ABSTRACT

of the dissertation for the degree of Doctor of Philosophy (PhD) in educational program 8D07106 – Thermal power engineering

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Low-temperature cell for studying vibrational spectra of hydrocarbon fuels in the mid-IR range

General characteristics of the work

The dissertation presents the results of the development and testing of a low-temperature cell for an IR Fourier spectrometer operating at atmospheric pressure and designed to study the vibrational spectra of hydrocarbon fuels.

Relevance of the topic

To further advance energy trend, reliable results on the properties and behavior of hydrocarbon fuels under various conditions are needed. Based on theoretical and experimental data obtained as a result of such research, innovations in this field will make it possible to create various energy-efficient fuel mixtures, optimize precursors for new fuels, expand the operating conditions and applicability range of hydrocarbon compounds, thereby improving the capabilities of the thermal power industry.

New research on the thermal energy properties of hydrocarbons is focused on either low-temperature studies under vacuum or normal conditions, i.e., room temperature and atmospheric pressure. However, data on the low-temperature properties and behavior of hydrocarbon fuels at atmospheric pressure are either absent or very rare, leading to a lack of information in the thermal energy literature regarding hydrocarbons. This lack of data on hydrocarbons at low temperatures could lead to a slowdown in technological and energy progress, which is unacceptable within the context of the current scientific paradigm.

The development of the thermal power industry based on the use of hydrocarbon fuels is crucially determined by the depth of study of their physicochemical properties, combustion mechanisms, heat and mass transfer, and behavior under various operating conditions, such as low temperatures and atmospheric pressure. Systematic research into phase transitions and structural changes in fuels allows for increased energy efficiency, reduced environmental impact, and enhanced process and industrial safety.

Expanding the experimental dataset in this area allows for significantly improved prediction accuracy for changes in the physicochemical properties of hydrocarbon fuels at cryogenic temperatures and atmospheric pressure. This is particularly important for accurately modeling ignition and combustion processes, as well as for ensuring the stability of thermal and power plants under extreme operating conditions. Such research is of strategic importance for aerospace engineering, including within the framework of NASA (National Aeronautics) missions. and Space Administration (USA) and ESA (European Space Agency, Europe), where fuel is exposed to extremely low temperatures. Furthermore, a better understanding of the cryogenic behavior of fuels is critical for the reliable operation

of energy systems in the Arctic and subarctic regions of the Earth, where temperature anomalies directly impact combustion stability, equipment lifespan, and energy efficiency. Condensation, icing, and changes in fuel properties at low temperatures are a pressing issue.

The aim of this work is to develop and create a special low-temperature cell for conducting studies of infrared spectra of various hydrocarbon fuels at atmospheric pressure.

Research objectives

To achieve this goal, the following tasks are planned:

1 Develop a low-temperature sample holder for the diffuse reflectance attachment of the FSM 2203 Fourier transform spectrometer for high-resolution IR spectrometric studies at temperatures down to 80 K. Create an inert and IR-inactive environment for obtaining high-quality spectral data due to high radiation intensity and low noise due to the absence of impurities, moisture, and unwanted condensation on the samples.

2 Test the setup using IR spectrometric studies of petroleum hydrocarbon products in the characteristic vibration frequency range. Based on the obtained FTIR spectra of alkanols and other hydrocarbons, present results on the effect of temperature on the position, amplitude, and thickness of absorption bands corresponding to the characteristic vibrational modes of the functional groups of the molecules of the substances being studied.

3 Compare the data with the results of other authors in this field and confirm reproducibility, as well as demonstrate the feasibility of the developed technology and method for low-temperature hydrocarbon measurement at atmospheric pressure.

The object of the study is hydrocarbon fuels.

The subject of the study is cryogenic capillary system with a low-temperature cell.

Research methods

To achieve the stated goal and complete the established tasks, the following methods were used:

Infrared Fourier spectrometric method for studying vibrational spectra of hydrocarbon fuels;

Diffuse reflectance infrared beam method for surface analysis of crystalline hydrocarbons;

Cryogenic method of cooling the studied substances for the analysis of changes in absorption properties depending on temperature.

The novelty and originality of the dissertation work lies in the fact that it

1 A cryogenic capillary system with a low-temperature cell for the diffuse reflectance attachment of the FSM 2203 IR Fourier spectrometer has been developed for the first time, ensuring stable cooling and obtaining FTIR spectra of hydrocarbon fuels at atmospheric pressure;

2 The newly developed low-temperature cell was tested by studying the IR spectra of hydrocarbon fuels obtained at atmospheric pressure;

3 For the first time, the high reproducibility of new IR spectra of hydrocarbon fuels obtained using the developed low-temperature cell at atmospheric pressure has been demonstrated based on comparisons with the results of other researchers.

The main provisions submitted for defense:

1 The developed low-temperature cell based on copper (Cu) and polylactide (C3H4O2)n enables low-temperature measurements down to (80.0 ± 0.7) K and the acquisition of mid-IR Fourier spectra (400-4000 cm-1) of hydrocarbon fuels and alcohols at atmospheric pressure.

2 Validation of the developed low-temperature cell demonstrates the successful identification of natural characteristic vibrational modes of the functional groups of ethanol (C2H5OH), kerosene (C12H26), and methanol (CH3OH) with an accuracy of ±0.936 cm^{-1} when studying the obtained high-resolution FTIR spectra.

3 The values of the wave numbers of the characteristic bands of the stretching vibrations of O-H and C-H bonds C2H5OH, C12H26 and CH3OH, detected using the developed low-temperature cell in the cryogenic range of 80-100 K at atmospheric pressure, correspond to a reproducibility of 96-97%.

The level of reliability and interpretation of the results and conclusions made in the work

The reliability of the results obtained during the dissertation work is confirmed by the consistency of the data obtained using a set of modern physical and chemical research methods, as well as the presence of publications in highly rated foreign journals above the 25th percentile according to CiteScore, in scientific publications recommended by the Committee for Quality Assurance in Science and Higher Education of the Republic of Kazakhstan, in the materials of international scientific and practical conferences, and patents of the Republic of Kazakhstan for a utility model.

Correspondence to scientific development areas and government programs

This dissertation research corresponds to priority areas of energy development and was completed within the framework of research and projects AP25794643, AP26104451, and AP19680205.

The author's personal contribution includes independently conducting the research process, conducting experiments, writing sections of the dissertation and scientific publications, computer 3D modeling of the setup, and quantitative evaluation of the experimental results. In collaboration with scientific advisors, the goals were defined, objectives were set, and the results of the work were discussed.

Articles in journals included in the international scientific database Scopus and Web of Science

1 Turlybekova G., Kenbay A., Aldiyarov A., Korshikov Y., Lesbayev A., Nurmukan A., Yerezhep D. Cryogenic system for FTIR analysis of hydrocarbon fuels at low temperature and atmospheric pressure // Applied Sciences. – 2025. – Vol. 15, No. 14. – 7944. https://doi.org/10.3390/app15147944 (Web of Science "Engineering, Multidisciplinary" JIF – 71.7 percentile, Q2; Scopus "General Engineering" CiteScore – 79 th percentile, Q1) .

2 Kenbay A., Yerezhep D., Aldiyarov A. Development of low-temperature cell for IR Fourier-spectroscopy of hydrocarbon materials // Eurasian Physical Technical Journal. – 2025. – Vol. 22, No. 2 (52). – P. 88–96. https://doi.org/10.31489/2025N2/88-96 (Scopus CiteScore "General Engineering" – 26th ^{percentile} , Q3) .

Articles in journals recommended by the Science and Higher Education Quality Assurance Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan:

1 Kenbay A.A., Aldiyarov A.U., Yerezhep D.E. Cryogenic setup for FTIR spectroscopic study of the behavior of hydrocarbon compounds at atmospheric pressure // Bulletin of Toraighyrov University. Energetics Series. – 2025. – No. 1. – P. 188–200.

2 Kenbay A., Yerezhep D., Aldiyarov A. Analysis and comparison of kerosene FTIR spectra using the developed cryogenic-capillary system with low-temperature cell // Recent Contributions to Physics. – 2024. – Vol. 91, No. 4. – P. 64-76. (Web of Science "Physics, Multidisciplinary" JIF – 4.8 percentile, Q4) .

3 Kenbay A.A., Golikov O.Yu., Aldiyarov A.U., Yerezhep D.E. Low-temperature cell for IR Fourier spectrometric investigation of hydrocarbon substances // Scientific and Technical Journal of Information Technologies, Mechanics and Optics. – 2023. – Vol. 23, No. 4. – P. 696–702. (Scopus "Mechanical Engineering" CiteScore – 19th percentile , Q4) .

Abstracts from the materials of international scientific and practical conferences

1 Kenbay A.A., Yerezhep D.E. Analysis of spectrometric measurements in the field of hydrocarbon fuels // Proceedings of the international conference of students and young scientists "Farabi Alemi", Almaty, Kazakhstan, April 6–8, 2022. – P. 255.

2 Kenbay A.A., Yerezhep D.E. Development of a cell for low-temperature measurements of optical properties // Proceedings of the international conference of students and young scientists "Farabi Alemi", Almaty, Kazakhstan, April 6–8, 2022. – P. 256.

3 Kenbay A.A., Yerezhep D.E. Analysis of IR spectra in measuring the optical properties of hydrocarbon compounds at low temperatures , // Proceedings of the international conference of students and young scientists "Farabi alemi", Almaty, Kazakhstan, April 6–8, 2023. – P. 206.

4 Kenbay A.A. Spectroscopic analysis of materials at nitrogen temperature // Proceedings of the II International Conference in Memory of Academician E.G. Boos, Collection of Abstracts of the 2nd International Conference on High Energy Physics, Materials Science and Nanotechnology (ICHEPMS -2024), February 15–16, 2024 – P. 102–103.

5 Kenbay A.A., Yerezhep D.E., Golikov O.Yu., Aldiyarov A.U. New method for obtaining low-temperature IR spectra of hydrocarbon fuels at atmospheric pressure // Proceedings of the International Scientific and Practical Conference " Satbayev International Conference 2024 (Satpayev Readings – 2024). Integration of science and technology: the path to sustainable development", April 12, 2024. – P. 512–518.

6 Kenbay A.A., Yerezhep D.E. Low-temperature spectroscopy of hydrocarbons using kerosene as an example in cryogenic capillary system // Collection of abstracts of the international conference of students and young scientists "Farabi Alemi", Almaty, Kazakhstan, April 3–5, 2025. – P. 144.

Utility model patents

1 Patent. 7284 Republic of Kazakhstan. Low-temperature measuring cell for diffuse reflectance in the mid-IR range / Yerezhep D.E., Aldiyarov A.U., Golikov O.Yu., Kenbay A.A.; patent holder Yerezhep D.E. – No. 2022/0443.2; declared . 19.05.2022; published . 15.07.2022. – 5 p.

2 Patent. 9621 Republic of Kazakhstan. Modernized low-temperature sample holder for IR spectroscopy / Kenbay A.A., Yerezhep D.E., Aldiyarov A.U.; patent holder Kenbay A.A. – No. 2024/0911.2; declared . 19.07.2024; published . 25.07.2025. – 6 p.

Volume and structure of the dissertation

The dissertation contains an introduction, a main body consisting of three sections, a conclusion, and a list of references. It is 102 pages long and contains 29 figures, 19 formulas, 7 tables, and 157 bibliographic references.