mitigating errors introduced by uncertainties in upstream raw materials and downstream products in traditional LCA, thereby ensuring accuracy and robustness in carbon footprint assessment. (3) Multi-objective low-carbon optimization advantages: The constructed optimization model integrates economic profit maximization and carbon emission minimization into a unified framework, achieving coordinated optimization of production performance and environmental performance. Under a carbon tax scenario, the method translates carbon emissions into economic costs, providing quantitative support for low-carbon operational strategies. Furthermore, combined with the high-efficiency predictive capability of the PINN-assisted surrogate model, computational effort and time consumption in the optimization process are significantly reduced, enhancing the reliability and implementability of optimization decisions while maintaining product yield and carbon emission accuracy.

5.5.2. Limitations and Future Work

Despite the significant advantages demonstrated by the PINN-assisted surrogate model combined with PLCA for low-carbon optimization in FCC units, several limitations remain. First, the model's training and validation rely on high-quality, comprehensive historical production data. In cases of insufficient data or measurement errors, prediction accuracy and generalization may be limited, particularly under extreme operating conditions or novel process scenarios, where reliability requires further verification. Second, the current proxy model primarily considers mass balance constraints, whereas energy conservation, non-ideal kinetics, and catalyst deactivation have not been fully integrated, which may affect prediction accuracy under high-load or long-duration operations. Finally, carbon emission quantification in the optimization model focuses mainly on CO₂, with other greenhouse gases such as CH₄ and N₂O not fully covered, limiting the comprehensive assessment of low-carbon performance and environmental impact.

Future work can focus on three directions: (1) Incorporating multi-source data fusion and real-time sensor data to enhance prediction accuracy and applicability under complex operating conditions. (2) Integrating energy conservation, catalyst deactivation, and multiphase reaction kinetics constraints into the PINN model to improve physical consistency and long-term prediction stability. (3) Expanding carbon footprint assessment to include CH₄, N₂O and other greenhouse gases for comprehensive evaluation of low-carbon performance.

5.5.3. Application Expansion

Although the methodology proposed in this study is primarily applied to FCC units, its underlying principles and technical framework exhibit broad applicability and generalizability, rendering it suitable for a variety of industrial sectors and application scenarios: (1) Complex industrial processes: The approach can be extended to chemical synthesis units, high-temperature gasification, metallurgical processes, and power generation systems, enabling high-precision prediction and optimized control of carbon emissions and product performance. (2) Energy systems and renewable energy: In wind, photovoltaic, biomass, and energy storage systems, the method can be integrated with life-cycle assessment to quantify carbon emissions and energy consumption, facilitating efficient operational optimization and the development of low-carbon dispatch strategies. (3) Urban infrastructure and building energy management: By enabling high-fidelity simulation and optimization of carbon emissions and energy consumption in urban heating, building energy use, and transportation systems, the framework provides a scientific basis for low-carbon design,

intelligent management, and policy formulation. In the future, through integration with artificial intelligence-based optimization algorithms, digital twin platforms, and real-time monitoring systems, this methodology is expected to support cross-industry, multi-scale low-carbon optimization and intelligent decision-making, thereby contributing to sustainable development.

Additionally, the proposed methodology is suitable for implementation in industrial FCC units and other process systems, contingent upon the availability of operational and process data of adequate quality. Successful deployment entails integration with existing process control and data acquisition infrastructures, complemented by systematic calibration and periodic validation to preserve model fidelity across varying operational conditions. These requirements are compatible with conventional industrial computing capabilities, indicating that the methodology is practically deployable while maintaining reliable predictive performance and enabling high-precision, low-carbon process optimization.

6. Conclusions

This study addresses the challenges of inaccurate carbon emission quantification, difficulty in implementing low-carbon operational optimization, and slow solution of complex kinetic mappings in FCC units. A PINN-assisted low-carbon operational optimization approach was proposed. Specifically, a single-unit carbon footprint model was developed based on PLCA, enabling high-resolution quantification of direct and indirect carbon emissions. Subsequently, a multi-objective low-carbon optimization model under a carbon tax scenario was constructed, integrating carbon emissions and associated carbon tax costs into the optimization objective, achieving coordinated optimization of economic performance and low-carbon operation. Finally, a PINN-based surrogate-assisted model was developed, embedding mass balance constraints into neural network training, providing efficient approximation of complex product yield kinetics and improving computational efficiency and predictive reliability for optimization. The proposed method was applied to real operational data from an FCC unit at a refinery production site. Optimization results showed an increase in hourly profit from 2,256,226.922 CNY/h to 2,268,275.773 CNY/h. CO₂ emissions decreased from 457,853.904 kgCO₂eq/h to 456,764.983 kgCO₂eq/h. Steam consumption decreased from 64,648.246 m³/h to 64,323.965 m³/h, improving energy efficiency. Yields of light diesel and oil slurry increased from 22.396% and 4.584% to 22.629% and 4.656%, respectively, while low-carbon light fraction yields slightly decreased, demonstrating effective carbon flow redistribution and high-value product yield improvement. The surrogate model validation indicated that the PINN model achieved an average R^2 of 0.9968 and average RMSE of 0.1482, significantly outperforming other models.

The PINN-assisted low-carbon operational optimization approach provides three key advantages: (1) high-resolution carbon quantification with physical consistency, ensuring reliable optimization results; (2) multi-objective optimization with carbon tax scenario analysis, achieving coordinated economic and low-carbon performance and providing quantitative decision support for industrial low-carbon operation; and (3) proxy-assisted modeling, which significantly improves computational efficiency, enabling feasibility for online optimization of complex industrial units. Future work will focus on: (1) integrating energy conservation, catalyst deactivation, and multiphase reaction kinetics constraints to enhance predictive accuracy and long-term stability under extreme conditions; (2) expanding carbon footprint assessment to include CH₄, N₂O, and other greenhouse gases, enabling comprehensive evaluation of low-carbon performance and exploring cross-industry, multi-scale low-carbon optimization and intelligent decision-making applications.

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