



ISSN: 1813-162X (Print); 2312-7589 (Online)

Tikrit Journal of Engineering Sciences

available online at: <http://www.tj-es.com>
TJES
Tikrit Journal of
Engineering Sciences

Production and Characterization of Synthetic Diesel Fuel from Coal via Fischer–Tropsch Indirect Liquefaction

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Keywords:

Coal liquefaction; Fischer–Tropsch synthesis; Synthetic diesel fuel; Gasification; Cobalt catalyst; Fuel properties; Emission reduction; Energy security.

Highlights:

- The developed process achieved a synthetic diesel cetane number of 72, which significantly exceeds conventional diesel benchmarks.
- The variation in synthesis pressure enabled precise control of product distribution, increasing the diesel fraction yield up to 61.8%.
- The produced fuel demonstrated exceptional long-term stability with minimal oxidation over 180 days of accelerated aging.

ARTICLE INFO

Article history:

Received	09 Jul.	2025
Received in revised form	17 Sep.	2025
Accepted	18 Oct.	2025
Final Proofreading	13 Dec.	2025
Available online	19 Dec.	2025

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Citation: Astanakulov KD, Quttymuratova YA, Sevryugina NS, Dorofeev EM. **Production and Characterization of Synthetic Diesel Fuel from Coal via Fischer–Tropsch Indirect Liquefaction.** *Tikrit Journal of Engineering Sciences* 2025; 32(Sp1): 2633.
<http://doi.org/10.25130/tjes.sp1.2025.15>

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Abstract: This study investigates the production of synthetic diesel fuel from coal through indirect liquefaction using Fischer–Tropsch synthesis. A series of experiments was performed, starting with coal gasification in a vertical reactor at 1270°C and 22 bar to produce synthesis gas containing approximately 51.4% of carbon monoxide and 43.7% of hydrogen. After purification, the synthesis gas underwent catalytic conversion in a high-pressure reactor using a cobalt–zirconia catalyst. Under baseline conditions of 227°C and 25 bar, the average liquid product yield was 12.6 kg over 6 hours, with the diesel and kerosene fractions of 57.4% and 31.2%, respectively. Increasing the pressure to 30 bar enhanced the diesel fraction to 61.8% and improved the total liquid yield by 7.5%. The resulting synthetic diesel exhibited superior properties compared to petroleum-derived fuel, including a cetane number of 72, sulfur content below 2 mg/kg, and aromatic hydrocarbons limited to 3.2%. Stability tests conducted over 180 days confirmed excellent oxidation resistance. These findings demonstrate that indirect coal liquefaction can deliver high-quality diesel fuel with significant potential to reduce environmental impacts and enhance energy security. The cobalt–zirconia catalyst was prepared in-house as a bulk CoO–ZrO₂ granulate and pre-reduced in situ before synthesis. Under 225–230 °C and 25–30 bar, the system consistently delivered 57.4–61.8 wt% diesel within the liquid products with stable operation. The process configuration is compatible with pre-combustion CO₂ capture units, providing a clear pathway for integrating CCS in future scale-up.

1. INTRODUCTION

In the modern world, the issues of ensuring sustainable energy supply and reducing dependence on traditional hydrocarbon resources are becoming increasingly important. The growth of global fuel consumption, the deepening energy crisis, and the desire to reduce greenhouse gas emissions are driving a sustained trend towards the search for development and deployment of alternative fuels. One of the priority areas in this context is the production of liquid coal fuel, which is considered an important strategic measure to diversify energy resources and improve the energy security of several countries. At the same time, this problem is especially relevant for countries with significant coal reserves and limited oil reserves, which is clearly demonstrated by the historical and contemporary experience of Germany, South Africa, China, and the USA [1-5]. Today, two main technological approaches are used for the production of liquid coal fuel, each with its own advantages and limitations. The first approach is based on direct liquefaction of coal, in which the feedstock is crushed and interacts with water, reagents, and hydrogen under high temperatures and pressure. As a result of the chemical transformation, the coal mass is converted into hydrocarbons suitable for subsequent purification and use in internal combustion engines. The advantages of the direct liquefaction method include the relative technological simplicity of the process and the possibility of obtaining fuel with characteristics close to those of petroleum diesel. However, this process requires extensive preliminary preparation of coal, in particular demineralization and strict control of fractional

composition, and is also associated with elevated carbon dioxide emissions during combustion of the finished product [6]. These factors significantly limit the prospects of this method, particularly in light of increasingly stringent environmental regulations and national commitments to reduce anthropogenic CO₂ emissions [7,8]. The second approach, indirect coal liquefaction, is based on the principle of gasification of solid fuel and the subsequent synthesis of liquid hydrocarbons using the Fischer-Tropsch reaction (Fig. 1). First, coal undergoes partial oxidation to form synthesis gas, which is a mixture of carbon monoxide and hydrogen. Then, under the action of catalysts such as iron or cobalt, the gas mixture is converted into liquid hydrocarbons, which are cooled, purified, and divided into desired fractions, including diesel fuel, kerosene, and propane. One of the key advantages of this method is the ability to obtain fuel with improved performance properties compared to oil analogues: a higher octane number, minimal sulfur content, and an almost complete absence of aromatic hydrocarbons. In addition, the combustion of such fuel is accompanied by substantially reduced harmful emissions. An important advantage of indirect liquefaction is the ability to utilize by-products such as steam, steam for electricity generation, as well as chemical compounds used in the production of plastics, synthetic fibers, and lubricants [9-13]. Comprehensive treatments of coal gasification unit operations and FT catalyst selection are provided in standard references and recent reviews, which frame the present process choices.



Fig. 1 The Plant for the Production of Synthetic Diesel Fuel from Coal.

At the same time, despite the obvious technological and environmental advantages, the indirect liquefaction method requires significant capital investments in the construction of gasification plants and synthesis reactors, highly qualified personnel, and customization of the technology to coal-specific characteristics. An equally significant factor is the need to develop and implement effective systems for CO₂ capture and utilization during gasification and synthesis. In gasification-based FT configurations, pre-combustion CO₂ removal from syngas using physical-solvent or amine systems allows for routinely achieving high capture rates at elevated CO₂ partial pressure, while keeping the energy penalty manageable at the CTL scale. We therefore consider the present setup (already featuring partial upstream CO₂ removal and tail-gas CO₂ at ~8.4 vol%) as a suitable basis for integrating a dedicated capture unit (e.g., Selexol/Rectisol or advanced amines) targeting $\geq 90\%$ of the overall CO₂ capture in subsequent pilot work. The compliance of the technology with modern environmental standards depends on the successful solution of these problems. In recent decades, interest in indirect coal liquefaction has increased significantly, which was facilitated by examples of successful industrial applications of FT synthesis. Historically, the most indicative experience is Germany, where several dozen plants were built during World War II, providing a significant part of the country's transport fuel requirements. Later, the unique experience of South Africa in the conditions of the international oil embargo demonstrated that indirect coal liquefaction could become the basis for a sustainable national fuel balance. Today, similar projects are being implemented in China, Australia, and the United States. A number of other countries, and authoritative international organizations, including the International Energy Agency and the World Coal Institute, recognize the development of synthetic coal fuel production as a priority area of energy policy [14-19]. In this regard, the direction chosen in the study seems justified and extremely relevant. The use of the indirect coal liquefaction method using the Fischer-Tropsch reaction allows not only the creation of additional sources of liquid hydrocarbons for transport and industry, but also increases energy security by mitigating dependence on oil price volatility and the risks of supply shortages. An important feature of this technology is its high flexibility, which allows processing coals of various qualities and even carbon-containing waste, which creates the prerequisites for the efficient use of mineral resources. In addition, in the case of the current trends in decarbonization and the transition to more environmentally friendly types of fuel, the

development of systems for capturing and subsequent use or utilization of carbon dioxide as part of the coal gasification process is an important condition for reducing the carbon footprint of synthetic fuels. Therefore, the presented direction combines technological maturity, proven industrial efficiency, and prospects for further improvement in the context of modern environmental challenges. The purpose of this work was to study the technology of producing alternative liquid coal fuel by indirect liquefaction using FT synthesis, to analyze its fuel and energy characteristics, including a comparative assessment with traditional petroleum fuels, and to consider the possibilities of using the resulting product in various sectors of the economy.

2. RESEARCH METHODS

As part of the methodology of this study, a series of experiments was conducted to comprehensively study the process of indirect coal liquefaction by gasification with subsequent synthesis of liquid fuel using the Fischer-Tropsch technology. The primary objective of the experiments was to produce a stable synthesis gas, perform catalytic hydrocarbon synthesis, and subsequently analyze the quality of the final fuel and by-products. For coal gasification, a vertical gasification unit of the GSP-1200 brand was utilized, equipped with a reaction chamber lined with heat-resistant ceramics and an oxidizing agent supply system [20-22]. The chamber had a working volume of 0.85 m³ and allowed processes to be carried out at temperatures of up to 1450 °C and pressures of up to 35 atmospheres. Coal gasification was carried out in the partial oxidation mode at a temperature of 1250–1300 °C and an excess pressure of 22 atmospheres. Oxygen and steam supply were regulated by an automated dosing system with a step of 0.5 kg / h. The feed rate of the coal-water mixture was 15 kg/h, which ensured a stable concentration of carbon monoxide and hydrogen in the synthesis gas (Fig. 2). After gasification, the resulting synthesis gas was purified from sulfur compounds and carbon dioxide using an ACF-250 continuous adsorption column loaded with activated carbon and a zeolite sorbent. The adsorption process was conducted at a temperature of 45°C and an operating pressure of 18 atm. According to the results of gas analysis, the impurity content did not exceed 0.02%. Catalytic synthesis of liquid hydrocarbons was carried out in an HTCR-500 high-pressure reactor with an internal coating of the Inconel 625 alloy, resistant to the effects of aggressive components of the synthesis gas. The working volume of the reactor was 160 liters. To implement the process, a cobalt catalyst modified with zirconium oxide was used at a concentration of 25% of the charge

weight. Synthesis was carried out at a temperature of 225–230 °C and a pressure of 25 atm; the synthesis gas feed rate was maintained at 220 Nl/h. Cobalt catalysts promoted with ZrO₂ are well established in Fischer–Tropsch synthesis; Zr has been shown to enhance C₅⁺ selectivity and activity on alumina and related supports. In this study, the novelty does not lie in claiming a new formulation, but in deploying a bulk granulated CoO–ZrO₂ composite (1.8–

2.2 mm, 128 m² g⁻¹) under a coal-derived syngas at 225–230 °C and 25–30 bar, achieving high diesel selectivity without noble promoters. We position our contribution as optimization of the process-window using an industrially relevant catalyst morphology, consistent with the state of the art on Zr-promoted cobalt systems [23–26]. During the reactions, the CO/H₂ ratio and the liquid phase accumulation rate were simultaneously monitored.

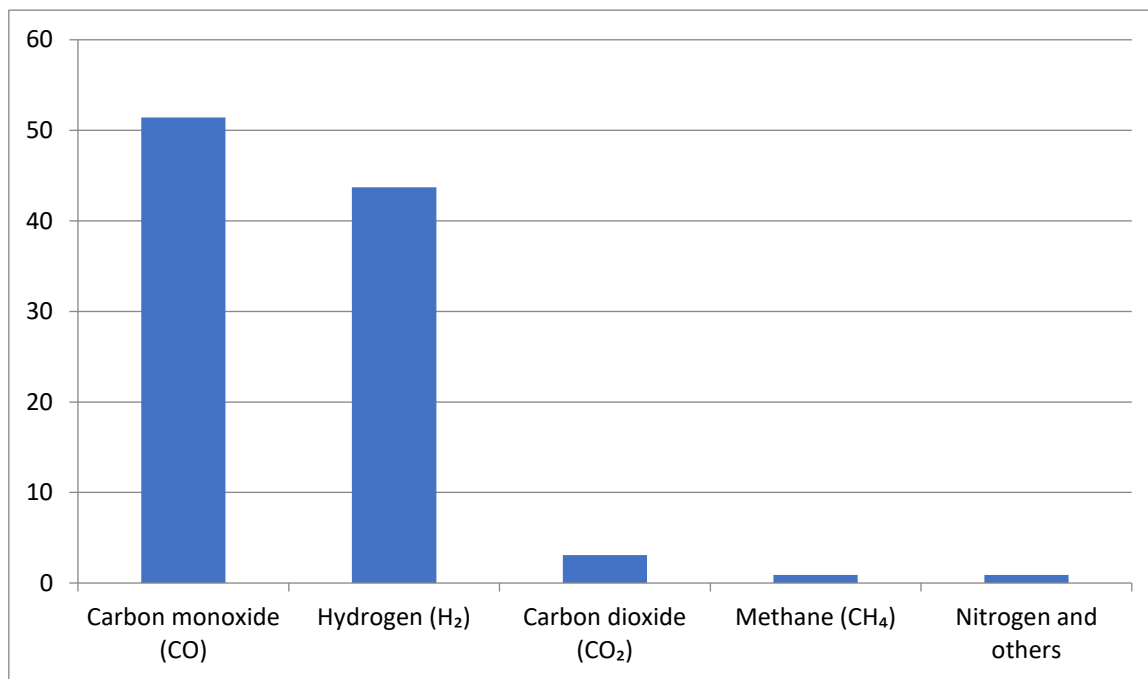


Fig. 2 The Composition of Synthesis Gas after Gasification and Purification.

To assess the physicochemical characteristics of the obtained fuel, fractional composition analyzers were used, including the Crystek-7000 device, which ensures the determination of the initial boiling point and the final distillation point. An additional experiment was conducted to study the effect of changes in the synthesis pressure on the yield of diesel and kerosene fractions. For this purpose, the synthesis was carried out at pressures of 20 and 30 atm while maintaining a constant temperature and catalyst composition. All key measurements were performed in triplicate on independent batches ($n = 3$). The 6 h liquid yield at 227 °C/25 bar was 12.6 ± 0.4 kg (RSD = 3.2%). Fraction yields at 25 bar were 57.4 ± 1.3 wt% (diesel), 31.2 ± 0.9 wt% (kerosene), 6.8 ± 0.4 wt% (light hydrocarbons), and 4.6 ± 0.3 wt% (waxes). At 30 bar, the total liquid yield was 13.5 ± 0.5 kg with 61.8 ± 1.1 wt% diesel; at 20 bar, it was 11.4 ± 0.4 kg with 52.6 ± 1.5 wt% diesel. The diesel density was 0.792 ± 0.003 g cm⁻³ at 20 °C; aromatic content was 3.2 ± 0.2 wt%. Sulfur was below the LOQ method of 2 mg kg⁻¹ (repeatability was verified using a 3 mg kg⁻¹ spike, with RSD < 5%). Unless otherwise stated, values were mean \pm SD. Additional tests were conducted to obtain by-product

chemicals, including synthetic wax and light hydrocarbons, and to evaluate their suitability for use in lubricants and the polymer industry.

3. RESULTS AND DISCUSSION

The study employed a comprehensive experimental approach to systematically investigate the technology of indirect coal liquefaction to obtain synthetic hydrocarbon fractions. Preparation of coal feedstock involved pre-crushing in a VM-850 vibration mill to a particle size of less than 80 μ m. To ensure stable combustion and uniform feed to the gasification unit, a coal-water suspension with a concentration of 62% coal by weight was prepared. The prepared suspension was dosed using an automated feeder with a feed capacity of 15 kg/h. Gasification was carried out in a vertical unit equipped with a 0.85 m³ reaction chamber and a refractory ceramic lining. The process was carried out at a temperature of 1270 °C and a pressure of 22 atmospheres. The oxidizing agent was supplied as a mixture of oxygen and superheated water vapor in a mass ratio of 1:1; the gas feed rate was 24 Nm³/h. The output was synthesis gas characterized by a carbon monoxide content of 51.4% and hydrogen of 43.7%. Impurities in the form of carbon dioxide and methane were less than 4%

by volume. To remove acidic components and traces of sulfur, the mixture was passed through an adsorption column operating at 45°C and a pressure of 18 atmospheres. Following purification, the synthesis gas was fed to a high-pressure HTCR-500 reactor for catalytic conversion via the Fischer-Tropsch process. The catalyst was a granulated mixture of cobalt oxide and zirconium oxide with a grain size of 1.8–2.2 mm and a specific surface area of 128 m²/g. Catalyst preparation and activation were as follows. A bulk unsupported CoO–ZrO₂ granulate (1.8–2.2 mm; BET 128 m² g⁻¹) was prepared in-house by co-precipitating aqueous Co(NO₃)₂·6H₂O and zirconyl nitrate (analytical grade, Sigma-Aldrich or equivalent) with the pH of 9.0 ± 0.2 (NH₄OH), aging for 2 h, filtration, drying at 120 °C (overnight), wet granulation, and calcination at 400 °C for 6 h in air. The resulting composition corresponded to 20 wt% of Co (as CoO) with ZrO₂ as the matrix; no additional support was used. Before the FT operation, the bed was reduced in situ under 10 vol% H₂/N₂ (3 NL min⁻¹) with a 1 °C min⁻¹ ramp to 350 °C and a 6–8 h hold, then cooled to 225–230 °C under H₂ and switched to syngas. This activation protocol is consistent with the best practice for Zr-promoted Co catalysts that favor higher C₅⁺/diesel selectivity. The synthesis reaction was carried out at a temperature of 227°C and a pressure of 25 atm, with a gas feed rate of 220 nl/h. An automated system continuously recorded process parameters, including temperature, pressure, a gas flow rate, and liquid phase mass at 30-second intervals. During additional experiments, the effect of pressure on product selectivity was investigated by conducting experiments at 20 and 30 atmospheres, while maintaining all other conditions constant. The purpose of this part of the work was to determine the effect of pressure on the selectivity of diesel and kerosene fraction formation. The effect of the gas contact time

with the catalyst on the yield of liquid hydrocarbons was also studied separately. In these experiments, the gas feed rate varied from 160 to 280 nl/h, which corresponded to a change in the contact time ranging from 2.1 to 4.5 s. Additionally, a series of experiments was conducted to study the possibility of isolating and utilizing by-products, primarily synthetic wax and light hydrocarbons. To determine the fractional composition, part of the resulting liquid was processed in the Crystek-7000 fractional distillation unit. Using fractional distillation, the liquid was separated into three fractions: light hydrocarbons (the boiling point of up to 180°C), diesel hydrocarbons (180–320°C), and waxy components (over 320°C). Each fraction was weighed and analyzed for carbon, sulfur, and aromatic compounds. Our findings demonstrated that under conditions of 25 atmospheres and 227°C, the continuous operation of the reactor for 6 hours yielded an average of 12.6 kg of the liquid phase hydrocarbons. For clarity, the total liquid yield at 25 bar was 12.6 ± 0.4 kg (n = 3), and 13.5 ± 0.5 kg at 30 bar; the diesel fraction at 25 bar was 57.4 ± 1.3 wt% and 61.8 ± 1.1 wt% at 30 bar. Of these, the share of diesel fraction was 57.4%, kerosene was 31.2%, light hydrocarbons were 6.8%, and wax was 4.6%. Physicochemical analysis showed that the density of the obtained diesel fuel was 0.792 g/cm³ at 20°C, the flash point was 62°C, the mass fraction of sulfur did not exceed 2 mg/kg, and the total content of aromatic hydrocarbons was only 3.2%. Increasing the pressure to 30 atmospheres resulted in a 7.5% increase in total liquid hydrocarbon yield compared to baseline conditions. This was accompanied by a higher proportion of the diesel fraction, which reached 61.8% of the product weight. On the contrary, a decrease in pressure to 20 atm led to a decrease in the total yield of the liquid phase by 9.2% and an increase in the proportion of light hydrocarbons to 11.4% (Table 1).

Table 1 The Fractional Composition of the Liquid Synthesis Product under Different Pressure Conditions.

Pressure, atm	Diesel fraction, % mass	Kerosene, % mass	Light hydrocarbons, %	Wax, %
20	52.6 ± 1.5	29.8 ± 1.0	11.4 ± 0.6	6.2 ± 0.4
25	57.4 ± 1.3	31.2 ± 0.9	6.8 ± 0.4	4.6 ± 0.3
30	61.8 ± 1.1	28.0 ± 0.8	5.0 ± 0.3	5.2 ± 0.4

Varying the gas-catalyst contact time, it was observed that increasing the contact time from 2.1 to 4.5 s, shifted the selectivity toward heavier hydrocarbons. In particular, the yield of waxes increased from 4.1 to 7.9%, while the proportion of light hydrocarbons decreased to 3.2%. This demonstrates that product distribution is highly sensitive to the hydrodynamic conditions of the process. In a separate series of experiments, the energy potential of gasification and the utilization of

the released steam were evaluated. When the gasification unit operated at a temperature of 1270 °C for 8 hours, steam was generated in the amount of 164 kg, which was sent to the heat exchange module and made it possible to generate about 78 kW h of electricity used for the equipment's needs. A comparative analysis of the obtained properties of synthetic fuel with traditional petroleum diesel showed that the initial boiling point was on average 8–10 °C lower, which confirms a narrower hydrocarbon

spectrum. The cetane number was 72 units, which exceeds the average values of petroleum diesel (about 48–52 units). This can be regarded as better ignition properties and higher thermal efficiency (Table 2). Owing to near-zero sulfur ($< 2 \text{ mg kg}^{-1}$) and low aromatics (3.2 wt%), Fischer–Tropsch diesel typically yields lower regulated tailpipe emissions than conventional petroleum diesel in unmodified engines does. The literature

indicates reductions of particulate matter (PM) by ~20–30%, NO_x by ~5–12%, and CO and HC by ~20–60%, depending on duty cycle and after-treatment configuration. With our measured fuel properties, we expect comparable benefits for the present coal-based FT diesel. (Data synthesized from IEA AMF Annex 31 reviews and chassis-dyno tests by NREL/WVU on neat FT diesel.)

Table 2 Comparative Characteristics of Synthetic and Petroleum Diesel Fuel.

Parameter	Synthetic fuel	Petroleum diesel
Cetane number	72	48–52
Density at 20°C, g/cm ³	0.792	0.82–0.84
Mass fraction of sulfur, mg/kg	< 2	Up to 350
Flash point, °C	62	55–65
Content of aromatics, % by weight	3.2	15–35

In addition, during the experiments, data on the oxidation stability of synthetic fuel were obtained. The tests were conducted with the samples stored for 180 days at a temperature of +35°C, which simulated accelerated aging. The analysis showed no noticeable changes in color, odor, or viscosity. The acid number increased only from 0.01 to 0.04 mg KOH/g, which characterizes the fuel as stable during long-term storage. Independent studies from the United States and South Africa have demonstrated comparable yields of liquid hydrocarbon fractions. For the context, under LTFT conditions (220–240 °C, 20–30 bar), iron catalysts typically exhibit stronger WGS activity and lower diesel-range selectivity during comparable conversions, while being more sensitive to carbide phase changes. Representative studies report C_5^+ selectivities around 40–55 wt% with faster deactivation than that of Co systems. Commercial Co/Al₂O₃ or Co/SiO₂ catalysts generally achieve 55–70 wt% C_5^+ with stable operation over 100–500 h. Against these benchmarks, the present diesel fraction of 57.4–61.8 wt% at 25–30 bar places our bulk Co–ZrO₂ granulate within the upper tier of Co-based performance for the investigated window and above typical Fe-based values in this regime. For example, in the studies performed on installations with cobalt catalysts under conditions of 230°C and 20 atmospheres, the liquid-phase yield was approximately 10–13 kg over 6 hours. However, in the present study, owing to the use of a catalyst modified with zirconium oxide, higher selectivity for the diesel fraction and a smaller proportion of impurities were noted. In addition, during the extended series of experiments, the features of by-product formation were assessed. In particular, the methanol content in the light hydrocarbons fraction reached up to 1.8% wt% in individual experimental runs, while the content of ammonia compounds did not exceed 0.3%. The

composition of gas emissions after gasification was also assessed. The average content of carbon dioxide in the tail gases was 8.4%, confirming the effectiveness of the partial CO₂ capture stage. Analysis of the totality of the obtained data allowed us to conclude that the technology of indirect coal liquefaction in the selected modes ensures a high yield of synthetic diesel fuel with performance characteristics superior to oil analogues. The use of variations in pressure and time of gas contact with the catalyst allows us to regulate the composition of the products, which makes it possible to adapt the process to various consumer requirements. The results obtained demonstrate the significant industrial potential of the technology in the context of ensuring sustainable fuel resources and reducing the environmental burden.

4. CONCLUSION

Our findings demonstrated that the indirect coal liquefaction via Fischer–Tropsch synthesis enables the production of synthetic diesel fuel with performance characteristics superior to those of conventional petroleum diesel. Under the baseline synthesis conditions (the temperature of 227°C and pressure of 25 atm.) the average liquid-phase yield was 12.6 kg for 6 hours of continuous reactor operation, with the diesel and kerosene fractions accounting for 57.4% and 31.2%, respectively. An important feature of the obtained product was its extremely low sulfur content, which did not exceed 2 mg/kg, almost 175 times lower than the upper limit of the sulfur content in standard petroleum diesel, where this figure can reach up to 350 mg/kg. The cetane number of the synthetic fuel was 72, significantly exceeding the typical range of 48–52 units typical of the petroleum analogue, and directly indicates higher ignition properties and increased thermal efficiency. The fuel density at 20 °C was 0.792 g cm⁻³, lower than the typical 0.82–0.84 g cm⁻³ range for petroleum diesel, which is

consistent with the narrower hydrocarbon distribution reported above. This characteristic can contribute to reduced fuel consumption when used in internal combustion engines. Experiments involving variation of synthesis pressure revealed a pronounced influence of this parameter on process selectivity. Increasing the pressure from 25 to 30 atm resulted in 7.5% increase in the total liquid hydrocarbon yield, with the diesel fraction rising to 61.8%. On the contrary, reducing the pressure to 20 atmospheres, led to a 9.2% decrease in the total liquid yield, while the proportion of light hydrocarbons increased by more than 1.5 times and amounted to 11.4%. Our data highlights the adaptability of the technology to specific tasks: for example, maximizing the production of diesel fractions or targeted production of light hydrocarbons and synthetic waxes. Similar trends were observed upon variation of the synthesis gas–catalyst contact time: increasing this time from 2.1 to 4.5 s led to an increase in the proportion of heavy components, in particular waxes, from 4.1 to 7.9%. Particular attention was paid to the analysis of the physicochemical stability of the obtained fuel. Storage simulation tests conducted over six months at a temperature of +35°C showed an extremely low tendency to oxidation, with the acid number increasing from only 0.01 to 0.04 mg KOH/g, indicating high resistance to aging. Comparisons with the international studies confirm the competitiveness of the developed technology: the obtained yields of liquid fractions (12.6 kg in 6 hours) are comparable or even slightly exceed the data from the USA and South Africa, where at similar temperatures but lower pressure (20 atm.) the yield was about 10–13 kg. A significant advantage was recorded in terms of the level of purification from sulfur and the content of aromatic compounds: in the obtained fuel, their total content was only 3.2%, while in petroleum diesel, this share can exceed 15–35%. Finally, the energy potential of the gasification stage further validated the approach: in 8 hours of operation of the gasification unit, 164 kg of steam were generated, enabling the production of 78 kW·h of electricity used for the equipment's own needs. Looking forward, integration of a dedicated pre-combustion CO₂ capture unit (e.g., physical-solvent absorption) is expected to raise overall capture to ≥ 90% in CTL-FT configurations, further strengthening the environmental case for the present diesel product. Overall, the study demonstrates that the indirect coal liquefaction using a modified cobalt catalyst allows obtaining environmentally friendly, stable, and efficient diesel fuel, offering high flexibility in controlling the fractional composition and efficient utilization of auxiliary energy streams.

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