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SYNTHESIS OF FUEL COMPOUND BASED ON LIGHT DISTILLATE OF COAL TAR

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Abstract. The paper considers the process of fuel compound production on the basis of light distillate of coal tar (CT). The analysis of group and individual composition of CT fractions is carried out, the main components including aromatic hydrocarbons, phenols, heteroatomic compounds and asphaltenes are revealed, and their physical and chemical characteristics are established. The technique of stabilisation of mixtures of CT distillate and petroleum fuel oil using a surfactant - acrylic acid - has been developed. It is shown that surfactant introduction provides a high degree of homogeneity and stability of fuel compositions, preventing the formation of precipitates even during long-term storage. Optimal ratios of light distillate and fuel oil (70:30 and 50:50) allow to obtain fuel compounds, the characteristics of which meet the requirements for boiler and furnace fuels. The obtained results demonstrate the promising application of light distillate of CT for creation of highly efficient fuel products, which opens new opportunities for processing of coal-chemical raw materials. The proposed approach contributes to improving environmental safety, reducing the toxicity of the final product and expanding the raw material base for fuel production.

Key words: coal tar, light distillate, fuel compound, surfactant, fuel oil, boiler fuel.

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1. Introduction

Coal tar (CT), a by-product of coke production, has a significant industrial potential due to its complex chemical composition, including condensed aromatic hydrocarbons and other high molecular weight compounds [1-3]. However, its multicomponent nature, high reactivity, and the presence of carcinogenic and toxic compounds make its processing technologically challenging. With the growing global demand for alternative fuel sources and high-yielding chemical products, the processing of CT becomes an important area of scientific research and industrial application.

Current global trends demonstrate high activity in the field of development of coal tar processing technologies for obtaining fuel compounds and valuable chemicals. For example, in China, industrial plants for the production of diesel fuel from CT have been introduced, which allows not only to effectively utilise waste, but also to solve the issues of energy balance [4,5]. Similar studies are actively conducted in the EU countries, where special attention is paid to the creation of environmentally safe recycling processes [6-12].

This paper studies the possibilities of using light fractions of coal tar produced by “Shubarkol Komir” JSC for the synthesis of fuel compound. The study is aimed at developing an innovative approach to the processing of tar, including the use of hydrocarbon component and surfactants, with an assessment of the performance characteristics of the resulting products.

The results of the work have not only practical value for the industry of Kazakhstan, but also correspond to the world trends in the field of creation of effective and environmentally friendly technologies for processing of carbon-containing waste, as the results of the study lays the foundation for the formation of competitive technologies that can ensure sustainable development and diversification of industrial production.

2. Experimental part

Objects and methods. Medium-temperature coal tar (CT) produced by Shubarkol Komir JSC was used for the study. The fractionation process was carried out using nitrogen to prevent secondary reactions and improve heat transfer.

The component composition of the fractions was analysed using IR spectroscopy and chromatography-mass spectrometry. NICOLET 5700 spectrophotometer (FT-IR) with Fourier transform in the range of wave numbers

400-4000 cm-¹ was used to determine the qualitative composition of CT. The spectra were processed and interpreted using OMNIC software.

Chromatographic analysis was performed on an Agilent 6890 N instrument (Agilent Technologies, USA) with a DV-1 capillary column (27.5 m, 0.32 mm, 10 μm).

Fuel oil of 100 grade with boiling point of 350-360 °C was used as a hydrocarbon component.

The calorific values of fuel compositions based on light distillates of coal tar were determined using Elementar Vario Micro Cub and calorimeter B-08NA ‘K’.

Toxicity indicators of fuel compositions were determined in accordance with the interstate normative document GOST 12.1.044-2018 ‘Fire and explosion hazard of substances and materials’ (paragraph 13), which allowed to establish the hazard class of the samples under study.

3. Results and Discussion

The distillation results showed that the lightest fraction of CT (up to 170°C) is 3.6% of the initial resin mass, and the main yields come from the absorption (19.3%) and anthracene (17.2%) fractions [13]. The residue - pectic - was 36.5% of the mass of CT, with characteristics corresponding to GOST: softening point 127°C and volatile content 50.6% [13].

The analysis of IR spectra showed that the light fraction is characterised by a high content of aromatic hydrocarbons, including benzene and its derivatives. This fact is associated with the formation of azeotropic mixtures and complexes in the composition of CT. In this connection, phenol and naphthalene impurities appear in the benzene fraction, and naphthalene is contained in the phenol fraction, etc. Figure 1 compares the IR spectra of the distillation fractions of CT with the IR spectrum of the initial CT and determines their convergence coefficients (Table 1).

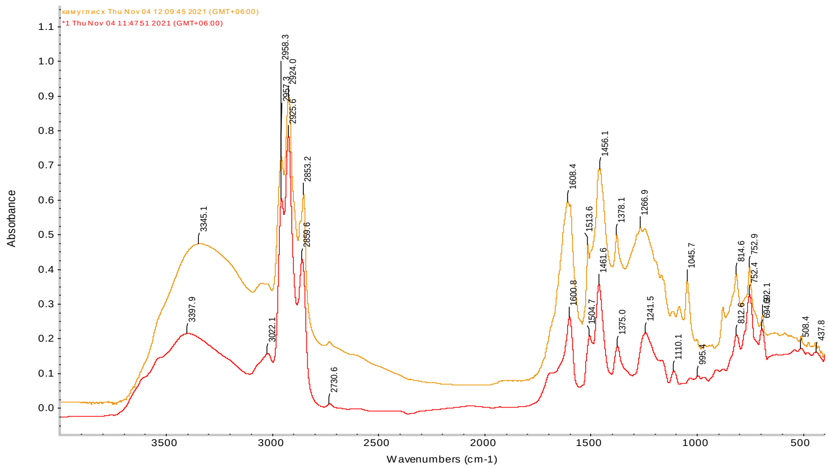

Figure 1 – Comparison of IR spectra of initial CT and light (benzene) fraction

Table 1 - Coefficients of convergence of IR spectra of fractions of CT distillation with IR spectrum of initial CT

№	Fractions	Convergence coefficient, %
1	Light, %	68
2	Phenolic, %	78
3	Naphthalene, %	74
4	Absorbent, %	83
5	Anthracene, %	86

Fractions 4 and 5 are the closest to the initial resin in terms of chemical composition, which indicates the predominance of hydrocarbons in this fraction, constituting the organic mass of CT. Thus, the basis of the fraction ‘organic bases’, according to the data of chromatography-mass-spectral analysis are nitrogen-containing heterocyclic compounds of quinoline and carbazole types with an admixture of aromatic amines and carbonitriles. The phenolic fraction contains mainly phenols with the number of rings from 1 to 4, furans and long-chain alkanes C_{18}-C_{26}. Asphaltenes include arenas of various degrees of condensation with predominance of three- and four-ringed ones, as well as sulphur-, nitrogen- and oxygen-containing heteroatomic compounds - thiophenes, quinolines, furans. Oils, the dominant fraction of CT, include mainly aromatic compounds of hydrocarbon composition, including unsaturated ones of indene series. Neutral resins are a mixture of nitrogen- and oxygen-containing heteroatomic compounds - quinolines, carbazoles, carbonitriles, furans and ketones.

According to the results of group chemical analysis, the main fractions of CT are oils (63.6 %) and asphaltenes (11.7 %). The total share of other group fractions is less significant - 24.7 %. It should be noted that among the majority of valuable, expensive individual hydrocarbons constituting these fractions, CT also contains substances that give it carcinogenic (pyrene, benz(a)pyrene, benzfluoranthene, benz(a)anthracene, etc.) and toxic (carbazole, carbonitrile) properties. This fact complicates the classified use of coal tar and its distillates.

Nevertheless, the obtained data on group and individual compositions of CT fractions confirm the necessity of their use as a raw material source for obtaining a variety of commercial products. In particular, for obtaining fuel compound on the basis of fractions of CT with achievement of significant reduction of its toxicity and carcinogenicity by mixing with commercial fuel oil.

It is known that petroleum fuel oils and coal tar are mutually insoluble. When they are mixed together, a precipitate precipitates, presumably salting occurs. In addition, the surface tensions of fuel oil and coal tar are different. Between petroleum and tar oils there is, for equal viscosity, a difference in surface tension of about 10 dyne/cm. The mixture was therefore stabilised by the introduction of surfactants. Acrylic acid was tested as a surfactant.

Light distillate (n.k.-360°C) and fuel oil are dispersed systems, the state of which depends on the temperature of experience, heating temperature, in connection with what, at mixing, the same temperature of components 60-80 °C was chosen. Light distillate, surfactant and fuel oil were mixed sequentially. Duration of mixing 10-60 minutes to obtain a homogeneous mass. The ratio of components (light distillate:fuel oil) in the fuel compound was, % - 30:70, 50:50 and 70:30. Surfactant was introduced in the amount of 0.5; 0.6; 1.0 or 4.0 %. As a result of homogenisation we obtained highly dispersed fuel compounds with high stability to stratification during long-term storage. Fuel compound of composition light distillate: fuel oil 70:30, as well as 50:50, have characteristics commensurate with those of commercial fuel oil and heating oil shown in Table 2.

Table 2 - Quality indicators of the developed fuel compositions.

№	Indicator	Normative document	Indicator value			
			Fuel composition L4 (70% light distillate + 30% fuel oil) + 0.6% surfactants)	Fuel composition L5 (50% light distillate + 50% fuel oil) + 0.6%	Fuel oil commercial M-100; GOST 10585-99	Domestic heating oil; ST RK 2951-2021
1	Kinematic viscosity at 20°C, not more than, mm^2/s	GOST 33-2016	-	-	-	8.0
2	Kinematic viscosity at 50°C, not more, mm^2/s	GOST 33-2016	14.51	23.04	-	-
3	Kinematic viscosity at 80°C, not more, mm^2/s conditional, °VU:	GOST 33-2016	5.388	7.598	11.84	-
4	Kinematic viscosity at 100°C, not more	GOST 33-2016	3.416	5.208	5.0	-
5	Flash point in open crucible, not less than °C	GOST 4333-2014	116	102	110	-
6	Ash content, not more, %	GOST 1461-75	0.1	0.006	0.14	0.02
7	Mass fraction of water, not more %	GOST 2477-	0.4	0.7	1	traces
8	Coking ability, %, not more %	GOST 19932-99	1.77	2.40	-	0.35
9	Content of water-soluble acids and alkalis	GOST 6307-75	Weakly alkaline	absence	absence	absence
10	Mass fraction of sulphur, not more, %	ST RK ASTM D 4551-	0.02	0.02	0.5 – 3.0	0.5 (GOST R 51947)

One of the most important technical characteristics of fuel is its calorific value. Heat of combustion of fuel is the amount of heat released during complete combustion of fuel. Values of heat of combustion of fuel compositions on the basis of light distillates of coal tar make 39517 - 42 000 kJ/kg that correspond to the interval of value of working lowest heat of combustion of furnace fuel oil (Qrn = 35 500 - 42 000 kJ/kg) and boiler (furnace) fuel (Qrn ~ 40 000 kJ/kg). Thus, the obtained fuel compositions, by many quality indicators, meet the requirements and norms for boiler (furnace) fuel and by some indicators - for commercial fuel oil. Toxicity indicators were determined and on their basis the hazard class of fuel compositions in accordance with the interstate normative document GOST12.1.044-2018 ‘Fire and explosion hazard of substances and materials’, item 13 (Table 3).

Table 3 - Toxicity indicators and hazard class of fuel compositions according to GOST 12.1.044-2018 ‘Fire-explosive hazard of substances and materials’, item 13.

№	Composition	Toxicity index, $H_{CL_{50}}$, g/m^3	Hazard class, (T_h)	Name of the category of fuel composition hazard class
1	(30 % Light distillate + 70 % Fuel oil) + 0.6 % surfactant (acrylic acid)	72.36	(T2)	Moderately hazardous
2	(50 % Light distillate + 50 % Fuel oil)+ 0.6 % surfactant (acrylic acid)	43.22	(T2)	Moderately hazardous
3	(70 % Light distillate + 30 % Fuel oil) + 0.6 % surfactant (acrylic acid)	37.44	(T3)	Highly hazardous
4	100 % Light distillate (original)	55.72	(T2)	Moderately hazardous
5	100 % Fuel oil (commercial)	30.33	(T3)	Highly hazardous

Analysis of the data in Table 3 shows that according to the value of the toxicity index of combustion products, the initial light distillate belongs to moderately hazardous materials.

4. Conclusion

The results of this study confirm the prospects of using light distillate of CT as a basis for fuel compounds production. The study of the group and individual composition of CT fractions showed a wide range of valuable hydrocarbon compounds, including aromatic hydrocarbons, phenols, heteroatomic compounds (quinolines, carbazoles, furans) and asphaltenes, which can be used in various technological processes. A key limitation of the use of CT distillates remains the presence of carcinogenic (pyrene, benz(a)pyrene) and toxic compounds (carbazole, carbonitrile), which requires additional measures for their processing or neutralisation. Nevertheless, the proposed method of producing fuel compounds using surfactants such as acrylic acid, oleic acid and waste coolant allows to significantly reduce the toxicity and carcinogenicity of the final product. It has been experimentally established that the introduction of surfactants in concentrations from 0.6% ensures the stability of the obtained fuel compositions, preventing the formation of precipitates even during long-term storage. Optimal ratios of fuel compound components (light distillate: fuel oil) in the range of 70:30 and 50:50 provide characteristics comparable to commercial boiler and furnace fuels. The resulting fuel compounds exhibit a high degree of homogeneity, thermal and chemical stability. Their properties such as viscosity, density and heat of combustion meet the regulatory requirements for liquid fuels. In addition, the proposed approach to the processing of CT allows to minimise waste and expand the raw material base for the production of fuels.

Thus, the proposed technology of obtaining fuel compounds on the basis of light distillate of coal tar represents an environmentally and economically justified solution that allows to process secondary products of coal chemistry into high-quality commercial fuels.

Conflict of Interest: The authors declare that there is no conflict of interest requiring disclosure in this article.

СИНТЕЗ ТОПЛИВНОГО КОМПАУНДА НА ОСНОВЕ ЛЁГКОГО ДИСТИЛЛЯТА КАМЕННОУГОЛЬНОЙ СМОЛЫ

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Резюме. В статье рассмотрен процесс получения топливного компаунда на основе лёгкого дистиллята каменноугольной смолы (КУС). Проведён анализ группового и индивидуального состава фракций КУС, выявлены основные компоненты, включая ароматические углеводороды, фенолы, гетероатомные соединения и асфальтены, а также установлены их физико-химические характеристики. Разработана методика стабилизации смесей дистиллята КУС и нефтяного мазута с использованием поверхностно-активного вещества (ПАВ) – акриловой кислоты. Показано, что введение ПАВ обеспечивает высокую степень гомогенности и стабильности топливных композиций, предотвращая образование осадков даже при длительном хранении. Оптимальные соотношения лёгкого дистиллята и мазута (70:30 и 50:50) позволяют получить топливные компаунды, характеристики которых соответствуют требованиям к котельным и печным топливам. Полученные результаты демонстрируют перспективность применения лёгкого дистиллята КУС для создания высокоэффективных топливных продуктов, что открывает новые возможности для переработки углехимического сырья. Предложенный подход способствует повышению экологической безопасности, снижению токсичности конечного продукта и расширению сырьевой базы для производства топлива.

Ключевые слова: каменноугольная смола, легкий дистиллят, топливный компаунд, ПАВ, мазут, котельное топливо.

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КӨМІР ШАЙЫРЫ ЖЕҢІЛ ДИСТИЛЛАТЫНЫҢ НЕГІЗІНДЕ ЖАНАРМАЙ ҚОСЫЛЫСЫНЫҢ СИНТЕЗІ

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Түйіндеме. Мақалада жеңіл көмір шайырының дистилляты (КШ) негізіндегі отын қоспасын алу процесі қарастырылады. КШ фракцияларының топтық және жеке құрамына талдау жүргізілді, негізгі компоненттер, оның ішінде ароматты көмірсутектер, фенолдар, гетероатомды қосылыстар және асфальтендер анықталды және олардың физика-химиялық сипаттамалары белгіленді. ББЗ (беттік белсенді зат) – акрил қышқылын пайдалана отырып, КШ дистилляты мен мұнай мазутының қоспаларын тұрақтандыру әдісі әзірленді. Беттік-белсенді заттарды енгізу отын құрамының жоғары біртектілігі мен тұрақтылығын қамтамасыз ететіні, тіпті ұзақ сақтау кезінде шөгінділердің пайда болуына жол бермейтіні көрсетілген. Жеңіл дистиллят пен мазуттың оңтайлы арақатынасы (70:30 және 50:50) сипаттамалары қазандық және пеш отындарына қойылатын талаптарға сәйкес келетін отын қоспаларын алуға мүмкіндік береді. Алынған нәтижелер көмірдің химиялық шикізатын қайта өңдеудің жаңа мүмкіндіктерін ашатын жоғары тиімді отын өнімдерін жасау үшін жеңіл дистиллятты КШ пайдалану уәдесін көрсетеді. Ұсынылған тәсіл экологиялық қауіпсіздікті жақсартуға, соңғы өнімнің уыттылығын төмендетуге және отын өндірісінің шикізат базасын кеңейтуге көмектеседі.

Түйін сөздер: көмір шайыры, жеңіл дистиллят, отын қосындысы, беттік белсенді зат, мазут, қазандық отын.

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