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Thermal dissolution of coal with organic solvents

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ABSTRACT

The results of the study of the process of converting brown coal from the Kiyakty deposit under supercritical conditions and at boiling points of solvents, in media containing acetone and ethanol are presented. The features of the hydrocarbon composition of brown coal extracts using IR-Fourier spectroscopy were revealed. Aliphatic, aromatic, and oxygen-containing hydrocarbon compounds were found in the IR-spectra of acetone and ethanol extracts obtained under supercritical solvent conditions. The IR-spectra of acetone and ethanol extracts obtained at the boiling point of solvents differ in the presence of nitrogen-containing and unsaturated hydrocarbons. Thus, extracts obtained under supercritical solvent conditions differ from extracts obtained at the boiling point of solvents in the absence of nitrogen-containing compounds and cumulated double bonds. The above data show that the optimal conditions for the extraction process are applied to both options of extraction processing of brown coal. However, when coal is dissolved in acetone and ethanol media under supercritical conditions, a deeper destruction of the organic mass of coal is observed.

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1. Introduction

With the sharp reduction in the amount of oil and increasing demand for energy, the conversion of coal to liquid fuels, chemicals and carbon materials is attracting increasing attention. Brown coals, due to their higher content of oxygen-functional groups than anthracites and hard coals, have advantages as raw materials for liquid fuels, petrochemical, and fine organic synthesis. Extraction of brown coal is an affordable version of the conversion of raw materials into a soluble species and is suitable for use chemicals. By studying the structure and composition of liquid products in coals, researches can get important information about the structure of coals and facilitate the use of liquid products [1].

Many studies have been conducted using extraction methods to obtain useful components from brown coal, such as supercritical fluid extraction [2], supercritical liquid extraction, extraction with mixture of solvents [3,4], sequential extraction, and hydrothermal extraction [5].

Coal extraction using solvents is widely used for various purposes, including determining the structure of coal. It is generally recognized that the organic part of coals is a collection of macromolecules connected to each other by intermolecular forces that are weaker than covalent bonds. According to the data, it is known that some macromolecules in coals were extracted with solvents, and the amount of extractants varies greatly depending on the types of coals, as well as on the types of solvents. It is generally believed that extraction of coals by solvents under milder conditions breaks only weaker intermolecular bonds than covalent bonds, and molecules that dissolve in solvents do not react with each other [6].

The authors investigated the process of extraction of mechanically treated coal using a benzene. IR-spectroscopy revealed an increase in the intensity of absorption bands for hydroxyl groups of phenols at 3200–3400 cm^{-1} [7].

The composition of the product obtained by extraction in a tetralin medium, then by sequential extraction with chloroform, was also studied. According to the results of the analysis, the spectra at 2854, 2923 cm^{-1} and 1427, 1376 cm^{-1} are characteristic of valence and strain fluctuations of C–H bonds in saturated aliphatic compounds. At 1599 and 1504 cm^{-1}, the bands with maxima correspond to aromatic structures. Intense absorption bands in the regions of 860 and 814 cm^{-1} show that substituents are present in the aromatic rings. A maximum of 1702 cm^{-1} in the area of

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1700–1750 cm^{-1} proves the presence of significant amounts of lactones, acids and esters in coal. The high-frequency band at 3393 cm^{-1} is characteristic of hydroxyl groups. And in the area of 1000–3000 cm^{-1} can be found aliphatic alcohols, phenols and derivatives of esters [8].

This paper presents the results of a study of the IR-Fourier spectra of brown coal extracts obtained under supercritical conditions and at the boiling point of solvents. Previously, we conducted research on the extraction processing of brown coal in the works [9–12].

2. Experimental part

Brown coal from the Kiyakty deposit in Central Kazakhstan with the following characteristics was used for the extraction process (wt. %): W^{daf} 9.5; A^{daf} 11.1; V^{daf} 41.2; C^{daf} 74.3; H^{daf} 4.7; O^{daf} 19.3; N^{daf} 0.8; S^{daf} 0.9. Thermal dissolution of coal was performed in a rotating autoclave with a volume of 250 ml in the temperature range 236 ^{0}C-241 ^{0}C at a pressure of 4.7–6.3 MPa. The coal extraction process was carried out in the soxlet apparatus for 6–8 h, bringing the solvent to the boiling point. Acetone and ethanol were used as solvents. The physical and chemical characteristics of the solvents are shown in Table 1.

The IR-spectra of coal products were taken on a Spektrum 65 model Fourier spectrophotometer ("Perkin Elemer" company) in the range of 4000–450 cm^{-1}. KBr with a diameter of 3 mm was used as a tablet. The ratio of coal to KBr is 1: 200.

3. Results and discussion

The IR-Fourier spectrum of an acetone extract obtained under supercritical solvent conditions is shown in Fig. 1.

According to the IR-spectrum of the acetone extract obtained under supercritical solvent conditions, bound hydroxyl groups were detected at 3407 and 1222 cm^{-1}, alkanes at 2925, 2851, and 1379 cm^{-1}, amino acids containing an amine group at 1614 cm^{-1}, alcohols at 1031 cm^{-1}, ketones at 1713 cm^{-1}. The hydroxyl group in carboxylic acids (930 cm^{-1}), alkyl substitutes in the benzene ring (763 cm^{-1}), and alkynes (618 cm^{-1}) were also identified.

The IR-spectrum of the acetone extract obtained at the boiling point of the solvent differs in the presence of primary amines (3436 and 3451 cm^{-1}), allenes (1950–1970 cm^{-1}), alkenes (3019 and 1635 cm^{-1}), aromatic compounds (1525 cm^{-1}), aromatic aldehydes (1710 cm^{-1}), a carbonyl group in carboxylic acids (1215 cm^{-1}), and amine salts (2322 and 2400 cm^{-1}) (Fig. 2).

IR-Fourier spectroscopic study of ethanol extract of brown coal obtained under supercritical solvent conditions showed that this extract contains hydroxyl groups (3395 and 2900 cm^{-1}), alkanes (2977, 1453, 1382 cm^{-1}), alkenes (1646 and 694 cm^{-1}), alcohols (1087 and 1047 cm^{-1}) and alkyl substitutes in a benzene ring (879 cm^{-1}) (Fig. 3).

The IR-Fourier spectrum of ethanol extract obtained at the boiling point of the solvent differs in that it contains primary amines (3435 cm^{-1}), amine salts (3130–3030 cm^{-1}), esters (2830–2815 and 2850 cm^{-1}), allenes (1970–1950 cm^{-1}), isonitriles (2144 cm^{-1}) and aromatic compounds (1575 cm^{-1}) (Fig. 4).

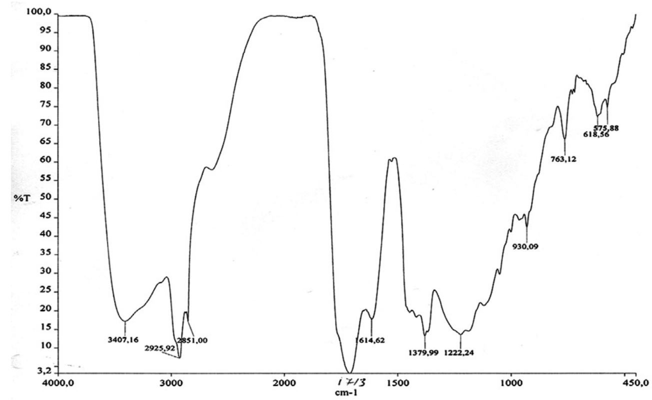

Fig. 1. IR-Fourier spectrum of acetone extract obtained under supercritical solvent conditions.

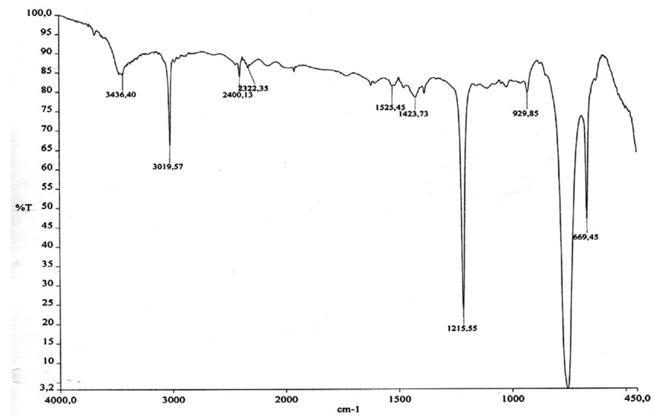

Fig. 2. IR-Fourier spectrum of acetone extract obtained at the boiling point of the solvent.

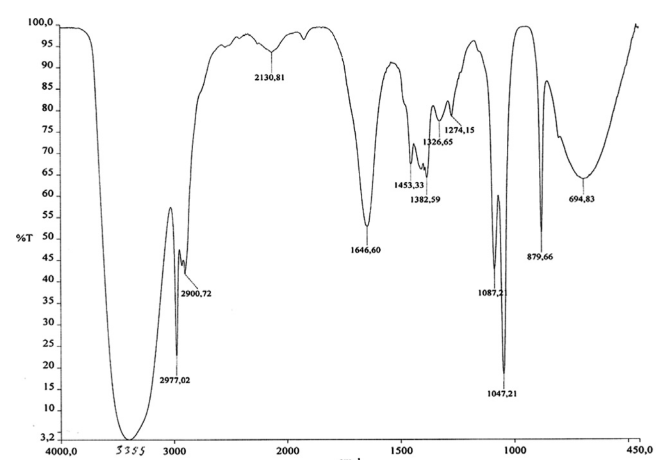

Fig. 3. IR-Fourier spectrum of ethanol extract obtained under supercritical solvent conditions.

Table 1
The physical and chemical characteristics of the solvents.

Solvent	t_{boil}, °C	t_{melt}, °C	t_{crit}, °C	P_{crit}, MPa	d_4^{20}, g/cm^3
Acetone	56.1	−95	235.5	4.7	0.7899
Ethanol	78.4	−114.3	241	6.3	0.7893

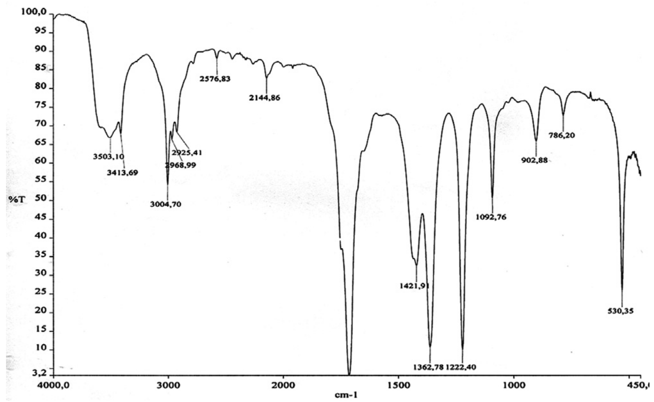

Fig. 4. IR-Fourier spectrum of ethanol extract obtained at the boiling point of the solvent.

Thus, extracts obtained under supercritical solvent conditions differ from extracts obtained at the boiling point of solvents in the absence of nitrogen-containing compounds and cumulated double bonds. The above data show that the optimal conditions for the extraction process are applied to both options of extraction processing of brown coal. However, when coal is dissolved in acetone and ethanol media under supercritical conditions, a deeper destruction of the organic mass of coal is observed.

CRediT authorship contribution statement

Zh.T. Yeshova: Conceptualization, Methodology, Software, Data curation, Writing - original draft, Supervision. **A.M. Manabayeva:** Writing - review & editing, Visualization, Investigation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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