International Journal of Energy
ISSN: 2957-9473 | Vol. 6, No. 1, 2025

Research on the Common Determination Methods of Material Composition and Trace Elements in Pingdingshan Coal Mine Coal

Dongdong Chen [1], Qianqian Zhang [2], Chunpeng Li [3], Yipeng Li [4]

[1] School of Resources and Environment, Henan University of Technology, Jiaozuo, Henan, 454000, China
[2] China Pingmei Shenma Group Nylon Technology Co., Ltd., Pingdingshan, Henan 467200, China
[3] China Pingmei Shenma Group Tianzhuang Coal Preparation Plant, Pingdingshan, Henan 467200, China
[4] Henan Shenma Hydrogen Chemical Co., Ltd, Pingdingshan, Henan 467200, China

Abstract: Pingdingshan Coal Mine is located in Pingdingshan City, Henan Province. Coal is an important energy mineral in China and a strategic resource for the country's economic and social development. The study of the material composition characteristics of coal is of great significance for the comprehensive utilization of coal. With the rapid development of social productivity, China's demand for coal in industrial production and people's daily lives is increasing, and the pattern of coal as the main energy source will not change in the short term. Due to the high content of trace elements in coal, trace elements will be released into the surrounding environment in different forms during coal mining and use, causing serious damage to the ecological environment. Therefore, we need to master the determination methods of trace elements, accurately grasp the composition and content of trace elements in coal, take corresponding prevention and remediation measures for the release of harmful trace elements, and protect the ecological environment. The coal produced during coal mining has a complex material composition and contains various trace elements. In order to accurately understand the content of trace elements in coal, appropriate determination methods need to be used for analysis. As a research object, Pingdingshan Coal Mine needs to focus on the content of trace elements and select appropriate measurement methods for accurate determination.

Keywords: Pingdingshan Coal Mine; Coal Material Composition; Trace Elements; Measurement Method.

1. Chapter 1: Study on the Composition of Coal Materials in Pingdingshan Coal Mine

1.1. Sample and Coal Element Determination Method

1.1.1. Sample

The samples were taken from the Wu and Ji groups of Pingdingshan Coal Mine. The sampling locations and sample descriptions are shown in Table 1.

1.1.2. Elemental Determination Method for Pingdingshan Coal Mine Coal

In the preprocessing process, the first step is to perform the inlaying machine process to produce coal bricks with separate labels for future use. Next, use a handheld XRF elemental analyzer for testing, and standardize the instrument by taking standard samples to ensure accuracy. After the standardization of the instrument display is completed, measure according to the sample number to be tested. Align the handheld XRF element analyzer gun head with the sample, press the measurement switch, maintain the alignment position for 1-2 minutes, and record the content of each element. This step ensures accurate measurement of the content of each element in the coal brick sample.

Table 1. The sampling locations and sample descriptions

Sample Number	Sampling Location	Sample Description
PDS−1	Wu9.10-12160 mining face	bright mirror coal, with a small amount of mica and uneven fracture surfaces
PDS−2	Wu9.10-21192 machine roadway head-on	semi bright coal, with low hardness, soft texture, and a large amount of moisture
PDS−3	Wu 9.10-20160 Wind Lane Frontal	Semi Bright Bright Coal, with a small amount of calcite filling and a stepped fracture surface
PDS−4	Wu 10.11-20192 tail	bright coal with stepped fracture and sliding surface
PDS−5	Wu 10.11-20102 mining and arranging 25 sets	bright mirror coal with stepped fracture surfaces
PDS−6	Ji 17-22320 mining and arranging 45 sets	bright mirror coal with sliding surfaces
PDS−7	Ji 15.16-22290 Machine Lane	Bright Mirror Coal, with a stepped fracture surface
PDS-8	Ji 15-24080 mining and discharging machine tail	Ji 15-24080 mining and discharging machine tail
PDS-9	Ji 15-24080 mining head	bright mirror coal, containing a small amount of muscovite, with stepped faults

1.2. Determination Results of Elements in Pingdingshan Coal Mine Coal

In the laboratory, a portable handheld XRF elemental analyzer was used to measure the content of constant elements in the coal bricks obtained from the coal samples. The data obtained was analyzed by mathematical statistics Table 2. The portable handheld XRF elemental analyzer here is a portable device that can quickly achieve qualitative and semi quantitative analysis of elements. This device can quickly obtain the content of various elements in coal samples, and the data obtained through mathematical statistical analysis can provide the constant element content of coal bricks, providing data support for further analysis in the future.

Table 2. Mathematical Analysis Results of Constant Elements in Pingdingshan Coal Mine

Element	maximum	minimum	mean	median	standard deviation
S	15485	2557	4828	3565	11363
K	2535	345	989	721	2116
Ca	105901	0	17051	3958	96398
Ti	3219	272	1651	1679	2701

1.3. Discussion

1.3.1. Coal Element Analysis and Hydrocarbon Generation Significance

Coal resources play an important role in the development of Chinese society. As one of the main energy minerals, the utilization of coal resources inevitably accompanies the emission of pollutants, which have a negative impact on the environment and human health. With the introduction of advanced analytical instruments and methods, China's research in coal geochemistry has rapidly developed. The constant elements in coal include C, H, O, N, Na, S, Mg, Si, K, Ca, Al, Ti, P, and Fe, which play an important role in the coal combustion process, coking energy, and coal to hydrocarbon generation process. For example, Fe is mainly present in sulfide minerals, while Ca is present in various compounds. Changes in the content of these elements can affect the pyrolysis characteristics of coal and the process of hydrocarbon generation. Therefore, the transformation and migration of elements in coal are important issues for the environment and health.

1.4. Conclusion

Based on the analysis of the elemental content of Pingdingshan coal mine coal, the following conclusions are drawn:

The coal samples in Pingdingshan coal mine exhibit high contents of elements such as Ti, Fe, S, K, Ca, etc. Among them, Fe and S elements are particularly prominent, with an average content of about 1977ppm and 4828ppm, respectively. This phenomenon may indicate the presence of pyrite in coal, a chemical component that may catalyze the coal's hydrocarbon generation process, thereby improving the coal's hydrocarbon conversion rate. For example, Fe element can promote the oxidation-reduction reaction of coal under certain conditions and increase the rate of oxidation-reduction reaction; And S element may form sulfide reactions, react with organic matter to generate organic sulfur, and play a role in the hydrocarbon generation process.

2. Chapter 2 Research on Trace Elements in Pingdingshan Coal Mine Coal

2.1. Research Status

According to reference [2], Lu et al. used atomic fluorescence spectroscopy (AFS), inductively coupled plasma atomic emission spectroscopy (ICP AES), and graphite furnace atomic absorption spectroscopy (GF-AAS) to detect trace elements in seven coal samples from China. They believed through cluster analysis that the distribution of trace elements in different coals is related to the geophysical and chemical factors of coal formation. This study can serve as a marker for coal seam comparison, which is of great significance for finding ways to reduce pollution, control pollution, and achieve green coal utilization in the process of coal combustion and processing. At the same time, they mentioned the research results of using physical washing methods to basically remove toxic elements significantly related to sulfides. In another study, according to reference [3-4], Ren Deyi et al. used ICP-AES and INAA to determine trace elements in the Shenbei coalfield, and combined with correlation and cluster analysis as well as scanning electron microscopy energy dispersive spectroscopy (SEM-EDX) analysis results, concluded that only a few elements such as P and V showed organic affinity, while Ba, Sb, Se were related to carbonate minerals, and Cu, Ni, Cr were related to sulfides to a certain extent. These research results provide important scientific basis for the utilization of coal resources. In addition, the determination results of harmful trace elements such as As, Hg, F, Cl, Cr, Cd, Mo in coal by Song Dangyu, Zhang Junying, etc. showed a significant correlation between Hg and As and pyrite, providing strong support for the study of pollutant emission characteristics during coal combustion.

2.2. The Occurrence Forms of Trace Elements in Coal

The occurrence states of trace elements in coal include chemical binding states and physical distributions. Chemical forms include ionic bonding, covalent bonding, and adsorption in pore water. The physical forms include discrete minerals, dispersed elements within minerals, and trace elements in organic valleys. For example, trace elements bound by ionic bonds can exist in the form of Na^+, K^+ions; Trace elements that are covalently bonded can form covalent bonds with atoms such as sulfur, nitrogen, and oxygen through shared electrons. In coal, trace elements may exist in the form of solid solutions, such as Fe^{2+}which can dissolve in the lattice of pyrite.

Liu Feiyan [5], Liu Guijian [6] and others have conducted research on the characteristics of element occurrence in coal and how to develop and utilize trace elements in coal. The occurrence forms of trace elements in coal are shown in Table

3: Trace elements in coal include various elements, such as iron, copper, zinc, nickel, etc., which exist in different forms in coal. For example, iron can exist in coal in free or organic bound forms. The occurrence forms of these trace elements have a significant impact on the development and utilization of coal.

Table 3. Occurrence Forms of Trace Elements in Coal

	trace element
Sulfide	Ag,Cd,Co,Ni,Pb,Sb,Sn,Ti,Zn,Hg,Cu,Ni,Cr,As
Halide	Br,Cl,F
Carbonate	Cu,Hg,Mn,Ni,Sb,Ba,Se
Arsenate	As
Silicate	Ba,Ni
Phosphate	P
Oxide	As,Cr,Sn,Th
Complex	Co,F
relatedto organic matter	Ag,Be,B,Br,Cd,Cu,Hg,Mn,Ni,Sb,Sn,U,Zn,P,V
related to pyrite	As,Hg,Sb,Se,U,Cu,Zn,Ni,Cr,Cd,Pb,Th
related to clay minerals	Be,Tl,V,Zn
related to adsorption in pores, etc	Cl,Hg

2.3. Reasons for the Formation of Trace Elements in Coal

Some organic substances present in coal have the ability to enrich trace elements. With the passage of time, the degree of coal conversion will gradually increase, and the functional groups of humic acid will gradually weaken. The enriched trace elements will be released in various ways. Part of it exists in the coal seam in the form of individual minerals, while the other part combines with organic matter in the coal and becomes a part of the coal. This indicates that trace elements in coal can be released as the degree of coalification increases, which is of great significance for the utilization and application of coal.

2.4. Changes in Trace Elements during Coal Conversion Process

2.4.1. Conversion Behavior of Trace Elements in Coal Combustion Process

The distribution and enrichment behavior of trace elements during combustion can be roughly divided into three categories: the first category of trace elements is distributed in equal amounts in fly ash and bottom ash, including Be, Co, Cr, Cs, Ga, Li, Ti, etc. These elements usually have a strong affinity for oxygen and are often associated with silicate minerals. They are melted during combustion and, due to their high boiling point, are not easily volatile. They aggregate with aluminosilicates to form a component of slag and fly ash. The second type of trace elements is significantly enriched in fly ash and significantly lacking in bottom ash, and the enrichment degree becomes more pronounced with the decrease of fly ash particle size. These trace elements include As, Cd, Mo, Co, Pb, Sb, Se, Zn, etc. These elements usually have a strong affinity for sulfur and exhibit significant volatility during combustion. As these elements exist as sulfides or in sulfide ores, high temperatures during combustion break sulfur-containing chemical bonds, causing these elements to partially or completely evaporate. The third type of trace elements have strong volatility and are not even enriched in fly ash. They are almost entirely emitted into the atmosphere in gaseous form, including Hg, Br, F, etc. The distribution of most trace elements in coal is related to the migration and distribution of the main mineral elements in coal, because trace elements are removed from the gas phase by condensation or adsorption of fly ash with high specific surface area. Quick [7] compared the release behavior of trace elements after the combustion of washed coal and raw coal, and concluded that the purification of coal effectively removes silicate minerals from coal, while the trace elements in coal do not decrease proportionally. Although the total amount of fly ash generated by the combustion of washed coal has decreased, the content of trace elements in fly ash has increased. Furimsky [8] established a model based on the principle of thermodynamic equilibrium to describe the transition characteristics of trace elements in combustion systems, which is consistent with experimental results within a certain range. This model is used to estimate the distribution trend of trace pollutants such as As, Pb, Cd in fly ash and bottom ash, which is consistent with experimental data. In terms of the enrichment pattern of trace elements in combustion products, domestic and foreign scholars have achieved consistent research results, that is, most trace elements are enriched in fly ash and bottom ash, and their enrichment and distribution coefficients are dominated by multiple factors.

2.4.2. Conversion Behavior of Trace Elements During Gasification Process

The volatilization behavior of trace elements under gasification reduction conditions is different from that under combustion oxidation atmosphere. Under reduction conditions, some trace element hydrides are generated, such as B_2H_4 SeH_2, AsH_3, etc. can increase their volatility. Helble [9] studied the volatility of trace elements during gasification, and the results showed that several elements such as As, Se, Sb, Pb, and Zn partially volatilized during gasification and were enriched in small particles. Elements such as Cr, Ni, Co, Mn, and U had very low volatility, while Hg was almost completely gasified. Thermodynamic analysis shows that under gasification reducing conditions, As, Sb, Pb, Hg, and Se exist in the gas phase in the temperature range of hot gas purification operation (500-600℃). As mainly exists in the gas phase in the form of AsO; Se exists in the form of gas-phase Se H_2; Pb exists in the gas phase in the forms of PbCl, $PbCl_2$, and Pb; Hg exists in the gas phase at all temperatures. Diaz somoano [10] classified trace elements into three categories based on their volatility during gasification according to thermodynamic equilibrium calculations: the first category had the weakest volatility and existed almost entirely in condensed form during gasification or gas purification, such as Mn; The third type of element has strong volatility and exists in gaseous form under most conditions, such as Se, Hg, B; Most of the remaining trace elements belong to the second category of volatility between the above two categories, such as Sb, As, Cd, Pb, Zn, Ni, Cr, V, etc.

3. Chapter 3 Common Methods for Determining Trace Element Content in Coal

3.1. Common Methods for Determining Trace Elements in Coal

3.1.1. Chemical Analysis Methods

According to the laboratory chemical analysis methods of China's coal system, comprehensive operations are carried out on trace elements such as phosphorus, arsenic, gallium, chlorine, uranium, etc. through colorimetric or volumetric methods. Colorimetry is a method of determining substance content by comparing the color of the test solution with the color of a standard solution. The colorimetric method can be applied to analyze various substances, such as metal ions, organic substances, etc. The volumetric method is a method of determining the content of a substance to be tested through titration, which is suitable for determining the content of a certain substance in colored solutions. The volumetric method is commonly used for the determination of acidity and alkalinity, as well as for the determination of trace elements. For example, in coal analysis, we can use the volumetric method to determine the content of trace elements, ensuring the accuracy of chemical analysis.

3.1.2. Atomic Emission Spectroscopy (AES)

The advantage of AES is that its equipment and analysis costs are relatively low, which means that using AES for elemental analysis is relatively cost-effective and particularly suitable for analyzing large amounts of samples. For example, in industrial production, AES is an economical and effective choice for quickly analyzing the composition of a large amount of raw materials. However, it should be noted that AES analysis has low precision and belongs to a semi quantitative analysis method, so it may not be applicable in high-precision analysis scenarios. For example, in the field of strict control and testing of the composition of high-end raw materials, other more precise analytical methods may be required. Specifically, AES can analyze Be B, Na, Mg, Al, Si, P,S,K,Ca,Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Ga,Ge,As,Sr,Y,Zr,Nb, Mo,Ru,Rh,Pd,Ag These elements include most of the elements that are often analyzed in industrial production. However, for situations where high accuracy is required for the analysis of trace elements, AES may not be suitable. For example, in the field of trace metal composition analysis or precision analysis, it may be necessary to choose other more precise analysis methods, such as ICP-MS or AAS. AES is therefore often used for "census" work on a large number of samples. This means that it is more suitable for basic element analysis of large quantities of samples, and in cases where high-precision analysis of individual samples is required, careful selection of analysis methods is necessary.

3.1.3. Atomic Absorption Spectroscopy (AAS)

Atomic absorption spectroscopy is a commonly used technique in analytical chemistry, which involves dissolving a sample and exciting it with a flame to produce vapor. The elements are then detected using methods such as flame atomic absorption spectroscopy, graphite furnace atomic absorption spectroscopy, cyanide generation atomic absorption spectroscopy, and cold atomic absorption spectroscopy. Among them, flame atomic absorption spectroscopy (FAAS) is a relatively mature, low-cost, and easy to operate analytical method. But its disadvantage is that it cannot process solid samples, and even if processed, the preprocessing of the samples is quite cumbersome. For example, for solid samples, dissolution treatment is required before detection can be carried out.

3.1.4. Neutron Activation Analysis (NAA)

Neutron activation analysis is a commonly used method for analyzing coal and its related substances. It includes activation analysis technology, thermochemical neutron technology, and INAA technology in instruments, with the first technology being widely used. The capture of elemental isotopes in coal can be achieved through the formation of radioactive isotopes, resulting in radiation. The types and intensities of these rays can be used to detect the content of elements. For example, through neutron activation analysis, we can accurately determine the content of multiple elements in coal solid samples, and the substrate effect is relatively small. It is worth noting that one of the drawbacks of neutron activation analysis is the need for a neutron reactor and a long analysis period, as well as the inability to analyze light elements such as O, N, and Si.

3.1.5. X-ray Fluorescence Spectroscopy (XRF)

X-ray fluorescence spectroscopy uses X-rays generated by external excitation to determine the atomic number of an element. Under specific conditions, the intensity of characteristic X-rays is directly proportional to the concentration of the excited element. The advantage of this method is that the equipment cost is relatively low and it is widely used. However, its disadvantage is its low sensitivity to trace elements.

3.1.6. Spark Source Mass Spectrometry (VNet)

Mass spectrometry is an analytical technique, and spark source mass spectrometry uses a high-frequency activated ion source. This technology has the advantages of high sensitivity, small selection effect, and simple structure, and is particularly suitable for solid sample analysis. For example, spark source mass spectrometry can be used to analyze various metal elements, including iron, copper, zinc, etc.

Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES) and Inductively Coupled Plasma

Mass Spectrometry (ICP-MS) are two commonly used analytical techniques that can be used to analyze the elemental composition and content in various samples. ICP-AES uses atomic emission spectroscopy to quantitatively analyze elements in samples, while ICP-MS uses mass spectrometry technology for analysis.

Inductively Coupled Plasma (ICP) is a novel spectroscopic technique used for Atomic Emission Spectroscopy (ICP-AES) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS). ICP-AES uses high-temperature (5000K) plasma generated by radio frequency electromagnetic field as the excitation light source, which ensures efficient excitation of elements and improves the precision and detection limit of analysis. Compared to traditional spectroscopic methods, ICP-AES has higher detection limits, higher accuracy, smaller systematic errors, and lower interference levels. ICP-MS is an ion source for mass spectrometry analysis using plasma. Its advantages include high selectivity, high sensitivity, low detection limit, the ability to detect multiple elements simultaneously, and fast testing speed. However, ICP-MS instruments are expensive and sensitive to analyte signals and plasma stability.

List several methods for determining trace elements in coal, as shown in Table 4.

Table 4. Determination methods for trace elements in coal

Element	Method Name	Standard Number
As	arsenic molybdenum blue spectrophotometric method, hydride atomic absorption spectrometry	GB/T3058-2019
Se	hydride atomic fluorescence spectrometry	GB/T39538-2020
Hg	hydride atomic fluorescence spectrometry	GB/T39538-2020
Pb	chemical titration method	GB/T16658-2007
P	spectrophotometric method	GB/T216-2003
Cl	high temperature combustion hydrolysis electrochemical determination method	GB/T3558-2014
Cd	hydride atomic fluorescence spectrometry	GB/T39538-2020

4. Chapter 4 Conclusion

By studying the material composition and trace elements in Pingdingshan coal mine, we have gained a deeper understanding of the constant and trace elements in coal. This study helps us gain a deeper understanding of the basic chemical composition and trace element content in coal. With the deterioration of the ecological environment, when studying the constant and trace elements in coal, people have also linked environmental science and ecology to deeply analyze the impact of the elements released during coal mining and processing on the surrounding geological and atmospheric environment, laying a good theoretical foundation for formulating environmental protection strategies in the future. With the increasingly prominent environmental issues, the impact of substances released from coal mining and processing on the surrounding environment is becoming more prominent, prompting people to link the release of elements in coal and its environmental impact with ecology and environmental science, providing stronger theoretical support for environmental protection and sustainable development. Studying the occurrence characteristics, enrichment mechanisms, and migration patterns of trace elements in coal from a geochemical perspective not only has theoretical and practical significance for preventing the impact of harmful elements on the environment and human health, protecting the ecology and human living environment, but also for developing new types of mineral resources. Studying the occurrence characteristics, enrichment mechanisms, and migration patterns of trace elements in coal from a geochemical perspective is of great significance for preventing the impact of harmful elements on the environment and human health, as well as for developing new mineral resources. The study of the geochemistry of constant and trace elements in coal has become a hot topic in energy, environmental science, and new resource research, which is one of the forefront topics internationally and an inevitable requirement for China to achieve environmental protection and sustainable development. Studying the geochemical characteristics of constant and trace elements in coal has become an international research hotspot and an urgent need for China to achieve environmental protection and sustainable development.

References

[1] Dai Shifeng, Ren Deyi, Tang Yuegang. The occurrence characteristics and research significance of major elements in coal [J]. Coalfield Geology and Exploration, 2005, 33 (2): 1-5.

[2] Lu X H, Zeng H C, Xu T et al.Chemometric studies of distribution of trace elements in seven Chinese coals[J], Fuel, 1995,74(9).

[3] Ren Deyi, Xu Dewei, Zhang Junjun, etc Distribution characteristics of associated elements in coal from Shenbei Coalfield Journal of China University of Mining and Technology, 1999, 28 (1).

[4] Song Dangyu, Zhang Junjun The geochemical characteristics of harmful trace elements in coal in Guizhou Province Coal Conversion, 2007, 10, 30 (4).

[5] Liu Feiyan, Zhu Zhimin, Shen Bing. The occurrence and development of trace elements in coal in China [J]. Conservation and Utilization, 2006, 22 (5): 467-468.

[6] Liu Guijian, Peng Zicheng, Wang Guiliang, et al. Research progress on trace elements in coal [J]. Advances in Earth Sciences, 2002,17(1): 53-62.

[7] Quick W J,Irons R M A,Trace element partitioning during the firing of washed and untreated power station coals[J], Fuel, 2002, 81(5).

[8] Furisky E. Characterization of trace element emissions from coal combustion by equilibrium calculations[J]Fuel Processing Technology,2000, 63.

[9] Helble J J, Mojtahedi M,Jyyranen J,et al Trace element partitioning during coal gasification,Fuel,1996,75(5).

[10] Diaz-Somoano M,Martinez-Tarazona M R,Trace element evaporation during coal gasification based on a thermodynamic equilibrium calculation approach[J],Fuel,2003,82(2).