



Assessments of Chemical Composition and Properties High-Viscosity Oil Based on Elemental

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Abstract: Analysis of the chemical composition of asphaltines in high-viscosity oils using elemental analysis and IR spectroscopy provides important information about their molecular structure, functional groups and elemental composition. This data helps optimize oil production and refining processes, solve operational problems, ensure high quality products and contribute to the development of the oil and gas industry. Continued research and advances in analytical techniques will contribute to an even greater understanding of asphaltines and facilitate more efficient and sustainable use of high-viscosity petroleum resources.

Key words: high-viscosity oil, chemical composition, elemental analysis, IR spectroscopy, molecular structure, functional groups, elemental composition, oil production.

Introduction

The world's reserves of highly viscous oils are quite significant, but their exact quantities can be difficult to estimate due to different classifications of oils and data variability. However, according to the International Energy Agency (IEA), as of 2021, global reserves of high-viscosity oils amount to about 1.6 trillion barrels [1-3]. This is approximately 10% of the world's total oil reserves. Most of the high-viscosity oils are located in Canada, Venezuela and Russia. Canada has reserves of Atlantic high-viscosity oil (tar sands) estimated at more than 170 billion barrels. Venezuela has reserves of highly viscous Orinoco oil, which are estimated at more than 300 billion barrels. Russia has reserves of West

Siberian high-viscosity oil, which are estimated at more than 50 billion barrels [2-4]. In Uzbekistan, this number hovers around 100 million tons.

Extraction of high-viscosity oil can be difficult and costly due to its special properties [5]. The properties of high-viscosity oils can also vary, but they are generally characterized by high viscosity, density, and viscoplastic properties. This means that it can be difficult to extract and requires special technologies and equipment to pump and process it. In addition, highly viscous oil may contain large amounts of water and solids, which also complicates its processing.

Therefore, for evaluation purposes, assessing the chemical composition of asphaltenes in high-viscosity oils using elemental analysis and IR spectroscopy is of great importance in several aspects of the oil and gas industry [6,7]. Since IR spectroscopy is a universal method and is used to study oils and petroleum products in different areas of the infrared spectrum [8-10]. Methods for analyzing multidimensional data in the near-infrared range are the basis for express analysis of oil, oil refining and petrochemicals [10-12]. The use of IR spectra makes it possible to more reliably determine functional groups and structural fragments of hydrocarbon and non-hydrocarbon compounds [13-15]. The use of Fourier transform infrared spectroscopy has significantly expanded the capabilities and boundaries of analysis in the IR range [6-15]. Fourier transform infrared spectroscopy has high performance and allows you to work with low-transparent objects, such as oil and petroleum products. It supports optimization efforts, quality control, regulatory compliance, risk mitigation, research and development, predictive modeling, intellectual property and knowledge sharing. Using this information, companies can make informed decisions, improve operational efficiency and innovate in the use of heavy oil resources, which ultimately contributes to the sustainable and efficient development of the industry [16-26].

The purpose of the work is to assess the chemical composition and properties of high-viscosity oil asphaltenes based on elemental analysis and IR spectroscopy.

Material and research methods: samples high viscosity oil Ashalchinskoye deposit (Almetyevsky district, Tatarstan) and products of their processing.

1. Experiments on processing high-viscosity oil were carried out in an Autoclave with varying temperature and catalyst (Figure 1). Aquathermolytic reactions were carried out under high-pressure conditions of a thermoreactor connected to a gas chromatography (GC) system.

2. Liquid adsorption chromatography techniques have been used to study the group composition of samples derived from rocks and transformed asphaltenes.

3. The structural and group composition of extracts from rocks and asphaltenes was determined using Fourier infrared spectroscopy on a Vector 22 infrared spectrophotometer (Bruker) in the range of $4000\text{--}400\text{ cm}^{-1}$ with a resolution of 4 cm^{-1} .

4. The individual hydrocarbon composition of saturated fractions of oil and bitumen, including n-alkanes and acyclic isoprenoids, was studied using an AutoSystem XL chromatograph from Perkin Elmer using a flame ionization detector (FID) and a high performance SE 30 phase quartz capillary column.

5. The elemental composition of asphaltenes was determined using the combustion method on a semi-automatic CHN analyzer.

6. The results obtained were subjected to statistical processing.

The results obtained and their discussion

After the aquathermolysis process, a large amount of gases is released. On the other hand, the presence of sodium nanoparticles and its interaction with water [1] leads to the release of a significant amount of hydrogen and the formation of sodium hydroxide (see Table 1).

1-table

Content of released gases after aquathermolytic upgrading of heavy oil in the absence of sodium.

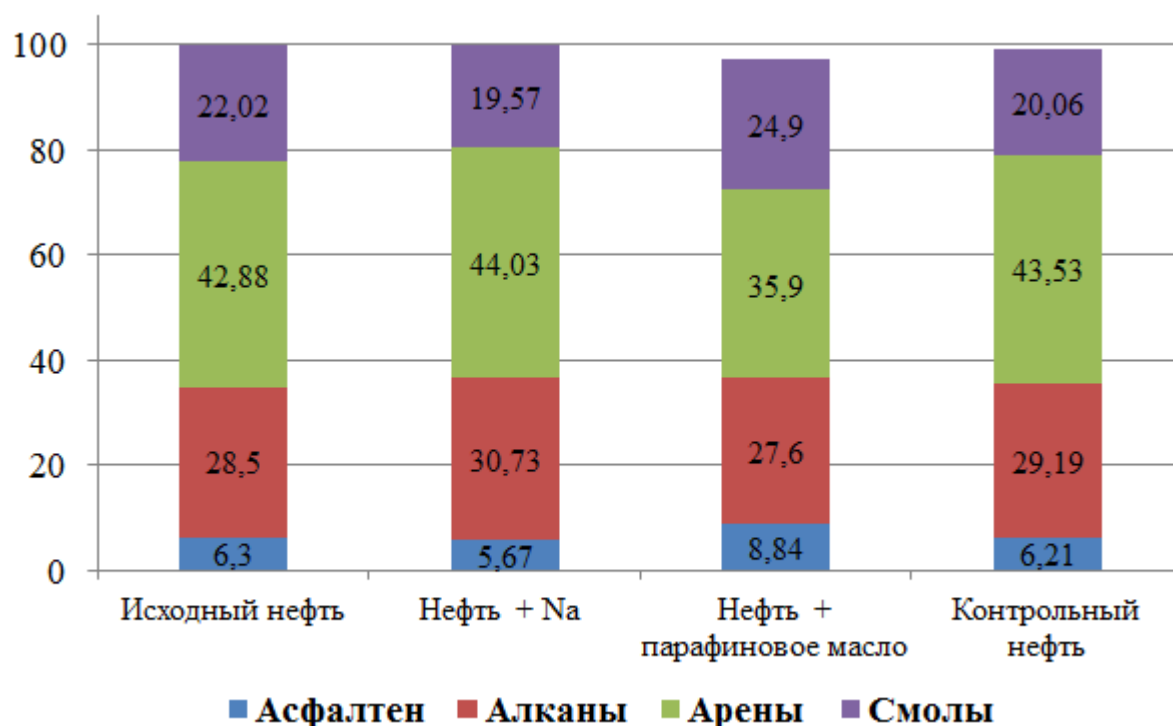
Sample	Share, %									
	C1	C2	C3	C4	H ₂	CO ₂	H ₂ S	N ₂	O ₂	Total
Oil-250, control	0.016	0.017	0.019	0.029	0.015	0.154	0.099	99.58	0.071	100
Oil-250 with sodium suspension	0.017	0.024	0.025	0.041	0.805	0.009	0.001	99.02	0.063	100

Thus, the analysis of the released gases after aquathermolysis from heavy oil samples in the presence of Na nanoparticles showed an increase in the hydrogen content (from 0.015 to 0.805 wt. %) and a decrease in the content of hydrogen sulfide and carbon dioxide compared to the control sample to 99% and 94%, respectively. The initial pressure is created by nitrogen, and, therefore, its maximum content is observed in both samples.

Carbon dioxide content was significantly reduced after hydrothermal treatment using Na nanoparticles, indicating its chemical conversion in the presence of excess free hydrogen gas. Therefore, hydrogenation of carbon dioxide in reservoir conditions can be considered as a possible technology for special utilization of carbon dioxide. The gas composition of the samples was analyzed at a temperature and pressure of 32°C and 11.3 bar, respectively. Aquathermolysis of heavy oil was carried out for 24 hours at a temperature of 250°C and the initial pressure created by nitrogen gas was 10 bar (at an ambient temperature of 25°C).

To study the fractional composition, the extracts were divided into a hydrocarbon part and two groups of resins: benzene and alcohol-benzene, passed through a chromatographic column (Fig. 1) and collected into fractions. The number of fractions was determined by the gravimetric method. The results obtained in the form of histograms are shown in Fig. 1.

From the analysis of the data in Fig. 1, it is clear that the addition of Na to oil leads to a decrease in the concentration of asphaltenes and resins, and an increase in the concentration of alkanes and arenes. This is due to the interaction of Na with asphaltenes and resins, which leads to their decomposition.



1-fig. Fractional composition of oil before and after treatment

The addition of paraffin oil to petroleum also causes changes in the concentrations of the components. In this case, there is an increase in the concentration of asphaltenes and resins, and, accordingly, a decrease in the concentration of alkanes and arenes. This is due to the dissolution or mixing of paraffin oil with asphaltenes and resins, which leads to an increase in their concentration.

The control oil shows some changes compared to the original oil, but these changes are not as significant as when adding Na or paraffinic oil.

Overall, data analysis indicates that the addition of Na and paraffinic oil to oil causes changes in the concentrations of asphaltenes, alkanes, arenes, and resins. These changes may be due to chemical reactions or physical interactions between the components of the oil and the added substances.

The results of elemental analysis of heavy oil samples before and after upgrading are summarized in Table 2. The data shows an increase in the content of carbon, hydrogen and nitrogen, while the sulfur content was reduced. It is well known that CS bonds have the lowest dissociation energy - 66 kcal/mol and are easily destroyed even at a temperature of 180°C. Therefore, a decrease in sulfur content in the samples was expected. It is important to note that sulfur is released in the form of H₂S.

2- table.

Elemental analysis of the original oil and after aquathermolysis with and without a catalyst.

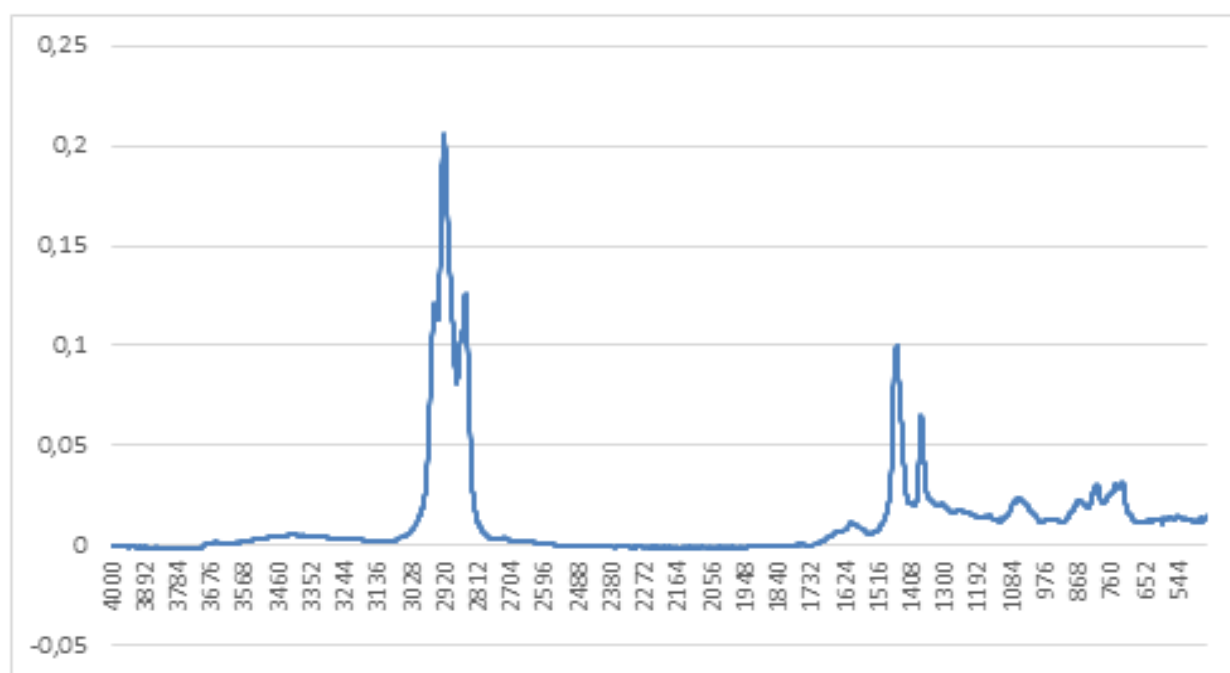
Sample	Share, %				
	C	H	N	S	H / C
Initial oil-250	81.49	12.08	0.00	4.6	1.77
Oil-250, control	82.02	12.15	0.02	4.48	1.77
Oil-250 with Na suspension	82.12	12.80	0.04	4.40	1.86

Elemental analysis provides insight into the composition of asphaltines by determining the relative concentrations of various elements. In table Figure 2 presents elemental analysis data for oil samples after autothermolysis with and without a catalyst. Samples include Original Oil -250, Oil-250 control, and Oil-250 with Na slurry .

By comparing the percentages of carbon (C), hydrogen (H), nitrogen (N) and sulfur (S), it is apparent that all samples have the same elemental composition with minor differences. The H/C ratio provides an important measure of the aromaticity and stability of asphaltines . Original oil-250 and control oil-250 had the same H/C ratio of 1.77, while oil-250 with Na slurry had a slightly higher ratio of 1.86. This suggests that the presence of a sodium catalyst enhances the release of lighter hydrocarbons during aquathermolysis .

IR spectroscopy provides information about the functional groups and chemical structure of asphaltines. The IR spectra presented in Fig.2 cover three ranges: from 3028 to 2812 cm^{-1} , from 1624 to 1300 cm^{-1} and from 1084 to 652 cm^{-1} .

Further analysis of IR spectra in these ranges can provide additional information about the chemical composition of asphaltines . Detailed study of specific absorption bands and their corresponding wavenumbers can help in identifying the functional groups and molecular structures of asphaltines .



Rice. 2 . IR spectrum of the Oil-250 sample with Na suspension

For example, in the range from 3028 to 2812 cm^{-1} , the presence of intense absorption bands indicates the presence of CH stretching vibrations, suggesting the presence of aliphatic and aromatic hydrocarbons in asphaltines . The intensity and shape of these bands can provide information about the degree of unsaturation and branching of hydrocarbon chains.

The range from 1624 to 1300 cm^{-1} corresponds to the stretching vibrations of carbonyl ($\text{C}=\text{O}$). The presence of absorption bands in this region indicates the presence of carbonyl functional groups in

asphaltenes. The specific wavenumbers and intensities of these bands can provide insight into the nature of carbonyl groups, such as ketones or esters, and their content in asphaltenes.

In the range from 1084 to 652 cm^{-1} , known as the fingerprint region, characteristic vibrations of various functional groups can be observed. By analyzing specific absorption bands in this region, it is possible to identify additional functional groups present in asphaltenes, such as aromatic rings, sulfur-containing compounds, and other heteroatoms.

Overall, assessing the chemical composition of asphaltenes in high-viscosity oils using elemental analysis and IR spectroscopy is a vital step towards understanding and optimizing the use of heavy oil resources. Continued research and advances in analytical techniques, coupled with interdisciplinary approaches, will help unlock the full potential of high-viscosity oil reserves and develop sustainable and efficient solutions for their extraction, processing and use in the energy industry.

Conclusion

Thus, assessing the chemical composition of asphaltenes in high-viscosity oils using elemental analysis and IR spectroscopy provides important information about their molecular structure, functional groups and elemental composition. This knowledge helps optimize oil production and refining processes, solve operational problems, ensure product quality and contribute to the development of the oil and gas industry. Continued research and advances in analytical techniques will further improve our understanding of asphaltenes, paving the way for more efficient and sustainable use of high-viscosity petroleum resources.

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